THE INFLUENCE OF CLIMATE ON THE HYDROGEN-ION BUDGET OF UPLAND CATCHMENTS: A HYDROLOGICAL APPROACH

by
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CERTIFICATE OF ORIGINALITY

I certify that I am responsible for the work submitted in this thesis, that the original work is my own except as specified by the acknowledgements or by the references, and that neither the thesis nor the original work contained therein has been submitted to this or any other institution for a higher degree.

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ABSTRACT

Clear links are known to exist between the terrestrial characteristics of catchments and the chemistry of their surface waters. During the last decade it has been established that atmospheric pollution, in the form of acidic deposition, can also influence the chemistry of waters draining sensitive upland sites. Furthermore, recent studies have suggested that reductions in these anion loads can have marked consequences for the surface-water quality of acidified catchments. However, many of these field experiments and model estimates have neglected other, potentially important realms of atmospheric influence.

This thesis proposes that climate change over periods of up to one century can alter the hydrogen-ion budget of a catchment in two ways. First, variations in the relative frequency of large-scale synoptic features may significantly modify catchment chemical budgets by changing existing spatial and temporal patterns of acidic deposition. Secondly, as each major class of weather type is characterised by distinct precipitation and temperature regimes, the seasonal magnitude and frequency of acidic episodes may also be affected by long-term adjustments to the catchment water-balance.

A hydrological perspective was employed in order to investigate these potential hydrochemical relationships. This involved hydrological modelling and hydrogen-ion budgeting, statistical analyses of climatic trends, the application of weather classification schemes, and the generation of synthetic input data from observed and historic meteorological data. These elements were combined by the development of a robust and comprehensive computer package (the Shifting Climate and Catchment Acidification Model, or SCAM) which enables the manipulation of a wide range of atmospheric and catchment properties.

The model was calibrated and validated against data obtained from the Beacon experimental catchment in the East Midlands and then transferred to three contrasting watersheds in the Llyn Brianne region, Mid Wales. Using multiple climate and pollution scenarios, modelling experiments revealed that variations in the predominance of three key weather types modified the mean annual wet-deposited acid load by ±20% and the mean surface-water acidities by up to ±15%. Under the most extreme scenario the frequency of daily flows of less than pH 4.5 was increased by +90%. Whilst recognising the simplicity of the hydrologically-driven soil model, a feature common to all of the catchments was the exaggeration of existing seasonal discharge and acidity regimes. The sensitivity of individual catchments to a given climate change was found to be highly variable, depending upon the complex interaction of hydrology and catchment characteristics.

It was concluded, therefore, that the effect of reduced emissions of acidifying substances on catchment recovery can be modified by climate change. Furthermore, acid-sensitive

species occupying marginal sites, could be affected by the changes envisaged under the proposed BASE scenario. This underlines the need for a definition of the term 'critical load' that embraces desirable ecological responses with the required acidic deposition rates, for a given climatic context.

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Thine, O Lord, is the greatness and the power
and the glory and the victory and the majesty.
All that is in heaven and on earth is thine.
All things come of thee, O Lord,
and of thine own do we give thee.

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CHAPTER ONE

INTRODUCTION

"*One of the most important - and yet least well-understood - consequences of future changes in climate may be alterations in regional hydrologic cycles and subsequent changes in the quantity and quality of regional water resources*" (Gleick, 1987b, p 137).

1.1 STUDY CONTEXT

A scientific consensus is emerging that water resources are sensitive to environmental change and that a dominant factor affecting such systems over the next 50-100 years will be the greenhouse effect (Hulme and Jones, 1989; Jones and Henderson-Sellers, 1990; Beran 1989a/b). Recent evidence suggests that the observed warming can not be attributed to solar forcing alone (Kelly and Wigley, 1990) and that the expected changes will be distinct from the natural variability of the climate system (Wigley and Raper, 1990). However, the scientific community (or rather the mathematical models) are far from being in agreement as to the precise magnitude and rate of CO_2-induced climate change (Bach, 1989). Furthermore, it has become apparent that the Global Circulation Models which have been used to predict the response of the atmosphere are often limited in their capacity to describe many sub-grid scale processes (eg Entekhabi and Eagleson, 1989). Unfortunately, it is the regional context which is precisely of greatest interest to politicians, policy-makers and planners alike. In particular, *regional hydrologic* impacts of climate change may have profound effects on society by disrupting: water supply; energy supply from hydropower and thermal power plants; inland and coastal navigation; coastal protection; flood control; urban drainage; irrigation; soil salinity; agricultural production; soil erosion and water pollution control (DOE, 1988; Lemmela et al., 1990).

Against this background, acidified catchments provide a unique opportunity for evaluating changes in the *quality* of regional water resources because many have been the subject of intensive hydrochemical studies over recent and historic timescales (UKAWRG, 1989). As well as being a major environmental problem of current concern, the acidification of surface waters also has serious implications in terms of land-management practises, loss of fisheries, detrimental effects on water resources and the economic cost of implementing ameliorative measures. But above all, acidic catchments may be sensitive to both the direct and indirect effects of climate change as manifested by altered *hydrologic cycles* and, by dynamic temporal and spatial patterns of acidic deposition respectively.

1.2 BACKGROUND TO THE ACIDIFICATION DEBATE

Acidified catchments have been studied for around two centuries, with a gradual increase in knowledge that has accelerated greatly in the last 60-70 years (Gorham, 1989). In 1757 Home applied the concept of acids, bases and neutral salts to soils, whilst by 1852 Smith had attributed acid rain to coal combustion in Manchester, and in 1872 was the first to use the term "acid rain". However, it was not until the late 1950s that acid rain was related more specifically to sulphur-dioxide emissions from fossil-fuel combustion. In 1968 Oden noted for the first time the controversial potential for ecosystem degradation by acid deposition arising from the long-range transport of air pollutants across national boundaries. A landmark in the development of the acid precipitation theory was established by the final Report of the SNSF-project (Drablos and Tollan, 1980) which identified the main causes of the regional acidification of lakes and rivers in Scandinavia. Since the beginning of the 1980s the main concerns have been to determine more precisely the mechanisms of soil and surface water acidification, and to predict the long-term effect of various emission scenarios and land-management strategies. Mathematical models have since become prominent in the latter areas as heuristic tools for integrating process-level research and understanding of long-term catchment response (Hauhs, 1988).

Despite growing evidence linking the emission of sulphur dioxide to acid rain and thence to damaged ecosystems, the UK Central Electricity Generating Board disputed its liability as late as 1985 (Anon, 1984; Beardsley, 1984; Pearce, 1985). Two factors were eventually instrumental to the emerging British scientific consensus during what has been termed the decade of the "acid wars" (Pearce, 1990).

The first arose from diatom analysis of sediment cores which established the temporal coincidence between acid deposition and lake acidification at remote upland sites (Battarbee et al., 1985, 1987). The method depends upon establishing a quantitative relationship between the measurable diatom communities and lake pH of present day samples, and the preserved fossil assemblages of dated sediment horizons. Whilst a number of the reconstructed pH time-series have identified that acidification has occurred naturally in some lakes since the last Ice Age (eg Pennington, 1984) a majority of cores taken from sites around the British Isles have revealed that the most recent rapid phase of acidification pre-dates 20th century afforestation and upland drainage (Battarbee et al., 1985). In general the trend towards lower pH values began around or shortly after 1850 and typically involved a pH decline of between 0.5 and 1.5 pH units from a pre-Industrialisation level of 5.5 to 6.5 (UKAWRG, 1989). Furthermore, these trends have often been accompanied by a rising influx to lake sediments of heavy metals and carbonaceous particles, both of which are clearly indicative of increasing atmospheric contamination (Rippey, 1990; Oldfield and Richardson, 1990; Wik and Natkanski, 1990).

Although many palaeoecological reconstructions have been used to discredit the 'land-use change' or 'afforestation' hypotheses (Birks et al., 1990; Patrick et al., 1990; Battarbee et al., 1985) there is chemical evidence from the Lake District (Bull and Hall, 1986), Wales (WWA, 1987) and central Scotland (Harriman and Morrison, 1982) that streams of similar calcium content draining forestry plantations are more acid than streams draining grassland or moorland (Barth, 1988; Reynolds et al., 1988, 1989; UKAWRG, 1989). According to Hornung's (1988) review of the subject these disparities arise from a combination of interactive processes such as : the enhanced 'filter' effect of certain species of spruce; increased nitrogen fixing by species such as alder; changes to the production, composition and decomposition of humus under coniferous forest; increased soil solution concentrations due to greater evapotranspiration losses; the addition of acidifying nitrogenous fertilizers to peats or podzols; the net removal of base cations by cropping; the oxidation of sulphides and the mineralisation of organic nitrogen by the ploughing and drainage of peatlands; and finally, increased drainage-network efficiency leading to reduced residence times and a higher proportion of acidic, near-surface runoff. Therefore, it is now clear that the primary cause of acidification in the UK is acid precipitation (wet, dry and gaseous deposition) and that the large scale afforestation of sensitive catchments or the cessation of liming may significantly contribute to the acidity and aluminium concentrations of upland runoff.

The second line of scientific enquiry to establish the link between emissions and surface water acidity was mathematical modelling. Although acidification models have been constructed for a range of applications (hydrochemical, biological, economic and experimental), timescales (from the storm-period response to mean annual trends), and localities (principally North America, Scandinavia, and the UK) there has been growing concurrence as to the key processes involved (Reuss et al., 1986). The dominant hydrochemical controls for acid waters are currently thought to be: sulphate adsorption and desorption by soils; carbon-dioxide degassing; cation-exchange reactions; the saturation of some ecosystems by nitrate; the enhanced mobility of certain heavy metals (eg Mn, Fe, Cu, Zn, Cd and Pb) with increased acidity; hydrological pathways as regulators of acid buffering; the complicated non-linear behaviour of aluminium solubility and speciation with pH (UKAWRG, 1989). At the same time, studies of processes such as those governing the mobilisation of aluminium have highlighted the need for continued experimental research to challenge established, yet unrealistic ideas concerning, for example, thermodynamic stability/ solubility controls (Neal et al., 1989). Nonetheless, the modelling of acidification processes and, more importantly, of 'critical load' impacts is being conducted with increasing confidence as model predictions have been verified retrospectively (Jenkins et al., 1990), against manipulated catchments (Wright et al., 1990) and by recent field evidence (Battarbee et al., 1988; Dillon et al., 1986; Forsberg et al., 1985).

If the main achievements of the 1980s may be regarded as the quantification of the atmospheric and terrestrial phases of the catchment acidification process, the challenge of the 1990s will be to act upon the information obtained from long-term model predictions. This will involve the inclusion of the wider ecosystem response (eg Schindler et al., 1989) to hydrochemical forecasts, and hence the implementation of the most cost-effective or appropriate remedial actions. These might include: drastic emission reductions (of the order of 60-90% [Christophersen et al., in press]); sensitive land-management and drainage techniques (Hornung, 1988); or catchment liming (Grieve, 1990; Warfvinge and Sverdrup, 1988; Davis and Goldstein, 1988). The inclusion of ecological processes within acidification models may also lead to the emergence of a global dimension to the study of acid rain, with boundary conditions such as climate assuming increasing importance (Rodhe and Herrera, 1988; SCOPE 29, 1986). For example, Webster et al. (1990) have recently shown that reduced groundwater inputs related to sustained drought or to global warming increase the risk of acidification to many softwater systems. As well as reducing the planet's biodiversity, acid rain may have indirect impacts on greenhouse warming itself by disrupting soil 'sinks' for methane; by increasing CO_2 uptake through the eutrophication of ocean ecosystems; and by promoting the production of dimethylsulphide cloud seeds and hence modifying the planetary albedo (Wigley, 1989; Charlson et al., 1990; Pearce, 1990).

Not withstanding the above advances during the past two decades, a major gap in research has therefore been to assess the impact of climatic variations over historic timescales on the qualitative hydrological response of river basins. It is also clear that if greater reliance is to be placed upon simulations for the justification and implementation of remedial actions, there is an urgent need to examine the sensitivity of model forecasts to the boundary conditions of climate, landuse and patterns of acidic deposition. This thesis will seek to address these important issues.

1.3 THESIS AIMS AND STRUCTURE

Four fundamental aims of this thesis are identified below:

1) To **construct** a robust hydrochemical model that is capable of simulating the key features of the surface water acidity and hydrology of an experimental catchment in the East Midlands using minimal data inputs.

2) To calibrate, validate and then **utilise** the model to assess the relative sensitivity of catchment hydrochemistry to a range of climate scenarios (over 10-100 years).

3) To **predict** - on the basis of a single BASE scenario - the long-term hydrochemical response of a range of catchments, to account for any spatial variations in the sensitivities, and to assess the likelihood of their recovery under these conditions.

4) To **assess** the qualitative impact of the BASE scenario on the aquatic ecosystems of each of the four catchments and to outline future avenues of research in this respect.

The first section of this thesis presents a brief overview of the acidification debate; the following chapter will examine in greater detail the background to, and possibilities for coupling climate and hydrochemical systems via mathematical models. Within this context **Chapter 2** will also highlight the extent to which the heuristic capabilities of models have been exploited in all three fields of climate, hydrological and acidification research.

Chapter 3 then proceeds to describe the theoretical and practical development of the Shifting Climate and Catchment Acidification Model (SCAM). This algorithm is intended to be conceptually realistic yet sufficiently robust to withstand transfers to a range of atmospheric and catchment conditions.

Chapter 4 deals with the theoretical constraints imposed on model calibration and verification by the actual model design, parameter sensitivities, data quality and optimisation routines. The central requirement to modelling of lengthy, detailed, accurate and varied data sets is then pursued further in **Chapter 5** by a review of the techniques involved in the collection and collation of the SCAM calibration data-base.

Chapter 6 provides an opportunity for comment on the main features and patterns emerging from the experimental and secondary data sources in relation to the SCAM model assumptions. Following a brief description of the pertinent features of each of the selected catchments, **Chapter 7** provides the first quantitative test of the model forecasting ability. A range of objective tests are applied to assess the model performance under varied conditions and an attempt is made to account for any discrepancies between the observed and simulated time-series.

A sensitivity analysis of the model parameters provides a firm basis on which to evaluate the relative significance of climate versus terrestrial processes to runoff acidity in **Chapter 8**. Using a range of climate and pollution scenarios the first half of this chapter will examine the detail of the forecasted equilibrium and transient response(s) of the Beacon catchment. The second section investigates the inverse situation: namely, the spatially varied (seasonal to super-annual) responses of the four calibrated catchments to a single BASE scenario.

The results obtained from these two separate approaches then provide the input to the discussion in **Chapter 9**. This chapter will address the issues of catchment and ecosystem recovery under fluctuating climate conditions. The discussion will also highlight the degree to which spatial factors such as land-use or soil structure ultimately govern the sensitivity of a catchment ecosystem to a given climate change.

Finally **Chapter 10** concludes the thesis with a review of the most significant contributions made by the study and confronts some of major model limitations. A number of suggestions are made for future research - in particular the need for acidification models that incorporate quantitative and realistic descriptions of whole ecosystem responses. Further research into the qualitative implications of climate change on the water supplied by upland catchments is also advocated.

1.4 SUMMARY

This thesis will test the hypothesis that climate change over time-scales ranging from days to decades will have 'significant' consequences for the hydrogen-ion budget of acidic catchments. The empirical and theoretical basis of the SCAM model, its design, calibration, verification and eventual application, provides the experimental framework within which this hypothesis is to be challenged. Given the growing credence of greenhouse warming and the length of time required to simulate the recovery of acidified catchments (cf. Neal et al., 1986; Whitehead et al., 1988a/b), the possibility that boundary conditions or model inputs (that were once considered stable) may actually change justifies serious attention (Alcamo and Posch, 1986; Streets et al., 1985). Should the hypothesis be vindicated, the implications for water quality would be far reaching, making climate change a mandatory consideration in the setting of 'critical loads'.

CHAPTER TWO

MODELLING CLIMATE-HYDROCHEMICAL INTERACTIONS

"Climates change - this much can be said without contradiction. While there is uncertainty about mechanisms and magnitudes it is at least clear that the traditional perception of a static climate is not tenable.......It is therefore impossible to regard climatic and hydrological series as unchanging, and it is against this background of continuous climatic variability that we must view the new risks (and conceivably benefits) of a man-induced climate change " (Beran, 1989a, p 1).

2.1 INTRODUCTION

The following literature review is not intended to be comprehensive nor does it seek to examine in any great detail the different modelling approaches involved. Rather the cited examples have been chosen to reflect the contemporary issues, objectives and concerns of the three modelling areas included within the design of the Shifting Climate and Catchment Acidification Model, namely: catchment-climate interactions, catchment hydrology, and catchment acidification. Two unifying themes are examined. The first identifies the centrality of water as a medium by which acidic ions are transported, deposited, stored, released and redistributed in time and space. The second investigates the advantages and limitations of model building as a means of quantifying these varied processes. Catchment acidification and the hydrologic response of watersheds to climatic changes have been selected as the focal points since these processes operate at comparable temporal scales and provide a management perspective to the overall discussion of climate-hydrochemical interactions.

2.2 MODELLING THE REGIONAL HYDROLOGIC CONSEQUENCES OF GLOBAL CLIMATE CHANGE.

Largely on the basis of evidence from homogenised data series, it is now accepted by the scientific community that rising CO_2 concentrations since the Industrial Revolution have induced a warming of the Earth's surface temperatures (Jones et al., 1986, 1988) and brought about concomitant changes to surface pressure patterns and annual rainfall amounts (Bradley et al., 1987). Recent remotely sensed data obtained by the AVHRR NOAA

(Advanced Very High Resolution Radiometer) satellite suggests that the rate at which these climate changes are occurring may even have accelerated over the most recent decade (Strong, 1989). However, of less certainty is the precise interpretation of these physical changes to the atmospheric system in terms of the potential human societal and hydrologic consequences. This uncertainty arises from two related issues pertaining to future climatic changes. Firstly, it is not clear as to when and by what magnitude changes of climate will occur in the future in response to elevated CO_2 concentrations. Secondly, it has yet to be fully established, the extent to which ecological feedback mechanisms and interactive responses of water resource systems are able to mitigate the effects of these direct and indirect climate changes. Therefore, if any confidence is to be placed in regional hydrologic forecasts these two issues must first be fully addressed.

The impact of climate changes on hydrologic systems was recently the subject of the International Conference on Water and Climate (Lemmela et al., 1990) and the XV General Assembly of the European Geophysical Society (EGS, 1990). At the former venue two schools of thought concerning the forecasting of future atmospheric conditions were aired: mathematical modelling and climatic analogues. The use of General Circulation Models (GCMs) for the prediction of the impacts of climatic change on regional hydrosystems is seen to depend primarily upon their ability to reliably depict the seasonal and geographical distribution of the changes in surface climate variables (Gates, 1985; Mitchell, 1983; Wigley and Raper, 1990). Seasonally specific regional results require either a specified, non-interactive sea surface temperature or more realistically, an interactive mixed-layer ocean (Lough et al., 1983). As Schlesinger (1988) has shown from a recent review of different modelling approaches (eg. Energy Balance Models [EBMs], Radiative Convective Models [RCMs], and GCMs) the predicted climates can vary significantly as a result of their differing physical processes, structures and parameter values. The subsequent projections of CO_2-induced surface temperature change are therefore highly sensitive to the actual model design. Whilst there is a general consensus between the different GCMs that the global near-surface atmosphere warms by 2-4 °C when CO_2 is doubled, there are still significant differences arising from the interpretation of ocean-atmosphere coupling and the role of cloud feedback mechanisms (Cattle, 1989; Slingo, 1990).

The CO_2-induced changes of annual precipitation amounts are even more problematic, as the variability of rainfall in both space and time is due largely to convective-scale processes. Due to the grid-scale of the current generation of GCMs these mechanisms must be represented parametrically in terms of the large-scale distribution of temperature and humidity (Entekhabi and Eagleson, 1989). Regional and microclimatic effects arising from, for example, changes in relief and the distribution of ocean currents are not easily represented by these methods. This is also unfortunate because overall confidence in the performance of GCMs must ultimately rely on the degree to which they are based on physical principals (Mitchell, 1988).

This limitation of model resolution and grid-scale is perhaps the most pervasive deterring factor in the application of GCM climate forecasts to regional and catchment scale impact studies. As Schlesinger (1988) observes the physical processes that may be of importance to climate and climatic change span 14-orders of magnitude from the planetary scale (10^7m) to the cloud microphysical scale (10^{-6}m). Yet contemporary computers permit the resolution of physical processes over just two orders of magnitude; a thousand-fold increase in computer speed would allow the resolution of only one more order of magnitude ! Thus the spatial resolution of the best current climate models are 400 km^2, a scale which does not enable the detailed investigation of regional or local climatic impacts. Similar limitations are also imposed on the temporal resolution of GCMs as they must reconcile two distinct sets of variables: fast response variables such as land-surface temperatures and humidities (0.05 - 5 years); and slow response variables such as the deep ocean temperatures and the extent of continental ice-sheets (100 - 10,000 years) (Saltzman, 1988). Furthermore, existing GCMs are almost entirely devoted to determining the equilibrium response of the climate to instantaneous increases in CO_2-levels rather than the transient response which is generally of greater relevance to watershed sensitivity studies. Consequently, with the exception of a few examples (eg. Mitchell, 1983) current GCM outputs tend to be limited to annual, bi-annual (summer-winter) or perpetual monthly (eg. January only) statistics.

Therefore, in order to be of value to water-resource planners, regional hydrologic assessments should include: a focus on shorter time-scales such as months and seasons rather than annual averages; the formulation of hydrologically significant variables such as runoff and soil moisture, rather than simplified accounts of temperature and precipitation; and the incorporation of regional hydrologic characteristics such as snowmelt, topography, soil properties and land-use impacts on the water balance (Gleick, 1987b; EGS, 1990). Clearly, these criteria are beyond the scope of even the most advanced GCMs and require the implementation of alternative modelling strategies. One promising approach involves the coupling of regional/ local impact models (which function at the sub-grid scale) to the grid-scale output of existing GCMs (Hulme and Jones, 1989; Cohen and Allsopp, 1988; Gleick, 1986). This method was successfully applied to the Sacramento Basin, California using a number of temperature and precipitation scenarios predicted for the region by three GCMs (GFDL, GISS and NCAR CCM) in conjunction with a monthly water-balance model (Gleick, 1987a). The results indicated large decreases in summer soil-moisture and runoff due to a heightened evapotranspiration demand, increases in winter runoff, and shifts in the timing of average-monthly runoff arising from the faster disappearance of winter snow pack. An alternative solution to the 'climate inversion' problem involves the use of regression techniques to establish a statistical relationship between, for example, precipitation changes predicted at the GCM grid-scale and, anomalies at each locality within an area comparable to the grid element (Gates, 1985). In either case, the resultant local responses could potentially be aggregated to determine the regional-scale or even global impact.

Climatic analogue methods provide a further option for the determination of local and regional hydrometeorological variables (Lough et al., 1983; Budyko, 1989). This approach involves the use of regional and seasonal patterns of past warm climates (derived either from lengthy proxy or empirical data records) to construct warm-world scenarios as an analogue for future CO_2-induced climate changes. This method of scenario construction makes the fundamental assumption that given the same boundary conditions (as represented by the oceans, biosphere and cryosphere), the general atmospheric circulation responds in a similar manner to different forcing mechanisms (Lough et al., 1983). If however, the boundary conditions are not in fact stable - as would seem most likely - different episodes (such as the Medieval warm phase) should not strictly be representative of future near-surface meteorological characteristics. Conversely, a major advantage of the method is that it enables the use of the natural variability of real past climates at a temporal and spatial resolution not yet achieved by GCMs. Furthermore, it can be argued that the main impact of climate and weather on hydrologic systems is through changes in variability, particularly in the frequency of extreme events, rather than through changes in the mean (Parry, 1985).

Both the analogue method and the use of mathematical models are therefore subject to uncertainties arising from natural and man-induced feedback mechanisms within the climate system. Examples of these processes include climate-biosphere interactions (Rosenzweig and Dickinson, 1986) and ocean-cryosphere-atmosphere systems (Ramantham, 1988). In terms of the hydrologic consequences, a number of recent water balance studies have shown (using both conceptual and deterministic models) the direct influence of carbon-dioxide concentrations on evapotranspiration rates and hence streamflow (Aston, 1984; Wigley and Jones, 1985; Bultot et al., 1988; Lankreyer and Veen, 1989). For example, increases in streamflow of 40-90% obtained by a distributed deterministic process model were attributed by Aston (1984) to the direct effect of elevated CO_2 concentrations in increasing vegetation stomatal resistances. However, whilst it is recognised that CO_2 enrichment can alter physiological processes such as plant growth, photosynthesis and canopy density, none of these models (as yet) have included terms which enable the counterbalancing of reduced evapotranspiration rates with increased leaf areas and hence a greater number of stomata. This omission has been justified to a certain extent by the argument that plant physiological responses appear to be more sensitive to temperature and rainfall perturbations, and nutrient limiting factors, than the direct effects of a CO_2-enriched atmosphere (Bultot et al., 1988). But it is now generally accepted that countervailing hydrometeorologic features such as evapotranspiration feedbacks should be included in any regional assessment of climate-impacted hydrological systems. The global perspective should also examine the feedback which exist between climate and the changing distributions of entire biomes (Rosenzweig and Dickinson, 1986; Prentice and Fung, 1990).

Another factor which can serve to mitigate the effect of changing precipitation patterns and the seasonal timing of evapotranspiration is catchment geology. Bultot et al. (1988) demonstrated using three catchments in Belgium, that where the geology allows rapid infiltration increased groundwater storage, baseflow and total flow throughout the year would result from a warmer/ wetter climate. Conversely, where catchment geology promotes surface flow, an increased flood risk in winter and reduced summer streamflow and groundwater storage is to be anticipated. Similar results were obtained for Britain using a regression model developed from 214 small catchments during the FREND project (Arnell and Reynard, 1989).

At the individual catchment scale the situation becomes still more complex. Vegetation, soil structure, geology, land-use changes and management practises are all capable of mitigating the potential water-balance impacts associated with climate change. Situations may even arise where it is very difficult to distinguish between gradual climate change effects and progressive alterations made to hydrologic systems by human activities within catchments (Alley et al., 1989). Nonetheless, numerous potential impacts to catchment hydrosystems have been identified (Beran, 1989a/b; EGS, 1990; Hulme and Jones, 1989; Cohen and Allsopp, 1988), not least of which are: soil moisture changes (eg. Gleick, 1987a/b); snow and ice cover (eg. Collins, 1989); river regimes and flooding (eg. Nobilis, 1989); groundwater recharge (eg. Thomsen, 1989); urban and industrial water supply and drainage (eg. Law, 1989; Niemczynowicz, 1989).

From the preceding discussion it is clear that there are two main difficulties involved in quantifying the impact of climatic change on hydrologic systems. Firstly, the problem of articulating global-scale atmospheric variables in a format and resolution that is compatible with catchment-scale hydrologic processes. For example, it is not currently possible to obtain extreme events directly from GCM output and there is no formalised approach for estimating the future incidence of flood, drought, rapid snowmelt, intense storms and high winds (Beran, 1989a). Secondly, whilst the significance of vegetation has been qualitatively assessed, there is still great uncertainty as to its quantitative role in mitigating the effects of climatic change and as a regulator of the regional hydrologic response. For catchment- or regional-scale impact studies - where long instrumental records permit - the analogue approach facilitates the formulation of climate scenarios at a resolution currently exceeding that of GCMs. However, further research is needed into techniques for bridging the disparity between what climate modellers can provide and what hydrologists require (Beran, 1989a; Hulme and Jones, 1989).

2.3 CATCHMENT HYDROLOGICAL MODELLING

"Despite its clear definition as a science, in most cases hydrology is still viewed and practised as a technology. Its mission is not seen as improving the understanding of the water cycle, but as solving the many urgent practical problems involving water, by any means available, including baseflow separation, unlikely results of maximum likelihood estimates, random numbers and worse" (Klemes, 1988, p6).

This perspective is upheld by the historical legacy of 'hydrological problem solving' (eg. Biswas, 1970). The earliest known hydrological endeavours of Mesopotamia and the Nile Valley (c3000 BC) were concerned with regulating and controlling unpredictable natural elements through localised impoundment and irrigation schemes. The origins of the quest for hydrological understanding have been accredited to individuals such as Plato, Aristotle and Leonardo da Vinci. However, it was not until the seventeenth century that the necessary instrumentation was available to lend support to, or falsify some of these earlier hypotheses about the hydrological cycle. This 'quantitative revolution' in hydrology laid the foundations of subsequent water engineering and design practise of the second half of the nineteenth century, much of which still persists in the form of the 'rational method'. The empirical solutions of this era arose in direct response to the prevailing engineering problems of urban sewer design, land reclamation drainage systems design and reservoir spillway design (Todini, 1988). Much effort in the first half of the twentieth century was devoted to modifying these rational methods in order to cope with the nonuniform distribution of rainfall and catchment characteristics in space and time. Increasingly however, the models became divorced from the real world mechanisms and were superseded in the 1960s by rainfall-runoff models which attempted to describe the hydrologic cycle using conceptualised expressions of the key processes involved (eg. Stanford Model IV [Nash and Sutcliffe, 1970]). During the 1970s a growing awareness of issues such as land-use impacts, the dewatering and incursion of saline water into aquifers, pollutant dispersal and soil erosion prompted the development of spatially distributed models such as the Systeme Hydrologique Europeen (Abbott et al., 1986a,b) as a means of assessing the integrated effect of the internal and external processes affecting catchment behaviour. Finally, the 1980s have witnessed the advent of real-time forecasting models

(Wood and O'Connell, 1985) as a response to the need for flood forecasting and as a management tool for hydraulic structures and reservoirs.

Clearly, the historical perspective supports the assertion that hydrology has evolved as a technology to meet the needs of society rather than as a science (Klemes, 1988). Contemporary hydrological expertise may therefore be divided into three complementary sub-disciplines, namely: applied hydrology (or hydrological technology), hydrological support and pure hydrological research (or the science of hydrology).

The literature abounds with examples of hydrological models which have been devised in order to meet the demands of water resources management or decision making. Furthermore, these models are not restricted to any single category or model-type. For example, Pirt's (1983) Ungauged Catchment Model, utilising regression equations of catchment variables (such as the network density) to derive the parameter values of the conceptual model, is able to predict the timing and magnitude of flood events in catchments for which the available data is minimal. Similar intentions motivated the Flood Studies Group (NERC, 1975) to derive a parametric equation of the mean annual flood of an ungauged catchment. At the opposite end of the data-requirement spectrum are the physically-based distributed catchment models (Beven, 1989; Bathurst, 1986; Rushton et al., 1982) which have forecasting potential in all of the following areas: the effect of spatially variable inputs and outputs on surface and groundwater resources; the hydrological consequences of different basin land-use and management practises; the movement and storage of pollutants and sediments; and the hydrological response of ungauged catchments. However, it is important to weigh against these benefits the considerable expenditure required in terms of programming, computer resources, data preparation and field experimentation, and economic cost.

This latter point is really the crux of the issue concerning hydrology as practised by technologists as opposed to scientists. That is, managers have to make decisions within the context of the available resource support, time, data quality and information with respect to the anticipated impact. Many hydrologists have responded to these demands by devising models of a range of complexity, data-requirements and accuracy. This point is amplified by Beven (1987, p 396):

"*........we have inherited and continue to develop a plethora of incompatible and inadequate models of catchment response without the tools to choose between them in any rigourous way. They all work (to some extent); equally, they are all falsified.*"

Considerable interest has therefore been focused on the theoretical and technical means of improving and discriminating between the forecasts of competing models. These aspects of hydrological support may be further subdivided into three key development areas: the improvement of model design; the assimilation of modern data-handling and collection technologies; and numerical calibration and validation techniques.

A central theme of contemporary debates concerning model design and theory has been the question of scale (Gupta et al.,1986; Pilgrim, 1983; Beven, 1988; Mancini and Rosso, 1988). The concept of the Representative Elementary Area and the use of catchment morphology as a surrogate for the multitude of hill-slope processes is also gaining prominence (eg. Beven et al., 1988). Associated with this awareness of catchment heterogeneity rather than homogeneity, is the assertion that rainfall-runoff processes must be considered stochastic instead of deterministic in nature due to the inherent "unknowability" of hydrologic systems (Beven, 1987). In the case of the physically-based models, the interaction of grid scale with model operation is also recognised to be important but relatively little research has so far been conducted on this matter. Two areas which require particular attention have been identified (Bathurst and Wicks, 1988): firstly, measurement techniques need to correspond as far as possible with the model grid scale; secondly, recognition of the fact that model grid scale may typically exceed the spatial scale at which key processes (such as point erosion) are operative. In this latter respect, many current applications of physically-based models use them as lumped-conceptual models at the grid scale (Beven, 1989).

The development of high-resolution, multi-channel, remote sensing techniques potentially offers a solution to the task of detailed and representative sampling of spatially-distributed systems (van de Griend, 1985; Ottlé and Vidal-Madjar, 1989). It may be argued that the long-term feasibility of the physics-based models as integrating catchment modelling tools will hinge on advances being made in this direction. However, satellite technology also brings with it new difficulties such as the need for ground-truth experiments, consideration of the image resolution in relation to model design, the limited range of hydrological parameters to which the method is amenable, and inevitably cost (Kite, 1988).

Another technical innovation which has played an increasingly important role in the progress of hydrology as a science and technology, is computer hard- and soft-ware. According to Abbott (1988) the state of the art is such that it is reasonable to consider the possible applications of fifth-generation or Expert Systems to the modelling and management of hydrologic systems. This in turn will place new demands upon research establishments to meet on the one hand the social requirements placed upon modelling services and the concomitant complexity of the models, and, on the other hand, the training and expertise of practitioners in these fields (Abbott, 1988).

The final aspect of hydrological support pertains to the computational and numerical analyses required to optimise the performance of many hydrological models. A cynical review of the advances being made in these techniques proposes that though satisfactory from a mathematical point of view, the process of calibration does not encourage the rejection of 'unrepresentative' models (Beven, 1987). Thus, the emphasis has been directed towards specifying measures of "closeness" between the model and catchment outputs, at selecting appropriate or more efficient methods of optimising elusive parameters, and, deriving unique and conceptually realistic parameter sets (Sorooshian, 1988). However, relatively little has been done to quantify the confidence limits that accompany flow predictions and which are associated with uncertain parameter values (Roger et al., 1985; Lee et al., 1990).

In one respect the inadequacy of many existing rainfall-runoff models should act as a strong stimulus of pure hydrological research. For a start there has been a call by some for greater "intellectual honesty" and the rejection of hydrologic pseudoscience (Hall, 1971; Beven, 1987; Klemes, 1988). For example, methods of baseflow separation are still being advocated (eg. Shaw, 1983) despite the contradictory (and now well established) evidence concerning the isotopic composition of storm hydrographs (Dewalle et al., 1988).

With regard to the questions surrounding scale-effects, some authors have argued that there is an over-riding need to discover hydrologic laws at the catchment scale (Pilgrim, 1983). Furthermore, DeCoursey (1988, pp 24) asserts that concurrent development of hydrologic models and research watersheds is necessary for the adequate development of both. Hence, strategic research:

"........should have its roots in the needs of the decision maker......[it] may be fundamental in character, but it must respond to some gap in knowledge needed to improve the decision makers ability to make decisions based on adequate information."

Some of the scientific issues that should be addressed then include: the transfer of processes between different temporal and spatial scales; the need to couple chemistry and biology with the physics of water movement; the impact on the food web of toxic substances in water; the use of statistics to determine confidence levels in scientific understanding and engineering applications; and finally, the development of algorithms which enable the evaluation of the socio-economic consequences of extreme hydrologic events (National Research Council, 1983).

Therefore, rather than advancing along separate lines of enquiry, future pure and applied hydrology should become increasingly united in order to sustain their mutual value to the decision maker. A good example of the fruitfulness of this stance - in which research watersheds and policy/ decision making have advanced simultaneously - has been the modelling of surface water acidification.

2.4 MODELLING SURFACE WATER ACIDIFICATION

"Mathematical models used by researchers are generally constructed for two purposes, the first being for the testing of hypotheses and the second for making predictions from the effect of altering current conditions. Models for surface water acidification are no exception" (Stone and Seip, 1989, pp 192).

Mathematical models of surface water acidification have undoubtedly made significant contributions to the set-up and testing of hypotheses. As the examples cited below will illustrate these numerical models have often been subjected to critical review by carefully designed field experiments in order to assess their prognostic potential. Although the models vary enormously in their complexity and data-requirements they may be broadly divided into two categories: those which have been designed to investigate the short-term hourly or daily response of catchments, and are essentially flow-driven; and secondly, those which are concerned with the long-term mass-balance of key ions and are driven by the flux of strong anions through the soil profile.

Possible exceptions to this simplistic twofold division are the empirical models which have enabled the systematic interpretation of large amounts of data and led to a focus on the key processes. For example, Henriksens (1979) empirical model of lake acidification was developed on the basis of water chemistry data collected from a survey of 719 lakes in southernmost Norway. Based on the hypothesis that the acidification process can be described as a large scale titration (in which a bicarbonate solution is titrated with strong acid), the model indicates that the acidification process is dominated by a limited number of cations and anions. At the same time the model has also highlighted a major uncertainty: whether or not the rate of chemical weathering is a function of the loading of strong acid (Wright, 1984). The answer to this question, for instance, is crucial to the long-term predictions of the Enhanced Trickle Down (ETD) model (Nikolaidis et al., 1988).

However, one of the earliest conceptual models of streamwater chemistry was developed for the Birkenes catchment in Norway to simulate the day to day variations and seasonal flux of sulphate through acidic, upland soils (Christophersen and Wright, 1981; Christophersen et al., 1982). This research confirmed the importance of mobile ions such as SO_4 and Cl as the vehicles by which cations are transported through the catchment. The model was a land-mark in catchment hydrochemical modelling because it incorporated for the first time a systematic description of numerous ion-exchange processes including: cation exchange, weathering, dissolution/ precipitation of gibbsite, sulphate adsorbtion/ desorbtion, and sulphate mineralisation. Furthermore, the intensive catchment input-output field studies associated with the project revealed a number of recurring patterns, most notable of which was the coincidence of high acidity and aluminium concentrations with periods of high discharge (Wright, 1984).

More recently conservative tracers such as ^{18}O have been used to investigate the hydrological stores and pathways of the Birkenes model (Hooper et al., 1988). The results indicate that as a descriptor of solute pathways the sub-model is not entirely satisfactory and that one passive store, rather than two, more accurately represents the hydrochemistry of the catchment. Similar conclusions followed an analysis of the model's inability to describe the Cl in streamwater issuing from two upland catchments of the River Severn, Mid-Wales (Neal et al., 1988). The authors suggest that the stochastic properties of water movement and chemical processes operating at the microscale account for the observed, deterministic streamwater chemistry responses at the catchment scale. This complies with the concept of "unknowability" arising from the heterogeneity of the system (Beven, 1987) and implies that simple time-series approaches which incorporate key catchment processes may suffice (eg. Whitehead et al., 1986). The opposing view argues that efforts to incorporate hydrologic effects into surface water acidification models should address the relationship between the spatially distributed mechanisms of runoff generation and the resultant spatial variations in watershed biogeochemistry (Lawrence et al., 1988; Bishop and Grip, [in press]; Christophersen et al., [in press]; Wheater et al., [in press]). For example, the existence of ephemeral soil pipes may exaccerbate stream acidities by enabling acidic precipitation to bypass most of the soil matrix and thereby reducing the potential for buffering (WWA, 1987). Recent models of 'representative' hillslopes within the Birkenes catchment have been developed with some of these pathways in mind, allowing water originating from the various soil horizons to mix (Christophersen et al, [in press]).

Detailed investigations of the Birkenes model have therefore indicated the limit to which lumped representations of complex and spatially distributed chemical reactions in soils can efficiently describe the gross chemical behaviour of whole catchments. These spatial variations have been incorporated within the design of the ILWAS (Integrated Lake Watershed Acidification Study) model (Chen et al., 1984) by the assumption that heterogeneous systems can be represented more realistically by a network of homogeneous compartments. Thus, the model divides a lake-watershed system into subcatchments, river segments and a lake, and further describes canopy, snowpack, soil and lakewater processes within each compartment in order to calculate the concentrations of 16 chemical constituents. The main processes considered by the model include plant respiration, nutrient uptake, nitrification, decomposition of litter, cation exchange and dissolution of aluminium. Although the ILWAS model is the most comprehensive model of its kind developed to date, Reuss et al. (1986) assert that for many catchments insufficient data will exist for utilising the complete model without resorting to obtaining parameter values via calibration. Perhaps the most significant contribution to understanding made by the model is the stressing of the importance of basin characteristics, flowpaths and residence of water in the soil for determining lake water chemistry (Goldstein et al., 1984).

Whilst the Birkenes model was developed primarily to describe the contemporary 'steady state', models such as MAGIC (Cosby et al, 1985a/b) and RAINS (Alcamo et al., 1987) have been applied to longer-term management questions such as "what changes in the lake or watershed can be expected from various emission scenarios ?" and "what is the time frame over which such changes will occur ?" (Chen et al., 1984). This capability is founded on the assumption that in the absence of long-term calibration data sets, the ability of the model to predict future water chemistry, may be assessed by its performance at describing the dynamics of the contemporary system. The problem associated with this philosophy was expressed succinctly by Reuss et al. (1986, p 927):

"It must be recognised that the ability to reproduce short-term dynamics does not guarantee accuracy of long-term prediction. Policy needs will not allow luxury of postponing predictive uses until long-term verification is accomplished. We must therefore accept some uncertainty in predictions made for this purpose."

As a means of verifying the likelihood of its predictions, the MAGIC (Model of Acidification of Groundwater in Catchments) has been used in conjunction with historical data to retrodict the pH record of lakes inferred from diatom remains in dated core samples (Jenkins et al., 1990). MAGIC is primarily concerned with evaluating the relative significance of terrestrial and atmospheric sources of surface water acidity over time-scales of 10-100+ years and has been applied to a number of catchments, most recently Loch Dee, Scotland (Neal et al., 1986), Plynlimon, Central Wales (Whitehead et al., 1988a) and Llyn Brianne, Wales (Whitehead et al.,1988b). The results obtained from both forest and moorland sites showed that while atmospheric deposition is the primary cause of stream acidification, conifer afforestation can also enhance stream acidity. This effect was attributed to the forest root system, leaf litter layer and drainage ditches which can modify hydrochemical pathways (Hornung, 1988). Furthermore, there was also a localised enhancement of occult deposition due to the filtering effects of forests on the atmosphere (Fowler, 1984), whilst evapotranspiration increased the concentration of solutes entering the stream network. Changes to the hydrological characteristics of a catchment such as altering the ratio of baseflow to surface soil flow can also significantly affect the stream quality (Whitehead et al., 1986). However, the MAGIC model has a number of shortcomings (Warren, 1988): it uses estimated historical emissions as a surrogate for acid deposition; it contains no hydrological element and so cannot account for changes in the intensity and frequency of sub-annual events; it lumps soil chemistry on a catchment basis and thus does not address processes resulting from 'fine scale' heterogeneity.

By contrast the ILWAS model has incorporated a rudimentary level of spatial heterogeneity by dividing a lake-watershed system into sub-catchments, river segments and a lake but has not been as extensively tested as the MAGIC model. Nonetheless, an important application of the ILWAS model has been to simulate the response of acidic catchments to various liming mitigation strategies (Davis and Goldstein, 1988). Results obtained for the Adirondack Lake Watershed, New York State, indicate that the magnitude and duration of the response of the lake is a function of the seasonal timing, particle size, intensity and spatial distribution of the lime applications. The most effective results are generally obtained by liming the contributing areas of the tributary streams entering the lake (Warfvinge and Sverdrup, 1988). However, a major obstacle to the interpretation of such simulations is the difficulty involved in adequately representing 'real' forestry practises such as selective cropping, ditching and other factors such as the age of the stand, localised soil and parent material properties - all of which are known to effect the success of catchment liming.

The majority of simulation models have been concerned with evaluating the impact of different emission control strategies - these have tended to focus upon the variable inputs to catchment ecosystems rather than land-use practises. The most ambitious attempt at constructing a fully comprehensive source-receptor-water quality model is the RAINS (Regional Acidification Information and Simulation) model (Alcamo et al., 1987). The model is sulphur-based and currently incorporates factors of energy consumption, economics, abatement technology, quality of fuel and generating capacity to calculate the spatial pattern of emissions over the whole of Europe for a standard period 1960-2040! Atmospheric transport, deposition, soil-, lake-, groundwater-acidification and forest impact sub-models are the used to evaluate the terrestrial impacts of different European-scale control strategies. Alternatively, the model is able to determine the most cost-effective scenario for reducing sulphur emissions given certain ecological criteria. Whilst the model assumptions may be challenged on numerous fronts (cf. Kauppi et al., 1986) RAINS represents the first attempt at synthesising multidisciplinary scientific and policy components within a single model in a format that is readily understood by non-technical decision-makers.

An assumption implicit to all of these process models is that surface water acidification is in fact reversible and that degraded systems are therefore amenable to the implementation of appropriate management strategies. According to Hauhs' (1988) review of the topic, the response of water acidification to reductions in deposition is likely to be hysteretic, whilst the silicate weathering rate will largely determine a soils recovery potential. Additional factors affecting the reversibility of water acidification include the sensitivity, depth and whether or not equilibrium has been reached between current deposition levels and the base saturation of soils. The validity of these conclusions have been supported to a certain extent by the experimental results of the Project Rain (Wright et al., 1986, 1990) conducted at the Risdalsheia catchment, southern Norway. The watershed was covered by transparent panels and treated with deacidified rain; the resulting runoff concentrations were 20-30% lower for SO_4 and the pH was 0.1-0.3 units higher than a neighbouring (untreated) catchment after just one year. The greatest uncertainty in predicting the long-term recovery rate of acidified soils using models such as MAGIC and RAINS appears, therefore, to relate more to the uncertain future acid inputs than to the exact soil mechanisms involved (Warren, 1988; Georgakakos et al., 1989).

From the previous discussion it is clear that mathematical modelling has proved to be a valuable tool in the quantification as well as qualitative description of the controversial "acid rain" debate. Within the context of soil acidification processes, for example, Reuss et al. (1986) have observed a significant convergence of thought concerning the key processes of anion mobility, sulphate adsorbtion, ion exchange, and the dissolution of Al-bearing minerals. However, it should also be fully appreciated that the model predictions for future scenarios are still highly tentative and depend as much on the model structure and quality of data used as the forecasted emission levels. The satisfactory description of key hydrological pathways has also been shown to be a necessary prerequisite to subsequent hydrochemical simulations. As in the case of applied hydrological modelling (section 2.2) there has been a 'substantial divergence in modelling philosophy' (Reuss et al., 1986) that reflects the spatial and temporal scales of interest, the available data base and computational resources. Whilst there is some uncertainty as to the exact nature of acidified catchment recovery, the use of models in conjunction with experimental and palaeoecological data can point the way towards cost-effective treatments of these damaged ecosystems. Proxy data sources can also help meet the underlying need for long data series with which to validate model predictions (eg Battarbee et al., 1988 a/b).

2.5 DISCUSSION OF CLIMATE-HYDROCHEMICAL COUPLING

The preceding sections have examined in relative isolation some of the motivating factors and modelling tasks of three distinct, yet inter-related environmental disciplines. These three areas are united by their common interest in water dynamics and by a need to make long-term predictions of the effects of acid deposition on terrestrial and aquatic ecosystems. The climate represents the vehicle by which acidic ions are transported and ultimately deposited to terrestrial systems. Furthermore, meteorological factors which determine the occurrence of rainfall and evapotranspiration are the key driving variables of catchment hydrology (Georgakakos et al., 1989). Changes to these atmospheric boundary conditions may therefore lead to significant perturbations of annual runoff regimes, and to the timing and magnitude of individual hydrologic events. The exact form of the hydrological response will in turn be a function of catchment properties such as parent material, land-use and vegetation type. However, for acidified catchments, the indirect effect of climatic changes may be sufficient to modify sensitive hydrologic pathways and hydrochemical processes to such an extent that the possibility of recovery - even with significant reductions in the inputs of acidifying ions - is brought into serious question.

The previous sections have also highlighted the immense potential of mathematical modelling as a predictive and heuristic tool, whilst acknowledging the inherent technical and theoretical difficulties associated with each approach. However, to re-echo the words of Reuss et al. (1986) *policy needs will not allow the luxury of postponing predictive uses* until these obstacles have been overcome. As an interim measure, the mathematical coupling of climate and hydrochemical systems is considered to be a valid means of assessing the possible response(s) of surface water chemistry to (CO_2-induced) climate changes. With particular reference to acid catchments , this claim may be supported on four different fronts of scientific enquiry.

Firstly, as was stated above, the water chemistry of acidified catchments is 'driven' to varying degrees by atmospheric processes. It is now clear that the year-to-year variability of acidic loading is not controlled by emissions on the local or even the regional scale, but rather by atmospheric transport processes which are determined by climatic variables and are considered to be equal to, if not more significant than source emissions in determining deposition fluctuations (Campbell and Turk, 1988; Cape et al., 1984; Streets et al., 1985). This view was expressed succinctly by Bradley (1986, p 107):

"Acid deposition is a consequence of atmospheric processes acting on air pollutants. As such the phenomenon is subject to the variability of the atmospheric system on both short

(meteorological) and long (climatological) time scales. In assessing trends in acid deposition, climatic trends must be an implicit part of the assessment."

Clear evidence in support of this assertion has been provided by recent studies of the links between acidic deposition and synoptic meteorology (Davies et al., 1986; Farmer et al., 1989; Fowler and Cape, 1984; Wilby, 1989). The significance of climatic change to acid deposition becomes apparent when considered in the light of the pronounced long-term trend of decreasing westerly air flows since the 1920's (Jones and Kelly, 1982; Lamb, 1972). Since westerly weather types are associated - for the British Isles in general - with trajectories of 'clean' Atlantic air, it is possible that the concentrations of non-marine ions in precipitation were lower some decades ago (Davies et al., 1986). The implications of this are that as climate changes so too does the spatial distribution of acid deposition, even in the absence of alterations to European emissions. Furthermore, individual synoptic weather types have characteristic rainfall and temperature properties (Jones and Kelly, 1982; Sowden and Parker, 1981; Wigley and Jones, 1987; McCabe et al., 1989; Haagenson, 1985; Wilby, 1989); changes in the relative frequency of different synoptic types - whether or not as a product of the 'greenhouse' effect - therefore have the potential to dramatically modify existing hydrologic regimes and acid deposition rates.

Changes to hydrologic processes at the sub-annual scale provide the second justification for coupling atmospheric (meteorological) and terrestrial (hydrological) systems. Until now the establishment of such links within a single modelling framework has largely been confined to real-time rainfall-forecasting coupled with flood prediction models (eg. Georgakakos and Foufoula-Georgiou, 1988). Whilst desirable for some plot-scale applications (eg Wheater et al., [in press]), the level of (hourly) resolution contained in these models is not necessary for the evaluation of the changing frequency of hydrochemical source/ pathway activation. Within the context of long-term climatic changes, a daily time-step is considered more than adequate. This would enable an investigation of secular changes to the relative significance of stormflow and baseflow contributions, and the consequent trends in stream water acidities (cf. Whitehead et al., 1986). This in turn would enable the construction of detailed flow duration and stream water acidity excedence curves for the estimation of the frequency of lethal concentration doses (for selected biota). This intra-annual detail is currently beyond the scope of existing models such as MAGIC and RAINS which operate on an annual time-step (Cosby et al., 1985; Alcamo et al., 1987). This may be a serious omission as it is changes to the magnitude and frequency of acidic episodes, rather than to the annual mean streamwater acidity, that are potentially of greatest significance to aquatic biota (Warren, 1988; Harriman et al., [in press]; Morris and Reader, [in press]).

The third reason for climate- hydrochemical coupling is the need to establish the sensitivity of surface water acidity to changes in long-term atmospheric, hydrological and soil-chemical parameters (Lee et al., 1990; Georgakakos et al., 1989). This task is most efficiently undertaken when all contributory factors are included within the design of a comprehensive mathematical model. Furthermore, it will also provide the means of standardising the impact of annual emission totals for selected regions in accordance with the prevailing climatic and meteorological conditions.

Finally, the coupling of climatic changes to surface water acidity, provides an appropriate experimental framework within which to assess the extent to which catchment acidification is currently (or likely to be) enhanced/ reversed by changes to atmospheric boundary conditions. There is a growing body of experimental and theoretical evidence that demonstrates that the reversal of catchment/ lake acidification is possible under 'favourable conditions', and can even be quite rapid (Wright et al., 1988; Neal et al., 1988; Forsberg, 1985; Hauhs, 1988; Dillon, 1986). Whilst the potential for catchment recovery is beyond question, the precise mechanisms by which it proceeds and can vary between sites, are still unclear (eg. Dillon, 1986). In most instances improvements in the quality of the surface water have been attributed to reduced sulphurous and nitrogenous emissions, and the associated declines in the acid depositions (eg. Wright et al., 1988). But it has also been shown that other factors such as the soil-base status, sulphate adsorption and release mechanisms, weathering rates and hydrological variables play a key role in mitigating the effects of acid depositions (Neal et al., 1988).

However, two questions remain unanswered. Firstly, to what extent could changing emissions rather than changing climate variables be linked to the observed, declining acid deposition in certain regions ? Secondly, what are the relative significances of reduced acid loads and variable hydro-meteorological factors in determining the long-term reversibility of acidified catchments ? The answers to these questions would go some way towards understanding the long chain of events between the emission of acidifying substances and the ultimate effects on aquatic biota (Mason, 1985).

2.6 SUMMARY

Climate change has significance for acidified catchments in two key respects: as a variable source of acidic compounds, and as a regulator of the frequency and magnitude of hydrochemical pathway activation. From section 2.2 it was concluded that specific questions concerning the reversibility of catchment acidification are more readily answered by using the analogue method as a source of future climate scenarios. This approach in turn demands that a highly robust hydrochemical model be adopted: conceptual modelling offers a moderate degree of process description and does not presume the existence of a highly detailed data base (sections 2.3 and 2.4).

The "reversibility" debate provides a distinct and topical point at which to focus efforts at coupling climate and hydrochemical systems. Within this context the literature reviews of sections 2.2 - 2.4 have underlined the value of mathematical modelling in enabling the asking of "What if ?" questions. In addition to the testing of hypotheses, the development of these tools in response to specific environmental problems has often aided the formulation and testing of effective management solutions. Bearing these points in mind, the following chapter describes the theoretical and empirical development of one such tool: the Shifting Climate and Catchment Acidification Model (SCAM).

CHAPTER THREE

THE SHIFTING CLIMATE AND CATCHMENT ACIDIFICATION MODEL

"All models seek to simplify the complexity of the real world by selectively exaggerating the fundamental aspects of a system at the expense of the incidental detail. In presenting an approximate view of reality, a model must remain simple enough to understand and use, yet complex enough to be representative of the system being studied" (Anderson and Burt, 1985, p1).

3.1 INTRODUCTION

The previous chapter presented a selection of historical and philosophical arguments for the use of mathematical models in the evaluation of a wide range of environmental issues, not least of which were climate change and catchment acidification. The following chapters will now establish the theoretical basis of one such 'selective' and 'approximate' representation of these two complimentary issues. However, before describing the functional attributes of the Shifting Climate and Catchment Acidification Model, several criteria for evaluating the applicability of water-balance models to climate impact assessments are briefly presented (Gleick, 1986).

Firstly, the inherent accuracy of the model is of utmost importance. Having said this, simpler, more **robust** models can often yield better results particularly when the quality of the input data is low. Secondly, attention should be paid to the precise methods of deriving **model parameters**, especially those which may be time-dependant. An example, that was mentioned in section 2.2, is the extent to which the transient response of vegetation to both the direct and indirect effects of climate changes are incorporated by hydrological models. Thirdly, the availability and quality of the input **data** should be considered within the context of model calibration and verification. The confidence placed in model forecasts will ultimately depend on the reliability of the values assigned to sensitive model parameters. Fourthly, the model should be **versatile**, easy to use and readily applicable to a wide range of catchment and climate conditions. And finally, the model should ideally be **compatible** with existing GCMs or more specifically their output statistics. This reflects the need to link hydrological and hydrochemical responses at the regional and even catchment scale to global climate changes.

Thus having established the criteria by which the design of a climate impact model should be evaluated, the remainder of this chapter will present the requirements placed upon the SCAM model, the chosen modelling strategies, and descriptions of the 'fundamental' processes included. Firstly, however, in order to provide an overview of SCAM, the model structure is briefly described.

3.2 MODEL STRUCTURE

Reference to Figure 3.1 shows that the SCAM model has basically two parallel modes of operation: calibration and simulation. The calibration mode utilises the data base (described in Chapters 5 and 6) to obtain the optimised values of a total of around 15 hydrological and hydrochemical parameters (cf. Table 3.4). The theoretical background to, and the methodological procedures involved in this task are discussed in Chapters 4 and 7 respectively. Broadly speaking the daily data required to 'run' the model (precipitation amount and acidity, and mean temperature) are input to the four simulation modules (climate, evapotranspiration, hydrology and hydrochemistry), and the resulting output data are compared statistically with the observed streamflow properties by the 'model performance' sub-routine. The parameters are then further modified or stored according to these results. Summary statistics are also supplied both to the screen and to external files for further analysis.

Having first optimised the hydrologic parameters using the empirical data base (cf. Chapter 7), it is then possible to derive hydrochemical forecasts for the same catchment using the second, simulation mode. This mode enables the program user to selectively manipulate the parameter values of a second parameter set according to the specifications of the desired forecast scenario. So for example, it is possible to adjust the parameters which describe the synthetic temperature regime - mean annual temperature, daily anomalies, rate/ direction of annual trends and seasonalities - either individually or corporately. Typical catchment output variables include: daily discharge, streamflow acidities and Al-ion concentrations, catchment base-status and soil moisture deficits etc. Although it is possible to change over 100 different parameters in this way, default values and suggested ranges are provided in every case - these having been established previously from a combination of empirical and historical sources (Chapters 5 and 6). These parameters are then used to generate the necessary input data, which as before, is supplied to the catchment hydrochemical systems. Furthermore, it is also possible to manipulate the catchment parameter values , so that a wide range of soil, hydrological and geochemical conditions may be embraced. A record of the parameter values entered for each simulation is maintained by the 'datasheet' file

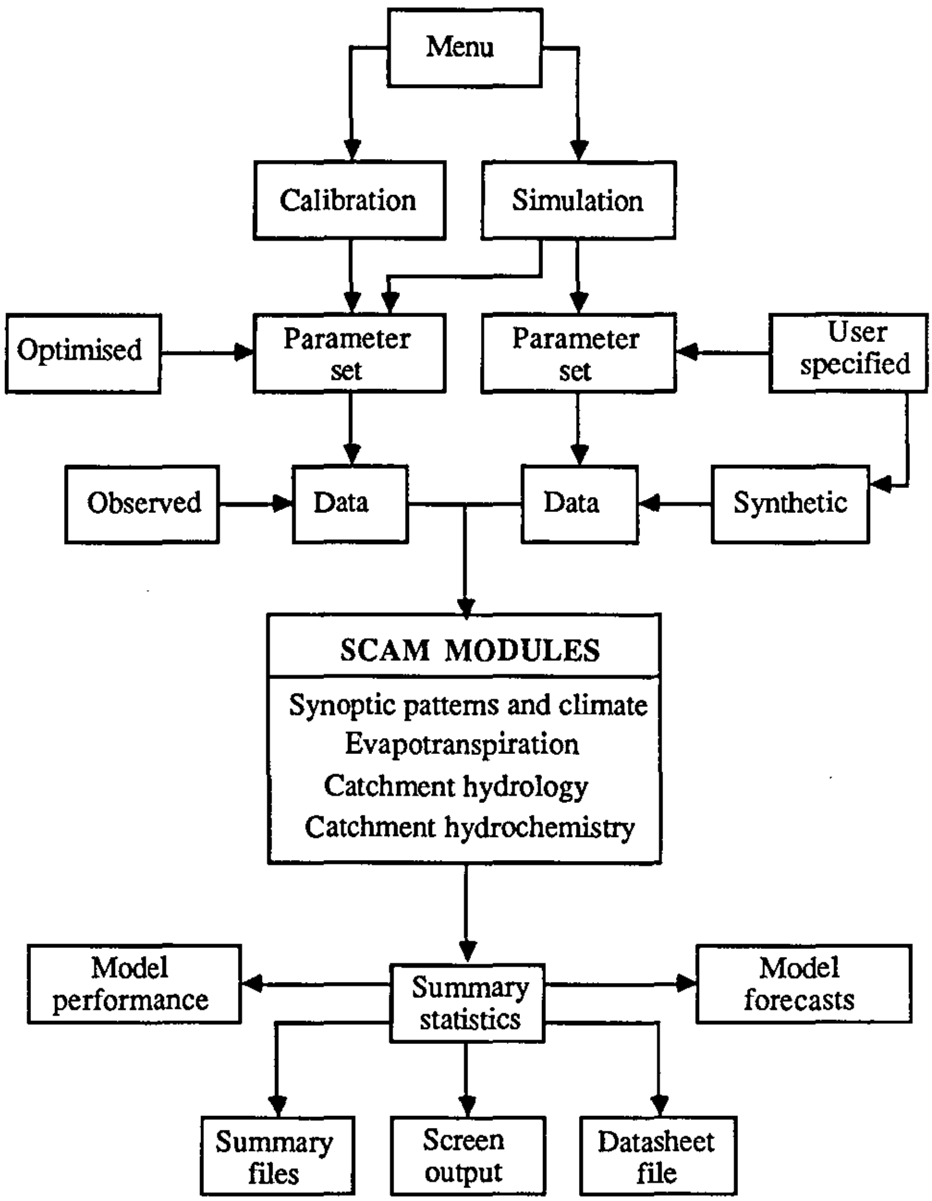


FIGURE 3.1 The main components of the Shifting Climate and Catchment Acidification Model (SCAM)

alongside the simulation results for future reference. An example of the output held in the 'datasheet' file is shown in Table 3.1.

In summary, the calibration mode uses 'real' data to derive optimum parameter values for the terrestrial responses to atmospheric inputs (precipitation, acid load and temperature), and to define the parameter default values, and probabilities used in the second mode of operation. On the basis of these values, the (second) forecasting mode generates 'synthetic' atmospheric data - for future climate regimes - and determines the hydrochemical response of the catchment to the user-specified climate scenario. The precise means by which these procedures are implemented are described in section 3.4, prior to this, it is necessary to first provide the theoretical basis and justification of the SCAM model design assumptions.

3.3 BACKGROUND TO THE MODEL COMPONENTS

As the opening quotation so eloquently implied, models represent 'selective', 'exaggerated', 'simplified' and 'approximate' views of reality - and in this sense they are a very personal, even subjective interpretation of real-world complexities. What processes, therefore are worthy of inclusion, or by the same argument, exclusion ? The answer to this question is undoubtedly determined by factors such as available data, technical resources, time and socio-economic constraints rather than scientific rigour *per se*. This perspective was clearly supported by the main themes discussed in the previous chapter, and particularly with reference to recent developments in hydrological modelling (section 2.3). The SCAM model is not likely to be an exception to this general rule, so in the following sections an attempt has been made to examine in closer detail, the theoretical background and alternatives to the existing SCAM model assumptions. These same assumptions should be viewed in the light of the modelling objectives (2.6) and the external constraints and criteria mentioned above. Each of the four SCAM modules are discussed in turn.

3.3.1 Synoptic climatology

Some of the most significant limitations of Global Circulation Modelling were discussed in section 2.2. With respect to the SCAM model objectives, the opportunity for deriving realistic and detailed hydrologic scenarios using current GCMs output was considered unfeasible primarily due to the coarse temporal and spatial resolutions of these models. If it is required that the atmosphere must be regarded as a variable source of acidic compounds and as a regulator of hydrologic regimes, four conditions should first be satisfied by the chosen methodology, namely: the day-to-day meteorological controls of acidic deposition

VARIABLE INPUT PARAMETERS

No.days:10000 Start date:1/1/1988

Maxc: 15.6	Maxdc: 205	Meanc: 9.8	Trendc(pa): 0.00
Seed1: 30	Seed2: 180	Seed3: 120	Dddrate: 100.0

LWT PROBABILITY MATRIX

	A	W	C	N	NW	S	SW	OT	MRAIN	PRAIN	TANOM
A	0.680	0.040	0.030	0.010	0.010	0.010	0.030	0.190	3.413	0.110	0.150
W	0.080	0.370	0.080	0.000	0.070	0.000	0.090	0.310	3.346	0.593	1.830
C	0.110	0.070	0.390	0.020	0.070	0.000	0.020	0.320	4.539	0.750	-0.540
N	0.300	0.000	0.100	0.300	0.100	0.000	0.000	0.200	3.511	0.692	-3.300
NW	0.180	0.350	0.000	0.060	0.180	0.000	0.000	0.290	4.042	0.400	-0.100
S	0.290	0.140	0.000	0.000	0.000	0.000	0.140	0.430	4.100	0.556	2.640
SW	0.120	0.320	0.060	0.000	0.000	0.030	0.350	0.120	3.103	0.500	2.920
OT	0.200	0.150	0.120	0.020	0.030	0.040	0.050	0.390	3.819	0.456	-0.160

CATCHMENT PARAMETER SET

r(1): 547000.0	r(2): 0.9800	r(3): 75.0	r(4): 28.0
r(5): 0.1250	r(6): 0.017	r(7): 49.0	r(8): 1.085
r(9): 110.0	r(10): 2.0E8	r(11): 100.0	r(12): 6.35
r(13): 3.7	r(14): 100.0	r(15): 2.0E7	r(16): 476.0

SIMULATION OUTPUT STATISTICS

Total rain (mm): 15079.2	Total discharge (mm): 2739.4
Mean annual rain (mm): 550.8	Mean annual discharge (mm): 100.1
Mean daily temperature: 10.15	Number of westerly days: 1434
Number of cyclonic days: 1029	Number of anticyclonic days: 3477
Number of wet-days: 3964	Discharge-rainfall(%): 18.17
Total H-ion input (kg): 987.142	Total H-ion output (kg): 24.8460
Mean rain pH is: 4.099	Mean discharge pH is: 4.780
Initial base saturation: 0.100000	Final base saturation: 0.095977
Total Al-ion output (kg): 1603.7	Al-ion concentration (mg/l): 1.07
The frequency of LCDs: 4829	Ratio of H-ion out-in(%): 2.52

TABLE 3.1 Example of the DATASHEET output file showing the Lamb's Weather Type transformation matrix.

episodes; the magnitude and timing of individual precipitation events; changes to the seasonality of precipitation inputs; and finally, the inclusion of long-term trends (> year) within these time-series.

The modelling of acidic ion emission, transport, transformation and deposition to receptor sites via atmospheric processes have been investigated along four main avenues of research (Table 3.2). Of these, the synoptic approach was considered to be the most promising for a number of different reasons:

(1) Synoptic schemes pay equal attention to the effects of geostrophic wind direction and to large scale atmospheric motions, thereby acting as a surrogate for processes operating in three dimensions. For example, Haagenson et al. (1985) showed that the precipitation in the cold sector of a cyclone is often more acidic than other sectors of the storm since the air flows are generally confined to the 'polluted' boundary layer by the overlying warm sector.

(2) Long records of daily synoptic patterns are readily available and have been widely used for pollution studies, as well as indicators of climate change.

(3) Additional intra- synoptic-class refinements may be achieved by consideration of factors such as daily wind fetch and the persistence of key weather types.

The synoptic approach is also well placed for the description of other atmospheric phenomena such as precipitation mechanisms and temperature anomalies. For example, McCabe et al. (1989) used weather type analyses as a basis for stochastic precipitation modelling by identifying weather conditions associated with varying frequencies, intensities and amounts of precipitation. Elsewhere attempts have been made to relate seasonal (Perry, 1976) and super-annual changes (eg. Wigley and Jones, 1987) in precipitation variability to changes in large-scale forcing factors such as pressure gradients and weather-types. The main advantage that these approaches have over purely stochastic descriptions of precipitation generation is that they can introduce greater physical realism in the form of weather type persistence and its subsequent effects on regional rainfall totals (McCabe et al., 1989). In the case of long-term annual means (> 20 years), Wilby (1989) showed that a synoptic method of rainfall generation was capable of attaining a mean error of <5%, although errors of up to 10-25% were found for individual, extreme years such 1975/76.

Given the large number of different classification systems, the question then arises as to which synoptic scheme is most applicable to the simulation of regional rainfall and temperature characteristics. Several different schemes are currently available, ranging from

METHOD	EXAMPLES	ADVANTAGES	DISADVANTAGES
Empirical studies/ field observations.	Martin and Barber (1984); Skeffington (1984); Singh, Nobert and Zwack (1987); Raynor and Hayes (1982); Wolf et al. (1979); Buishand et al. (1988); Sperber (1987); Musold and Lindqvist (1983); Munn and Rodhe (1970).	Identification of pollutant sources; Associations between acidic ions; Seasonal and annual trends; Meteorological controls; Site specific details.	Essentially descriptive.
Back-trajectory models.	Fowler and Cape (1984); Smith and Hunt (1978); Henderson and Weingartner (1981).	Determination of most representative path; Physical status of air-mass; Explanation of pollution episodes.	Identification and weighting of pollutant sources; Limited predictive power; Relating emissions to acid depositions.
Physical models.	Hanna et al. (1984); Verkatram (1985); Maryon (1989); Jakeman (1988).	Prediction of ambient air and precipitation concentrations.	Data intensive; Parameterisation difficulties; Lack of standardisation. Coarse resolution.
Synoptic methods.	Davies et al. (1986); Farmer et al. (1989); Alcamo and Posch (1986); McCabe et al. (1989); Wilby (1989).	Seasonal and long-term trends; Meteorological basis; Applicable to range of variables; Inclusion of stochastic components.	Classification procedure; Definition of class boundaries; Number of classes required; 'Unclassifiable' or hybrid states.

TABLE 3.2 Alternative approaches to acid deposition modelling.

the computer-assisted, correlation-based systems (eg. Key [1986], Yarnel et al. [1988]) to the largely subjective classification methods such as the PSCM indices (Murray and Lewis, 1966), the *Grosswetterlagen* weather situations (Baur, Hess and Nagel, 1944), and the British Isles weather types (Lamb, 1972). The Lamb's Weather Type (LWT) system was deemed to be the most appealing method for further classifying daily precipitation characteristics (amount and acidity) and daily temperature anomalies (cf. Table 3.1). The LWT scheme was selected in preference to the other classifications because:

(1) The system has been well documented and numerous examples exist to support the versatility and efficiency of the approach.

(2) The daily sequence of air circulation patterns have been classified from 1861-onwards by one person using a strict methodology that guarantees that the register is at least lengthy and internally consistent.

(3) The inclusion of hybrid weather types by the scheme makes for greater objectivity by avoiding the forcing of marginal days into one of the seven main types and reduces the number of days which must be dismissed as being 'unclassifiable'.

(4) The hybrid classes may be divided and regrouped into the seven basic types for statistical study.

(5) The classifications were devised specifically for the British Isles.

Therefore, the Lamb's Weather Type register of the daily sequence of circulation patterns offers a convenient source of data and a methodology for detailed, coherent and long-term investigations of the climate regime of the British Isles. Furthermore, synoptic climatology has proven success in integrating and aggregating the range of meteorological variables that characterise regional weather patterns. The technique is equally valid for describing and synthesizing climate variables over timescales ranging from daily rainfall and temperature generation to the decade-by-decade evolution of the atmospheric system.

3.3.2 Evapotranspiration

Evapotranspiration is the loss of water into the atmosphere through evaporation from all surfaces, including evaporation from free-water surfaces, soil and man-made surfaces and transpiration from plants (Knapp, 1985). In the case of a vegetated land-surface evaporation consists of two main components: those losses occurring under wet canopy conditions due to rainfall interception; and transpiration from the biomass occurring under dry canopy conditions. Taken together, these two components are of immense significance to both land-use and water resource management practices.

The intercepted component of the total annual evaporative loss from a forest is largely a function of the frequency of rainfall events and is especially significant under conditions of prolonged canopy wetness. Interception losses may account for between 10-30% of the gross annual rainfall to temperate catchments (Gash, Wright, and Lloyd, 1980) depending upon the nature of the rainfall regime. Regional variations in the absolute magnitude of the interception loss between sites are often not so much a result of variations in the rate of evaporation, but rather of the size of the canopy capacity and the proportion of the time that the canopy remains saturated (Gash, Wright and Lloyd, 1980).

Process studies of forest evaporation conducted over the past fifteen years have contributed greatly to the development of a number of models of the interception process, ranging from simple regression type models (Jackson, 1975) to the sophisticated, physically-based, data-demanding model of Rutter et al. (1975). In an intermediate position are the analytical and numerical simulation models which assume that mean evaporation and rainfall rates apply for all showers (eg. Gash [1979]; Pearce and Rowe [1981]; Rowe [1983]; Bruijinzeel and Wiersum [1987]), thereby greatly reducing the instrumentation required for predictions.

There is, however, in the case of all of these models, some debate as to their physical basis; night-time studies of evaporation rates appear to indicate that evaporation from the wet canopy is driven by advected energy and not by radiation alone (Pearce and Rowe, 1980). Furthermore, Rowe (1983) has shown that seasonal differences in interception losses are also significant. For a beach forest canopy these range from 22% in winter to 35% in summer, reflecting changes in the evaporation rate from the wet canopy. The development of direct measurement techniques (such as gamma-ray attenuation [Calder and Wright, 1986]) may go some way towards resolving these issues.

The transpiration component of evaporation is widely recognised as being of far greater complexity than the interception process as it is influenced by many more factors; climate, forest age, species, structure and soil moisture conditions all produce large variations in forest transpiration. However, Roberts (1983) has suggested that forest transpiration may actually be a conservative process; that is to say, certain processes tend to equalise annual transpiration losses between forests. A comparison of annual transpiration losses from several European forests indicated very similar annual totals (c. 300 mm p.a.); and furthermore annual totals that were far below the potential amount. This was attributed to a number of factors: the buffering effect of forest understoreys; a feedback response mechanism operating between radiation and humidity deficit, stomatal behaviour and transpiration losses; and the fact that variations in soil water content, in most cases, have a negligible effect on transpiration rates, except under severe drought conditions.

The accurate estimation of transpiration rates is complicated by the fact that the process has an atmosphere-dependant and biosphere-dependant phase. Lysimetry, energy budget methods and physically based combination approaches are generally considered to be the most reliable, with an estimation error of less than 10% for intervals such as an hour. As Knapp (1985, p 551) points out:

"*......solar radiation is the major driving force behind the evapotranspiration process, and any reasonably accurate method for computing evapotranspiration should account for it.*"

Alternative, less data intensive and reliable methods, include soil moisture measurements, catchment water budget methods, crop coefficients and empirical equations. These methodologies are all designed to produce rough estimates of actual evapotranspiration in areas for which no detailed analysis is feasible. Within the dual constraints of available instrumentation and time, the empirical approach was considered to be the most viable modelling option available.

3.3.3 Hydrology

As was indicated previously, any hydrological model that has been developed primarily as a tool for investigating the potential impacts of changes to the 'driving' climate variables should be robust, versatile, compatible with existing climate models, and (ideally) responsive to vegetation-atmosphere feedback mechanisms (Gleick, 1986). Within the context of assessing climate change impacts on hydrological systems a number of different modelling approaches have recently been adopted (EGS, 1990; Lemmela et al., 1990). These range from the empirical (eg. Arnell and Reynard, 1989), through the conceptual/ water-balance approaches (eg Gleick, 1986, 1987a/b), and the stochastic (eg. Georgakakos et al., 1989) to the physically-based distributed models (eg. Alley et al., 1989). Each of these model classes have characteristic methodological and theoretical constraints as well as advantages (Table 3.3).

As may be seen from the selected examples presented in Table 3.3, there exists a fundamental trade-off between model complexity/ detail and the accompanying data/ resource demands. At one extreme, the empirical models require relatively little input data and in return yield monthly or 'average condition' statistics based upon simple linear

METHOD	EXAMPLES	ADVANTAGES	DISADVANTAGES
Empirical models/ unit hydrograph.	NERC (1975); Arnell and Reynard (1989); Shaw (1983); Sherman (1932).	Minimal data requirement; Applicable to ungauged catchments; Limited computational requirements.	Vary considerably in accuracy; Time invariant response; Equations are catchment specific; Provide limited number of output variables; Limited process explanation.
Conceptual/ lumped models.	Nash and Sutcliffe (1970); Gleick (1986/1987a/b); Pirt (1983); Blackie and Eeles (1985);	Moderate-low data requirement; Simplification of complex processes and reactions; Highly versatile.	Assumes homogeneous catchment conditions; Representative parameter values; Identification of critical processes; Scale and calibration problems.
Stochastic models.	Gupta et al. (1986); Wood and O'Connell (1985); Georgakakos et al. (1988); Todini (1988).	Requires no hydrology!; Real-time forecasting; Application to a wide range of enviromental issues.	Divorced from real processes; Updating transfer functions/ parameter values. Long time-series required for calibration. Catchment specific.
Physically-based distributed models.	Abbott (1986a,b); Bathurst (1986/1988); Beven (1985); Moore and Clarke (1981); Rushton et al. (1982).	Applicable to ungauged catchments; Investigation of complex hydrologic problems such as land-use change; Detailed hydrologic output; Inclusion of 'real' processes; Compatible with remote sensing.	Highly data- and resource-demanding; Model calibration and validation; Problems of scale and model structure; Fitting of precise models to imprecise data.

TABLE 3.3 Alternative approaches to catchment rainfall-runoff modelling.

regression techniques. At the other extreme, the physically based models are highly data intensive, require considerable technical back-up and computational facilities, yet are able to describe the hydrological properties at all points on a three dimensional grid representation of the catchment. According to Anderson and Burt (1985) the selection of the most appropriate model-type for a given hydrological task should be influenced by the water-balance terms that are of interest, the required interval, the desired level of accuracy and the amount of *a priori* information that is available for the catchment. Whilst the availability of data will often determine which class can be chosen, the accuracy and representativeness of individual measurements will define the level of confidence that may be placed in model forecasts.

On the basis of these considerations, the conceptual approach to catchment modelling was chosen as it represents the best available compromise between model complexity/ accuracy and concomitant data requirements. As the name suggests these models are:

"quasi-physical in nature, [and] rather than using the relevant equations of mass, energy and momentum to describe the component processes of the rainfall-runoff process, simplified but conceptual representations of these component processes are adopted" (Wood and O'Connell, 1985, p 506).

Although the approach enables the representation of complex processes by a few simplified, conceptually appealing ones, a major disadvantage is that the identification and delimitation of these critical processes is purely arbitrary. Furthermore, if these models are to be successfully coupled to hydrochemical interpretations of the catchment, it is essential that the hydrological interpretations on which they so heavily depend be compatible (cf. Hooper et al., 1988). This becomes especially poignant when the number and nature of the catchment stores and pathways are to be specified. Tracer experiments have, for example, clarified the significance of 'pre-event' water - that is water residing in the catchment prior to the onset of the storm/ flood event - to the hydrological and hydrochemical responses of the watershed (Hooper et al. [1988]; Dewalle et al. [1988]). As will be shown later the model structure itself can also give rise to features within the model parameter space which seriously hinder the location of a global optimum (Wheater et al., 1986). However, the versatility of the conceptual modelling approach, coupled with the moderate - low data requirements makes this model design the most attractive option for describing the impact(s) of climate change on hydrological systems.

3.3.4 Hydrochemistry

Soil and water acidification is now generally held to occur over two different rates: in the short-term (<year), in response to snowpack melting, storm episodes and variable hydrological pathways (eg. Morris [1988]; W.W.A. [1987]; Langan and Whitehead [1987]; Bache [1984]); and in the longer-term due to the inherent soil chemical processes and to acidic deposition (Reuss et al. [1987]; van Breemen et al. [1984]). These two timescales broadly correspond to what Reuss et al. (1987) have defined as equilibrium and flux relationships.

Long-term acidification and recovery is believed to progress through seven chemical stages (Cosby et al., 1985b). The first stage, or pre-acidification phase is the steady state prior to increases in atmospheric deposition. During stage two the soil is undersaturated with respect to sulphur resulting in a lag in the increase in the strong acid anion concentrations as the soils adsorb the sulphur. Thus, continued acid depositions increase the external input of strong acid anions such as SO_4 and NO_3 and their accompanying cations (largely H and NH_4). The H-ion then exchanges place with cations such as Ca, Mg and K at sites on the surface of clay-humus complexes. These cations are in turn leached from the soil profile by the strong, mobile, acid anions (SO_4) such that there is a progressive increase in the soil and soil-solution acidities. At $pH<5.5$ the rate of loss of basic cations is further accelerated by the dissolution of clay minerals and the subsequent release of Al into solution. If the external acid load continues unabated, the exchangeable base cations in the soil become so depleted by this process that further Al can not be exchanged and the surplus begins to increase soil water and runoff Al-ion concentrations. By stage three the soil sulphate adsorption sites are filled and a new dissolved-adsorbed sulphate equilibrium is established. The flux of high concentrations of anions through the soil continues to deplete the store of exchangeable cations until a new steady state at the higher levels of atmsopheric deposition is reached by the end of phase four. Stage five is initiated when the deposition rate is reduced to its original low level and the accumulated sulphur begins to be desorbed. As the anion concentration declines, so too do the base cation, hydrogen and aluminium concentrations required to maintain the ionic balance. After the anions have returned to their pre-acidification levels, a gradual recovery of the soil base saturation occurs during phase six, and is accompanied by a rise in alkalinity. Finally, stage seven, the return to the pre-acidification steady state is not achieved until some 280 years after the intial onset of acidification!

Thus the long-term flux of acids and bases through the soil is ultimately regulated by the rate at which weathering replenishes the supply of basic cations. Even moderate levels of sulphate deposition with the subsequent increased anion flux through the soil can significantly alter the flux of base cations from the exchange sites (Cosby et al, 1985b, Reuss et al., 1987). The long-term soil-solution equilibrium will therefore be a function of the base status and sulphate/ nitrate adsorbtion properties of the soil. Superimposed upon these processes, the actual amelioration of acidity is still largely dependant upon the extent to which runoff processes influence the possibility of input-rain water mixing with the soil solutions and its degree of contact with the solid phase of the soil (Trudgill, 1988).

Unfortunately no single catchment model currently exists that adequately reconciles these short- and long-term process time-scales. However, in order to investigate the freshwater impacts of climate change it is necessary to include hydrochemical processes that operate at both these temporal scales (cf. section 2.5). The processes governing short-term fluctuations in streamwater acidity need to be included since it is at the aggregated, daily-scale that changes in the 'driving' climate variables (of precipitation and temperature) will be felt especially by aquatic biota. Secondly, it is essential that the long-term geochemical mass-balance of acidified catchments be simulated, as climate change serves to regulate the total super-annual influx of acidic compounds.

Of the four types of model reviewed by Reuss et al. (1986) and discussed in 2.4, none were considered capable of satisfactorily incorporating the two operations outlined above. For example, the Birkenes model (Christophersen and Wright [1981]; Christophersen et al. [1982]) recognises that streamwater chemistry is highly dependent upon flow, but present versions do not include a mass balance for exchangeable cations, thereby limiting the direct use of the model to relatively short-term applications. Conversely, the MAGIC model (Cosby et al., 1985a) assumes that the routing of water within the catchment is of less importance and that a detailed hydrologic model is unnecessary for long-term (>100 year) predictions of water quality (Reuss et al., 1986). Recent formulations of the MAGIC model are therefore incapable of detecting subtle changes to the hydrochemical regime arising at the sub-annual scale (such as changes in the frequency of critical streamwater acidities). A further constraint imposed on the application of either of these two conceptual models is the need for detailed data concerning the ionic composition of the precipitation and of the streamflow.

A less data intensive alternative is offered by the acid neutralising capacity, mass balance and weathering rate models such as the steady state "Trickle Down" model (Schnoor, 1984; Nikolaidis et al., 1988). This model type assumes: that the weathering kinetics are fractional order with respect to input acidity; that the base export from exchange sites is replenished by chemical weathering; and that a sulphate input-output balance exists. These assumptions have been challenged on a number of fronts (Reuss et al., 1986).

Firstly, all of these models tend to give a linear response to the input acidities. Secondly, the exchangeable base reservoir is generally equivalent to 50-200 years of deposition inputs, meaning that a new steady state would be considerably delayed. Thirdly, hydrological processes are represented by a crude mass balance relationship. And finally, even if the sulphate input-output budget may be assumed to be in equilibrium, no account is made as to how nitrate should be handled.

Despite the short-comings of the mass balance models, their main appeals of conceptual simplicity and limited input data have lead to their inclusion in management tools such as the RAINS model (Alcamo et al. [1987]; Kauppi et al. [1986]). Once the more questionable elements of the mass balance approach have been excluded, and greater allowance has been made for the role of hydrological pathways, it is argued that this conceptual framework should be adopted in order to capitalise on the dual benefits of simplicity and data efficiency. The following sections will therefore describe in further detail the specific modifying assumptions made during the design of the SCAM model.

3.4 THE MODEL PROCESSES

In the following sections detailed descriptions of the SCAM modules are provided. The complete Fortran 77 program listing for use on the HP 9000 series 300/800 computer is presented in Appendix 2. The specifications for a demonstration program written in BASICA for use on IBM compatible microcomputers may be found in Appendix 3. A summary of the key model equations and variables is presented in Table 3.4 (below).

3.4.1 The synoptic climatology sub-model

The climate module computes the following variables: the prevailing daily synoptic weather type, the chance of precipitation occurring, the precipitation amount (if any), the precipitation acidity and the daily temperature anomaly associated with the given weather type. As Figure 3.2 indicates the operation of this module is centred on the use of a probability/ transformation matrix (an example of which is shown in Table 3.1). Since this module is concerned with the generation of synthetic/ stochastic atmospheric variables it is only activated when SCAM is operating in the forecast mode; otherwise these statistics are provided by the SCAM data base (Chapters 5 and 6).

As Figure 3.2 suggests, the generation of synthetic atmospheric data is initiated by the selection of an appropriate climate scenario (cf. Chapter 8). On day one of the simulation

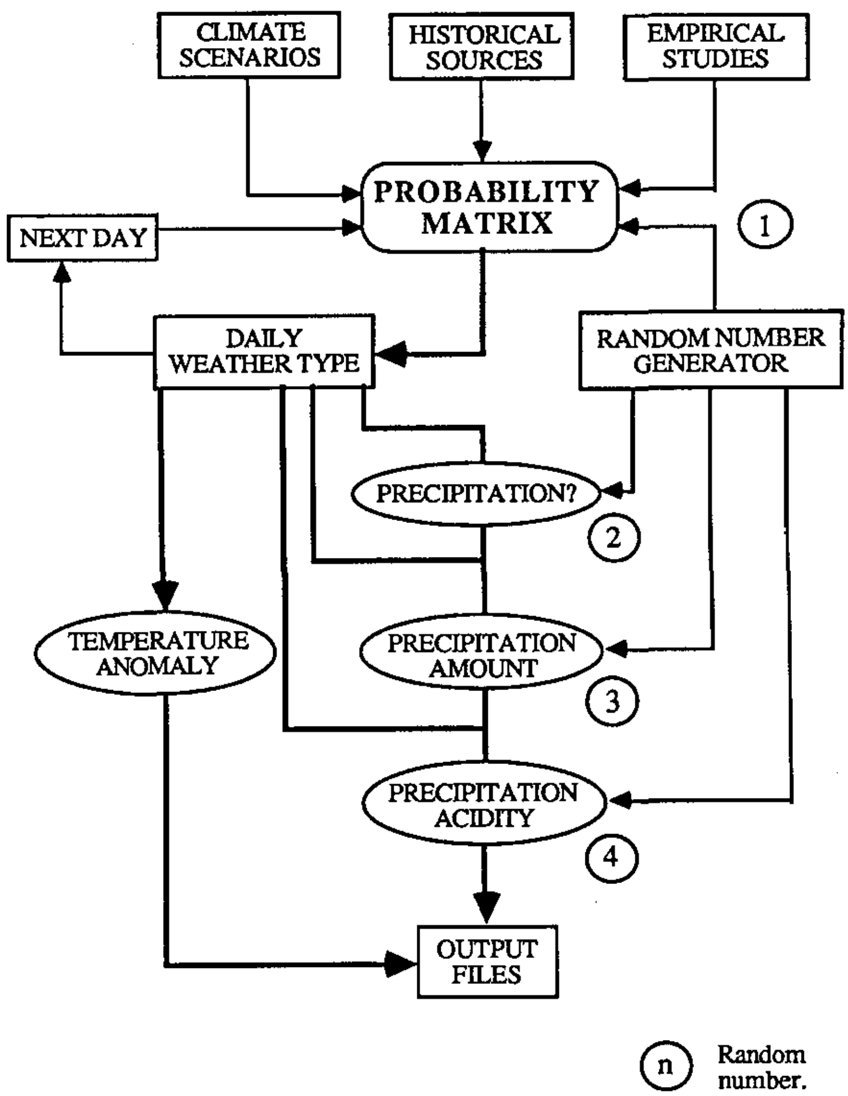


FIGURE 3.2 A conceptual representation of the SCAM model: the synoptic weather type and climate change module.

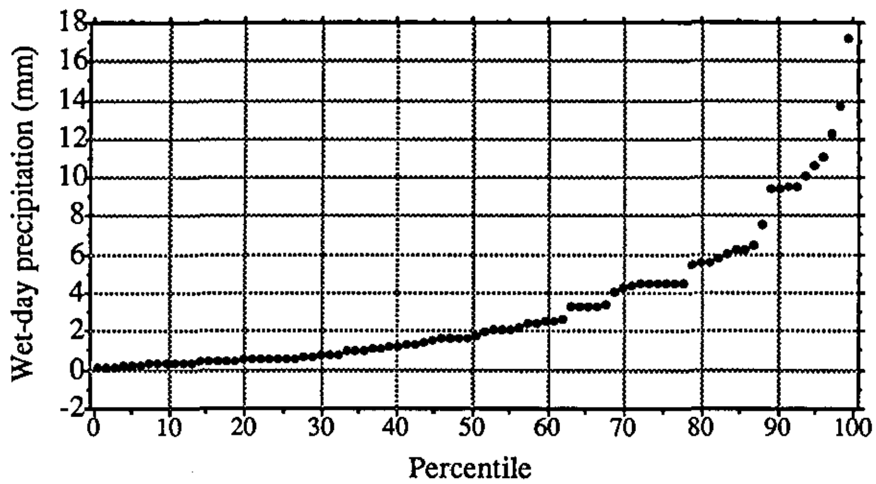
the weather type is assumed to be anticyclonic (A-type). In general, however, each of the eight weather-type categories represented in the transformation matrix (Table 3.1) has a 'variable' chance of occurrence that depends on the weather type of the preceding day. If for example, the weather-type of yesterday was the C-type (row=3), the probability of a W-type occurring on today would be 0.07 (row=3, column=2). Since each daily weather-type is a function of the weather that preceded it - a complex Markov chain - it is possible to simulate the 'blocking' situations that are associated with certain synoptic patterns. Thus, the probability of an A-type following an A-type (for the climate scenario envisaged by Table 3.1) is 0.68 (row=1, column=1), whereas, the chance of a C-type following an A-type is just 0.03 (row=1, column=3). The actual weather-type generated for any given day is determined by a linear random number generator which produces values between 0.0 and 1.0 (random number 1).

Once the prevailing weather type (or row number, Table 3.1) has been determined, it is then necessary to determine whether or not precipitation is likely to occur. The PRAIN parameter (column=10) gives the probability of precipitation occurrence for each of the eight weather-type categories. So for example, the chance of precipitation occurrence for the A-type is only 0.11, and that for the C-type 0.75. Again a random number (2) determines the exact outcome. This approach enables the simulation of 'wet-spells' associated with the persistence of rain-bearing weather-types such as the C-type. Conversely, long-periods of below average rainfall or drought conditions are simulated whenever the A-type predominates.

If it is determined that a 'wet-day' has occurred, the random number generator (3) then computes the precipitation amount of the day. The size distribution of precipitation events for specific weather-types were assumed to be exponentially distributed. Using equation [1] (Table 3.4) and the mean wet-day precipitation amount (MRAIN) for each LWT class it is therefore possible to simulate the overall rainfall distribution (Figure 3.3). For example, the probabilities that the C-type and W-types will yield a daily storm size in excess of 25 mm in any given year under present (1988-1989) conditions are 11 and 4% respectively.

Also if a 'wet-day' is indicated, it is necessary to compute the acidity of the precipitation event-day (random number 4). In general the precipitation acidity (pH) distributions are believed to be bimodal (Fowler and Cape, 1984; Martin and Barber, 1984) and this assertion was confirmed by the overall pattern for the 206 wet-days monitored between March 1988 and June 1989 (cf. Figure 6.5a). However as Figures 6.6a-c indicate there were considerable differences in the pH-frequency distributions between the various LWT classes. For example, the distributions for the anticyclonic and cyclonic types were positively skewed whilst the westerly (and south-westerly) types were clearly negatively

(a)



(b)

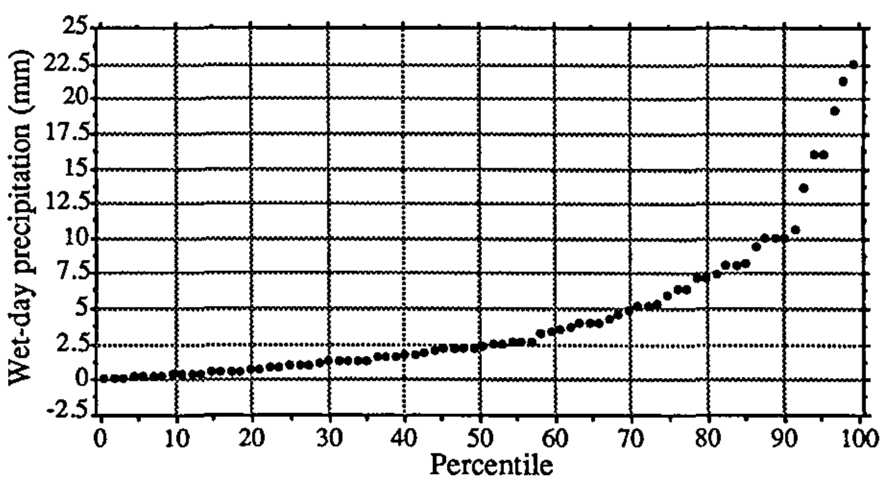


FIGURE 3.3 Wet-day precipitation amount distributions: a) westerly and, b) cyclonic weather types (1988-1989).

skewed. In view of the diversity of the histogram types encountered, second and third order polynomial equations were used to describe the cumulative frequency distributions (Figure 3.4). This approach was found to be both more convenient and computationally efficient than the use of the central limit theorem to simulate the observed normal and log-normal distributions. As Figure 3.4 reveals, the polynomial-fitting yielded highly significant descriptions of both the cyclonic and westerly precipitation acidity distributions.

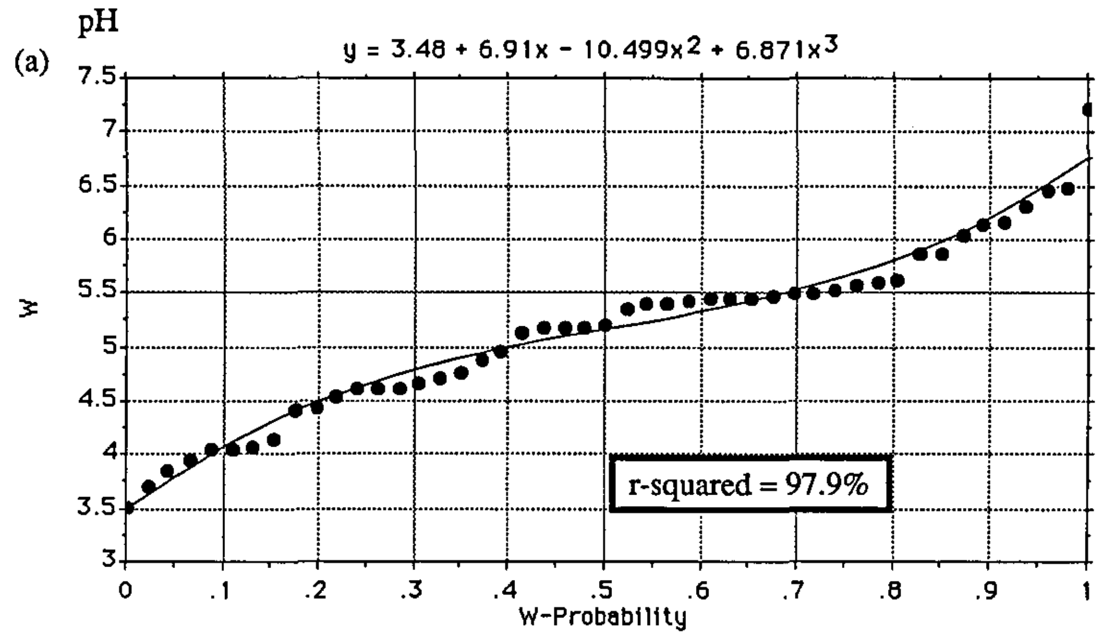
In the event of an occurrence of a 'dry-day', the acid load is given by the calibrated parameter value for the daily dry deposition amount (Table 7.2). This distribution was assumed to be time-invariant and reflects the aggregated effect of current (1988-1989) emission patterns of the regions from which each of the weather-types originate. For longer (>year) simulations the mean annual deposition rate may be linearly adjusted to compensate for any potential emission reductions.

The final operation of the transformation matrix (Table 3.1) is to yield the daily temperature anomaly (column=11) associated with each weather-type. Although, in the example, the A-type has a net TANOM value of only +0.15 (1988-1989) this annual mean obscures the fact that in the winter the A-type produces large negative anomalies and in summer, significant positive anomalies. However, this discrepancy may be offset by the seasonal weighting adjustments applied to individual mean monthly temperatures. By including daily temperature anomalies the model is able to represent the marked variations in air temperature which may occur as there is a shift in the prevailing weather-type. Furthermore, exceptionally warm/ cool months may result from the blocking activity of certain weather-types. The full importance of these 'unusual' temperatures becomes evident when the seasonal pattern of evapotranspiration is considered (see below).

Once these four variables have been generated they may be stored in a variety of different formats (daily, monthly, annual, total period statistics etc.). The entire sequence is then repeated for any specified number of daily time-steps with the output variables from each daily cycle being used to run their respective modules: temperature (evapotranspiration), precipitation amount (hydrology) and precipitation acidity (hydrochemistry).

3.4.2 The evapotranspiration sub-model

Daily potential evapotranspiration rates are computed using Linacre's (1977) equation which requires only the following variables: mean daily temperature, site latitude, site altitude, and mean daily dew-point (Table 3.4b, equs [2] and [3]). Although it is possible to compute the mean daily dew-point from an additional empirical equation, the daily



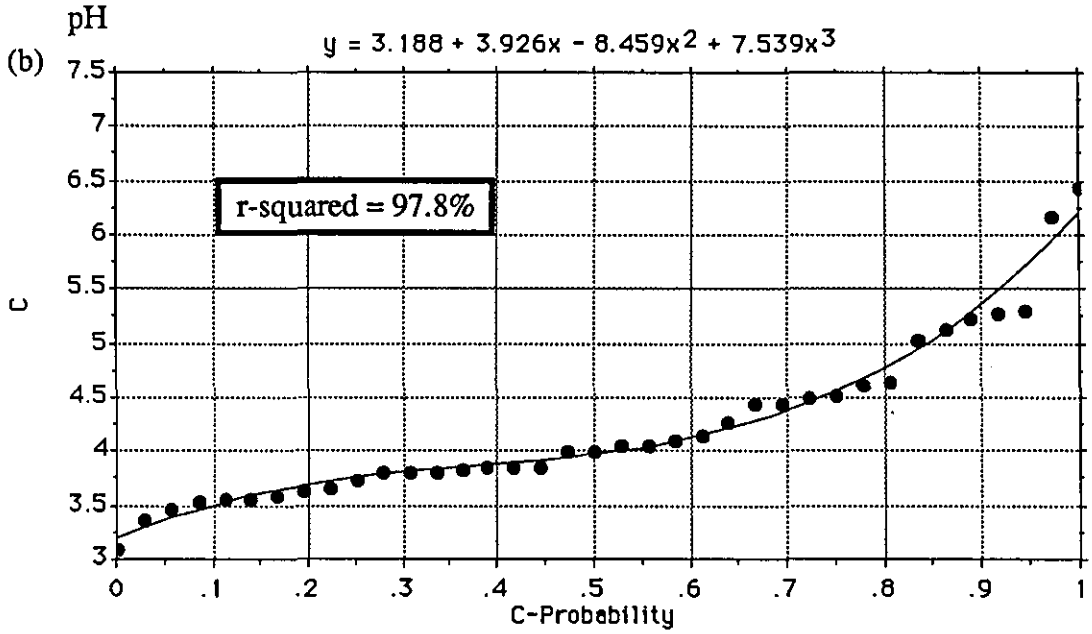


FIGURE 3.4 The pH probability distribution for (a) westerly-type, and (b) cyclonic-type precipitation (or wet) days [Loughborough, 1988-1989].

DAILY PRECIPITATION AMOUNT

$PPT_d = -Pmean*\ln(P)$ where $0 < P \leq 1$ [1]

DAILY TEMPERATURE

$T_d = [Tmean*\Delta T] + ([Tmax-Tmean]*\cos[-2\pi\{d-Dmax\}/L]) + Tanom$ [2]

DAILY EVAPOTRANSPIRATION

$$ET_d = \frac{r[2]*[\{10.64*T_d\} - 5.9]}{[80 - T_d]}$$ [3]

DAILY DISCHARGE

$SMD_d = SMD_{d-1} - PPT_d + ET_{d-1} + Q_{d-1}$ [4]

$Q_d = r[1]*((\{r[4] - SMD_d\}*r[5]) + (\{r[3] - SMD_d\}*r[6]))$ [5]

DAILY STREAMFLOW ACIDITY

$CES_d = CEC_{d-1} - \Delta H*[Hload_d + DDR_d] + r[11] + 10.0^{(6.0 - pHd-1)}$ [6]

$$BS_d = \frac{CES_d}{r[10]}$$ [7]

$$K = \frac{r[10]*\{r[12] - r[13]\}}{r[3]*r[15]}$$ [8]

$pH_d = r[13]*[BS_d*K*SMD_d]$ [9]

DAILY STREAMFLOW TOTAL ALUMINIUM CONCENTRATION

$AL_d = a + b*[pH_d] + c*[pH_d]^2$ where a, b and c are constants [10]

VARIABLE DEFINITIONS

PPT_d	Daily precipitation amount (mm)
Pmean	Mean storm size by Lamb's Weather Type (mm)
T_d	Mean daily temperature (°C)
Tmean	Mean annual temperature (°C)
ΔT	Linear temperature trend (°C/year)
Tmax	Maximum mean monthly temperature (°C)
d	Day number
Dmax	Day of maximum mean temperature (°C)
L	Wavelength of temperature regime (365 days)
Tanom	Daily temperature anomaly by Lamb's Weather Type (°C)
ET_d	Daily evapotranspiration (mm)
SMD_d	Soil moisture deficit (mm)
Q_d	Daily discharge total (mm)
CES_d	Number of available exchange sites ($\mu eq/m^2$)
CEC_d	Total number of exchange sites ($\mu eq/m^2$)
ΔH	Linear deposition trend ($\mu eq/m^2$/year)
$Hload_d$	Daily wet-deposited acidity ($\mu eq/m^2$)
pH_d	Mean daily stream acidity (pH units)
BS_d	Proportion of exchange site occupied
K	Catchment soil coefficient
AL_d	Mean daily stream total aluminium concentration ($\mu eq/l$)

TABLE 3.4a The SCAM model equations and variable definitions

Hydrological parameters:

r(1):	Catchment area (m^2).
r(2):	Evapotranspiration correction factor.
r(3):	SMD at which baseflow ceases (mm).
r(4):	SMD at which stormflow ceases (mm).
r(5):	Stormflow recession rate.
r(6):	Baseflow recession rate.
r(7):	Initial SMD (mm).
r(8):	Precipitation correction factor.
r(9):	SMD at which evapotranspiration restricted (mm).

Hydrochemical parameters:

r(10):	Total number of exchange sites.
r(11):	Daily weathering rate.
r(12):	Maximum soil pH.
r(13):	Minimum soil pH.
r(14):	Daily dry deposition rate.
r(15):	Number of occupied exchange sites.

TABLE 3.4b Listing of SCAM catchment parameters.

potential evaporation was adequately determined using a constant for the former variable (cf. Chapter 7). No attempt was made to include plant physiological controls on the evapotranspiration rate, although a very crude representation of soil moisture limiting was applied by setting the rate to zero at soil moisture deficits in excess of a predetermined threshold value.

The mean daily temperature (equ [2])is assumed to follow a sinusoidal wave-form at the annual scale, for which it is possible to define the annual mean, the amplitude, the phase displacement and the wavelength. The mean displacement of the sine-wave corresponds to the mean annual temperature. Long-term (> year) linear trends in the temperature regime are accommodated by systematically raising or lowering this mean value. The amplitude of the annual temperature regime is simply given by the maximum mean monthly temperature, whilst the phase displacement is represented by the day number on which this maximum occurs. The wavelength is set to equal 365 days. As mentioned in 3.4.1 it is also possible to weight summer/ winter temperatures so as to simulate changes to the 'extremes' of the annual temperature regime. Note that when the mean daily temperature reaches freezing point or below, the evapotranspiration rate is set automatically to zero.

From these parameters it is possible to simulate changes in the day-to-day and secular temperature regimes, and hence the daily potential evapotranspiration rate. This in turn affects the catchment soil moisture status and as a consequence the annual flow regime.

3.4.3 The hydrological sub-model

The hydrological module computes the catchment soil moisture deficit (SMD), stormflow and baseflow components on a daily time-step (equs [4] and [5]). The catchment soil-moisture store is envisaged as a single reservoir with no specific attempt being made to incorporate snow-melt or canopy processes (Figure 3.5) - experimentation with previous model versions indicated that the increased parameter dimensionality associated with an inclusion of these features was not justified by the marginal improvements made to the model's forecasting ability.

The evapotranspiration weighting factor (r[2]) is used to modify the Linacre (1977) equation so as to accommodate localised 'vegetation properties' - this parameter therefore enables a limited representation of canopy losses and 'atmosphere-biosphere interactions' etc. The stormflow (r[5]) and baseflow (r[6]) recession constants define the daily rate at which the soil moisture store is depleted by these two components of the total discharge. The stormflow SMD threshold value (r[4]) defines the moisture status of the catchment for

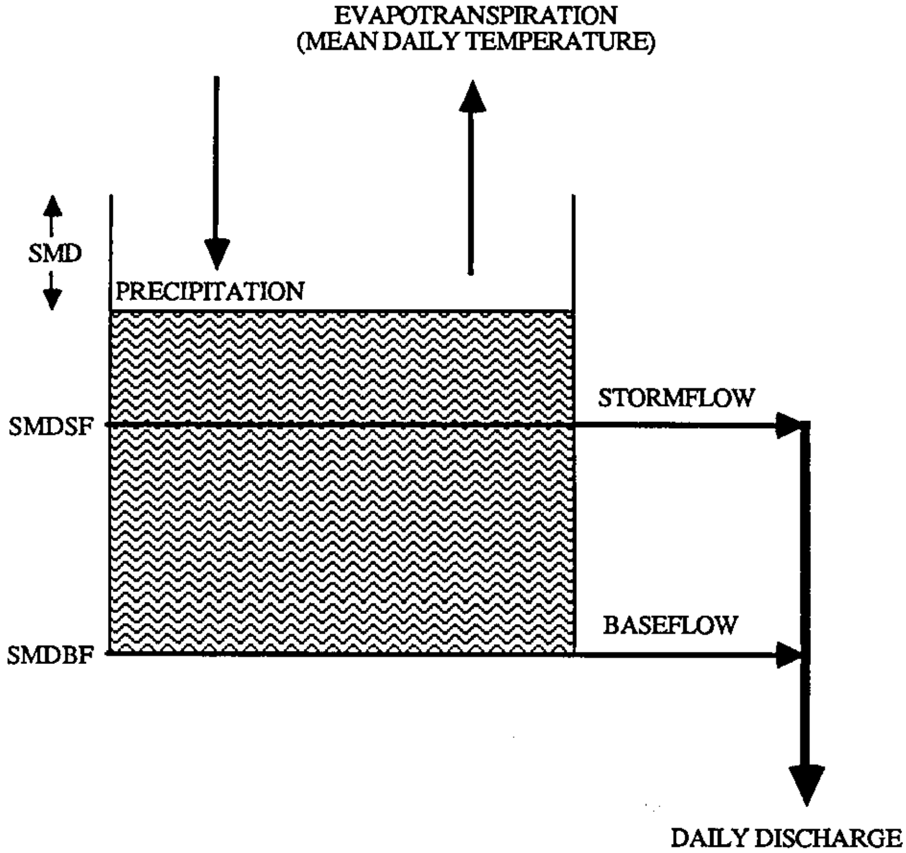


FIGURE 3.5 A conceptual representation of the SCAM model: the daily discharge and soil moisture module.

which a storm of given magnitude will not result in the production of a stormflow component to the total discharge. Similarly the baseflow SMD threshold (r[3]) identifies the point at which groundwater flow from the catchment ceases and is in effect the mean catchment storage capacity. The rainfall weighting factor (r[8]) enables the precipitation inputs to be adjusted according to the significance of local orographic effects (if the input is measured at a site outside of the catchment area). Finally, the catchment area and initial soil moisture deficit are self-explanatory (r[1] and r[7] respectively).

The daily precipitation amount reduces the soil moisture deficit whilst the daily evapotranspiration rate and discharge serve to increase it. The rate at which the two flow components release moisture to the surface channel network is inversely proportional to the overall soil column SMD (or the depth to the water-table, Figure 3.5). The stormflow component of the total discharge is envisaged not as 'rapid runoff', 'overland flow' or 'saturated overland flow' but rather as the displacement of water stored in the upper soil horizons to surface flow by the incident precipitation. This component is assumed to be equivalent to what has been termed 'near surface runoff' (Wolock et al., 1990). Conversely, the baseflow component is regarded as being 'old' water that has been displaced from deeper strata/ soil horizons by water percolating from above. The significance of these assumptions becomes clearer when the associated solute stores, pathways and ion-exchange processes are considered in the complimentary hydrochemical model (3.4.4). In the case of Figure 3.5 a dual soil-horizon situation has been portrayed, however, for more complex profiles it is possible to increase the number of threshold SMDs and flow components to represent for example, soil-piping or leaf-litter runoff mechanisms. Through a consideration of the two components of total flow the module in effect mixes discharge from two distinct hydrochemical horizons. This is not unlike the processes invoked by the End Member Mixing Analysis (EMMA) of Christophersen et al. (in press). Although the size of the "shallow soil" store (which produces the near surface runoff component) must be identified by means of parameter optimisation, summer storms that are not large enough to generate stormflow are a useful indicator of this value (Wheater et al., 1986). The size of the overall catchment store, however, must be determined from the entire discharge record. In essence the hydrological model is therefore a single conceptual store with one threshold to generate quickflow.

3.4.4 The hydrochemical sub-model

The hydrochemical module utilises the output variables of all three of the preceding sub-models to compute the mean daily streamflow concentrations of the H-ion and Al-ion, as well as the catchment soil "base-status". As the hydrological module before it, the hydrochemical model computes these variables by considering the catchment soil matrix as a grey-box system of inputs and outputs linked to daily precipitation and flow respectively. This system is envisaged as a single store whose ability to 'resist' acidification is a function of the initial base-status of the soil, the base production (or weathering) rate and the acid load to the soil (Table 3.4a, equs [6],[7],[8] and [9]). No internal mechanisms of proton production - such as the net assimilation of cations by vegetation - are thus considered by the model. The total Al-ion concentration is simply related to the computed streamflow acidity by means of a polynomial expression (equ [10]) which approximates the hypothetical cubic solubility control between the activities of Al^{3+} and H^+ (Neal et al., 1989; Driscoll et al., 1987). This ion was included within the model because of its significance to aquatic biota and ease with which it may be related to the H-ion. Had data been available for calibration purposes it would have been desireable to include Mg+Ca for the same reasons.

Fluctuations in stream water acidity are assumed to be the result of changes in a uniform soil column occurring at two distinct yet inter-related time-scales. Short-term fluctuations (daily-year) in stream water acidity reflect closely the computed soil moisture deficit (SMD) which is treated as a surrogate for the depth to the water source in the soil column. Hence when the water-table is high (ie low SMD), streamflow is predominantly composed of water draining from the highly acidic upper soil layers (cf. Figure 6.10) as well as the less acidic groundwater component. Conversely, when the SMD is high and the water table is low, the dominant source of flow is from the deep, weathered and base-rich groundwater zone. This is the main justification for viewing the streamflow as being composed primarily of 'old' water which has attained a certain degree of pH-equilibrium with the surrounding soil-matrix (3.4.3). Furthermore, this approach also enables the simulation of rapid changes in streamwater acidity that are frequently observed as a result of major storm events (cf. Figure 6.12). As Figure 3.6a indicates there was a strong linear relationship between the computed soil moisture status of the Beacon catchment and the observed streamflow acidities. The computed SMD therefore provides a proxy by which it is possible to integrate the dominant sources of flow (and hence acidity) at various stages in the hydrological year. Rather than viewing the stream chemistry as a function of two or three discrete sources as in the case of EMMA (Christophersen et al., [in press]), sources are denoted by the SMD technique as a continuum which is highly responsive to antecedent meteorological conditions.

This leads on to the second simulation mechanism representing long-term variations in stream water acidity (>year) which are considered to be a function of the chemical state of the soil. This arises from progressive changes to the base-status of the catchment soil horizons which are assumed to respond to changes in the balance between the acid-ion

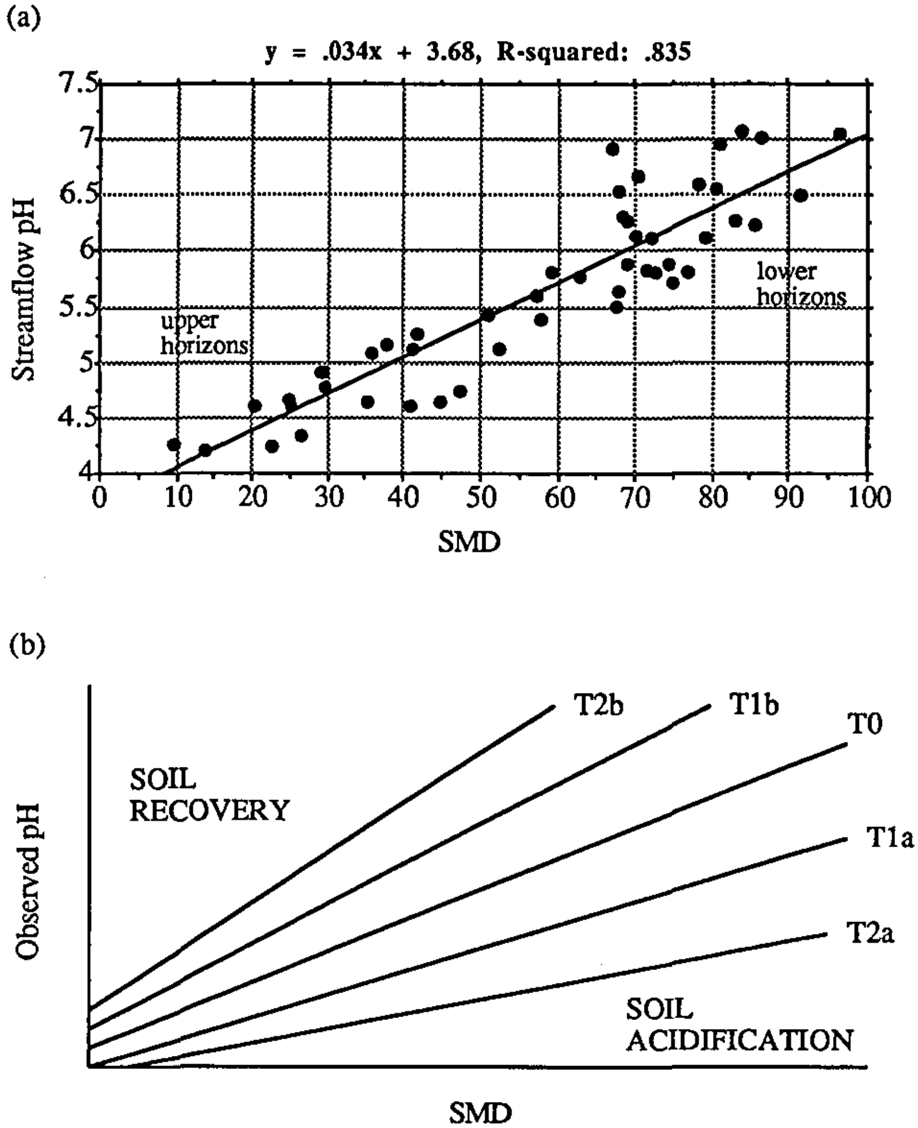


FIGURE 3.6 Streamflow acidity as a function of the computed catchment soil moisture deficit (SMD): a) short-term (<year) and, b) long-term (>year) variations

input-outputs (wet- and dry-deposition plus discharge) and, the replenishment of the base store and uptake of H-ions by the weathering of the parent material (equ [6]). This weathering progresses at a fixed daily rate (r[11]) that is independent of the base-status of the soil or of the soil/ stream water acidity. When the acid load exceeds the rate at which weathering occurs, soil acidification is under way; conversely, if the weathering rate exceeds the acid load rate, soil recovery results. Long-term changes to this ratio are introduced to the model in the form of the gradient of the SMD-stream pH relationship (Figure 3.5b): a steepening of the gradient being associated with soil recovery (eg. T0-T1b or T2a-T1a, Figure 3.6b). This process is readily conceptualised as a non-linear alteration of the soil acidity profile (Figure 6.10) in which there is a differential but systematic change in the soil pH at every depth (equs [7],[8],[9]). From equations [8] and [9] it may be seen that the form of the linear relationship is defined by the maximum and minimum observed soil acidities. The maximum streamflow acidity is assumed to occur at SMD = 0 and the minimum at the SMD value which defines flow cessation (r[5]). The constant which relates the gradient of this line to the soil base status is obtained by the calibration of the parameters r[3], r[10] and r[15] (Equation 8, Table 3.4). This constant therefore represents the physio-chemical properties of the soil matrix and ensures that the precise form of the long-term response will be catchment specific.

Finally, as a means of interpreting the short-term and secular changes to the surface water acidity in terms of the potential impact on biota, the module is able to record the frequency with which threshold values for Al-ion and H-ion are exceeded. By defining Lethal Concentration Doses (LCDs) sensitive 'biotic indicator species' may be targeted.

3.5 EVALUATION OF THE MODEL

Having presented the main working assumptions and processes included in the SCAM model it is now appropriate that these should be critically assessed and the model design evaluated within the light of existing studies. For the sake of convenience each of the four modules are discussed separately.

Two main questions arise concerning the assumptions made in the design of the climate module. First and foremost, how is climate change due to increased concentrations of atmospheric CO_2 (or for that matter any other secular trend in climatic boundary conditions) actually represented by the model ? Here the implicit assumption is made that the length of the LWT catalogue (Lamb, 1972) ensures that changes to the annual indices of key weather types are a consequence of (rather than the cause of) any long-term (>100 years) climate changes. By utilising different transformation matrices to describe different states and times in the evolution of the climate the transient nature of the atmosphere is readily simulated. This point will be discussed in greater detail in Chapter 8 within the context of establishing representative climate scenarios for the future.

The second issue concerns the supposition that the emission (and hence acidic deposition) levels are static in time. As Figure 3.7a indicates this has clearly not been the case where sulphur dioxide emissions are concerned. Furthermore, the model in its current form is unable to accommodate changes to the spatial pattern of emissions and hence to the precipitation acidities of certain weather types. Assuming that the emissions of sulphur dioxide from the U.K. will continue decline at the same rate, and that the model was calibrated against 1988-1989 precipitation data, the model forecasts must therefore be regarded as the 'worst possible' scenario. A potential exception to this would correspond to a pollution scenario in which increases to the levels of other compounds such as nitrogenous oxides (Figure 3.7b) offset the observed reductions in sulphur dioxide. By adjusting the value of the acid deposition weighting-factor accordingly, it is possible to make some allowance for these changes, and by relating this variable to the same LWT system as the precipitation acidity, the effect of changes to atmospheric circulation patterns would not be overlooked.

The previous chapter identified the potential significance of atmosphere-biosphere feedback mechanisms arising from elevated CO_2 concentrations to the catchment water balance (Aston [1984]; Wigley and Jones [1985]; Bultot et al. [1988]). Although it was suggested that the changing CO_2 levels could have a direct effect on plant biomass, respiration and stomatal conductance and hence soil moisture and streamflow, it may also be argued that these processes may in fact compensate for one another. For example, increased stomatal resistance may be offset by an increased number of stomata arising from greater Leaf Area Indices. The precise outcome of such interactive responses in terms of streamflow is largely determined by the ratio of the parameter values which are selected to represent the relevant plant physiological processes (Lankreyer and Veen, 1989). In the face of such uncertainty it is convenient to adopt the view of Roberts (1983) that the transpiration process is essentially conservative and that the annual total remains roughly the same from year to year. Andersson (1989) observes that due to negative feedbacks, the conservative nature of transpiration is described well by 30 year monthly means of potential evaporation. Only two important physical processes were shown to significantly improve model performances: the limitation of transpiration by low soil and air temperatures in spring and early summer, and the drainage of rainwater through unsaturated forest soils.

It is important to recognise that whilst the Linacre (1977) equation used in the evapotranspiration sub-model overcomes the relative complexity of the Penman formula

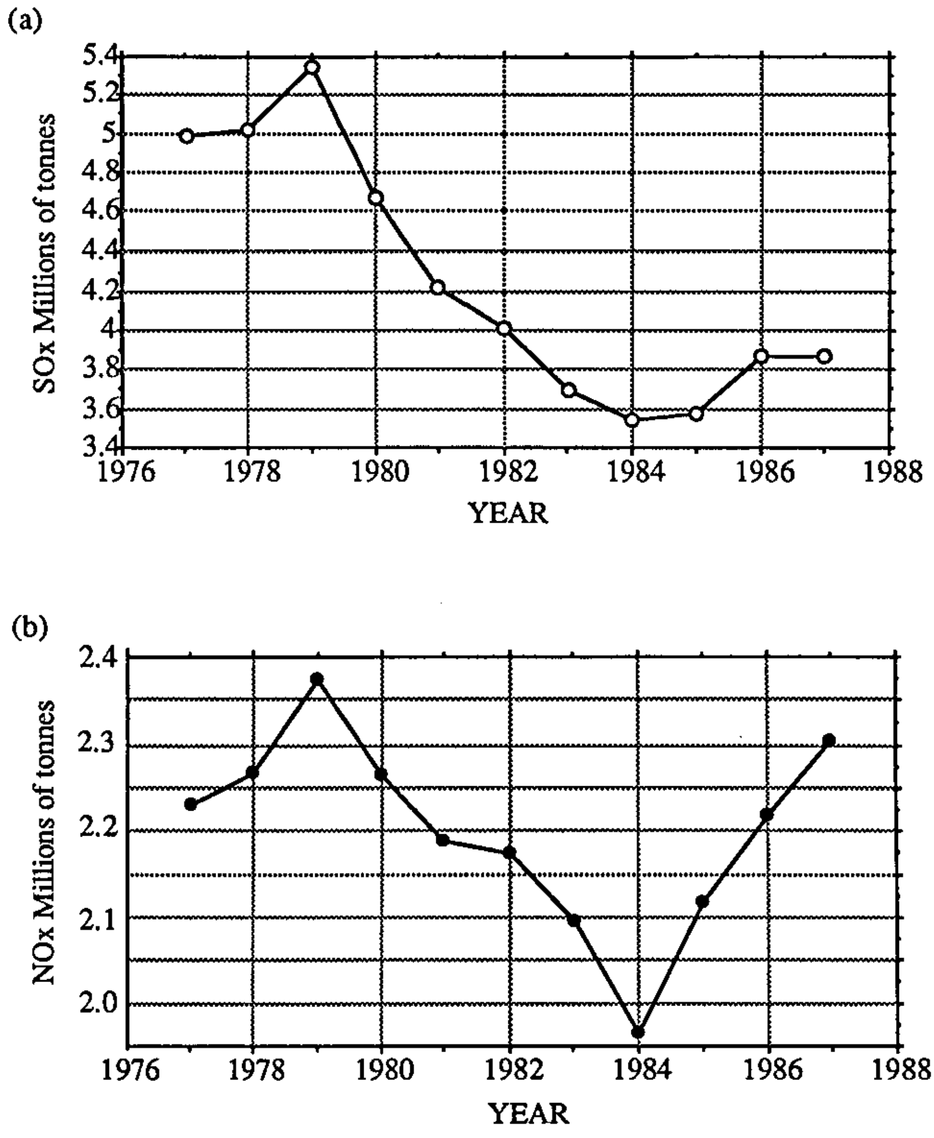


FIGURE 3.7 Total annual emissions 1977-1987 of a) SOx and b) NOx (Mt) (Source: Digest of Environmental Protection and Water Statistics, 1989, HMSO)

and its associated data requirements it only retains a physical basis by making four simplifying assumptions. Firstly, humidity is represented by a linear approximation of the saturated vapour pressure curve using a temperature function only. Secondly, the net-radiation flux-intensity is replaced by a consideration of the albedo of the surface and by a geometric modification of the global radiation flux-intensity. Thirdly, the diffusion resistance between water and air was found to be a relatively insensitive parameter that is a function of the inverse square-root of wind speed and is approximated satisfactorily by a fixed intermediate value. Finally, the psychrometric curve is represented by a chord between the mean daily and dew-point temperatures.

The reliability of empirical evaporation methods should be questioned on two main fronts. Firstly, since evaporation rates can not be measured directly, the validation of the Linacre (1977) model must inevitably rely upon indirect evaporation-pan measurements, or more sophisticated mathematical calculations (such as the eddy-correlation procedure of determining the flux of water vapour). Care should be taken in the interpretation of evaporation-pan data as uncertainties can arise from the 'oasis effect' or from micro-climatic ventilation factors that augment the pan evaporation. Furthermore, the readings have to be adjusted when rates of evaporation are required from surfaces other than a water-surface. Complex mathematical derivations of evaporation rates require considerable levels of instrumentation and it is uncertain as to the extent to which the increased complexity results in improved estimates.

Secondly, evaporation and transpiration can be highly sensitive to micro-climatic influences and may show considerable spatial variability (Knapp, 1985). Evapotranspiration estimation techniques may therefore be particularly inaccurate when transferring the empirical equations from one plant-soil community to another even under similar meteorological conditions. However, by taking field examples from a wide range of climates (and continents), Linacre's (1977) results indicate the immense versatility of the empirical equation outlined above and its robustness in the face of many varied applications. For example, on the basis of data collected from a well-watered grass plot in Copenhagen, the mean error between an evaporation pan and the equation predictions was found to be 0.5 mm per day. For the range of climates cited, the equation is consistently more accurate than the Thornthwaite procedure and only slightly less accurate than the Penman equation (a difference of approximately 0.1 mm per day).

The design of the hydrological module was also intended to obtain a fine balance between physical realism and simplicity. This has required the parameterisation of some processes most notably canopy interception losses and transpiration. The use of a single catchment store was justified on the basis of chemical/ isotopic tracer experiments conducted for other acidic watersheds (eg. Hooper et al. [1988]; Dewalle et al. [1988]; Neal et al. [1988]). For example, Dewalle et al. (1988) showed by means of a three component ^{18}O tracer model that soil water, groundwater and direct channel precipitation account respectively for 10-30%, 65-85% and 0-5% of the total observed event flows for a forest stream in the Appalachian Plateau. That is to say, the results support a 'piston flow' model of stormflow generation where stored soil water is discharged to the stream network by infiltrating event precipitation. Methods for calculating a runoff proportion (ROP) from indices of soil moisture status and precipitation amount, can therefore, grossly exaggerate the contribution made to stormflow by direct precipitation inputs. The relative amounts of soil water observed during a stormflow event does however relate to the antecedent soil moisture conditions (Dewalle et al., 1988). These findings lend credence to the decision to generate the soil water and groundwater contributions to total flow as a function of the catchment SMD. Piston flow is most conveniently simulated by treating the soil column as a single store.

In terms of applying the hydrological module to other catchment types it may be necessary to make certain stipulations. A basic requirement of all conceptually-based models is that there is a stable/ uniform distribution of vegetation, soil type and inputs due to the inherent 'lumping' of catchment characteristics. Clearly for watersheds exhibiting dynamic land-use and discharge source-area distributions, the model performance is likely to be severely impeded. This kind of model is therefore likely to be limited in its usefulness to experimental-size catchments of the order of <5 km^2. Furthermore in areas of complicated geology, non-uniform or artificially-drained soils, the computation of a mean catchment SMD may obscure the role of variable source areas.

As was stated earlier the principal concern of the hydrological module is to reproduce the gross hydrological behaviour of the catchment using minimal input data - the same argument supports the design of the single store hydrochemical module. It should also be stated that in both cases, the intention is not to reproduce the fine detail of all the known processes, but only those variables which might usefully be employed in the study of biological impacts. Hence in the case of the hydrochemical output variables, the principal concern is in the H- and Al-ion time-series (Drablos and Tollan, 1980).

In the absence of lengthy streamflow water quality data sets, the confidence placed in the reliability of model forecasts must be guaged by the model's ability to simulate contemporary conditions. From Figure 3.6a it is clear that there is solid empirical evidence linking short-term variations in streamflow acidity to the relative significance of the two components of flow (as represented by the SMD). Evidence in support of the proposed long-term changes to soil acidity profiles (Figure 3.6b) was supplied by data collected at a forest area in the south-west of Sweden from 1927 to 1982-1984 (Hallbacken and Tamm [1986]; Tamm and Hallbacken [1988]). Having accounted for the maturity of the forest stand at each site, the results indicated that between 1927 and 1982/1984 there was a reduction of 0.3 and 0.5 pH units in the humus layer (A_O) and the A_2/B horizons respectively (Figure 3.8). Although the decline in pH was not linearly distributed throughout the profile as is hypothesised in 3.4.4 (Figure 3.6) it was felt that the model assumptions provide a good first approximation of the observed changes. The departures from the hypothetical, linear-case were assumed to relate to the non-uniformity of the soil column geochemistry.

Whilst the proposed soil acidification mechanisms of SCAM clearly do not include all of the physical and geochemical processes mentioned in 3.4.4, the use of the SMD and soil profile relationships provides an efficient surrogate for many of the key hydrochemical processes which might be expected to respond to climatic change(s). The emphasis has therefore been placed upon the **hydrological controls of surface water acidity.** The inclusion of a simple cation-exchange accounting system enables the balancing of acidic inputs with their uptake/ adsorbtion by weathering products. By relating this variable base status of the soil to the overall profile acidities, the reversibility of acidification was assumed to be hysteretic rather than linear (Hauhs, 1988). The model does not pretend to be capable of explaining the fate of mobile anions such as sulphate or nitrate as this would necessitate a far more comprehensive data collection and chemical model. Thus, by means of a few relationships the hydrochemical sub-model recognises the importance of the acidic loadings, the weathering rates, base-status, size of the base reservoir and, above all , hydrological pathways that govern the short- and long-term trends in surface water acidification/ recovery.

3.6 SUMMARY

"Model building can be viewed as a sequential structuring of ideas concerning the workings of a system. It operates by the initial isolation of one or two simple components of the system under investigation followed by the study of their interrelationships" (Trudgill, 1988, p5).

In Chapter 2 the value of model building as a means of objective resource management and enquiry was illustrated using a number of topical environmental issues. This chapter has described the criteria, design assumptions, limitations and components of the hybrid SCAM model as a precursor to the calibration exercises, forecasts and simulations that follow in later sections. At each point in the theoretical development of the model an

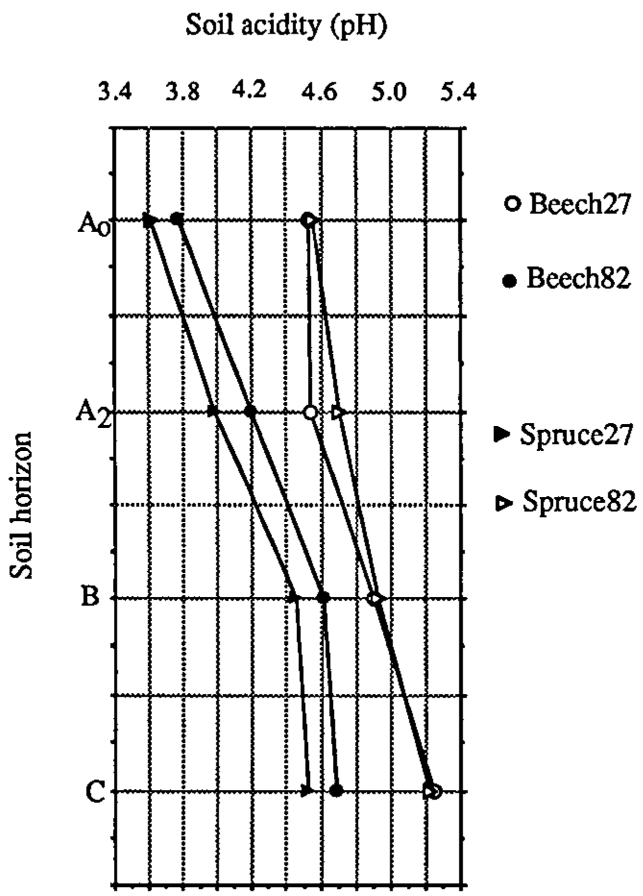


FIGURE 3.8 Changes in soil acidity between 1927 and 1982/1984 at a forested site in southern Sweden (based on data from Hallbacken and Tamm, 1986).

attempt has been made to present a range of competing ideas and perspectives alongside their concomitant resource requirements. Within the boundaries set by the often conflicting demands of theory and practise, the Shifting Climate and Catchment Acidification Model will, it is hoped, satisfactorily test the hypotheses for which it was devised. To this end the following two chapters discuss the theoretical aspects of model calibration procedures and the specific data requirements of the SCAM model.

CHAPTER 4

THEORETICAL ASPECTS OF MODEL CALIBRATION AND VALIDATION

"The degree of corroboration is a guide to the preference between two theories at a certain stage of discussion with respect to their then apparent approximations to the truth. But it only tells us that one of theories offered seems - in the light of discussion - the one nearer the truth " (Popper, 1972, p 103).

4.1 INTRODUCTION

At no point in the modelling exercise are issues concerning model structure and data set so intimately linked than during the calibration and validation stages. Once formulated the generalized structure of the conceptual rainfall-runoff model must be made site specific through the estimation of model parameters. These may have a physical basis, relating directly to catchment characteristics or conversely they may pertain to internal sub-processes operating within the catchment in which case they must be derived indirectly using optimisation techniques. In either case the model output is often largely determined by a few highly 'sensitive' parameters whose true value must be accurately determined if the model forecasts are to be reliable.

An initial sensitivity analysis of the model parameters (Figure 4.1) therefore represents a useful preliminary exercise in any assessment of the most economical techniques for collecting and using field data. Leading on from this, the quality, length and nature of the calibration data set establishes the foundation on which future predictions are ultimately based. A variety of techniques may then be employed to iteratively adjust or optimise the model parameters until the new set combines to give an 'acceptable' simulation of the observed streamflow; this entails the specification of a measure of the 'closeness' between model and catchment outputs. Finally the model must be validated using a second data set and, according to its performance additional modifications should be made to the model structure. Assuming that the performance during calibration and validation converges on a preset limit, the model and its parametric structure is then considered proficient enough (within certain bounds) to generate reliable forecasts of the system concerned. These 'bounds' which relate to the calibration and validation process will now be discussed within the framework set out in Figure 4.1.

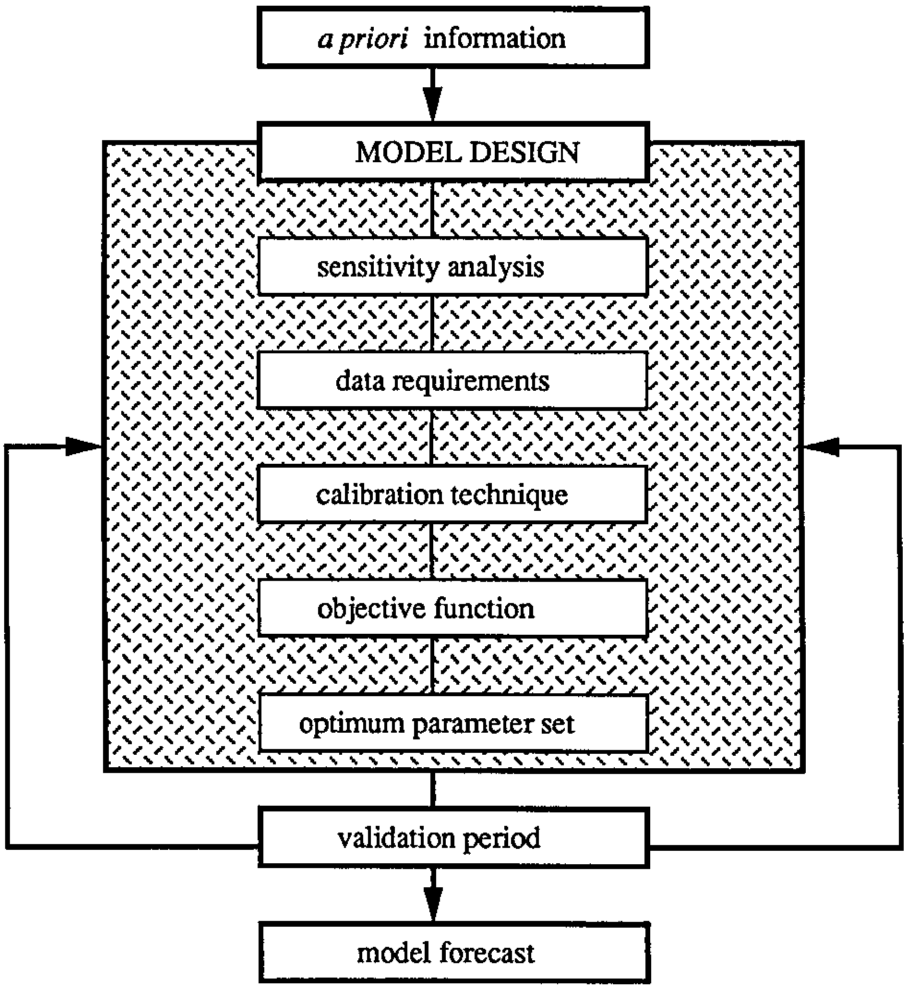


FIGURE 4.1 Stages in model calibration and validation

4.2 MODEL STRUCTURE

Sorooshian and Gupta (1983, 1985) and Gupta and Sorooshian (1985a) have pointed out the major problems associated with determining unique and consistent parameter estimates, and concluded that a major source of the problem is the poor 'identifiability' of the equations that constitute the model structure. Structural weaknesses in model design have also been linked with other aspects of the calibration methodology, namely: the indifference of the objective function to the values of threshold-type parameters; discontinuities in the response surface; and the presence of multiple, local optima (Johnston and Pilgrim, 1976).

The causes, consequences and possible solutions of structural non-identifiability have been exemplified by Gupta and Sorooshian (1983) using the percolation equation of the SMA-NWSRFS (National Weather Service River Forecast System) model. This particular model had been returning an extended valley in the response surface, making it difficult to calibrate with any precision whilst suggesting a high degree of parameter interdependence. Ideally the error function lines should be concentric (Figure 4.2a) indicating that the two parameters concerned are independent of one and another. In practise, however, a degree of interdependence will occur resulting in an elliptically-shaped response surface (Figure 4.2b). The occurrence of the worst case, the 'minimum error valley' (Figure 4.2c) in the SMA-NWSRFS model had two main implications for the calibrated version.

Firstly, the results of the calibration are highly dependent on the choice of the parameter values used to initiate automatic search algorithms.

Secondly, parameter interaction implies that there will be errors in the optimised values of other parameters which will tend to compensate for the initial error.

The most popular response to the difficult task of locating efficiently and consistently a unique global optimum, is to decrease the dimensions of the parameter space (Wheater et al., 1986). Advocates of simpler model formulations include Nash and Sutcliff (1970), Hornberger et al. (1985) and Pirt (1983). Alternatively the 'sensitivity ratio' has been proposed by Sorooshian (1988) as a means of assessing the level of parameter sensitivity and interdependence. In the case of the SMA-NWSRFS model, however, restructuring and reparameterisation of the offending equations lead to the largest improvement in the parameter estimations.

The Birkenes model of stream acidification (Christophersen and Wright, 1981) has also been investigated recently in order to evaluate the model structure. The results of a multisignal calibration methodology (Hooper et al., 1988) suggested that the hydrological

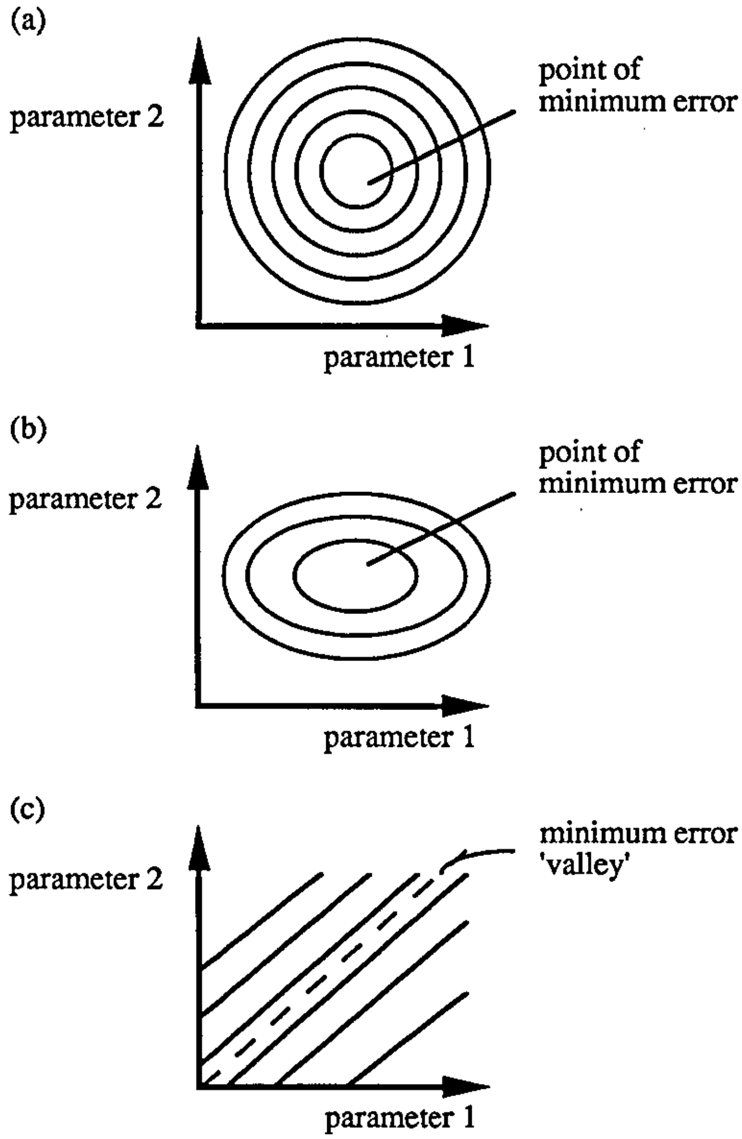


FIGURE 4.2 Relationships between parameters
(a) independence
(b) 'mild' parameter interdependence
(c) 'severe' parameter interdependence.
(Based on Kirkby et al., 1987, pp164).

model is overparameterised too, and that if the hydrologic structure of the model is to be determined from the hydrograph and a conservative tracer alone, it must be simplified to eliminate unidentifiable parameters. Considerations of model structure and parameter identifiability therefore have far reaching consequences not only for existing hydrochemical models but also for those seeking to justify more complex rainfall-runoff sub-models, since a change in one of the hydrological parameters can significantly influence the simulated streamflow chemistry.

4.3 PARAMETER SENSITIVITY ANALYSIS

A parameter sensitivity analysis is generally conducted by varying parameter values, each in turn, by a fixed amount in order to determine the effect on the model output of individual elements of the model structure. The results of a sensitivity analysis will therefore be a function of the initial parameter values, the sequence in which they are varied and the magnitude of the fixed amount. Furthermore, Gardner et al. (1980) have shown that sensitivity analyses must focus on both the importance of the parameter within the model mechanism, and on the uncertainty associated with the parameter value. Rather than using a fixed percentage change for each parameter value, new sensitivities in the model structure might be detected using the properties of the frequency distributions - such as the standard deviation of the mean - for each process parameter (Kirkby et al., 1987). Seasonal variations in the sensitivity of individual parameters should also be taken into consideration.

The advantages of conducting a sensitivity analysis at an early stage in model development are in determining which are the key parameters and which therefore merit particular attention during the collection of field data. Furthermore, two parameter sensitivity analyses may help to identify parameter interactions, regions of parameter influence and the presence of nuisance parameters (Simon, 1988). For a sensitive process parameter, the field-measurement programme should provide a sample of sufficient size to predict accurately the mean parameter value (Kirkby et al., 1987), since by implication, small changes to the true value of the parameter may lead to large errors in overall model performance. Conversely, an insensitive parameter is less affected by measurement and sampling errors, and hence requires less attention during data collection (cf. Booty and Kramer, 1984). Moreover, Pirt (1983) has advocated the omission of parameter equations that contribute little to model predictions or are infrequently activated during simulations; the General Catchment Model (Douglas, 1974) was reduced from 27 to 13 parameters. As well as increasing the parameter efficiency of the model this aspect of sensitivity analysis may also facilitate improved model identifiability.

4.4 CALIBRATION DATA

The importance of the interaction between model structure, parameter sensitivity and the type and quality of data can not be over-emphasised. Anderson and Burt (1985) considered four main areas in which the quality of information for hydrological forecasting impinges upon model operation, calibration and validation.

Firstly, the **availability** of data will determine which class or type of model may be used. It is important to recognize that the complexity of the various model classes (black box, stochastic, lumped conceptual and physically distributed) is paralleled by the size of the resource base needed to support development, calibration and operation of the model. Thus, real-time forecasts presuppose the existence of telemetry networks, rainfall radar and even satellite imagery. A major divide therefore exists between the modeling techniques and data demands of models devised for gauged and ungauged catchments. The available computational facilities and the accessible data base should also be considered within this context. However, the former case at least, may have diminished in significance with the widespread availability of relatively cost-effective and powerful desk-top computers.

Secondly, **valid** measurements should be employed, whereby conceptual model variables equate to real catchment properties such as soil moisture deficit. This aspect of the data is also particularly important when identifying realistic initial or boundary conditions prior to model calibration or simulations. In the case of parameters such as rainfall and discharge the definition is straightforward; other parameters such as the 'canopy storage capacity' are readily derived from empirical studies; whilst a parameter such as the 'maximum runoff percentage', although conceptually appealing, may actually have no 'real-world' analog or represent a range of field processes. For the latter category, Pirt (1983) applied a series of step-wise linear regressions to quantify the relationship between model parameters and a range of measurable catchment indices such as the stream frequency, catchment area or slope of the main stream. This approach effectively overcomes the problem of measurement 'validity' by tying specific catchment characteristics to otherwise, abstract model parameter values.

Thirdly, all sampling programmes must provide **representative** measurements of the parameters monitored by consideration of the temporal and spatial scales at which they are operative. Sorooshian et al. (1983) and Gupta and Sorooshian (1985) have pointed out that rather than length, the representativeness of the data set is related to the 'hydrologic variability' contained in the available information. That is to say, a data set containing a few large storm events may be less informative than a data set containing many storms of moderate size. This is because the precision of parameters improves directly as a function of the number of occasions on which a conceptual reservoir 'spills' and 'refills'. This 'switching frequency' applies to a wide range of hydrologic data-types such as storm intensity variations, inter-storm time interval and storm duration.

Hydrologic temporal and spatial scales - issues that have been the focus of much attention in recent years (eg Journal of Hydrology, August 1983; Water Resources Research, August 1986; Gupta et al., 1986) - also have a bearing upon the representativeness of catchment data. The problem arises from the fact that conceptual models must assign point measurements to non-point processes. Whilst remote sensing has the potential to facilitate a completely distributed approach to hydrologic data collection and modeling, even this tool is limited by issues such as the available ground truth measurements, pixel size, image resolution, interval between consecutive images and cost (Kite,1988). Elsewhere, it has been proposed (Dooge,1986) that there is a fundamental need to shift away from what many see as mere data fitting, to the discovery of hydrologic laws that operate at the catchment scale.

At present, however, the problem remains as to exactly when and where the point measurement(s) should be taken when faced by parameters that are temporally and spatially distributed by nature. Parameters which have received particular attention include: rainfall fields (Richards [1975]); hydraulic conductivity variations (Beven [1988]); solutional input networks (Granat [1976]); and dry deposition measurement (Pruppacher et al. [1983]). In the case of both temporal and spatial sampling, improved accuracy can of course be achieved by increasing the frequency and number of observations particularly during critical periods (such as high wind speeds, rainfall intensity or runoff). This reduces the need for temporal interpolation and has been attained to a certain extent by the advent of data-logging and telemetry networks. However, it should also be noted that there is also a point at which the collection of additional data contributes little more or nothing to our understanding of the observed process or parameter.

Bearing this in mind, Beven (1988) has explored the concept of the Representative Elementary Area (REA), a scale beyond which the hydrological response of subcatchments become more alike even though the patterns of properties (such as soil, hillslope and rainfall) differ within the catchment. This is due to the fact that as scale increases so does the sample of properties sampled in each statistically similar area. For example, the joint probability distributions, means and covariances of soil conductivity and rainfall characteristics were combined by Wood et al. (in press) using a version of the TOPMODEL to yield a REA of the order of 1 km^2 for these two mechanisms. Further beyond this scale and a new suite of conditions such as parent bedrock type tends to dominate the hydrological response. In theoretical terms, the REA therefore provides an indication of the minimum scale at which a given set of parameters will be adequately represented by a given sample density. However, the extent to which this understanding of scale and the REA will facilitate improved parameter or boundary condition estimates in samples designed for conceptual (as opposed to distributed) modeling is questionable.

Finally, the **accuracy** of field measurements must always be considered and if possible quantified at every stage of model design, calibration and validation. Assuming that the sample size and emphasis is appropriate to the spatial and temporal scale of the parameter, additional systematic and random errors may yet be introduced, particularly in the case of time-series data. For example, Rodda and Smith (1986) have examined the implications for acid rain studies of the consistent under-estimation of rainfall totals due to wind turbulence around standard rain-gauges. Similarly, Sorooshian (1988) has commented on the effects of heteroscedacity and autocorrelation in daily streamflow measurements. In the latter case, the presence of non-constant variance errors - particularly at high flows - has significance not only for flow forecasting (and consequently solute budget studies) but also for the actual calibration of rainfall-runoff models. Stochastic and systematic measurement errors have been shown to influence the shape of the response surface, with output errors producing a very rough surface with numerous local optima (Sorooshian,1988). In short, the goodness of fit cannot be better than the inherent errors and bias of the data set (Blackie and Eeles, 1985).

The available data base therefore influences the choice of the model type, the model structure, model calibration and model validation. Whilst the availability of data will often determine which class or type of model should be employed, the accuracy and representativeness of individual measurements will define the level of confidence that may be placed in model forecasts. Since all catchment models (whether hydrological or chemical) are heavily reliant for their success upon the ability to accurately describe the rainfall/stream hydrographs, the need for high quality data (of this type) is especially imperative.

4.5 CALIBRATION TECHNIQUES AND THE OBJECTIVE FUNCTION

Having considered the role of model structure, sensitivity analyses and data limitations in model formulation it is then necessary to 'fit' or test the model against observed data from the catchment to be simulated. Broadly speaking there are three main techniques of model 'fitting', namely: manual, semi-automatic, and automatic search algorithms. Each of these will be discussed in turn.

The purpose of all fitting techniques whether manual or fully automatic, is to iteratively adjust the parameter values until the response of all the model functions combine to give the best possible approximation of the observed time-series or process. By this means the model parameters are made specific to the physical properties of the system concerned. It is worth noting at this point that the parameters yielding the 'best-fit' during calibration may not necessarily result in the most accurate forecasts. Within this context Beven (1987, 1988) argues that parameter values and input data should be viewed in terms of sources of uncertainty rather than as physical values *per se*. Model forecast should ideally be accompanied by a statement concerning the level of certainty or confidence that can be placed in them (eg Rogers et al., 1985; Lee et al., 1990); this could then be incorporated directly within the decision-making process. Furthermore, without independent checks on parameter values, physically meaningless values - resulting from the effects of parameter insensitivity, internal correlations and errors in input data - may be allowed to persist, resulting in unrealistic forecasts.

Prior to the commencement of model calibration routines it is necessary to select a criteria of model accuracy - the objective function. The choice of the **objective function** itself can impact upon the shape of the response surface and is dependent upon the emphasis required from a particular catchment model. For example, the gradient of the criterion was found under identical conditions to be greatest for the Root Mean Square (RMS), intermediate for the Absolute value of the difference between simulated and observed flows (ABS) and least for the root mean squares of the Log-transformed flows (LOG) (Sorooshian, 1988). The LOG function places particular emphasis of the fit on low flows whilst the Sum of the Squares of the Residuals (SSR) is affected most by high flows. In all cases, however, when the value of the objective function reaches a turning point through the systematic modification of parameter values, the 'optimum' fit of the model generated flow on the observed discharge has been achieved.

As mentioned previously this optimum fit may be accomplished using one of the systematic approaches to parameter adjustment. The **manual calibration technique** relies upon the experience and subjective judgement of the modeller who adjusts parameter values each in turn on a 'trial-and-error' basis until the optimum fit is achieved (for example, Christophersen and Wright [1981]). Alternatively, parameter values may be estimated from available knowledge of processes or from direct measurements of the physical properties of the catchment. In either case, the main advantage of the manual method is that the analyst is able to direct the optimisation strategy according to a subjective view of how the field data should be interpreted. This overcomes a major short coming of automatic search techniques - namely there inability to reason hydrologically. It also enables the modeller to focus upon critical periods in the calibration data whilst allowing absolute control over the parameter values selected. The main disadvantage is that the method can be time-consuming especially for multi-dimensional investigations and the success or failure of the method can depend upon the initial or boundary conditions selected.

Semi-automatic approaches combine the advantages of the modeller's subjective interpretation of the data with that of a formalized 'objective' search algorithm. A recent example of this technique was discussed by Wheater et al. (1986) who used prior subjective interpretations of the discharge record to identify periods where different catchment behaviour such as baseflow recession were dominant. An objective function is then defined for each segment of the flow record that corresponds to a specific parameter. This enables the modeller to exploit the simplicity of the univariate search and by application only to tailored calibration periods results in improved performance with respect to sensitivity to structural and data errors, and convergence to the 'correct' parameter set. The method was particularly successful at retrieving the values of minor parameters which might otherwise have been lost in an objective function based on the entire flow record. On all occasions the method performed more efficiently than the Rosenbrock automatic search technique (discussed below).

Three main limitations of the technique and possible avenues of future research were identified (Wheater et al., 1986). Firstly, the actual selection and assignment of segments of flow record to specific model parameters is entirely subjective - more rigourous definitions of the segments are required. Secondly, the sequence of the parameters used in the univariate search is arbitrary, although further investigations should indicate an optimum sequence. Finally, the starting values used to initiate the optimisation strategy are again largely arbitrary.

Two of the most frequently used **automatic** or direct-search procedures include the Rosenbrock (1960) and simplex method (Nelder and Meade, 1965). To this group of methods it is possible to add a second but less popular set of derivative-based techniques (Gupta and Sorooshian, 1985).

The Rosenbrock algorithm activates each parameter in turn and commencing with the most sensitive, each parameter axis is searched until the lowest value for the objective function is located. At this point the value of the parameter is retained and the same strategy is applied to the next axis. The iteration is complete when all axes have been searched and produced a new minimum and retained their initial parameter setting (Blackie and Eeles, 1985). The method is particularly sensitive to gradients in the hyperspace topography and quickly locates the nearest local minimum. This means that the algorithm performs efficiently when the response surface resembles either case (a) or (b) in Figure 4.2. However, when the topography is less well defined and/or the boundary conditions are unclear, locally rather globally optimised parameters can be returned.

The simplex method searches the parametric space using a number of vertices that is one greater than the n-dimensional space. Thus a simplex in two dimensional space is a triangle and in three dimensions is a tetrahedron. The technique depends on the comparison of the objective function at the vertices and the replacement of the highest vertex by a new point. This new point is obtained by the reflection of the highest vertex around the centroid of the other vertices. According to whether it is less than, greater than or intermediate to the existing vertices the respective responses are to replace the highest point with the new point, conduct a second iteration or, to extend the search vector along the same line (Blackie and Eeles, 1985). Although the method searches a greater area of the n-dimensional surface than the Rosenbrock algorithm, it is just as likely to converge on a local as opposed to global optimum.

Derivative-based techniques rely upon the matrices of first and second derivatives of the gradient vectors to confirm that a minimum has been reached in the multi-dimensional parameter space. When the number of parameters to be optimised is large or when the model contains few threshold functions (ie. the hyperspace is smoothly analytic) the method performs very efficiently. However, for a data set containing errors and possible short term bias, derivative methods have been found to be especially vulnerable, and even more so when the response surface is roughly textured (Hendrickson et al., 1988).

From this brief discussion of the main optimisation techniques currently available it is clear that no single method is entirely satisfactory. Indeed, the selection of an appropriate parameter optimisation algorithm can represent yet another difficult decision facing the modeller. It is worth remembering, however, that the main differences relate to the strategy adopted in changing parameters and to testing the model against observed data. When deciding upon the type of optimisation technique required, the modeller should therefore consider other factors relating to the available computational and software facilities, the character and errors of the calibration data, the model structure and the simulation objective(s).

4.6 MODEL VALIDATION

The validation of a model can be viewed as an extension to the calibration strategy in that an objective function and a representative data set are still required to test the model within a forecasting capacity. The validation exercise is regarded by some as a form of hypothesis testing in which the combination of a particular model structure and its optimised parameters is assessed by reference to a set of independent conditions (Beven, 1988). In theory, this the stage in model development at which the model structure is either accepted fully, modified or rejected on the basis of previously specified, 'objective' criteria. In practise the model is seldom rejected out-right but rather modified in the light of any major disparities between observed and expected data.

The most common validation technique is to split the observed data set in two. The first part is used to calibrate the mode and the second to test the model's forecasting ability. This should ensure a reasonable degree of continuity in the data set whilst allowing the model to commence forecasting from a state in which the initial boundary conditions have been optimised. The validation period should then determine whether or not the chosen parameter values are conceptually realistic.

Since catchment models are often capable of producing a range of state variables (such as discharge, soil moisture status, groundwater storage and streamflow acidity) the modeller must specify the values of interest and apply the appropriate criterion of performance. A fundamental indication of the model's performance is usefully derived from a comparison made against the Zero Order Forecast (ZOF). For example, in the case of daily discharge, the ZOF for tomorrow's flow is the flow observed today - this the 'best' daily forecast with no model. Of far greater value, is to test the model accuracy under conditions of extreme or rapidly changing conditions. With reference to hydrological models, Sorooshian (1988, p30) has stated that:

"A model should be able to predict runoff, with a reasonable degree of accuracy, beyond the range of calibration and with input data exhibiting different properties than those used for calibration".

Since visual presentations of model forecasts against observed data can be deceptive, the use of a statistical test such as the percent bias (PBIAS) of the residuals is preferable. Should the model fail to meet an 'acceptable' level of performance (as defined by a suitable statistic), possible reasons for instability at this stage might include: parameter interdependence; discontinuities in the data (relating perhaps to a change of observers or instrumentation); a real change in the physical system that results in the activation of unforeseen or unmodelled processes; or model structure itself. Problems relating to the data base can be overcome by more effective quality control or by extending the data set to include a wider range of conditions. Where poor forecasts are due to the model or its parameter set, model restructuring (or even rejection) may be the only available options.

4.7 CONCLUDING REMARKS

From the preceding discussions it is apparent that the realm of model calibration and validation is characterized by a lack of standardisation. The choice of, for example, the optimisation method, objective function or validation criteria is inevitably based upon economic factors, personal experience and preferences, availability and reliability, as well as purely hydrological considerations and scientific rigour. Arising from this plethora of approaches are two main schools of thought. On the one hand there are those modellers (eg Lees et al., 1990; Rogers et al., 1985; Georgakakos et al., 1989) who attribute the uncertainty of model forecasts to errors within the data set, the actual structure of the model algorithm and to issues of parameter optimisation. The inherent assumption being that existing hydrological and catchment process theories are essentially correct - progress is therefore deemed to be heavily reliant upon advances made to overcome these numerical constraints. On the other hand, the second school of thought has argued that the whole modelling process is 'plagued' by uncertainties (eg Beven, 1987). There is also a lack of honesty about model performance and no objective means of choosing between the merits of different model types. Calls for a new paradigm in hydrological modelling have been made such that model forecasts should be regarded as being of a stochastic rather deterministic nature (Beven, 1987, 1989).

Both views are united by their common demand for a distributed approach to the collection of data and modelling of catchment scale processes. This is envisaged as occurring through increased exploitation and development of remote sensing and sophisticated ground-truth measurement devices (Sorooshian, 1988). To what extent this is (or will become) technically and economically feasible remains unclear. Either way, as Anderson and Burt (1985, p12) observe, in the final analysis:

".....data limitations may be paramount, for without good data the model must remain an untested theoretical structure rather than a reliable operational unit."

CHAPTER 5

SCAM DATA BASE

"*.......the physical geographer is educated 'through the soles of his boots'*"
(Haines-Young and Petch, 1986, p 176).

5.1 INTRODUCTION

The previous chapter emphasised the importance of assembling a valid, representative and accurate set of field measurements for model design, calibration and validation procedures. The following sections deal with the theoretical and practical aspects of data collection and analysis pertinent to the SCAM model. Because of its multidisciplinary nature, a wide variety of information sources and techniques have been employed, ranging from the direct and automated sampling of field processes, to laboratory analyses of field samples and the statistical interpretation of secondary data sources. Table 5.1 lists the main data requirements of SCAM and is conveniently divided into two main types: empirical observations concerned with short-term variations (< year); and long-term records (>10 years) which form the basis of model forecasts in Chapter 8.

Following a brief discussion of the theoretical background to the techniques involved in the assembly of each of the data sub-sets listed in Table 5.1, the main features of each of the field sites are briefly described. This section is then followed by an evaluation of the quantity and quality of the collected data and their implications for the SCAM design, calibration and forecasting potential.

5.2 METHODOLOGICAL CONSIDERATIONS

Prior to the commencement of data collection programmes it is advisable to consider the relative merits of the alternative sampling, and analytical requirements of a given field experiment. By evaluating the assumptions and possible sources of error associated with each sub-set of the SCAM data base, the level of confidence placed in, and the accuracy of individual measurements may be assessed. This section therefore provides a summary of the theoretical basis to the individual field monitoring experiments described in 5.4.

Empirical observations:

1. Daily meteorological observations.
2. Daily/hourly precipitation characteristics.
3. Daily/hourly recipitation acidity.
4. Daily/hourly stream discharge.
5. Mean daily/hourly stream acidity.

Secondary data sources:

6. Manley's Central England Temperatures (1659-present).
7. Nanpantan rainfall record (1879-present).
8. Lamb's Weather Type trends (1869-present).
9. Llyn Brianne catchments data

TABLE 5.1 Components of the SCAM model data base.

5.2.1 Meteorological factors

Whilst the SCAM model is primarily concerned with longer-term trends in atmospheric conditions, it was felt that useful insights might be gained from an improved understanding of the relative significance of the smaller-scale meteorological processes. In addition, although these insights have no direct input to the SCAM model, they do provide a basis by which the magnitude, direction and rate of inter-annual changes may be evaluated.

Numerous studies in recent years have been concerned with the effects of short-term meteorological variability on rainfall acidity (eg. Musold and Lindqvist [1983], Munn and Rodhe [1971], Wolff et al. [1979], Sperber [1987], Smith and Hunt [1977], Singh et al. [1987], Raynor and Hayes [1982]). A major objective of such studies has been to establish a definitive source-receptor relationship that can be used to evaluate the effectiveness of different control strategies (Bhumralkar, 1984). To this end, the meteorological aspects of acid rain are generally considered under the three main categories of transport, transformation and deposition processes. Meteorological data such as surface wind, upper air wind, hourly precipitation, pressure variations and temperature provide a common source of information for both empirical studies and theoretical (trajectory/transport) models alike.

5.2.2 Precipitation

The accurate *estimation* of daily precipitation inputs, both in time and space, is implicit to any hydrochemical model and therefore merits a detailed understanding of the uncertainties involved in its measurement. As Figure 5.1 suggests, numerous problems combine to reduce quantitative measurements of **rainfall at a point** to what can be best described as a good estimate of an areal process. Broadly speaking, four main categories of error may be identified: those which may be attributed to the siting and environment of the gauge; the design of the gauge itself; those that relate to the characteristics of the precipitation; and finally observer errors. These errors are compounded still further when the point values are extrapolated to provide inputs for catchment rainfall-runoff models. Each of these areas of uncertainty are now discussed in turn.

By far the most important source of error is the result of **aerodynamic interactions** between the falling precipitation, the wind, the gauge and its immediate surroundings (Ward, 1974). Since this is an area of uncertainty that may be significantly reduced by careful siting and exposure of the rain-gauge, considerable attention is normally paid to this during gauge installation. Turbulence and eddying about the rain-gauge result in an

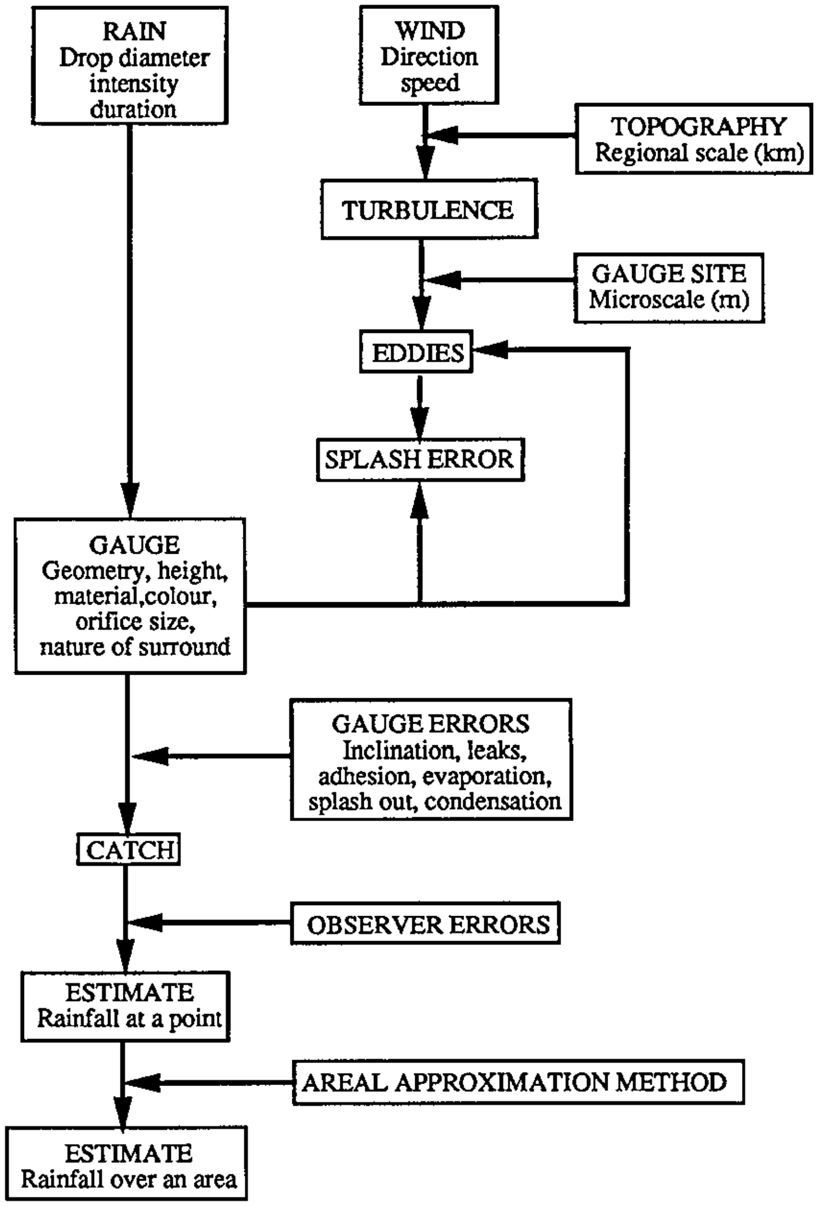


FIGURE 5.1 Uncertainties associated with point and areal rainfall measurements (based on Ward, 1974).

underestimation of the catch if the gauge is a prominent obstacle and wind speeds are high, or an excess catch if the gauge is set too low to the ground surface and insplashing occurs. For example, Rodda and Smith (1985) have shown that wind speeds as low as $4ms^{-1}$ can result in an underestimation of the rainfall catch by c.20% for a standard rain gauge. Furthermore, this loss of catch has a seasonal pattern and varies from storm to storm, being largest in winter when drop sizes are smallest and mean wind velocities are highest.

The actual **gauge design** will have some bearing on the size of the catch. Through varying degrees of eddy and turbulence generation, the gauge height is undoubtedly the most significant dimension. Comparisons between the standard installation height of 300mm (U.K.) and a properly installed ground-level gauge resulted in average catches of 6-8% less rain for the standard daily gauge (Rodda, 1967). Additional factors such as material, colour and orifice size will also influence the catch size through elevated rates of evaporation loss from the gauge funnel and from the collector inside the gauge (Shaw, 1983).

A major difficulty experienced in areas of high altitude or latitude is the accurate measurement of **snow, sleet or ice fall** into a rain-gauge. When snow has accumulated in the collecting funnel, the amount must be converted into liquid equivalents which will be dependent upon the density and nature of the snow flakes. Shaw (1988) describes a variety of techniques for measuring snowfall amounts, of which, gentle melting of the catch indoors is probably the most practicable. As in the case of rainfall, the actual efficiency of the snow catch is highly susceptible to wind turbulence and eddies. Fortunately, the East Midlands experiences snowfall on average only 15-20 days per year (or approximately 10% of precipitation events)[Atlas of Britain, 1963]. Of perhaps greater significance from the point of view of the solute flux associated with precipitation, is the incidence of dew fall, fog and ground frosts. Although the actual amount of water collected is insignificant in terms of the catchment hydrology, very high concentrations of acidifying ions are associated with these types of event. Precipitation 'types' of this kind are best grouped within the 'trace' rainfall category in terms of their ionic significance.

Finally, **observer errors** may be introduced, particularly at the point of reading the rain measure from the graduated flask or occasionally due to spillage. However, all of these errors (observer , gauge design and precipitation type) are usually small by comparison with the error due to wind and turbulence.

Having considered the possible errors of rainfall measurement at a point it is worth noting that an error of just 0.1 mm in the measured **rainfall averaged over a catchment** area as small as one hectare will result in a difference of +/- 1,000 litres! As Hall and Barclay (1975, p47) observe:

"Generally catchment rainfall derived from the normal sparsely gauged areas can only be regarded as an 'index' of rainfall, and this restricts our ability to successfully model the rainfall-runoff process."

Furthermore, due to the spatial variability of precipitation, different storm types (whether cyclonic, convectional, or orographic), the terrain and passage of storms between gauges, even dense networks can give only an approximate value of the areal precipitation. Numerous statistical techniques for calculating areal rainfall from a distribution of point rain-gauge measurements have therefore been proposed (Table 5.2) and are required by lumped and distributed catchment models alike. The purpose of all these varied methods is to maximise the usefulness of a very limited sample of the actual rainfall depth-area relationship.

In order to provide a representative sample, **gauge siting** for runoff prediction should pay attention to factors such as the size of the contributing area and the heterogenity of the rainfall over an area (Bras and Rodriguez, 1976). O' Connell (1977) makes two suggestions with respect to real-time flow forecasting given the existing network of rain-gauges in the U.K.. Firstly, it may be more advantageous to select those gauges having the strongest causal relation to river flows rather than using areal averages computed from all gauges in a catchment. Secondly, careful siting of gauges at hydrologically sensitive points within a catchment (such as the area contributing to the rising limb and peak of the storm hydrograph) might also be a more efficient means of managing a finite number of gauges. Furthermore, the 'storage effect' of catchments tends to alleviate the network design problem in that rain falling on more remote areas need not be sampled as the falling limb can be adequately simulated by an autoregressive flow component.

In summary, the main difficulties associated with point and area rainfall estimates for hydrological models appear to be best overcome by the judicious siting and maintenance of gauges at sensitive points in the catchment. Whilst estimates of areal precipitation will generally increase in accuracy as the density of the gauging network increases, the use of rain-gauge 'domains' (Catterall, 1972) defined by altitude, local relief and exposure, facilitates a more efficient usage of limited resources.

5.2.3 Precipitation acidity

The methodological difficulties associated with precipitation chemistry sampling are in many ways analogous to those of rainfall estimation and are characterised by even less

Method

1. Arithmetic mean.
2. Thiessen polygon.
3. Isohyetal method.
4. Hypsometric method.
5. Trend surface analysis.
6. Multiple regression.
7. Finite element analysis.

TABLE 5.2 Selected methods for determining areal rainfall totals (from Shaw, 1983)

Methodological difficulties

1. Network design for sampling solute fields.
2. Sampling frequency (time and space).
3. Sample collector (design, materials, site, etc.)
4. Sample component (bulk, wet-, dry-only).
5. Sample collection and storage.
6. Sample acidity measurement.

TABLE 5.3 Considerations for the sampling of atmospheric deposition.

Sample	Known value	No. labs.	Mean value	S.D.
A	6.18	17	5.45	0.74
B	6.15	18	5.53	0.76
C	6.20	17	5.54	0.52
D	6.07	18	5.56	0.41

TABLE 5.4 Results of WMORPS study (values in pH units) (based on Tyree, 1981).

technical standardisation. A list of the main problems associated with the assessment of atmospheric acid inputs to terrestrial systems is provided in Table 5.3

As in the case of rainfall estimation, the design of an adequate **network** of precipitation sampling locations will reflect the objectives of the research and the resources available. Networks have been maintained at a variety of scales ranging from the international (eg. European Air Chemistry Network [Granat, 1978]), the national (eg. Acid Deposition in the U.K. [Warren Spring Laboratory, 1987]), the regional (eg. South East England [Skeffington, 1984]) to the catchment level (eg. Trent Basin [Foster, 1987]) and address a range of issues. These include: the long-range transport of pollutants (Elliason, 1980), seasonal variations in solute inputs (Sutcliffe et al., 1982), deposition to forest canopies (Pruppacher et al., 1983) and numerous multidisciplinary catchment simulation projects (eg. RAINS model [Alcamo et al., 1987]). The extension of individual point values within larger networks to areal mean values of solute input is typically undertaken using the established techniques for the areal extension of point precipitation values (see 5.2.2), or by using spatially-weighted averages of point deposition values.

The **frequency** of sample collection in time is subject to similar considerations of scale. Studies which attempt to relate areal inputs to prevailing meteorological conditions (eg. Baker et al., 1981) are generally operated on an event-long or daily basis, and require only regional scale networks to demonstrate differences associated with prevailing air masses. Conversely, studies which focus upon the solute input contribution of a single source such as a coal-fired power station (eg. Patrinos, 1983) require a far greater number of samples both in space and time in order to detect the subtle changes. The question of the necessary **duration** of sampling required to characterize a solute deposition field relates to the area size and intra-area variability, as well as the separation of long-term deterministic trends from shorter (<1 year) random fluctuations (Cryer, 1986).

The design of an appropriate **sample collector** is in part a function of the solute 'component' of interest. For example, the most straight forward component to estimate is the 'bulk precipitation' acidity which includes wet- and dry-deposited material collected in the same container. The most popular type of bulk collector is simply a polythene funnel and bottle raised 1-2m above the ground and situated well away from tall vegetation and buildings. Considerable debate has surrounded the relative collecting efficiencies of different 'surrogate' surfaces and funnel designs (eg Dasch, 1983). These issues are particularly acute when attempts are made to separate wet- and dry-only components, and are made worse by the lack of any internationally accepted code of practise.

The **dry deposition** component is notoriously difficult to estimate being highly sensitive to the nature of the collecting surface. Furthermore, for vegetated surfaces, the rate of SO_2

deposition is known to vary according to the efficiency of uptake by stomata and cuticles and according to whether or not the canopy is wet (Fowler and Cape, 1983). Because of these practical difficulties a number of indirect estimation techniques have been devised. For example, the 'deposition velocity' represents a micrometeorological approach to the determination of the flux of gas or particles to a given surface down a concentration gradient. If the ambient concentration of pollutants, the prevailing meteorological conditions and the deposition surface characteristics are known, the dry deposition flux may be computed. However, as Businger (1986) has shown this technique is also not without its own set of sampling, instrumental and random errors which are compounded still further if the estimated dry deposition rates are extended over large temporal and spatial scales.

Unless steps are taken to rinse dry deposited material from funnel surfaces between rainfall events this can also represent a significant source of error in **wet-only estimates of acidity** (Fowler and Cape, 1984). Under certain conditions such as 'acid mists' or fog, high rates of 'occult deposition' can be accrued particularly by forest canopies (Unsworth, 1984). Due to the technical and theoretical difficulties of separating wet, dry and gaseous components of acid deposition, and the relative 'trap' efficiencies of different surfaces, the direct measurement of bulk precipitation remains the most extensively used method. Elsewhere, the dry-deposited component has been inferred from catchment ratios based upon the mass balance of conservative ions such as chloride (Wright and Johannessen, 1980).

In addition to the major difficulties involved in the collection of a representative sample of the total atmospheric acid input, further problems are involved in the **storage** and subsequent analysis of the collected samples. Precipitation samples may become contaminated in the field by small insects and bird excreta, or during transit by the sample container material. The latter problem is overcome to a large extent by the immediate laboratory analysis of the sample. However, when practical constraints require storage it is important to recognise that samples may be modified inadvertently by a range of processes such as reactions with active surface of the container, by temperature changes and by the activity of organisms present in the precipitation sample (Cryer, 1986). Whilst precipitation samples with a pH value of 4.5 or less are essentially self-preserving, Galloway and Likens (1976b) found that all samples could be 'adequately' stored in the dark at temperatures between 4°C and -4°C for a period of 7 months. Alternatively, chemical preservatives may be added to the samples, in which case great care should be taken to avoid contamination. Furthermore, a range of control tests should be conducted, comparing treated, untreated, blank, fresh and stored sample solutions.

Poor laboratory procedures with regard to sample storage and analysis can potentially offset any advantages gained in the prudent siting and maintenance of precipitation networks. Three methods for the determination of precipitation acidity are commonly applied, namely: pH, titration and ionic balances.

In a survey of 25 participating laboratories in the World Meteorological Organisation (WMO) network Tyree (1981) found considerable inaccuracy and lack of reproducibility in the pH measurements of **calibrated electrode systems**. A selection of the resulting data reports are shown in Table 5.4. Differences in ionic strength between pH buffer solutions and precipitation account for an error which is no more than 0.02 pH unit (Stum and Morgan, 1970). A significant factor contributing to the disparities shown in Table 5.4 is that the pH measures the concentration of *strong* acids plus 'some' of the *weak* acids present.

The reproducibility of **titrimetric** procedures appears to rest upon the choice of the endpoint pH, and as a consequence, the amount of weak acid measured. For example, for a titration of 50 micro-equivalents/litre of NH_4^+, with $Na^+ OH^-$, the ammonium ion would have consumed no sodium hydroxide in a titration to endpoint at pH = 5.6, but would have consumed 5 micro-equivalents/litre if the endpoint is at pH = 8.3 (Tyree, 1981).

Finally, the **ionic balance** method assumes that any charge discrepancy in favour of anions is due to the hydronium ion concentration. Clearly, this method requires that the concentration of all the principal ions found in precipitation samples (eg. Cl, SO_4, NO_3, NO_2, Na, Ca, Mg,K, NH_4) be determined. The accuracy and reproducibility of the method can therefore not exceed the degree of confidence that can be placed in the values for the individual ionic concentrations.

Tyree (1981, p58) concluded this critical review of contemporary measurements of precipitation acidity by stating:

"In the light of the foregoing analyses of the three methods, it cannot come as a surprise that the acidity data....are grossly inconsistent.....If a credible assessment of the acid precipitation problem is to be made, the first step might be to assure competent chemical advice and supervision of the data acquisition."

This lack of confidence in current analytical procedures epitomises the fundamental difficulty encountered at all stages of precipitation sample collection and of acidity measurement; namely, the absence of a standard methodology. To a certain extent this a reflection of the diversity of the issues being tackled but it is an area of uncertainty that should be resolved if any confidence is to be placed in the integrity of sample measurements and the 'inferred' effects upon biota.

5.2.4 Daily stream discharge

Having examined the main isssues concerning the atmospheric *inputs* to the SCAM model (daily temperatures, precipitation amount and acidity), the emphasis is now placed upon the catchment *outputs* (or responses). Within the context of the systems model approach, the discharge record provides a valuable source of information regarding the internal dynamics and 'mass-balancing' of the catchment ecosystem. A detailed record of the flow regime is also a necessary precursor of any attempt to explain catchment solute dynamics.

According to Herschy (1985) there are four criteria for establishing a hydrometric station: accessibility, adequacy, stability and permanency. The station should be accessible in all seasons and particularly during floods. The siting of the gauge should provide an adequate coverage of the full range of discharges that may occur. The chosen reach should ideally have: stable banks and bed alignment; a uniform cross-section and constant downstream slope; and a boundary resistance which does not vary with time as a result of vegetation growth. Finally the station should be located at a site which is unlikely to be disturbed, thereby ensuring a homogeneous and unbroken streamflow record.

Once the main requirements of a hydrometric station have been identified it is then necessary to implement a technique of streamflow measurement appropriate to that site. Comprehensive guidance and information in these respects have been provided by a number of authors (eg. Chow [1964], British Standards Institute 3680 [1983], Herschy [1985], Shaw [1988]). The actual selection of a method to employ at any proposed gauging station depends on a number of factors such as considerations of channel morphology and size, cost effectiveness and technical support. A full summary of the main decision-making factors involved is provided in Table 5.5.

A broad distinction exists between the techniques of discrete point and continuous streamflow measurement (Table 5.6). Point discharge measurements are (with the exception of dilution gauging) primarily concerned with the periodic sampling of channel flow velocities and cross-sectional areas. The instantaneous, open-channel discharge is then derived from the sum of the product of stream velocity, depth and distance between sample verticals. According to the depth and flow rate a range of velocity estimation techniques may be applied, including: use of a current meter; moving boat; or floats (British Standards Institute, 1983b). The measurement of channel depth is typically undertaken at

Governing factors

1. The available capital.
2. The size and morphology of the river.
3. The access, installation and maintenance facilities.
4. The hydraulic conditions of flow (eg. channel stability, river regime, channel geometry etc.).
5. Sediment transport conditions.
6. Operational constraints (eg. technical staff and equipment).
7. Gauging obstructions (eg. weeds, ice, log jamming etc.).
8. Data processing and telemetry facilities.

TABLE 5.5 Factors governing the choice of streamflow measurement technique (based on Herschy [1985, p8]).

Individual discharge measurements	**% Uncertainty[1]**
1. Velocity-area method	5
2. Dilution gauging	5
3. Slope-area method	10-20
Continuous discharge measurements	
4. Slope-stage-discharge or fall discharge	10-20
5. Notches, weirs and flumes	1-5
6. Ultrasonic (acoustic) or pressure gauging	5

TABLE 5.6 Methods for the measurement of open-channel discharge.

[1] Uncertainties for a single measurement of discharge at the 95% level (Herschy, 1985)

intervals of 1/15 of the width for regular and 1/20 for irregular bed profiles. Numerous methods are available for the computation of discharge from these channel depths and velocities. For example, in the case of stationary current meter measurements of velocity, discharge is calculated using: arithmetical methods (mean- and mid-section); graphical methods (depth-velocity integration or mid-section); velocity-area integration methods (velocity-contour method); and the mean section method (BS 3680 part 3a, 1980).

The dilution method (BS 3680 part 2, 1983) represents a useful alternative for gauging streams with steep gradients and high velocities, turbulent and rocky conditions. In this case measurements of concentrations of a tracer (such as radioactive isotopes or electrolyte) downstream of an injection point provides a direct discharge estimate of +/- 5% of the actual value (Herschy, 1985) without the need for cross-section data. Other modern gauging techniques derived for the measurement of flow velocity on difficult or unstable conditions include: the electromagnetic method, ultra-sonic method and the integrating float technique (Sargent, 1981). The first two developments also permit the continuous automatic monitoring of flow velocity rather than of stage (Herschy, 1985).

For many hydrological applications however, velocity area/point measurements of discharge tend to serve as a means of calibrating continuous flow measurements undertaken at fixed structures. The quasi-stable natural river section, is replaced by permanent control structures for which a theoretical and stable relation between head and discharge is derived mathematically. The choice of the actual structure design is conditioned by the range of discharges to be measured, the nature of the stream and the costs (Richards, 1982). A number of alternative designs (BS 3680 part 4h, 1986) are available to serve various purposes. For example, flumes - eg. rectangular throated, cut-throat, Parshall, Saniiri - are particularly suitable for small streams carrying a considerable fine sediment load, whereas weirs - eg. sharp-crested, thin-plate, broad-crested and rectangular - are highly versatile structures that can provide for measurements of discharges ranging from a few litres to hundreds of cubic metres per second. All of these structures are generally used for measuring low and medium flows; at flood flows increased downstream water levels can result in the drowning out of the flume or weir and the discontinuation of the stage-discharge relationship. However, within the 'modular' range flumes built to BS 3680 specifications can assess the discharge to within 1-2% without the need for any field calibration (Shaw, 1988).

For continuous records of stage upstream of the critical-flow section of a flume a means of automatically recording water-level variations is required. Conventional autographic devices involve a float in a stilling well (BS 3680 part 9b, 1981) which indirectly traces a line on a calibrated chart. Alternatively, pressure variations within the water column of the channel due to changes in stage may be used to activate a recording instrument via a diaphragm or transducer. When linked to a solid-state data-logging device, such an instrument can record and 'smooth' stage variations for any desired sampling interval.

Regular and continuous measurements of stage (whether in calibrated chart, digital or magnetic tape form) require a formalised system for the quality control or processing of data prior to its conversion to daily discharge statistics. Four major phases during which data quality can be checked (either manually or by a processing program) are typically recognised (Shaw, 1988):

(a) field data collection (check maintenance of instrumentation, reading and recording of the correct stage etc.)
(b) stream stage data (verification of unusual or extreme values)
(c) stage-discharge relation (check for shifting control or unstable channel conditions)
(d) daily discharges (check sensible agreement between rainfall and runoff records, and neighbouring catchments).

In general it is possible to detect and discard *spurious errors* attributed to human error or instrument malfunction. *Stochastic errors* cause the observations to deviate from the true mean in accordance with the laws of probability theory and may be approximated by a normal distribution. *Systematic errors* are potentially more serious - they cannot be reduced by increasing the number of observations - and if unchecked they may cause a marked error in the stage-discharge relation. Such errors may be attributed, for example, to the stage recording device.

The establishment and routine operation of an accurate gauging station therefore requires considerable forethought and rigorous procedures. Stringent criteria for the selection of a site, and the construction and installation of an appropriate gauging structure have been laid down in the International Standards; deviation from these specifications can result in considerable uncertainties arising in all aspects of continuous discharge monitoring. These uncertainties can then be introduced at the point of model calibration and verification with obvious implications for model performance.

5.2.5 Surface water acidity measurement and load computations

As implied by previous sections the catchment serves as a useful basic unit for studying the biogeochemical processes occurring within an ecosystem. Hence the estimation of solute input-output budgets for the catchment provides information for both hydrological operations - such as the origin of groundwater and rates of recharge - and for hyrochemical issues - such as land improvement by addition of fertilizers, point and areal pollution sources, and landuse changes etc. (Reynolds et al., 1987). As discussed in Chapter 3, the SCAM model is largely concerned with the input-output budgeting of the hydrogen-ion by the catchment ecosystem unit. Within this context the methodological issues associated with the monitoring of surface water acidity variations are reviewed under three main headings: sampling frameworks, ionic load computations and instrumentation. However, before commenting on the issue of solute **sampling frequencies** it should be recognised that:

"*Stream solute levels vary through time as well as in space because the catchment processes which generate streamflow and its dissolved content are dynamic rather than static in nature......stream solute levels will vary according to the hydrological pathways in operation and in response to changes in the type and rate of solute mobilization processes at different stages of the catchment water cycle*" (Walling and Webb, 1986, p 271).

The range of temporal and spatial scales of solute processes is reflected by the diversity of literature concerned with this aspect of water quality. At the global- and continental-scales broad environmental factors have been used to identify solute process-zones (eg. Gibbs, 1970; Douglas, 1972), whereas studies of spatial variations in river water chemistry at the regional-catchment scale have primarily been concerned with the effects of geology (eg. Imeson, 1973). Temporal variations in solute concentrations have also been examined at a number of different levels, for example: in relation to changes in stream discharge (Edwards, 1973); storm-period responses such as the 'flushing' and 'hysteresis' effects (Foster, 1979; Burt, 1979; Walling and Foster, 1975); diurnal oscillations in the concentrations of species such as Cl in relation to evaporation rates and water-table fluctuations (Hem, 1948); annual cycles of stream chemistry reflecting the discharge regime, summer accumulation and autumnal flushing of soluble material (Walling and Foster, 1975); long-term trends observed in species such as NO_3 (José, 1989) which often appear to be a complex response to cultivation practises; and finally, long-term catchment solute budgets and rates of denudation (Reynolds et al., 1987; Foster, 1987). From these examples it is clear that the selection of appropriate times and positions of sampling should reflect the nature of the individual study objectives. Furthermore, a clear, quantitative definition of the information required is essential to allow for a rational approach to the establishment of optimal sampling programmes (Hunt and Wilson, 1986); this in itself assumes the existence of a certain level of *a priori* knowledge about the processes to be monitored.

As an example of the significance of the sampling frequency, Walling and Webb (1982) used a detailed 5-year record of solute transport by the River Dart to show that estimates may often be only within ±10% or ±20% of the true mean concentrations for Mg and NO_3 respectively; in order to obtain an estimate within ±10% at the 95% level of confidence, sampling frequencies of 7 days and 2 days respectively would be required for these two ions. Similar results have been calculated for the Beacon H-ion concentration and presented in Figure 5.7 (section 5.4.5).

Related to the question of sampling frequency is the matter of the interpolation and extrapolation techniques adopted for the **solute load calculations** (Table 5.7). The performance of different procedures has been assessed by a number of authors: Walling and Webb (1982) found that in the case of Mg and NO_3 loads there was little difference between the extrapolation methods (rating curve vs load interval methods) although the interpolation methods (Table 5.7, procedures 4 and 5) produced the most accurate and precise results. The latter method assumes that the sampled concentration is representative of the sampling interval and calculates the total load as the sum of the products of sampled concentration and mean discharge for individual intervals (Walling and Webb, 1986).

As well as scale-factors and the level of accuracy/ precision required, the sampling programme should also be sensitive to the available resources and monitoring equipment. A number of sampling strategies are possible from which two extremes may be distinguished: random and systematic sampling. In random sampling, each time interval of the observation period has an equal chance of being sampled. The main advantage of this technique is that it provides unbiased estimates of statistics such as the mean ion concentration; however, in practise, it is an extremely inconvenient strategy to adopt for any length of time. Conversely, systematic sampling allows for the regular (hourly, daily, monthly etc.) collection of data and is therefore more suited to manual sampling strategies (Hunt and Wilson, 1986). A stratified or hierarchical sampling regime combines the advantages of both systems; periods of stasis or slow change may be sampled less intensively than 'active' periods such as occur during floods or snow-melt.

To a certain extent modern automatic data-logging systems have overcome many of the difficulties associated with the timing and frequency of sample collections/ analyses. These instruments may be pre-set to respond to an event of interest such as a flow of given magnitude, or alternatively, determinants may be monitored continuously through the use of ion-selective electrodes. The most attractive feature of these instruments being their simplicity and rapidity in providing data. However, when compared with

Method	Numerical procedure	
1	Total load = $K.(\Sigma C_i /n).(\Sigma Q_i /n)$	for i = 1 to n
2	Total load = $K.\Sigma (C_iQ_i /n)$	for i = 1 to n
3	Total load = $K.Q_r.(\Sigma C_i /n)$	for i = 1 to n
4	Total load = $K.Q_r.(\Sigma C_iQ_i) /(\Sigma Q_i)$	for i = 1 to n
5	Total load = $K.\Sigma (CiQpi)$	for i = 1 to n

Notation

K = conversion factor to take account of period of record
C_i = instantaneous concentration associated with individual samples (mg l^{-1})
Q_i = instantaneous discharge at time of sampling (l s^{-1})
Q_r = mean discharge for period of record (l s^{-1})
Q_{pi} = mean discharge for interval between samples (l s^{-1})
n = number of samples

TABLE 5.7 Load interpolation procedures (based on Walling and Webb, 1986)

spectrophotometry or atomic absorption spectrometry, the range of determinands covered by ion-selective electrodes remains relatively limited.

Referring specifically to the measurement of pH using electrodes, Mason (1985) has observed that special difficulties may arise particularly in weakly buffered solutions of low conductivity. Additionally, different commercial electrode assemblies can introduce systematic errors of up to ±0.2 pHunit due to difficulties associated with the liquid junction of the reference electrode. As has already been shown (5.2.3), the measurement of pH is characterised by a marked lack of precision and reproducibility that is largely dependent upon the individual analytical techniques employed (Tyree, 1981).

The combined effect of the uncertainties resulting from the problems of inadequate field sampling, inaccurate laboratory analysis and inappropriate computational procedures, necessitates that the calculated solute loads be viewed as estimates rather than in absolute terms (Walling and Webb, 1986). Even with the aid of sophisticated real-time monitoring systems it is apparent that it is not feasible to analyse all of the waters whose quality is of interest. A cursory glance at the previous four sections also reveals that this is equally true of meteorological observations, point and areal rainfall sampling, precipitation chemistry and daily discharge measurements. In each of these instances the complexity of the real-world situation requires that it be sampled at a finite number of discrete points in time and in space. Under these circumstances, the implementation of an appropriate sampling strategy - that maximises the cost-benefit relationship of the measurement programme - is of paramount importance to the quality and variability of the information contained in the resultant data-set.

5.3 FIELD SITE DESCRIPTIONS

Three categories of field site were utilised during the course of this study. The first, Loughborough University meteorological station provided the daily climate, precipitation and synoptic data required to 'drive' the model. The second group of sites provided the surface water quality and discharge data required to calibrate and validate the model performance. Finally, the Llyn Brianne catchments (LI1, LI6 and CI6) yielded an independent source of input-output data with which it was possible to assess the SCAM model's robustness in the face of unfamiliar catchment conditions.

5.3.1 Loughborough University Meteorological Station

Standard meteorological measurements have been conducted daily at the Loughborough University observation station (52° 46' N, 1° 11' W) since the beginning of 1988. The site is located at an elevation of 64 meters a.m.s.l. at the western end of the campus apart from major building structures and tree lines. The arrangement of the instruments complies with the specifications outlined in the Meteorological Office Observers Handbook (HMSO, 1983). Measurements routinely undertaken at the station include: daily maximum and minimum temperatures; surface pressure; precipitation amount, duration and intensity; geostrophic air-flow; daily surface wind speed and direction; and cloud-cover. Additional information regarding the synoptic situation at 12:00 is supplied for the Midlands by the European Meteorological Bulletin which is issued daily.

5.3.2 The Beacon Catchment, Charnwood, Leicestershire, U.K.

Charnwood Forest covers an area of approximately 65 square kilometres, and is conventionally defined as the area enclosed by the pre-Cambrian outcrops of the Charnian system. These rocks consist of Archaen granites, pyroclastics, quartzites and syenites which are highly resistant and rise to the surface as crags. Four main soil *associations* have been described and classified by Moore (1969). These include: the hill top 'tors' which are largely devoid of soil; the upper hillsides which are mainly brown rankers and acid brown soils of low base status; the lower hillsides which are mainly leached brown soils of higher base status and gleying; the valley floors which consist mainly of gleys.

The second field site was located within the Charnwood Forest area in the Beacon Hill catchment (Figure 5.2, Plates 1-6). This site has an elevation of approximately 150-250 meters a.m.s.l. and is situated 5km south-west of Loughborough. The catchment exhibits the first three soil associations and has an area of 66ha which is divided into the following land-use categories: bracken heathland (39%), mixed deciduous woodland (28%), open grassland (23%), coniferous plantation (6%), open deciduous and bracken understorey (2%), surface waters (<1%), and built up areas (<1%).

A tilting-siphon rain recorder and Snowdon rain-gauge have been operating on a north-facing slope at the southern edge of the catchment (Tomkinson's Farm, GR 515 142) since the start of 1988 and 1985 respectively. At the catchment outflow (Site 1, GR 521 149), stream water discharge has been gauged continuously using a V-notch weir and water level recorder since 1984. Also at this station a solid-state data-logger has been periodically installed to record hourly values of water temperature, pH, conductivity and stage particularly during periods of high flow.

In addition to the sites chosen to monitor the gross inputs (Tomkinson's Farm) and outputs (Site 1), the surface water acidity was monitored at a further six points within the catchment. The rationale behind the selection of these sites was as follows. Firstly, to maintain continuity in the monitoring programme with previous or existing studies of the Beacon (cf. Greenwood et al., 1986). Secondly, to undertake to assess the significance of spatial factors on the point acidity by comparing contrasting land-use and vegetation types. And finally, to evaluate the relative contribution to the total H-ion output made by the various zones of the catchment. A brief description of each of the Sites 1-7 is provided in Table 5.8.

5.3.3 The Llyn Brianne catchments, Mid Wales

Following growing concern over the loss of fisheries in upland Scotland and Wales a number of major studies were initiated in the UK and Scandinavia, principally under the auspices of the Surface Water Acidification Programme (Mason and Seip, 1985, 1990). Similarly a major multidisciplinary research programme was commissioned in 1984 by the Department of the Environment and Welsh Office to investigate episodically high acidity in streams of the Upper Towy catchment (Whitehead et al., 1988). Fourteen catchments were selected for intensive study in the Llyn Brianne area in order to assess the relative contribution of atmospheric and land-use factors in the acidification of surface waters, and

SITE	DESCRIPTION
1	*The catchment outlet.* Location of the gauging station, data-logging equipment and pump-samplers. Discharge is ephemeral.
2	*The stream network* (Plate 1). The point at which the mixing of the various water sources was assumed to be complete, providing confirmation of the acidity values monitored 30m downstream at Site 1. Discharge is ephemeral.
3	*The incised channel section.* A point at which to monitor flow re-emerging from a series of swallow holes, 100m further upstream. Discharge is ephemeral.
4	*The tile-drain outlet* (Plate 2). Possibly spring-fed source of base-rich flow all year round. Located at the edge of the mixed deciduous woodland zone (Plate 5).
5	*The plantation tributary.* This ephemeral source of flow emerges from a series of soil pipes and a saturated area at the boundary of the conifer and deciduous woodlands.
6	*Birches Pond* (Plate 3). The dominant source of flow is provided by a drain situated on the northern edge of the pond. Some flow is also supplied periodically by a vegetated ditch to the west. Discharges from the pond to the channel network (Site 3) are ephemeral.
7	*Frying Pan Pond.* Spring and rain-fed impoundment which may supply some seepage flow to the highly ephemeral surface drainage to the east. Situated at the foot of the Beacon summit (Plate 6).

TABLE 5.8 Beacon catchment sampling site descriptions.

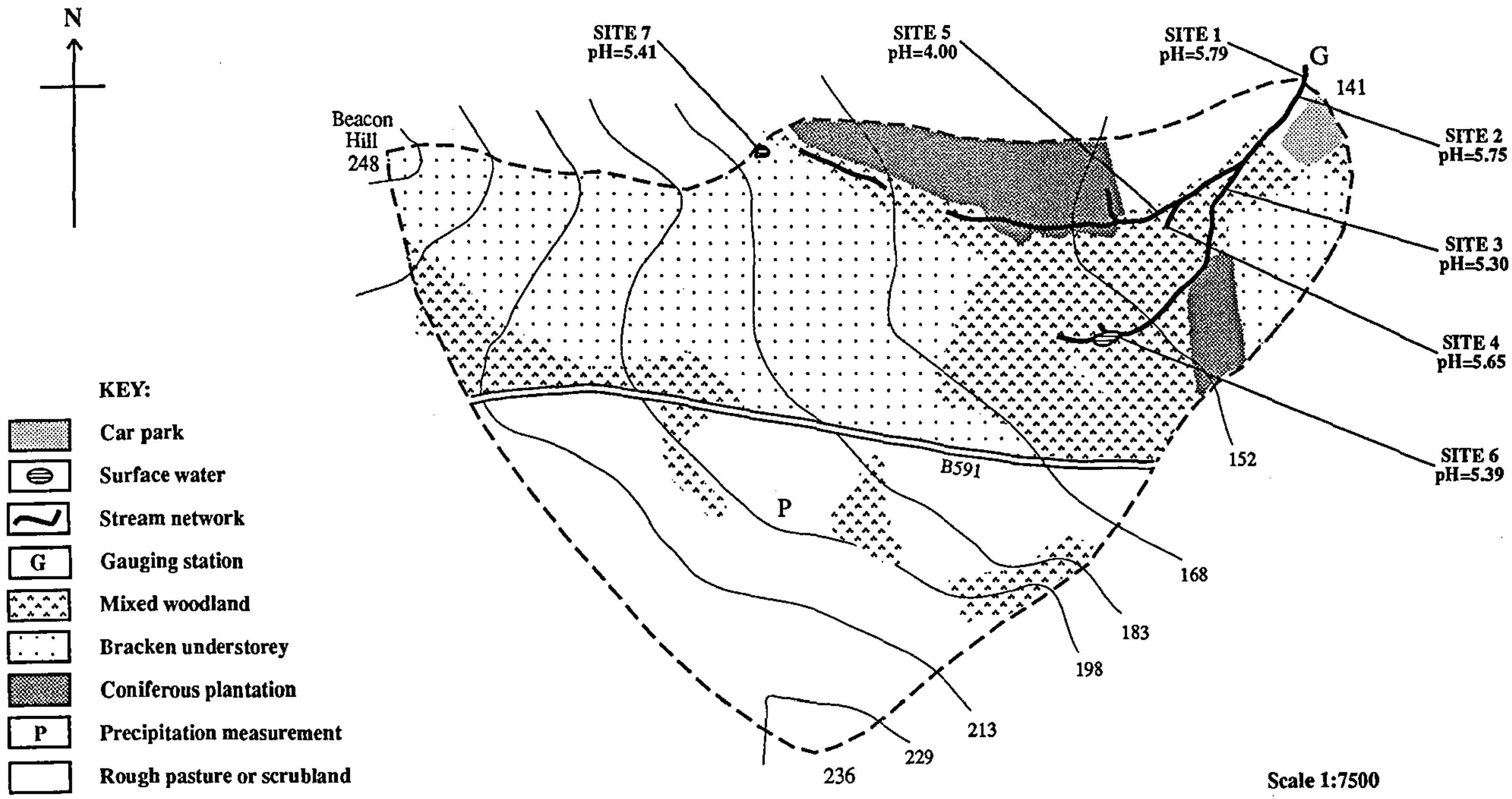


FIGURE 5.2 The Beacon catchment monitoring sites and mean surface water acidities (March 1988 to February 1989)

to develop practical solutions to the problem (WWA, 1987). Hydrometric, bulk precipitation and surface water quality data were kindly made available by the Institute of Hydrology (Jenkins, Waters and Staples, pers. comm.) for three of these catchments in order that the SCAM model might be more widely tested. A summary of basic information relating to each of these catchments is presented in Table 5.9.

All three catchments are underlain by Lower Silurian shales, mudstones and grits, with shales and mudstones dominant (Whitehead et al., 1988). LI1 is the largest of the fourteen catchments studied and comprises of brown podzolic soils, humic gleys and ferric stagnopodzols. The catchment has been totally afforested with Sitka Spruce with planting commencing in 1958. As a consequence, the storm water quality is highly acidic, with a pH averaging 4.87 and 25% of all spot samples taken registering at pH 4.6 or less. Aluminium concentrations are also very high, averaging 42 μeq/l with peak values of up to 94 μeq/l being recorded. Both these factors are thought to reflect the limited buffering capability of the drained forest floors, as well as canopy effects which tend to enhance evapotranspiration losses and the deposition of occult acidity (Whitehead et al., 1988; Hornung, 1988).

The unacidified moorland catchment LI6 is noteworthy for its high pre-storm baseflow, runoff coefficient, peak stormflows and recession limb flows relative to LI1 and CI6. These characteristics have been attributed to a combination of higher rainfall, high drainage density (2.74 km km^{-2}), compact watershed shape, lower evapotranspiration losses and the very steep channel gradients. Despite these hydrological conditions the stream acidity is very low with a mean value of pH 6.9. This arises due to the presence of calcite intrusions within the catchment which yield an abundant source of basic cations.

Finally the acidified moorland catchment CI6 is characterised by its short time to peak and high ratio of peak stormflow to pre-storm baseflow. The short response time has been attributed to the proximity of the catchments dominant contributing area to the watershed outlet. Unlike the incised channel of LI6, CI6 has a major zone of quasi-permanently saturated valley bottom peat in the lower reaches of the basin, which is capable of generating rapid runoff responses (WWA, 1987). The significance of this peak stormflow fraction relative to the moderately buffered pre-storm baseflow accounts for the very high peak acidities of pH 3.4.

PROPERTY	CATCHMENT LI1	LI6	CI6
Landuse	close canopy conifer forest control site	unacidified moorland control site	acidified moorland control site
Area (km^2)	2.55	0.735	0.607
Mean altitude (m)	441.8	437.4	410.3
Mean annual precipitation (mm)	1900	1900	1800
Channel gradient (m/km)	68	194	67
Time to peak (hrs)	3.5	3.1	2.4
Ratio peak storm:pre-storm flow	10.2	9.4	13.1
Pre-storm baseflow ($l/km^2/sec$)	24.7	43.3	17.0
Mean precipitation acidity (pH)	4.12	4.12	4.19
Mean runoff chemistry			
- mean pH	4.80	6.90	5.60
- pH range	3.4 - 7.1	3.4 - 7.1	3.1 - 6.9
- mean Ca (mg/l)	1.13	2.75	1.06
- mean total Al (mg/l)	0.36	0.07	0.10
Base saturation (%)	12.8 - 24.6	50.7 - 5.3	23.1 - 5.3
Cation exchange capacity (meq/100g)	14.45 - 3.21	16.53 - 4.40	16.53 - 4.40

TABLE 5.9 The Llyn Brianne catchments: basic hydrometric and chemical information (based on WWA, 1987 and Whitehead et al., 1987)

5.4 METHODOLOGIES

Having outlined the main features of the field sites the following discussion focuses upon the motives for their inclusion, the actual data collection procedures, some of the difficulties routinely encountered and precautions that should be observed. An additional appraisal is made in the section on secondary data of the Lynn Brianne data in relation to the SCAM model requirements.

5.4.1 Daily meteorological measurements

Comprehensive guidance and precautionary advice for all types of meteorological measurement is provided by the Observer's Handbook (HMSO, 1983). All readings were taken at a standard hour (09:00 GMT) and in a fixed order at the campus meteorological station. The 'meteorological day' is regarded as beginning at 09:00 GMT and lasting until the same time on the following day. Since rainfall and mean daily temperatures are the main inputs to the SCAM model (rainfall acidity aside) it follows that the hydrological day (and the mean daily stage, discharge acidity etc.) are also computed for this daily time interval.

Maximum and minimum daily temperatures are required to derive the mean daily temperature which in turn is used to compute the daily potential evaporation rate (cf. chapter 3). The sheathed-pattern maximum thermometer depends for its action on a small restriction in the bore of the tube, which splits the mercury column when the temperature falls below the highest temperature since it was last set. The minimum thermometer is a sheathed thermometer of the spirit-in-glass type which draws a dark marker towards the bulb as the temperature falls, and remains stationary at the lowest point reached as the temperature rises. The most common error encountered in the use of such thermometers is to misread the scale by +/- 5 or 10 ^{0}C; this would result in computed potential evaporation errors of 0.93 and 2.01 mm/day respectively. For an accuracy of +/- 0.1 ^{0}C in the reading of the daily temperatures the error is 0.09 mm/day.

Daily **pressure** (in millibars) was measured at 09:00 GMT using an open-scale barograph maintained in the meteorological station. From the daily readings the change in pressure was calculated for 24 hour intervals. The barograph requires little attention beyond changing the chart every week and ensuring that the pen is still working. The setting of the pen on the scale may be periodically checked against Met. Office regional forecasts.

The daily surface wind direction and wind speed should be measured at a standard height of 10 metres above the ground in open situations. The surface **wind direction** was estimated using a wind vane on a nine sector scale (eg. N-NE, NE-E,..etc.) where the ninth category refers to days for which the airflow was extremely weak and variable. This convention was adopted in preference to a 16-point degree scale as the objective of the measurements was to assist in the classification of the daily synoptic situation into the appropriate Lamb's Weather Type (chapter 3).

The mean daily **wind speed** was recorded using a cup counter anemometer fixed at an effective height of 2 metres - this required a correction to the standard height by a factor of +25%. With the exception of easterly winds, the the wind speed measurements were regarded as being highly representative of the surface run of wind and therefore a good indication of the 'ventilation factor' with respect to ambient pollutant concentrations. The wind fetch of easterly winds may be slightly underestimated due to the proximity of a tall hedge situated at the eastern edge of the station.

Finally **cloud cover** or cloud amount was estimated in oktas where 0 represents a completely cloudless sky and 8 a sky which is completely covered. An additional code figure 9 is reported when ever the sky is obscured due to fog or falling snow. The values assigned were a purely arbitrary record which can also assist in the classification of the daily weather type.

As previously mentioned, the European Meteorological Bulletin provided the basis of the daily **synoptic** and weather classifications. These charts were particularly useful for back-tracking pollutant 'episodes' to their general region of origin and proved invaluable in the classification of individual precipitation events. The meteorological data were divided into two sub-sets: wet- and dry-days, and then further subdivided into eight main Lamb's Weather Type (LWT) categories. Comprehensive guidance for this latter exercise is provided by Lamb (1972) who has detailed the characteristic surface synoptic features of seven main groups and a further twenty hybrid types (as discussed in Chapter 2). However, for the purpose of classifying the rainfall data described in 5.4.2 and precipitation acidities in 5.4.3, eight main LWT classes were selected. These were the cyclonic, westerly, anticyclonic, northerly, north-westerly, southerly, south-westerly and remainder. Having assigned each rain-day and its associated meteorology to one of these classes, the mean precipitation amount, probability of rainfall occurrence, precipitation acidity, H-ion load (in microgrammes per square metre) and daily wind fetch were than calculated (cf Chapter 6).

5.4.2 Precipitation

The daily precipitation amount is one of the key driving variables of the SCAM model, being essential for hydrological and geochemical simulations alike. The rainfall depths, intensities, durations and intervals between events are also of particular interest and represent a major component of the analogue approach mentioned previously (Chapter 2).

For both of the field sites it was assumed that the greatest errors are associated with wind and turbulence reducing the precipitation catch, and that through careful gauge siting these uncertainties may be minimized. Four gauges were involved, covering a catchment area of less than one square kilometre. The precise area of the catchment (in terms of the total volumetric inputs and outputs of precipitation) was determined using the contours of a 1:25,000 Ordnance Survey map (Sheet no. SK 41/51) and numerous visual surveys of the terrain. Having defined the superficial topographic boundary of the catchment, the area was calculated using tracing paper and a scaled grid underlay. The estimated area of 66.2 Ha was within 5% of previous values derived for the catchment (Greenwood, pers. comm.)

At both the meteorological station and Thomkinson Farm sites a tilting-siphon rain-recorder and one Snowdon rain-gauge were installed. Both sites were well-drained and the instruments regularly checked and maintained. Although situated at the centre of an open field, the Beacon gauges were not considered to be over-exposed due to the sheltering effect of the steep slopes. The gauges were also within 500 metres of what was deemed to be the main contributing area of the surface runoff, and within 800 metres of the discharge gauging station (see below). The tilting-siphon gauge recorded the timing, duration and approximate amount of rainfall at hourly intervals for a week; the Snowdon rain-gauge provided the actual rainfall amount and a means of calibrating the tilting-siphon recorder's trace. The Beacon gauges were checked once a week; those at the campus meteorological station daily. Any precipitation amount (including that arising from fog, condensation or very light rain) which was less than 0.05 mm was recorded as 'trace'.

As Figure. 5.3a indicates, the running total of inputs for the two sites are in close agreement (R^2 = 99%) as are the individual events (Figure. 5.3b) even though they are separated by a distance of 5km. The running total for the two sites consistently differs by approximately 10% whilst on average less than 5% of precipitation events were detected at one site only.The differences between the two sites was explained in terms of the site elevations - the Beacon is 134m higher - and in terms of local variations in aspect and in site exposure. This implies that with an appropriate 'weighting factor' of 1.1 the daily precipitation record of the meteorological station was readily (and conveniently) available as

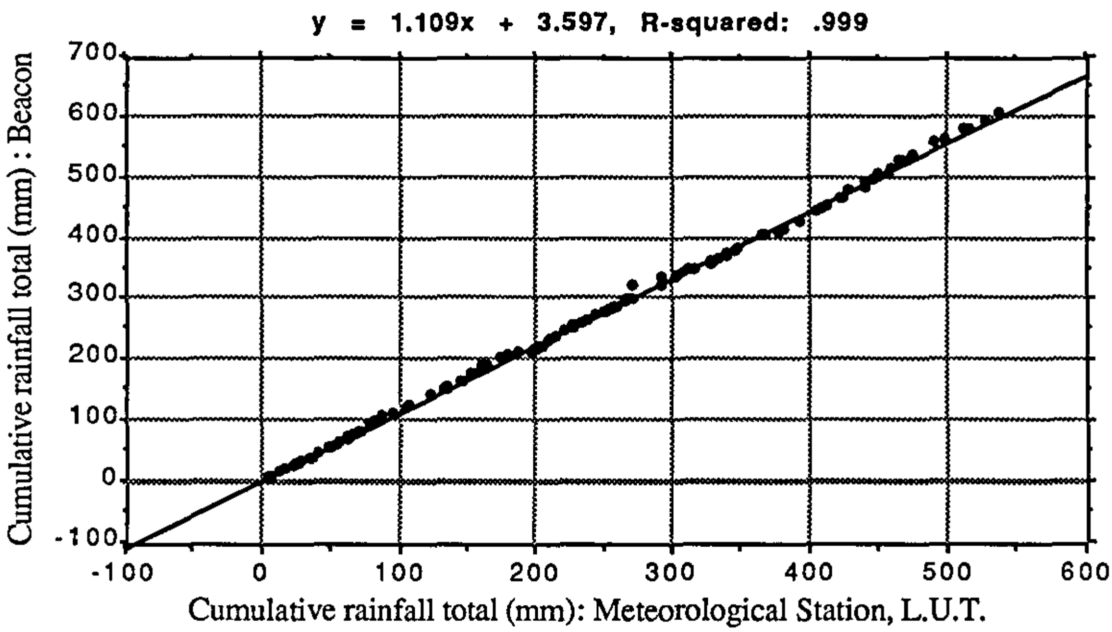


FIGURE 5.3a Comparison of the cumulative rainfall totals of the Beacon and Meteorological station, Loughborough (Mar 88-Jun 89).

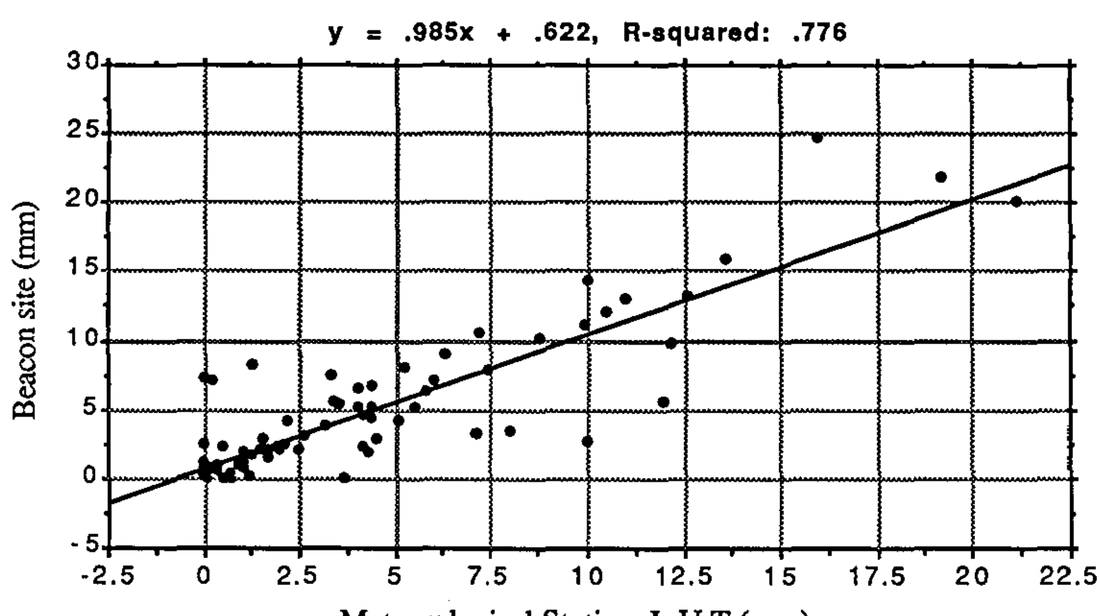


FIGURE 5.3b Comparison of the event rainfall totals for the Beacon and Meteorological station, Loughborough (Mar 88-Jun 89)

a source of input data for simulations of the 5km distant catchment. Furthermore, due to the limited areal extent of the catchment and the proximity of the Thompkin's Farm site to the main outflow point, the Snowdon catches at this site were considered to be particularly representative of precipitation inputs to the entire basin and therefore suitable for use in SCAM model calibration and validation.

5.4.3 Precipitation acidity

A record of the regional precipitation acidity was constructed on the basis of samples collected at the campus meteorological station (5.3.1). The site is well positioned for the collection of samples derived from a variety of sources (urban, rural, industrial, power generation and oceanic). Additional, complimentary information was provided by the meteorological observations also recorded at this site. The resultant precipitation amounts and acidity (in conjunction with published dry-deposition rates for the region [Warren Spring Laboratory, 1987]) provide the *regional acid load* input to the SCAM model and its temporal relation to the prevailing synoptic patterns.

According to the rainfall record each meteorological day was assigned to one of three precipitation categories: rainfall, trace, or dry. On days for which a **precipitation** amount of 0.05mm or greater was recorded by the Snowdon gauge, a precipitation sample was taken from each of two bulk collectors. These polythene bottle and funnel kits were housed in a protective box raised approximately 1.5 metres above the surrounding ground-level. A sample of the collected precipitation was transferred to a 'sterile' , 25 ml polythene bottle for subsequent laboratory analysis. If any sign of contamination was evident in either the funnel or collection bottle the entire sample was discarded. Having emptied the bulk collector, the funnel and bottle were then thoroughly rinsed with deionised water and replaced. The bottle was also routinely inspected and cleansed of any traces of algal growth.

Days which were included in the **trace** category typically represent conditions of very light rainfall (<0.05 mm), or condensation collected as a result of fog and mist droplets, frost or dewfall. As in the case of rain-days a 25 ml sample was taken, the kit was then rinsed with deionised water and replaced.

On days for which **no precipitation** was recorded, the funnels of the bulk collectors were 'washed' with 25 ml of deionised water and the 'rinse solutions' (incorporating a sample of dry-deposited material) were taken for analysis. By adopting this procedure, the contamination of 24-hour precipitation samples by dry-deposition between events was reduced to a minimal level. The actual precipitation sample collected after a dry spell may then be considered 'highly' representative of the actual precipitation event.

Regardless of the precipitation category, the 25 ml samples were immediately transported to the laboratory for analysis or cold (4°C), dark storage. Approximately 75% of all samples were analysed within 6 hours of their collection, and 90% within 48 hours. No samples were stored for longer than 7 days, a period well within the 7 month limit previously identified (5.2.3).

In all cases, the precipitation (and rinse) sample acidity was measured using a CORNING 120 pH Meter and Probe. The instrument was calibrated at least on a weekly basis using standard pH4 and pH7 buffer solutions. Prior to measuring the pH, the instrument was switched on and allowed to stabilise for at least 1 hour whilst the samples were warmed/cooled to room temperature.

Having thoroughly rinsed the pH probe with deionised water it was then placed in the sample and the reading allowed to stabilise for 1-2 minutes. The reading was recorded and the routine repeated for the following samples. Whenever possible, multiple samples of each precipitation, dry-day or trace event, were taken as a precaution against possible contamination. All readings were deemed to be within +/- 0.1 pH unit in terms of the reproducibility using the same instrument on different samples. Generally, the readings were within +/- 0.5 pH unit of similar measurements undertaken for multiple samples collected from sites 3-5 km distant from the meteorological station (Lee, pers. comm.). Since the same instrument was used for all measurements taken after May 1988 the data set should be internally consistent.

An additional experiment was also conducted periodically using the equipment shown in Figure 5.4, to determine the intra-storm precipitation acidity variability. Precipitation was collected by the funnel and passed into a 'mixing chamber' housing a pH probe immersed in pH7 buffer solution. The probe was connected to a data-recorder which plotted a continuous trace of the solution pH (measured at one minute intervals). As the chamber fills with 'fresh' rainfall, the excess 'old' sample is discharged via an overflow tube. Due to the tiny volume of the mixing chamber (approximately 5 ml) relative to the volume of the rainfall collected by the funnel (1 mm rain equals approximately 50 ml) the buffer solution and subsequent precipitation inputs are assumed to be completely displaced by 'fresh' rainfall. For time-intervals of one hour or greater the pH value indicated by the trace yields a good approximation of the actual rainfall acidity.

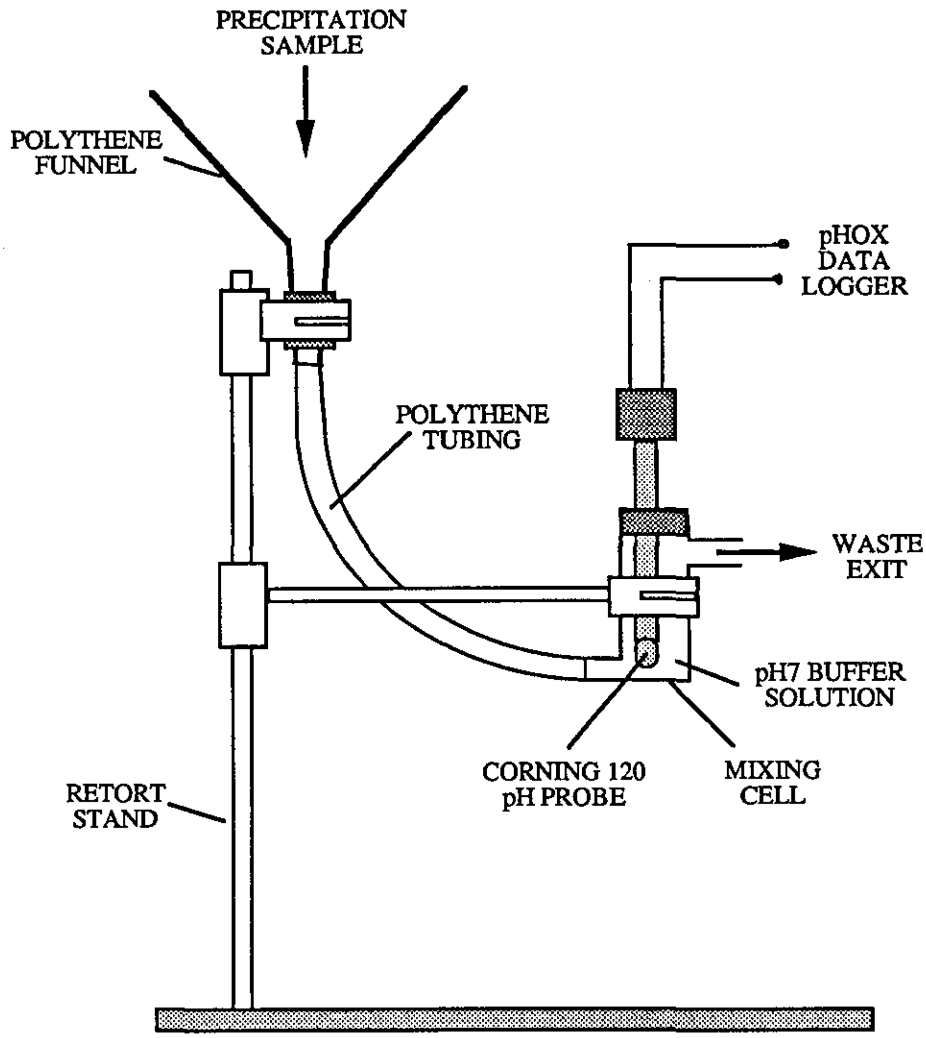


FIGURE 5.4 The design of the experimental continuously monitoring precipitation acidity probe.

A summary and evaluation of the precipitation acidity measurements taken for the period May 1988 - July 1989, particularly with regard to the prevailing meteorological and synoptic conditions is given in section 6.2.

5.4.4 Daily stream discharge

Deriving a continuous record of stage (and hence of discharge) was an essential aspect of first describing, then interpreting and finally, modelling the water budget of the Beacon catchment. The mean daily discharge and its associated acidity (5.4.5) represents the culmination of a complex sequence of processes which intervene between the moment of rainfall interception and its consequent passage to the channel network. Since it may be argued that streamflow is the only phase of the hydrological cycle for which direct measurements of any high degree of certainty can be made, the level of confidence placed in the predictions of a catchment model will largely reflect the length, accuracy, representativeness and variability of the discharge record against which it was calibrated.

The SCAM hydrological sub-model was calibrated using flow data collected at the lowest point of the Beacon catchment (cf. Figure 5.2 and section 5.3.2). A thin-plate V-notch weir and stilling well were installed and have operated continuously since the beginning of 1984. The structures are situated on a relatively straight section of channel with an average width of less than one metre. The channel bed is largely comprised of decaying organic debris overlying fine cohesive sediments; the channel network upstream of the weir is also congested periodically by log jams and dense riparian vegetation.

If the expense of the gauging station had not been a limiting factor, and if the difficulties associated with the in-channel (organic and sediment) debris had been taken into consideration, a flume (which is essentially self-cleansing) would have been a favoured alternative to the V-notch weir. But when factors such as the cost, accessibility to and maintenance requirements of the weir are considered, the facility represented the best available compromise.

In order to ratify the general equation of the thin-plate 90° V-notch weir:

$$Q = k\tan(q/2)H^{2.5}$$

(where Q is the discharge rate (in cumecs), k is a coefficient that accounts for the channel geometry and nature of the contraction, q is the angle of the V-notch, and H is the measured head) a calibration experiment was periodically undertaken. This involved measuring the length of time required for the discharge from the weir to fill a container of known volume and to then compare the measured discharge rate with the rate predicted by the theoretical equation. A range of stages were sampled and the results are presented in Figure 5.5. The slope of the regression line suggests that the equation underestimates all flows by a factor of 1.106 - 1.496 (95% confidence intervals) about a mean value of 1.361. This 36% discrepancy was attributed to the steepness of the channel gradient which resulted in an underestimation of the flow velocity at all stages by the general equation for the weir.

The autographic chart from the level recorder of the stilling well provided a continuous graphical trace of the stream stage. The clockwork mechanism of the recorder was regularly tightened and the charts changed on a weekly or fortnightly basis. At the beginning and end of each 7 day period, the head of water at the upstream side of the weir notch was measured manually. These values then enabled the scaling of the autographic chart for the interim duration. Under exceptional circumstances of very high flow, additional head readings were taken to improve the stage values obtained for the peaks on the chart. Furthermore, since June 1988 verification of the recorded stage on an hour-by-hour basis was possible as a result of the installation of an A.OTT ALGOMATIC Data Acquisition System and transducer pressure probe. Once correctly programmed this solid-state data logger required minimal attention with battery changes taking place on a fortnightly basis and memory cartridges exchanged every 1-6 weeks.

The parallel implementation of the two stage recording systems suggested that an average error of ± 0.5 cm in the hourly stage values was accrued. This equates with an error of 250,000 litres/day (± 5%) at a head of 0.25m and with an error of 25,000 litres/day (± 27%) at a head of 0.05m. A complete description of the distribution and relative significance of flow estimation errors is given in Figure 5.6. The error function - which takes into consideration the product of the flow estimation error and the frequency of occurrence of a given flow - suggests that the greatest compound error is associated with head values between 10-15 cm. These discharges occurred on 6% of the days in 1988 and had a mean flow estimation error of approximately ± 10%.

In general, the autographic flow data was used to calculate the mean daily discharge whilst the hourly data logger record was used as a convenient source of information relating specifically to flood events. The most accurate method for calculating the mean daily discharge is to convert each hourly stage value into discharge using the rating equation, and to then average the 24 discharges. The practise of averaging the stages and then converting this stage value to discharge is less accurate due to the parabolic shape of the stage-

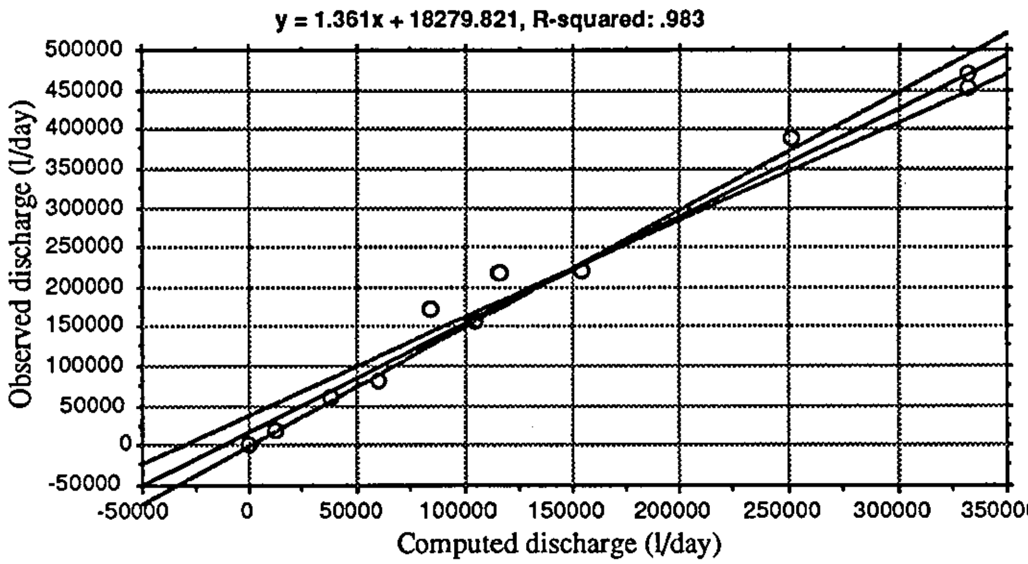


FIGURE 5.5 The thin plate weir calibration relationship (and 95% confidence intervals for the gradient): computed versus measured daily discharges.

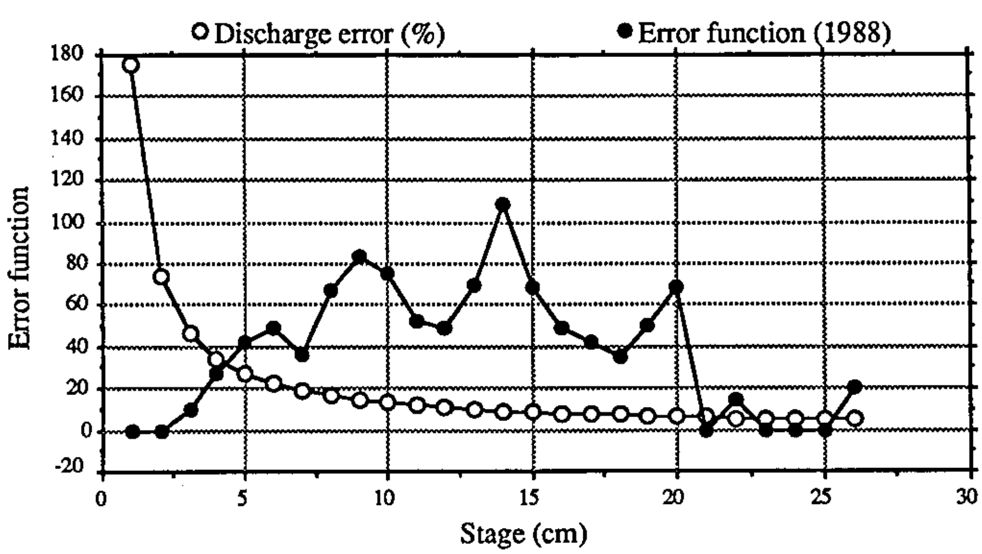


FIGURE 5.6 The distribution of computed discharge errors arising from uncertainties in the measurement of the daily stage.

discharge relation. However, in the case of the Beacon stream where the hydrographic response for flood events is somewhat damped and for much of the time relatively low and constant, the latter method was considered to be a more efficient means of manually converting the 12,000 hours of stage data. Even under conditions of extreme flow variability and at peak discharges the difference between the two methods never exceeded 1%.

A monthly summary of the resultant daily discharge data collected between March 1988 and May 1989 is presented in 6.2 alongside the respective rainfall and temperature statistics.

5.4.5 Surface water acidity sampling

The reproduction of a H-ion chemograph on the basis of inputs of daily meteorological conditions (5.4.1), precipitation amount (5.4.2) and acidity (5.4.3), alongside the forecasted daily discharge, is one of the culminating functions of the SCAM model. To this end, and more specifically, for the accurate derivation of the parameter values representing the catchment soil-weathering properties, data were required concerning the behaviour of the surface water acidity at different points in the hydrological year and within the Beacon catchment.

As indicated by Figure 5.2, water-samples were taken at weekly intervals from seven different sites within the catchment during the 70 week collection period (March 1988 - June 1989 inclusive). Using 'sterile' polyethylene bottles 25 ml samples were taken directly from each of the sites and transported back to the laboratory for analysis within 1-4 hours of collection. Contamination of the samples by sediments disturbed from the channel perimeter during the collection procedure was minimised by routinely taking the samples from the lowest point of the channel network first and then by working upstream. The analytical technique employed for the derivation of sample pH was identical to that used in the analysis of precipitation acidity (5.4.3). The results of these weekly samples (from the catchment outlet) were then used in conjunction with the daily stage data to compute the monthly H-ion input-output budget of the catchment. The interpolation procedure (number 5, Table 5.7) was employed because of its proven accuracy and simplicity (Walling and Webb, 1982). The results are presented in Figures 6.12 and 6.13.

In addition to the weekly samples, a continuous record of the stream acidity upstream of the gauging station was made possible (from July 1988 to June 1989) by means of a Multiprobe System 101 harnessed to a pHOX 100 DPM Multiparameter Water Quality

Monitor which in turn output information for logging on an A.OTT ALGOMATIC Data Acquisition System. The latter device was pre-programmed to sample the water pH, conductivity and temperature at intervals of one minute (and then to record the average hourly values) so that the detail of the catchment storm-response and rates of groundwater recharge/ recession could be investigated. During the 12-month period approximately 20 storm hydrographs of varying magnitude were monitored in this way (cf. Figure 6.12). Whilst it was possible to leave the equipment operating unattended for upwards of 14 days, the reliability of the results were increased by the regular cleansing of the sensor probes and by the recalibration of the pH-electrode. The weekly samples collected from the gauge site also provided a means of verifying the pH values obtained from the data-logger (and vice-versa).

As well as providing detailed information concerning the stream acidity during storm events, the hourly data (of which approximately 3600 hours are available) also enabled an independent experiment to be conducted into the sample frequency requirements - of a given level of accuracy and precision - of the H-load calculations. A two month subsample of 1500 hours of streamflow data was selected on the basis of its continuity and hydrologic diversity (cf. FIGS 6.12 a-d). This section of flow record was also equally divided between a period of rapid discharge fluctuation and a period of uninterrupted base-flow recession - making it ideal for the testing of different sampling frequencies. Figure 5.7 indicates that there is no clear pattern in the proficiency of different sample intervals where calculation of the H-load (via method 5, Table 5.7) were concerned. Although there was an overall reduction in the accuracy of H-loads with increased sampling intervals, the relationship is weak (r^2 = 31%) and demonstrates marked heteroscedacity. Beyond a sampling interval of 21 days the estimation error appears to reach a plateau value of c. 40%. It is worth noting that the uncertainties in the H-load estimates tended to be associated with the inability of the reduced sample frequencies to accurately represent the flow hydrograph; for instance, estimates of the streamflow acidity based on monthly samples were found to be within ±5% of the hourly mean value. The results shown in Figure 5.7 suggest, therefore, that weekly sampling of the H-ion yield from the Beacon catchment leads to load estimates to within ±20%; the daily sampling used to calibrate the SCAM model (Chapter 7) enables estimates of the H-load to within ±7%.

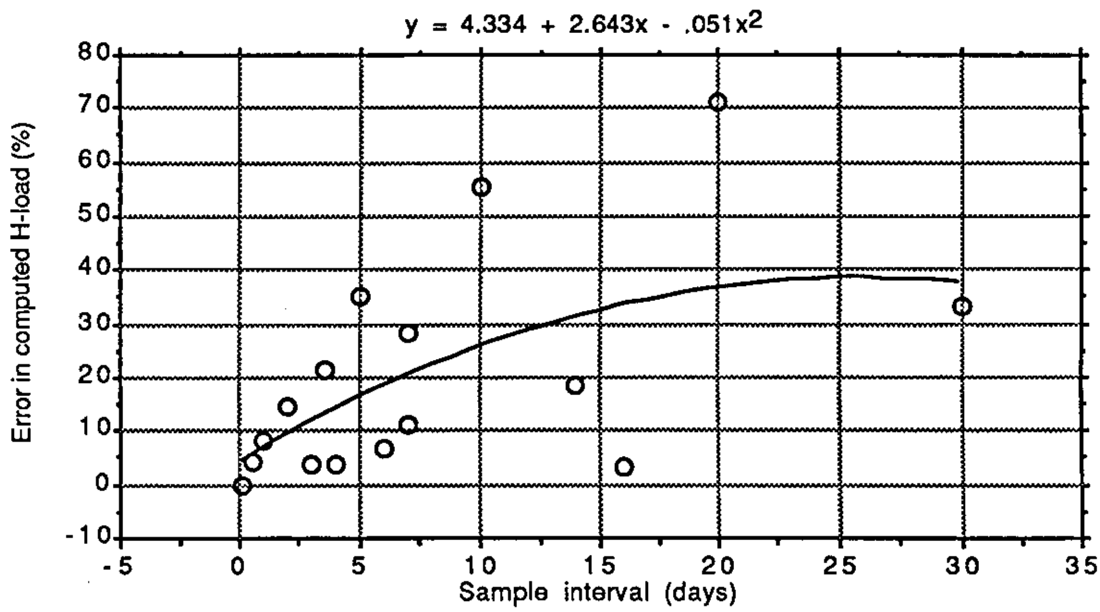


FIGURE 5.7 The effect of sampling interval on the calculation of H-ion loads. [The per centage errors were calculated with reference to the H-load derived from hourly pH and hourly discharge data].

5.5 SECONDARY DATA SOURCES

The first three sources of secondary data provided information concerning the long-term (>10 years) variability, the direction, the magnitude and the rates of change of three key climatic parameters, namely: temperature, rainfall and synoptic patterns. These series form the basis of the SCAM model scenarios and also enable the reconstruction of previous 'pollution climates'. Furthermore, by examining long-term records it is also possible to define realistic initial parameter values, and physically reasonable upper and lower boundaries to model parameters. The final data source provided by the Welsh Water Authority and the Institute of Hydrology provides detailed information on the hydrogen-ion input output budget for three catchments in the Lynn Brianne region, Wales.

5.5.1 Manley's Central England Temperature record (1659-)

The Manley (1974) series provides a unique long-term record of temperature derived from a wide selection of documentary, historical and scientific sources. However, it is important to view the Central England Temperature (CET) record within the context of the quality and reliability of the sources as the extension of records back in time is accompanied by diminishing instrumental and technical precision. Difficulties commonly encountered prior to 1881 include:

1.The need to 'bridge' gaps in the climatic record by the overlapping and standardization of data collected from a variety of sources.

2.Observer errors, inconsistent hours of temperature observation, exposure and design of the instruments.

3.Variations in the site conditions, exposure and proximity to expanding urban areas.

4.The need to convert readings taken under the Old Style or Julian calender.

Despite an abundance of records for London, the decision to provide monthly means representative of Central England was made on the basis of a number of additional considerations. Firstly, inherent difficulties associated with the growth of the built-up area in the south-east. Secondly, the fact that the Thames Basin is positioned such as to make it less representative of England as a whole. Thirdly, the best long series of monthly temperatures derived for any one place originates from the south midland record kept from 1815 onward at the Radcliffe Observatory at Oxford. There are also a number of valuable overlapping records for the west midland counties such as the one kept by Thomas Barker at Lyndon in Rutland (1736-1798). However, for the period 1659-1720 monthly values for the CET are generally based on 'uncertain' readings in south-east England, and were presented to within 0.5 ^{0} C. Prior to 1671 instrumental readings were few and therefore all values were rounded to whole degrees C (Manley, 1974).

5.5.2 Nanpantan rainfall record (1879-1981)

Daily measurements of rainfall have been undertaken close to the embankment of the Nanpantan reservoir, Leics. (GR 509 172) since 1879. Located at an altitude of 105 m (a.m.s.l.), this station is conveniently situated within 2500 metres of the summit of the Beacon Hill (5.3.2), and therefore provides an indication of the long-term rainfall receipt of the experimental catchment.

The original records provide some indication of the positioning, condition and design of the rain-gauge(s) which enables an evaluation of the quality of the rainfall record. Prior to 1926, the record should be treated with some caution: an entry in the log in 1881 suggests that the gauge was "in a bad state and not properly looked after". Between 1879 and 1925, at least four different types of gauge are known to have been used, whilst it is reported in 1883 and 1887 that the site was under-exposed due to sheltering by nearby buildings and vegetation. In 1887 the site of the gauge was also moved 40 feet south and to a slightly lower altitude - this site has been used ever since. After 1926, however, (when a 5" Snowdon rain-gauge was installed) only a few minor changes appear to have been made to the gauge height and in 1959 the site is described as having a "satisfactory exposure".

5.5.3 Lamb's Catalogue of Daily Weather Types (1861-)

The value of utilising synoptic-scale systems as a succinct means of accounting for recent changes to broad climatic variables such as the mean annual temperature (Sowden and Parker, 1981), annual rainfall totals (McCabe et. al., 1989) and precipitation chemistry (Davies et. al., 1986, Farmer et. al., 1989) has already been mentioned in Chapter 3. Of the alternative systems reviewed, the Lamb's Weather Type (LWT) register (Lamb, 1972) emerged as the most appropriate and convenient source of information regarding long-term trends in surface weather patterns.

The daily weather types contained in the register were based on some 150, 000 charts of surface pressure distribution, winds and weather. The main source of weather information came from the charts published in the Daily Weather Reports of the Meteorological Office. Earlier charts provided data on only limited periods of the day, which required an element of subjective judgement particularly with regard to fast-moving or developing systems near the British Isles. For example, during the years 1861-1873 (when no daily charts were available for the Atlantic) the cyclonic element was probably slightly under-estimated. Currently, four maps for each day (00, 06, 12 and 18 GMT) are available.

Lamb (1972) minimized the subjectivity of the classification procedure by recognising that some days are of a hybrid nature, some days are unclassifiable and that stationary large-scale pressure patterns are clearly identifiable. Moreover, the years were classified in a random order - so as to minimise the effect of any 'unconscious trends' - and the results were verified by second or third inspections some months later. The resultant register of daily LWTs provides an internally consistent and continuous record of the evolution and steering of circulation patterns across the British Isles 1861-1988. The major value of the record is not therefore in the classification given to any one particular day but -

".....the identification of the character of the general circulation and of similar sequences in different years, seasonal characteristics and spells of various lengths" (Lamb, 1972, p1).

5.5.4 The Llyn Brianne Acid Waters Project

Basic hydrometric amd water quality data were available for a period of 4 years commencing in 1984. Daily mean temperature and 24-hour precipitation totals were supplied by an Automatic Weather Station (AWS) situated to the west of catchment CI6. The bulk precipitation chemistry was monitored at two sampling sites in the area: the first being located in the Camddwr catchment, and the second between LI1 and LI6. Continuous monitoring instrumentation and automatic sampling equipment were used at all three stream monitoring sites since the summer of 1985. Measurements of stream pH were recorded using a pHOX 100DPM multimeter, whilst stream stage was converted in to flow using stage discharge relationships that had been previously established by dilution gauging (WWA, 1987). The aluminium-ion spot samples were taken at approximately weekly intervals and analysed at the former Welsh Water SW District Laboratory, Llanelli.

In general the reliability and continuity of the meteorological data far exceeded that for the stream monitoring, but some problems were encountered by the AWS during very low temperatures. Although the bulk deposition was not measured systematically, the data set was of sufficient length to determine a reliable estimate of the mean annual deposited acidity. The most serious limitation of the data set relates to the stream discharge and pH measurements. For instance, in the case of LI1, out of 1182 days of available information, streamflow measurements were lacking for 32% of the days. This meant that the maximum period of continuous flow data available for detailed model calibration and validation purposes was restricted to around 100 days in length. A detailed comparison of the discharge versus precipitation records also revealed that a number of (presumably) localised storm events were passing undetected.

However, given that the hydrochemical measurements were largely undertaken with the needs of the MAGIC model in mind (ie long-term mean annual statistics), the data set provides a firm basis for assessing the SCAM model's ability to reproduce the gross hydrochemical conditions at the outlet of each of the three catchments. Furthermore, the continuous daily time-series are of sufficient length and diversity to ensure that the storm-response simulations are adequately examined.

5.6 SUMMARY

To conclude this chapter, the 'uncertainty envelopes' associated with each of the empirical components of the SCAM data-base have been provided in Table 5.10. From the table it is immediately apparent that the greatest errors are anticipated for the areal precipitation amounts and rainfall acidity measurements. With such uncertain inputs and outputs to the catchment it is hardly surprising that during calibration the SCAM model should be unable to yield a perfect reproduction of the observed data-series. The performance of the model should therefore be reviewed within the context of these known, data-base uncertainties. With regard to the secondary data sources, the inherent error margins are not as readily derived. A limited assessment of the reliability of the data was made possible on the basis of the observer comments and the summaries provided by their respective authors. Whilst these data series are not used for direct calibration of SCAM (as is the case for the empirical data), they do represent the inputs to the forecasting mode and should be evaluated within this light.

The next chapter presents an overview of the SCAM data-base - in terms of the value derived from, and limitations imposed by the actual sampling period - for model calibration and verification. A description of the field data also provides an opportunity to assess some of the assumptions made during the design of the SCAM model.

Parameter	Error estimate
Mean daily temperature	±0.1 °C
Daily potential evaporation	±0.1 mm
Catchment area	±5%
Point rainfall measurement	±10%
Areal rainfall measurement	±15%
Precipitation acidity	±0.5 pHunit
Event H-ion load	±30%
Stage measurement	±0.5 cm
Daily discharge	±10%
Streamflow acidity	±0.5 pHunit
Weekly H-ion load	±30%
Annual frequencies of LWTs	±10%

TABLE 5.10 Summary of error estimates for each main component of the SCAM data-base.

CHAPTER 6

DISCUSSION OF THE DATA BASE

"The central mistake......is the quest for certainty" (Popper, 1972, p 63).

6.1 INTRODUCTION

The primary function of the empirical data set described in the previous chapter was to calibrate, test and explore the design of the SCAM model. The secondary data sources, by contrast, provide the basis for constructing realistic climate scenarios, and for applying the SCAM model to diverse catchment conditions. The accuracy of the individual data collection and measurement procedures were discussed under their respective methodologies; this chapter reviews the main features of the 16-month fieldwork period and assesses the representativeness and diversity of information contained in the data collection periods. This task is best achieved through the comparison of values obtained during the fieldwork period(s) with the corresponding long-term average condition(s) and through a broad discussion of the various components of the SCAM data-base assemblage. This discussion is supplemented by a section which considers the major features of the secondary data and their relation to the prevailing synoptic regimes.

Within this context of providing the SCAM model with realistic input parameters and a representative calibration data-base, the contribution made by the individual components described in 5.4 are now discussed.

6.2 THE EMPIRICAL DATA-BASE

Since each of the chosen catchments were regarded as 'grey-box' systems for modelling purposes, it is appropriate that the following discussion should make a broad distinction between data representing catchment inputs on the one hand, and outputs on the other.

6.2.1 Catchment inputs

Examination of the monthly temperature and rainfall regimes for the period March 1988 - April 1989 provides a useful explanation for the subsequent hydrological response of the catchment. Comparison of the **mean monthly temperature** with the standard values for the period 1941-1970 (Figure 6.1), suggests that between March 1988 and November 1988 the regime was very similar to the long-term average. The sinusoidal pattern conforms closely to the theoretical regime assumed in the design of SCAM (Chapter 3). The four month period December 1988 to March 1989 was however, anomalously mild, confirming the need for 'seasonal weighting parameters' when modelling 'real' temperature patterns. Reference to the Manley (1974) temperature record indicates that December 1988 was the 2nd warmest on record, January 1989 (6th), February 1989 (23rd), and March 1989 (7th) mildest since records began in 1659! From April 1989 to June 1989 the mean temperatures returned to conditions closer to the long-term average although May and April were respectively 2°C above and below the 1941-1970 mean for these months. The most outstanding feature of the 16-month period was therefore the very mild winter period (December 1988 - March 1989).

The 1941-1970 **mean monthly rainfall** record (Figure 6.2) indicates that the East Midlands region experiences no marked seasonal maximum with on average a difference of approximately 20 mm between the wettest (August) and the driest months (February). The data collection period, however, displayed a far greater range of monthly rainfall totals with a difference of 90 mm between the wettest (July 1988/ April 1989) and driest months (December 1988/May 1989). The period was also noticeable for its low aggregate total with only five months exceeding the mean monthly figures. The months August 1988 to February 1989 were particularly dry, as was May 1989: according to the Nanpantan rainfall record, November 1988 was the 12th, December and May 1989 the 10th, and January 1989 the 20th driest since 1881. Conversely, April 1989 was the 3rd and July 1988 the 8th wettest on record - this went some way towards mitigating what otherwise might have been an exceptionally low 16-month rainfall total.

The various components of the meteorological data-base (daily temperatures, rainfall intensity, pressure changes etc.) provide a valuable source of information with which to interpret the episodic and monthly totals of rainfall acidity (or hydrogen-ion load). Table 6.1 presents a summary of selected **meteorological variables** and their relation to dependent parameters. From Table 6.1 it is immediately apparent that there is a clear distinction between the significant meteorological factors operating at the monthly and daily time-scales. The monthly acidities (pH and H-ion loads) are primarily a function of the

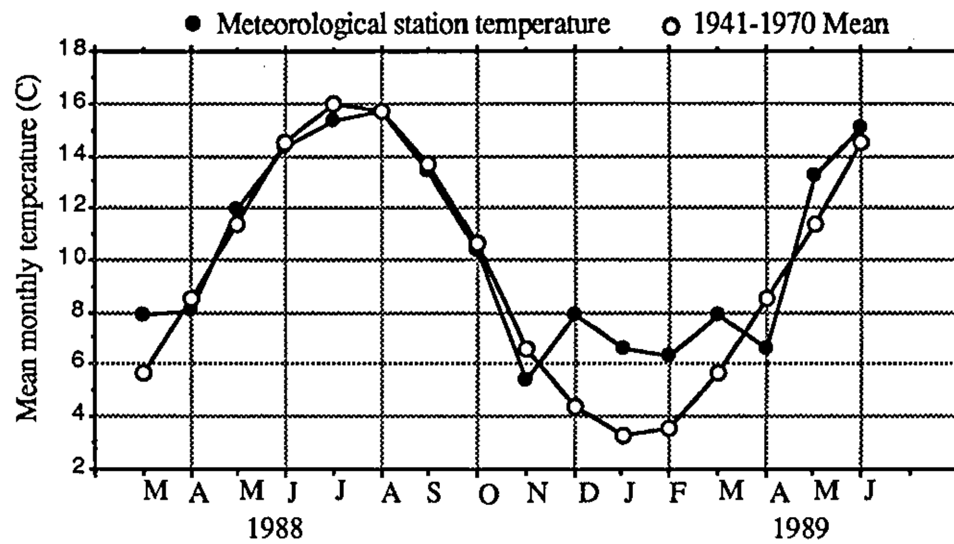


FIGURE 6.1 Comparison of the observed (Loughborough) mean monthly temperatures (Mar 88-Jun 89)with the 1941-1970 mean values.

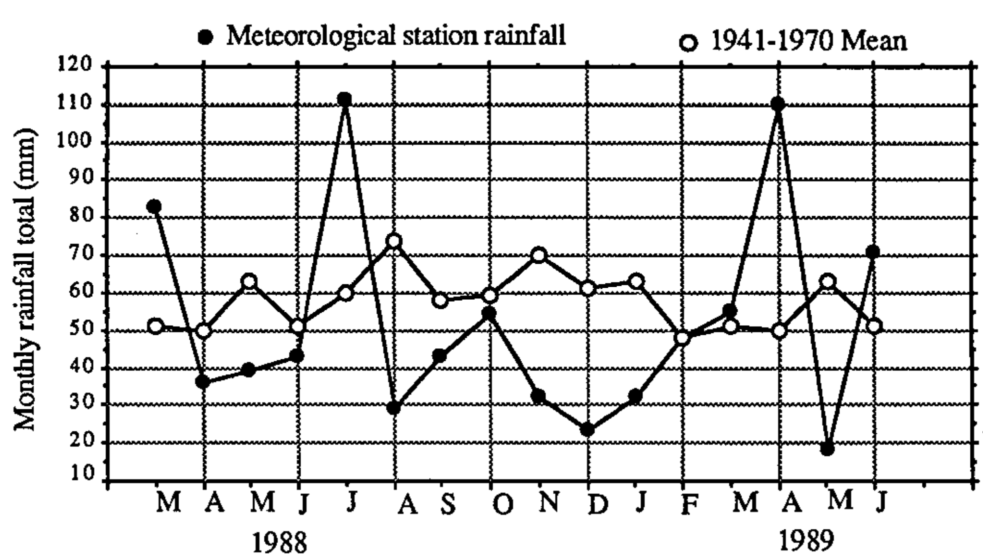


FIGURE 6.2 Comparison of the observed (Loughborough) monthly rainfall total (Mar 88-Jun 89) with the 1941-1970 mean values.

Dependent variable	Independendent variable	r-value	Confidence
Monthly means:	*Monthly means:*		
Volume-weighted pH	Wind speed	+0.502	90%
"	W-type rain-days	+0.631	99%
"	W-type frequency	+0.691	99%
"	A-type rain-days	-0.442	90%
H-ion concentration	Wind speed	-0.504	95%
"	W-type rain-days	-0.678	99%
"	W-type frequency	-0.614	99%
"	A-type rain-days	+0.437	90%
"	A-type frequency	+0.449	90%
H-ion load	C-type rain-days	+0.563	99%
"	C-type frequency	+0.695	99%
Daily values:	*Daily values:*		
Rainfall pH	Rainfall amount	-0.200	99%
"	Temperature	+0.224	99%
"	Wind speed	+0.292	99%
H-ion concentration	Temperature	-0.230	99%
"	Wind speed	-0.278	99%
H-ion load	Temperature	-0.163	99%
"	Wind speed	-0.218	99%

TABLE 6.1 Statistically significant correlations between selected meteorological variables.

Site	Rainfall (mm/yr)	Volume-weighted pH	H-ion load (k eq ha/yr)
Loughborough, 1988-1989	620	4.04	0.569
Tillingbourne, 1977-1981	1067	4.15	0.747
Rothamsted, 1969-1973	619	4.30	0.310
Holme, Norfolk, 1979	530	4.41	0.207
Rhyd-lydan, W.Wales, 1979	1421	4.70	0.284
Snake Pass, Derbys, 1979	1453	4.35	0.654
Cairnsmore, SW Scotland,1979	2000	4.42	0.760
Pitlochry, Scotland, 1976-1979	890	4.31	0.406
Birkenes, Norway, 1972-1978	1403	4.24	0.800
Storgama, Norway, 1974-1978	1108	4.28	0.580
Solling, W.Germany, 1969-1979	900	4.11	0.817
Hubbard Brook, USA, 1963-1974	1313	4.14	0.952

TABLE 6.2 Comparison of H-ion deposition at Loughborough with various sites (based on Skeffington, 1984).

larger-scale synoptic factors such as the anticyclonic (A-type) and cyclonic (C) LWTs which contribute to increased acid deposition, and the westerly-type (W) which results in lower concentrations. Within these broad classes, factors such as temperature and wind speed account for some of the day-to-day variability in the precipitation acidity. The mean wind speed is undoubtedly a surrogate measure of the daily 'ventilation factor' affecting concentrations of air-borne pollutants, whilst the temperature may indirectly reflect the predominance of summer-terrestrial as opposed to winter-maritime solute sources (Petts and Foster, 1985) or the influence of different sectors within individual cyclones (Haagenson et al., 1985; Raynor and Hayes, 1982). It is the daily summation of factors such as these which result in the different pH percentile distributions observed within each of the LWTs (cf Figure 6.6 below).

The sequential sampling of acidity within precipitation events illustrates the significant role of microscale atmospheric processes. **Hourly precipitation pH** data were collected for about a dozen higher magnitude events (> 5.0 mm) using the equipment shown in Figure 5.4. The acidities were found to vary significantly within most events with no common pattern seen: for some events the peak acidities were at the beginning of the event, for others, at the end or during the storm (Figure 6.3). There was no evidence of a seasonal pattern in the trends, nor were the changes particularly related to the precipitation intensity. Having obtained similar results for a site at Bottesford, E. Midlands from sequential rain samples, Martin and Barber (1984) concluded that the variations in concentrations arise because of variations in rain scavenging efficiency, because of variations in the gases and aerosols available for scavenging, and because of the evaporation of raindrops at the beginning and end of the event. These assertions are supported by the intra-storm pH variations shown in Figure 6.3 which suggest that the most acidic precipitation corresponds with the periods of most intensive precipitation (or scavenging). Although it is unlikely that such intra-storm variations in precipitation acidity will have any bearing on longer-term catchment chemistries, it is important to recognise that the single pH-value attributed to a given precipitation event actually represents an amalgam or synthesis of processes operating at a number of different scales.

The **episodic** nature of the wet-deposited acidity (Fowler and Cape, 1984) is clearly evident in the daily precipitation samples collected at the meteorological station. Ninety percent of the total wet-deposited acidity (measured between March 1988 and June 1989) occurred on 30% of the rain days (cf. Figure 6.4), with one event alone accounting for 15% of the period total. This latter event (which took place on the 24th of April 1989) further underlines the importance of daily meteorological, synoptic and precipitation processes in determining precipitation acidities. A Northerly synoptic pattern and surface wind direction allowed the air-mass trajectory to pass directly across the Nottingham-Derby

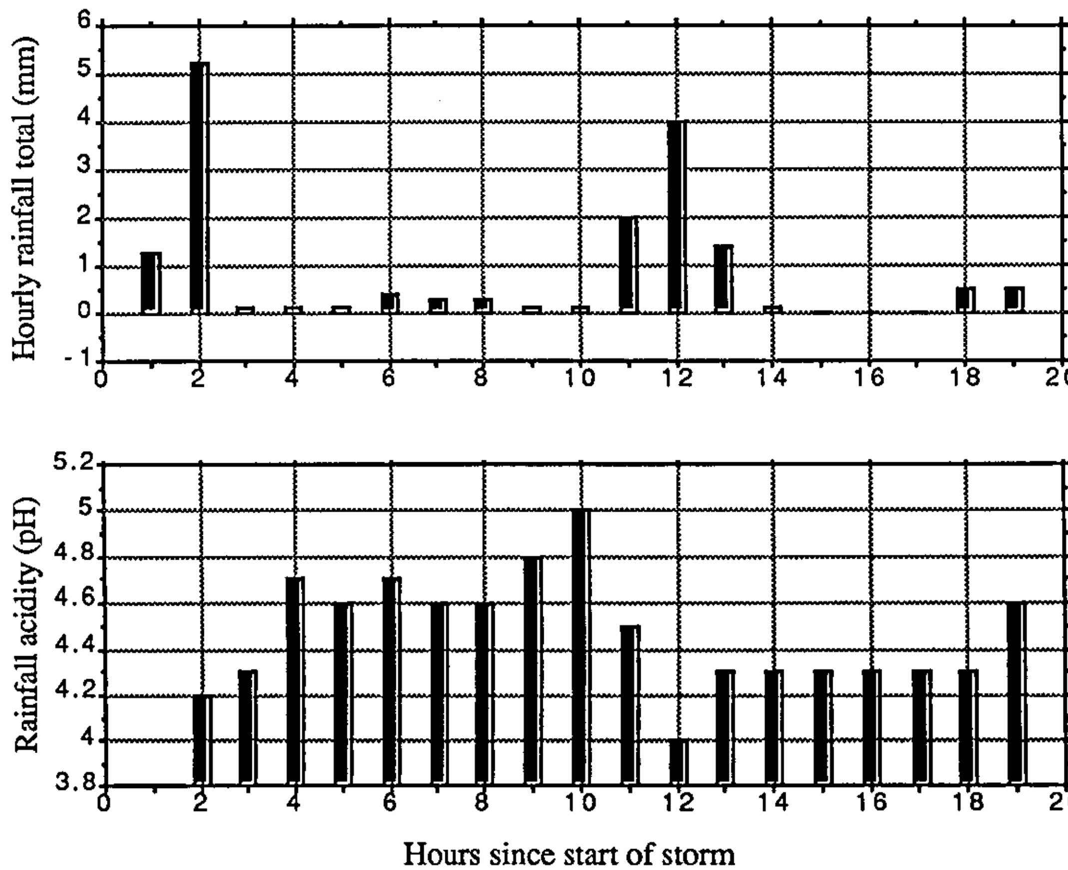


FIGURE 6.3 An example of within storm variations of acidity (pH) at Loughborough: the rainfall event of 3rd July 1988 .

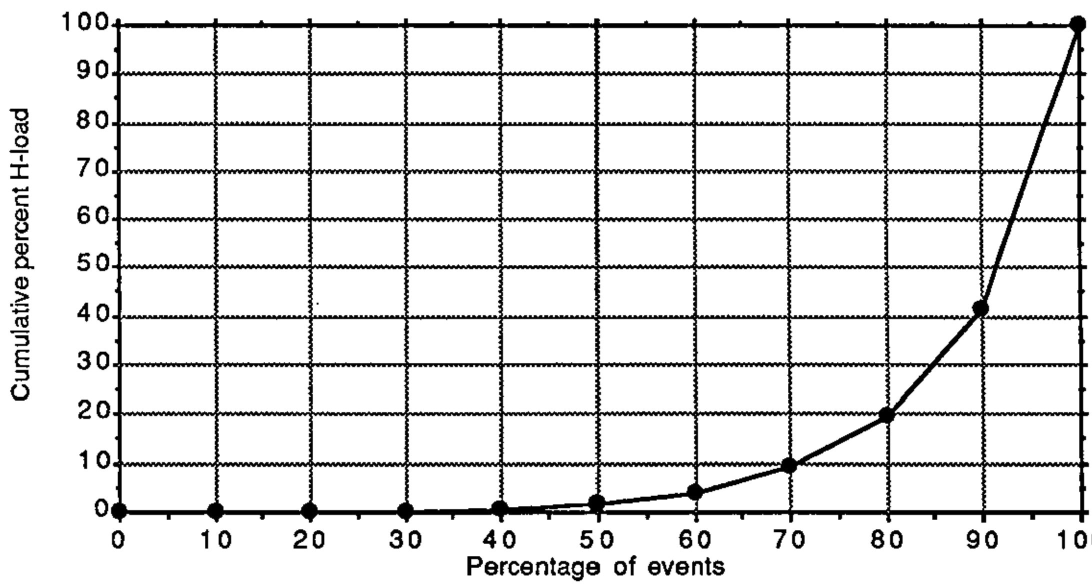


FIGURE 6.4 The cumulative per centage H-ion load against the proportion of precipitating events at Loughborough (March 88 to June 89).

conurbation and the Ratcliffe-on-Soar power-station, during which considerable quantities of the acidifying ions SO_4, NO_3 and Cl were ingested into its lower layers. The resultant precipitation concentrations for these ions were respectively 4.43, 9.87 and 9.81 mg/l (Black, pers. comm.). The heavy snowfall (approximately 12 mm) enabled the efficient scavenging of the polluted air-mass and provided an efficient receptor for occult deposition, thereby combining high H-ion concentrations with a large volume of precipitation. Over an area the size of the Beacon catchment this snowfall event was estimated to have deposited: 78 kg of Cl and NO_3, 35 kg of SO_4 and 7 kg of H-ion.

A comparison of the **mean-volume weighted concentration of H-ion** in precipitation collected over one year at the meteorological station (July 1988 to June 1989) with published data on other 'acidic sites' in the U.K., U.S.A. and Europe suggests that the rainfall in the East Midlands ranks alongside some of the most acidic. The mean pH value of 4.04 is lower than all sites given for the U.K., for Birkenes in Norway, for Solling in W.Germany and for the Hubbard Brook, NE U.S.A. (Table 6.2). The H-ion load for the 12-months was 0.569 keq/ha/yr; this represents an intermediate value when compared with the other sites and is a reflection of the lower annual rainfall experienced in the E. Midlands (Skeffington, 1984).

The overall frequency distribution of the monitored precipitation acidities was clearly bimodal (Figure 6.5a) as has been observed elsewhere (Fowler and Cape, 1984). However, the true extent of the rainfall acidity is borne out by the cumulative **percentile distribution** for all 206 precipitation events. Figure 6.5b indicates that approximately 90% of all the events had a pH of less than 6.0, 60% were below pH 5.0, and 25% were less than pH 4.0. The respective percentages for the daily pH values at Bottesford, E. Midlands between 1980-1982 were: 99%, 95% and 20% (Martin and Barber, 1984). Overall therefore, the rainfall at Bottesford appears to be of higher acidity with the exception of the lowest quartile (25-35%) which is more acidic at Loughborough. These differences are almost certainly due to the varying proximities of the two sites to major pollutant sources: Bottesford is located approximately 20 km due east of Nottingham and 25 km north-east of Ratcliffe-on-Soar power station. This site is therefore ideally located to receive a large proportion of the air-borne pollutants transported via westerly and south-westerly winds from the Trent valley sources. Conversely, for Loughborough to receive similar quantities of acidic compounds (as indicated by the precipitation pH), the rain-bearing winds must be of one of the less frequent northerly-types (Table 6.3). The greater proximity of Loughborough then facilitates higher H-ion concentrations during such extreme episodes.

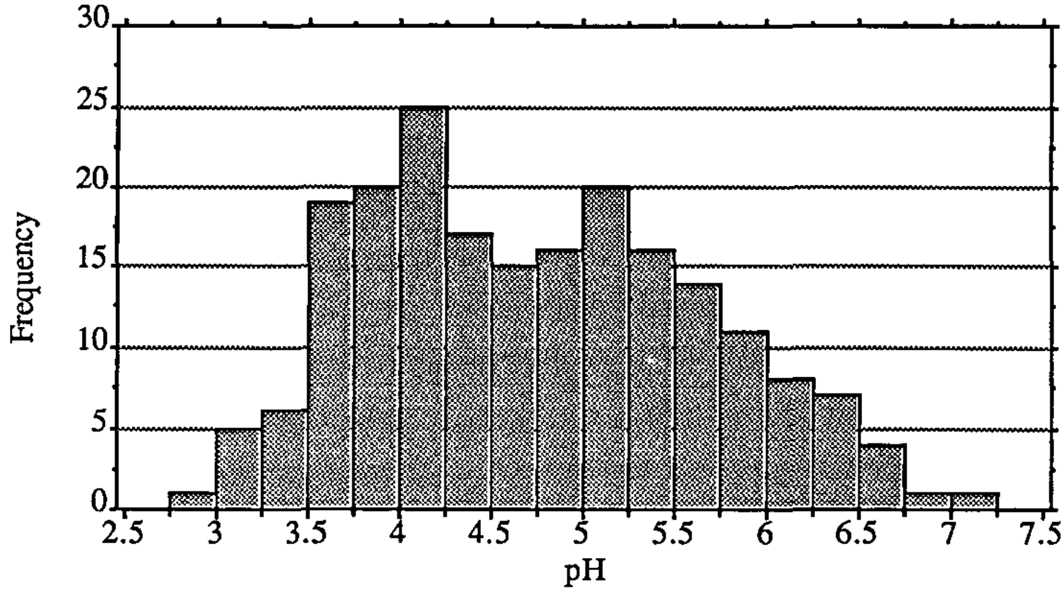


FIGURE 6.5a The frequency distribution of precipitation acidities monitored at Loughborough between March 1988 and June 1989.

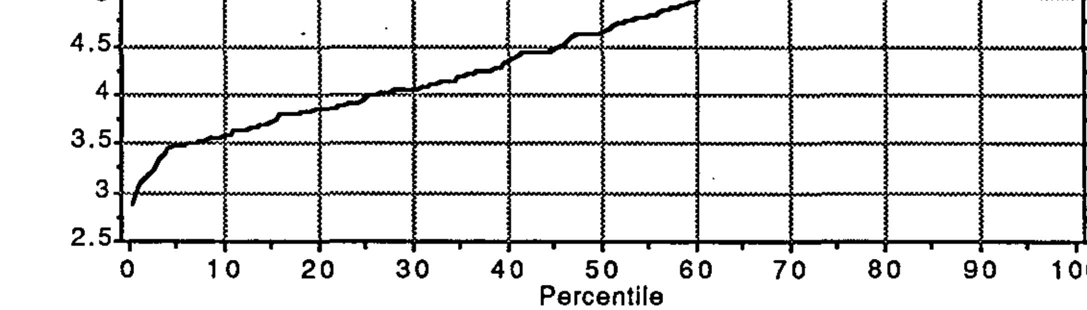


FIGURE 6.5b The cumulative percentile distribution of precipitation (day) acidities (or pH) observed at Loughborough (March 88-June 89).

LWT	n^0	$nraindays^1$	$probability^2$	mean $rain^3$	mean pH^4	mean $H\text{-}load^5$	km^6
W	91	54	0.593	3.346	5.13	177	380
C	64	48	0.750	4.539	4.62	440	279
A	136	15	0.110	3.413	4.28	467	186
N	13	9	0.692	3.511	3.63	1820	249
NW	15	6	0.400	4.042	4.37	461	347
S	9	5	0.556	4.100	4.79	152	269
SW	34	17	0.500	3.103	5.12	48	345
Other	114	52	0.456	3.819	4.60	304	247
Total	476	206	0.433	3.762	4.74	357	296

Notes:

0 Number of days assigned to the given Lamb's Weather Type category.

1 Number of precipitation days observed in each Lamb's Weather Type category.

2 Probability of precipitation occurring for the given Lamb's Weather Type.

3 Mean precipitation event amount (mm).

4 Arithmetic mean precipitation acidity.

5 Mean precipitation event H-ion load ($\mu gm/m^2$).

6 Mean daily wind fetch (or speed) (km/day).

TABLE 6.3 Daily precipitation statistics by Lamb's Weather Type for a site in Loughborough 12 March 1988 to 30 June 1989.

The **monthly** rainfall **hydrogen-ion concentrations** (pH values) were largely determined by the frequency of four main classes of Lamb's Weather Type (LWT), namely: westerly (W), cyclonic (C), northerly (N), and anticyclonic (A), of which the first three were the most significant (Table 6.3). The westerly, cyclonic and northerly classes alone accounted for 64% of the total acidity deposited between March 1988 and June 1989, and yet they were ascribed to only 35% of the days. With the exception of the northerly type, these 'acidifying classes' had mean precipitation pHs close to or exceeding the total mean pH; the significance of their respective H-ion loads are therefore attributed to their frequency of occurrence, probability of rainfall, mean rainfall amount and respective acidity distributions (Figure 6.6). For example, the northerly-type occurred infrequently but had the lowest mean rainfall pH and moderate rainfall amounts. Conversely, the anticyclonic class, despite having high H-ion concentrations (Table 6.3) and being prevalent on 29% of the 476 observation days, contributed just 9% of the total acidity. This was due to the low precipitation event sizes and very low probability of rainfall occurrence associated with this weather-type. Indeed, by calculating the product of the probability of occurrence of a given LWT, the likelihood of rainfall, mean event size and acidity it is possible to derive an index of acidifying tendency. This calculation reveals the following rank order for the weather types (from highest to lowest acidifying tendency): C>N>Other>W>A>NW>SW>S.

The results presented in Table 6.3 therefore support the assertion that inter-annual changes to the relative frequencies of these LWTs would have a large bearing on both the spectrum of over-lapping precipitation acidities and the long-term **acid load.** Figures 6.7a and 6.7b also reinforce the importance of considering the acid load as opposed to the mean monthly pH-values. Although the most acidic precipitation fell during April and November 1988 (mean pH<3.7), the greatest H-ion load was attributed to April 1989 which combined a moderate to low pH-value for the precipitation with a very high monthly rainfall total. At the opposite end of the spectrum, January 1989 recorded the lowest H-ion load of less than 0.394 mg/m^2 as a result of the highest volume-weighted pH-values and just 50% of the month's average rainfall total.

6.2.2 Catchment outputs

The combined effect of the unusually mild and dry period October 1988 to March 1989 is clearly evident in the **monthly discharge** totals (Figure 6.8): the recommencing of flow was effectively delayed by two months following the dry summer interlude, and did not resume average conditions until March 1989. Furthermore, the month of maximum

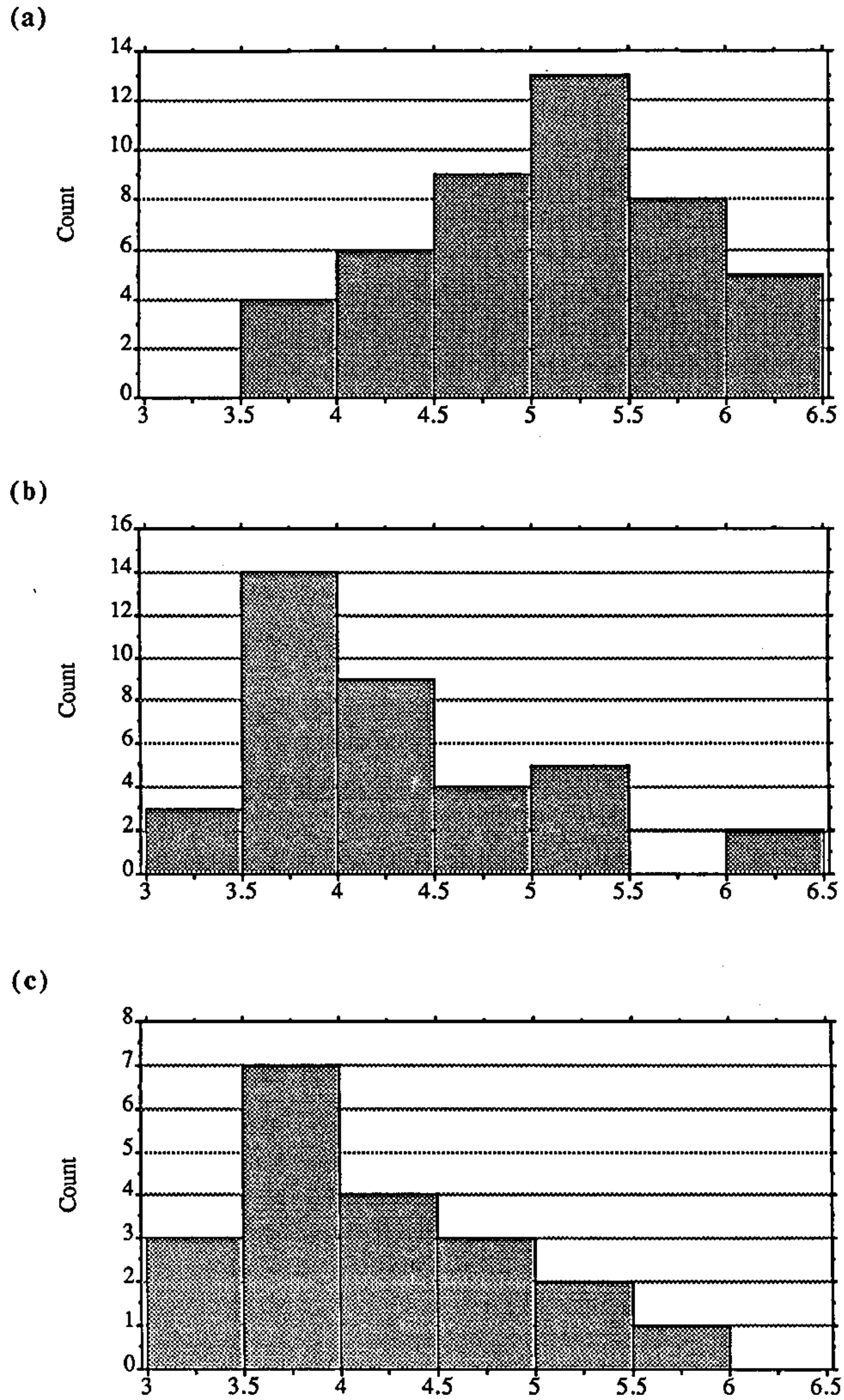


FIGURE 6.6 Precipitation acidity by Lamb's Weather Type: (a) westerly, (b) cyclonic and (c) anticyclonic pH distributions.

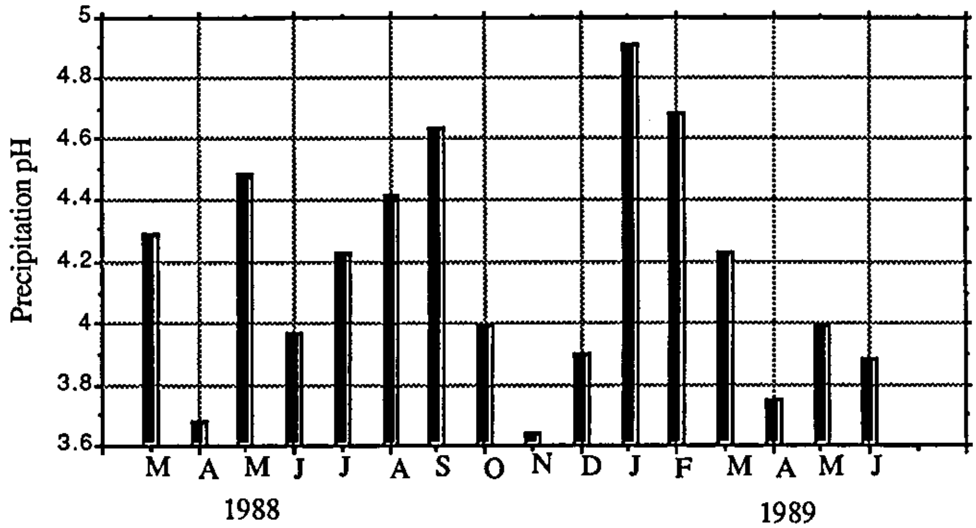


FIGURE 6.7a The monthly volume-weighted precipitation acidities measured at Loughborough (March 1988- June 1989).

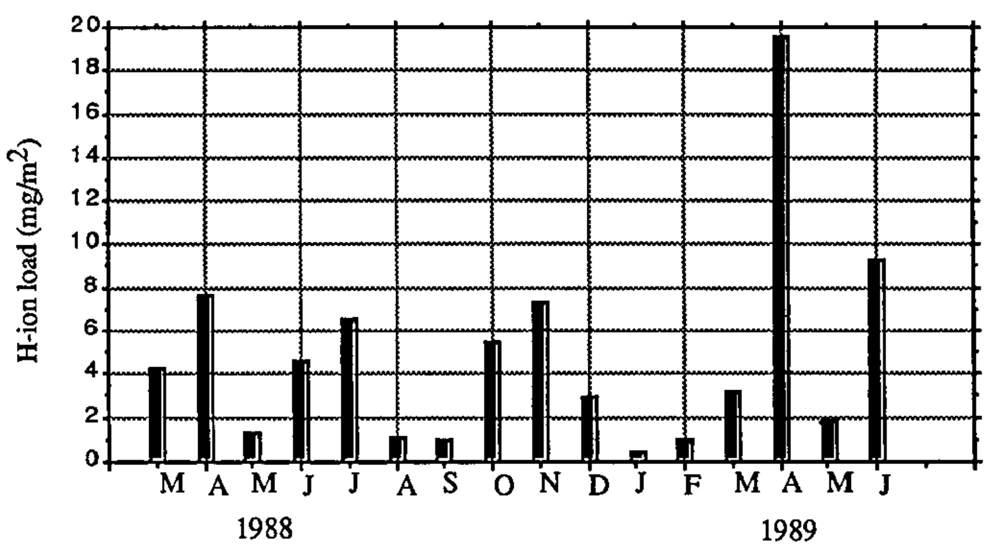


FIGURE 6.7b The monthly wet-deposited H-ion load observed at Loughborough (March 1988- June 1989).

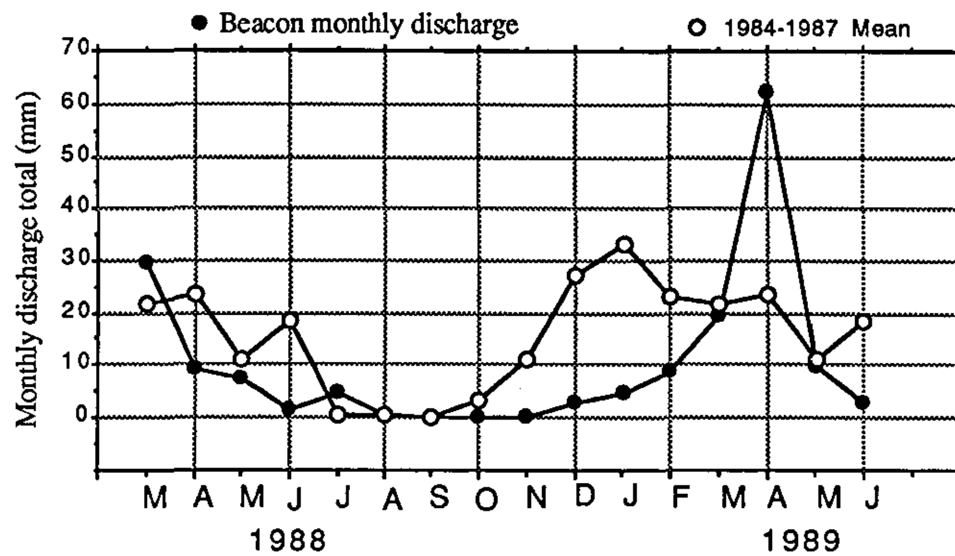


FIGURE 6.8 Comparison of the observation period (March 1988 to June 1989) Beacon monthly discharge totals with the 1984-1987 mean values.

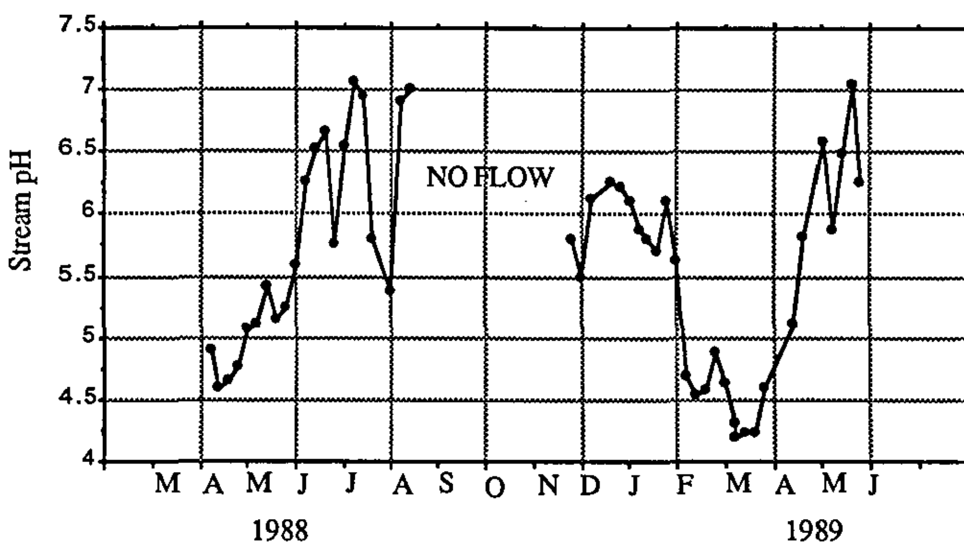


FIGURE 6.9 Weekly Beacon outlet streamflow acidities (March 1988 to June 1989).

discharge was postponed from January to April - a delay of three months. It is also interesting to note the effect of the very wet months (March 1988, July 1988 and April 1989) on the hydrograph. The latter month in particular was sufficient to 'switch' the catchment store from a state of drought in February 1989 to one of saturation by mid-April 1989. However, the warm-, dry-spell which occurred during the whole of May and the first half of June was sufficient to temporarily halt flow from the catchment one month ahead of average.

The **weekly** values of the **discharge pH** (Figure 6.9) support the assertion that there is a strong inverse relation ($r^2 = 85\%$) between the soil moisture status of the catchment (as indicated by the monthly discharge totals) and the surface-water acidity (Chapter 3). The effect of individual storms (detected at the weekly timescale) serve to punctuate the overall trend towards reduced acidities as the catchment soil moisture deficit increases. Conversely the progression towards saturated conditions in April 1989 from zero flow at the beginning of December 1988 was paralleled by a steady reduction of pH to a minimum of 3.7 (7th April 1989). The rapid fall in groundwater levels (and hence discharge) from the end of April 1989 and the increasing dominance of baseflow sources is clearly reflected by the rapid increase in the stream pH to a maximum of 7.05 (26th June 1989). Within the space of just three months the catchment fauna and flora were therefore subjected to H-ion concentrations across more than three orders of magnitude!

A possible explanation of this temporal behaviour - which relates the acidity of the streamflow to various indices of the soil moisture status - is provided by reference to a **soil-acidity profile** taken from the central portion of the Beacon catchment (Figure 6.10). Whilst this single profile should not be considered entirely indicative of the heterogeneous catchment soil properties it serves to illustrate a point. There is a clear progression from the highly-acidic, organic upper-horizon (0-20 cm) to the lower-acidic, parent material (150 cm). If the catchment moisture store is envisaged as a single vertical 'tank' it is apparent that when the store is full it will be supplying discharge predominantly from the upper acidic horizon (s); conversely, baseflow is supplied from the (relatively base-rich) lower layers of the profile when the store is low. Intermediate flows are therefore a 'mixed' combination of the two extremes.

Considerable **spatial variations** in the mean surface-water acidity were observed at a number of additional sites throughout the Beacon catchment (Table 5.8 and Figure 5.2). To a lesser or greater extent these sites also exhibited the seasonal acidity trend evident at the main sampling station (cf Figure 6.9). For example, Figure 6.11 compares the response of the surface-water acidity for two contrasting sites in the Beacon catchment to changes in the soil moisture (as indicated by the weekly gauging station stage levels). The two

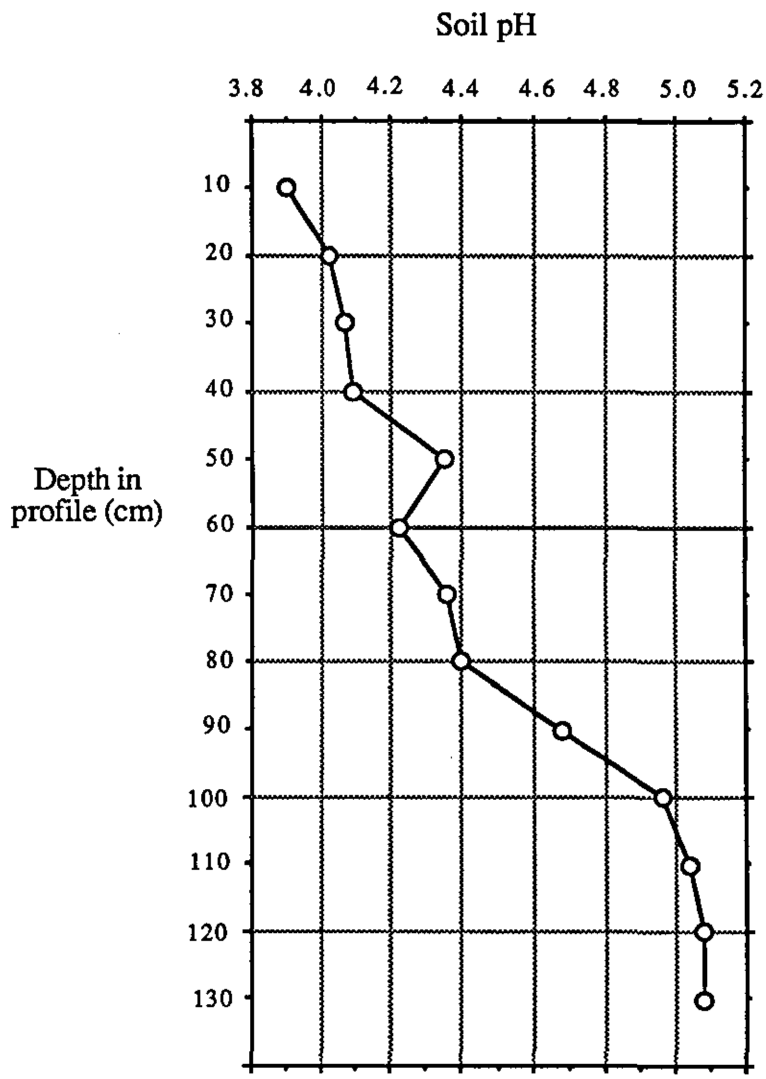
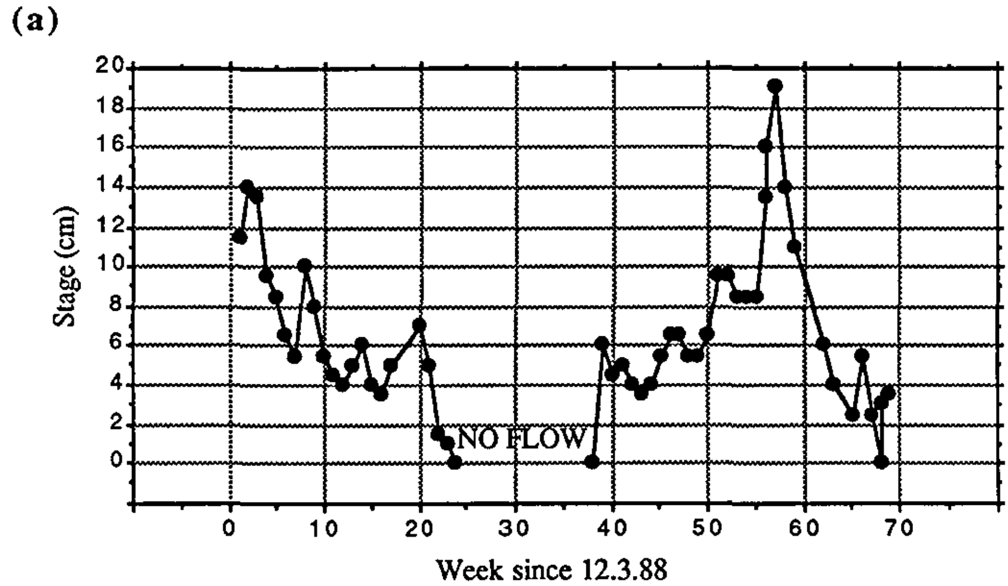


FIGURE 6.10 Soil acidity profile from a site in the Beacon catchment.



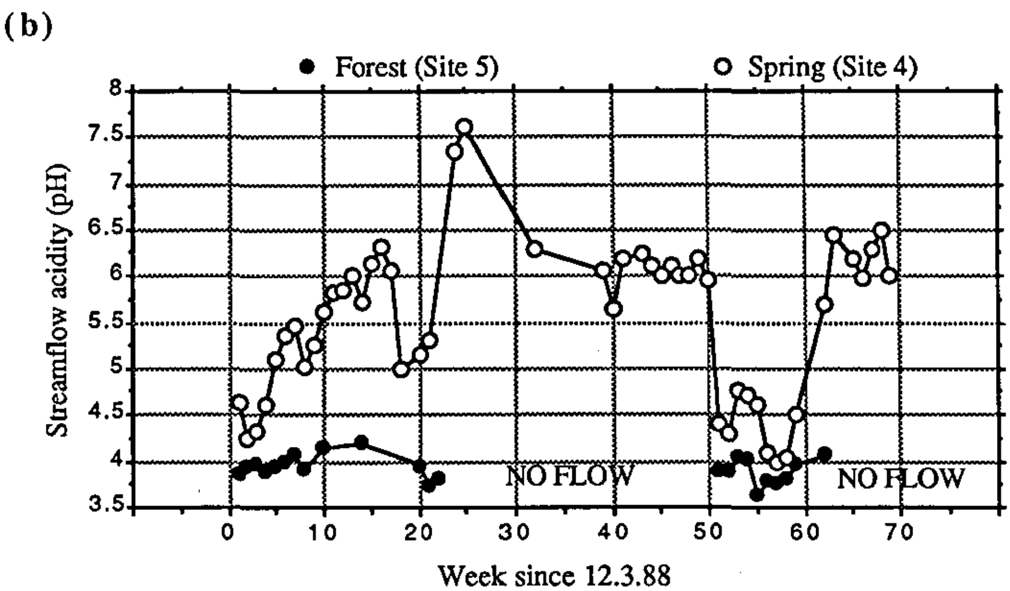


FIGURE 6.11 (a) Weekly stage at the gauging station (b) and weekly surface water acidity at two neighbouring sites in the Beacon catchment (March 1988 - June 1989)

sampling sites were separated by less than 10 metres yet demonstrated quite marked differences in their behaviour. Site 5 (Figure 5.2) is an ephemeral stream that drains the Beacon conifer plantation on the northern edge of the catchment. Site 4 is the discharge-exit of a sub-surface tile-drain/ spring from which flow continues throughout the year. The acidity of this site bears a greater resemblance to the catchment outlet (r^2 = 90%) suggesting that it is the dominant source of flow from the Beacon. The arithmetic means of the pH (and the standard error of the mean at the 95% confidence level) for Sites 5 and 4 were respectively 3.92 (± 0.06) and 5.45 (± 0.22) for the period March 1988 to June 1989. The greatest differences in the acidity of the two sites tended to occur during the period of baseflow recession (spring-summer drying). Under the saturated conditions of weeks 55-60, however, the responses of the two sites were very similar. Although discharges from Site 5 are limited on average to 25-30 weeks per year, this source assumes great importance when ever the saturated area of the catchment expands, thus providing the downstream network with highly acidic-, aluminium-rich flow.

The behaviour and characteristics of these two sites therefore exemplifies a fundamental weakness of the conceptual approach to catchment modelling (previously discussed in Chapters 2 and 3), that is, the lumping of spatially distributed factors such as land-use or soil-type. As has been demonstrated, dramatic changes can occur in the conditions and processes operating within a catchment even at an interval as small as 10 metres. Although it would be possible to calibrate the model against data obtained from any one of these sites, the catchment outlet remains a convenient point at which to simulate the composite effect of all contributing sources within the basin.

These micro-scale patterns of marked temporal and spatial change were borne out even more clearly by the **hourly** variations of **stream pH** during the rising and falling limbs of flood hydrographs (Figures 6.12a and 6.12b). Following an initial increase in pH - attributed to the 'flushing' of base-rich 'old' water into the channel - there followed a marked reduction in the streamflow pH. The minimum pH was in general found to lag 10-12 hours behind the maximum stage. These acid pulses of short duration which lag behind the peak flow have been attributed to the delay involved in forcing water from the upper layers of the soil profile into the surface water system (Mason and Seip, 1990). As the flood component subsides there is a gradual return to pre-storm levels of acidity, with a complete 'recovery' for the Beacon taking upwards of 500-1000 hours (Figures 6.12b,c and d). It should also be mentioned at this point that the storm runoff acidity has little (if any) relation to the acidity of the precipitating event(s). The correlation coefficient of r = 0.35 between the mean daily discharge acidity and precipitation acidity contrasts with that of r = 0.95 derived for the relationship established with the catchment soil moisture deficit (computed in Chapter 7). This behaviour suggests that the surface water chemistry of the

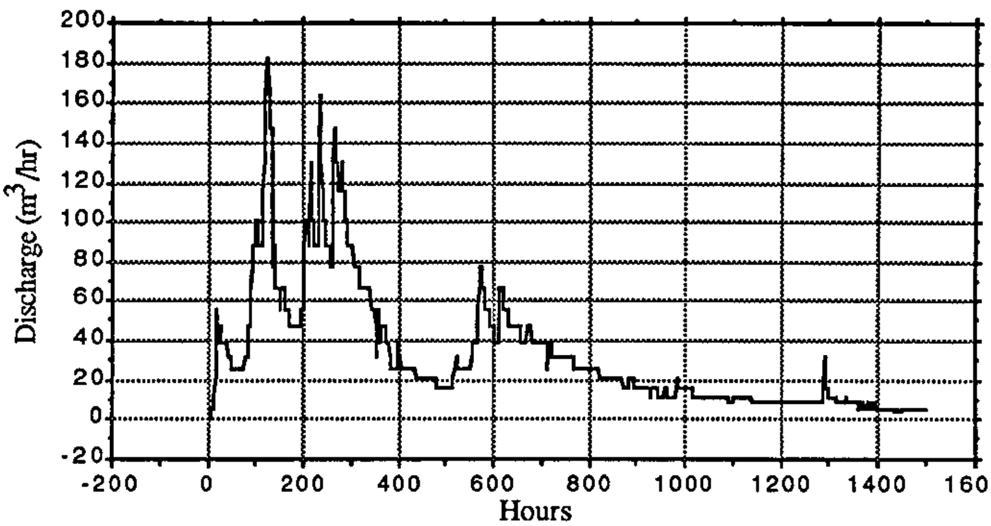


FIGURE 6.12a Hourly streamflow discharge from the Beacon (1.4.89 - 2.6.89)

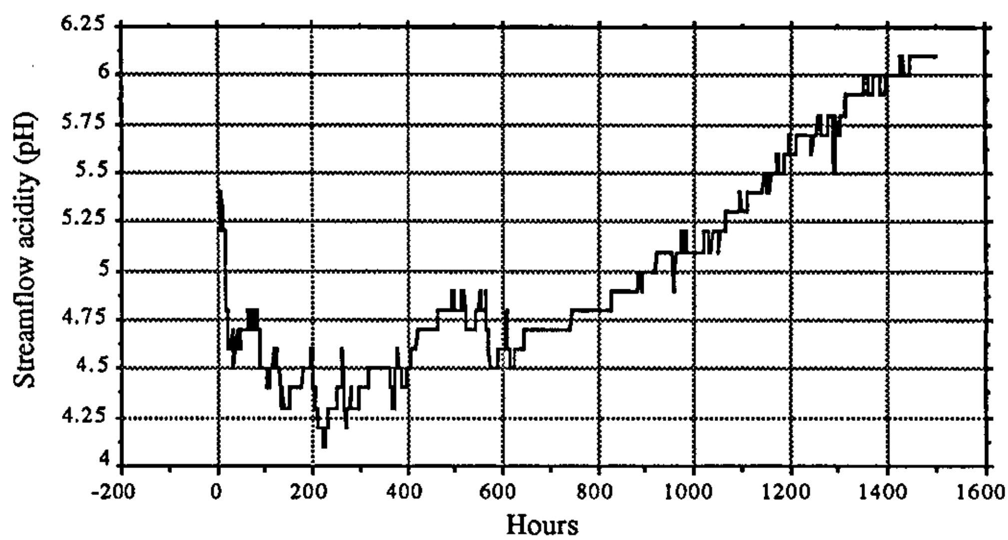


FIGURE 6.12b Hourly streamflow acidity on the Beacon (1.4.89 - 2.6.89)

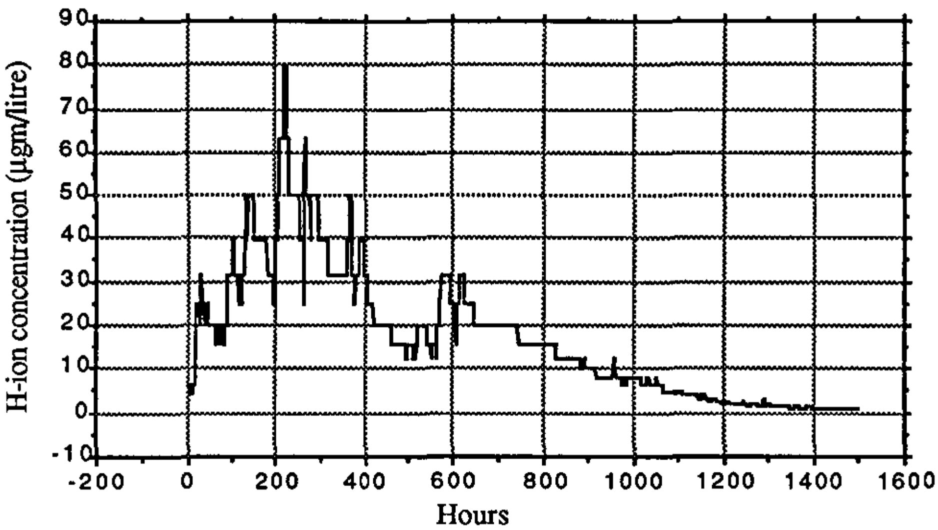


FIGURE 6.12c Hourly streamflow H-ion concentrations on the Beacon (1.4.89 - 2.6.89)

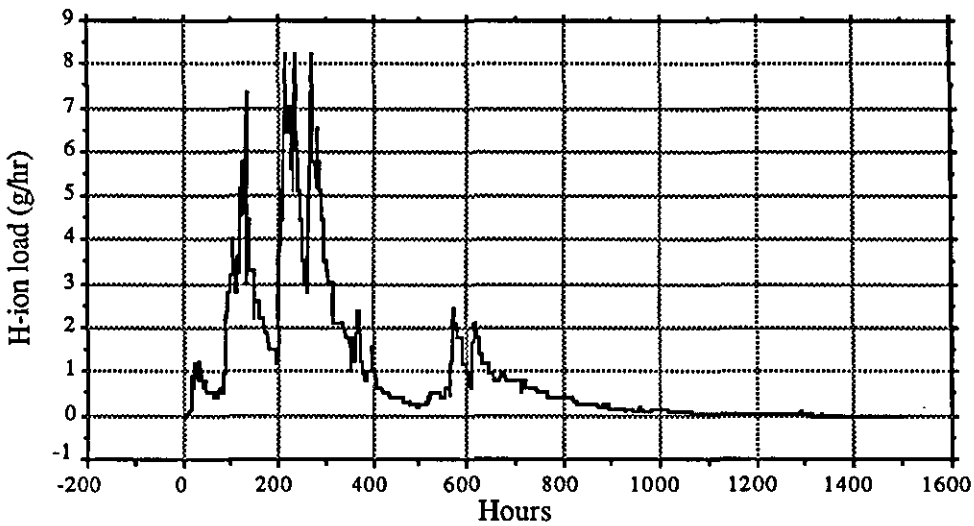


FIGURE 6.12d Hourly H-ion load discharged from the Beacon (1.4.89 - 2.6.89)

Beacon catchment (or more specifically the hydrogen-ion) is hydrologically as opposed to atmospherically 'driven'. That is to say, at the event-scale the terrestrial phase of the water-cycle has the greater influence on the emergent catchment water acidity.

This proposition was further supported by an investigation of the **monthly input-output** catchment-budget for the hydrogen-ion (Figure 6.13). Overall the Beacon catchment operates as an efficient sink for the hydrogen-ion (trapping 94.34% between March 1988 and June 1989). Whilst there was reasonable agreement between the monthly input and output H-ion loads (r^2 = 61.6%), this was largely attributable to the colinearity that exists between the H-load calculations and the monthly rainfall and discharge totals. It was possible to normalise these hydrological components by comparing monthly input-output acidities instead. Again, there was a stark contrast between the r-squared values obtained for the monthly input-output pH relationship (r^2 = 0.1%) and for the monthly discharge versus streamflow pH (r^2 = 93.4%). This is further evidence in support of the close relationship that exists between the seasonal pattern of H-ion assimilation and release from the catchment, and the monthly discharge regime. Furthermore, this link has already been established for other sites in the U.K., most notably in the Lynn Brianne region (Welsh Water Authority, 1987) and in the remote Galloway Hills, S.W. Scotland (Langan and Whitehead, 1987).

6.3 THE SECONDARY DATA SOURCES

A summary of selected periods of the CET record is given in Table 6.4, whilst a running mean of the annual temperatures (1659-1988) is presented in Figure 6.14. The statistics provided in Table 6.4 suggest that over the period 1659-1988 there has been a gradual warming by on average of 0.6-0.7 degrees Celsius in the Central England Temperatures. Within this long-term trend, five epochs may be arbitrarly identified: two periods of cooling (1659-1698 and 1951-1988), two of increasing temperatures (1699-1735 and 1891-1950) and one long period of relatively stable temperatures (1736-1890). Superimposed upon these broad zones, there is clear evidence in Figure 6.14 for 11- and 22-year (sunspot) cycles up until the 1930's and to a lesser extent a 200-250 year cycle (Gribbin, 1989). This visual interpretation of the data is also supported to a certain extent by Bain's (1976) power spectrum of CETs which indicated a strong spectral peak at a period of 23-years (the double-sunspot cycle).

In the light of recent discussions concerned with global warming (Idso, 1984) it is interesting to observe that the actual trend in the mean annual CET's since the 1950's has

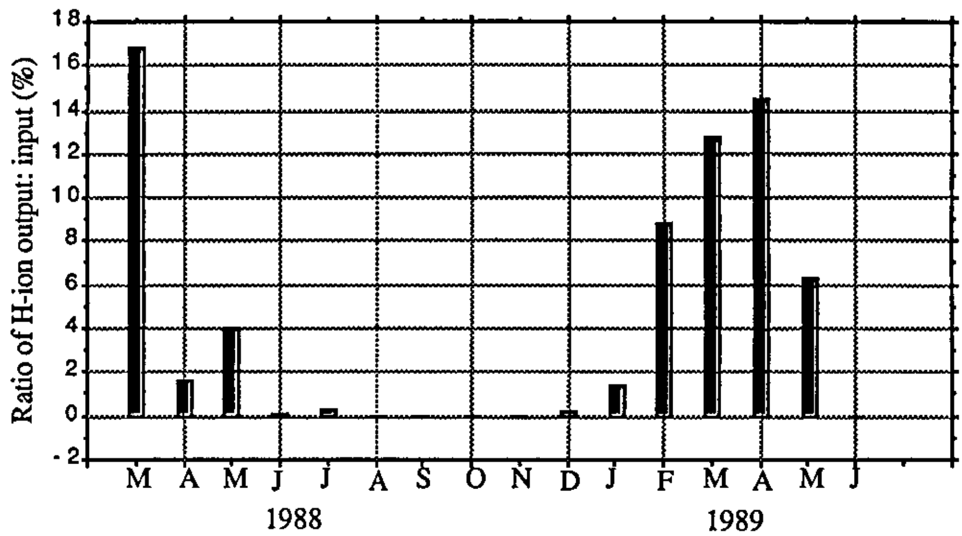


FIGURE 6.13a The H-ion input- output budget for the Beacon (March 88 to June 89).

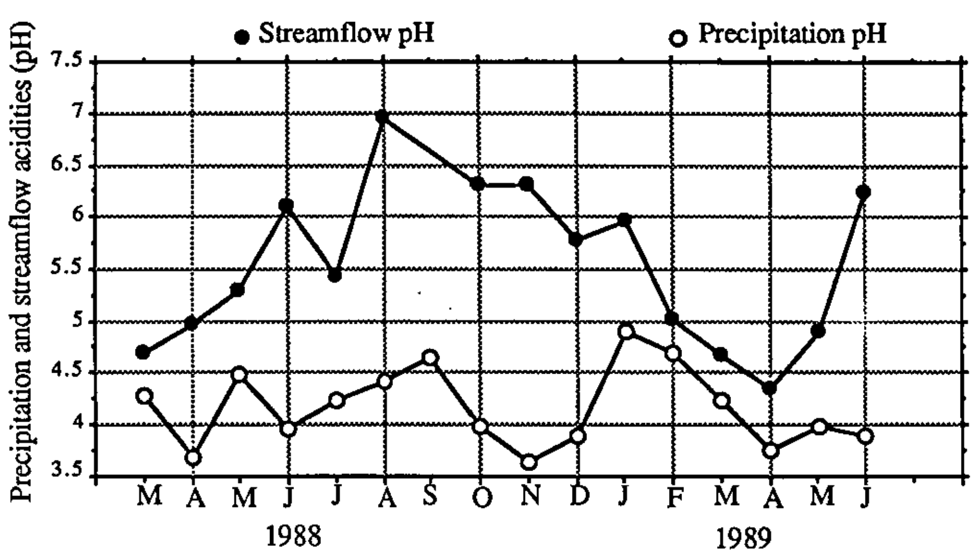


FIGURE 6.13b Volume-weighted input (precipitation) and output (streamflow) acidities (March 88 to June 89).

Period	Mean (°C)	S.D.(°C)	Trend (°C/pa)	Significance (%)
1659-1698	8.640	0.619	-0.030	0.02
1699-1735	9.311	0.448	+0.022	0.09
1736-1890	9.096	0.631	0.000	
1891-1950	9.388	0.508	+0.011	0.26
1951-1988	9.357	0.473	-0.007	
1659-1988	9.147	0.614	+0.002	0.01
1729-1738	9.87	Warmest decade		
1689-1698	8.06	Coolest decade		
1949	10.6	Warmest year		
1740	6.8	Coolest year		
1976	10.1	Drought year		
1988	9.8	(Loughborough)		

TABLE 6.4 Selected periods and extreme years from the Central England Temperature record.

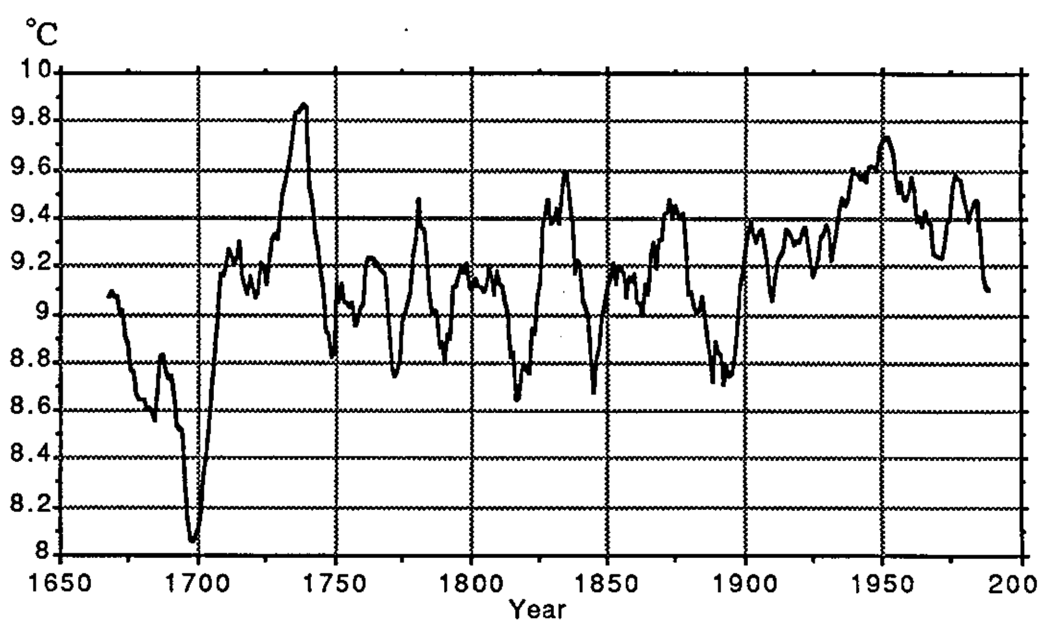


FIG 6.14 10-year running mean of the Central England Temperatures (1659-1988)

been one of gradual cooling. An investigation of the monthly statistics for the period since 1950 indicated that this decline in mean temperatures has been evident in all months with the exceptions of July, August, September and December which show a slight (statistically-insignificant) warming. The most significant cooling has occurred during April (82% confidence level) and May (93% level). For a slightly extended timescale, Sowden and Parker (1981) found that since 1900, the most significant changes appear to be in April cooling, and in October warming. However, despite these localised changes the underlying temperature trend for the entire record length is of the order +0.2°C per century.

Summary statistics for the rainfall recorded at the Nanpantan site (1881-1981) are provided in Table 6.5 and a 10-year running mean of the annual totals is presented by Figure 6.15. If the annual totals prior to 1926 are regarded as being of a suspect nature, the wettest and driest decades on record are centred on 1930 and 1945 respectively. With the exception of the period 1930-1945, the annual rainfall totals to 1988 have oscillated about a stable mean with no statistically-significant trend evident. As the standard deviations suggest, the year-to-year variability has been high during this period with decadal coefficients of variation close to or in excess of the long-term value.

On a seasonal and monthly basis (not shown) there has been an overall trend towards drier (late) summers /autumns (July-November) and wetter winters (December-March) between 1945 and 1988. The most marked changes have however, occurred during March and July (80 and 90% confidence levels respectively) with on average an increase of 15-25 mm in each of the months since 1945. The most significant decline in monthly rainfall has occurred during November (75% level) which for the 1980's was on average 15-20 mm drier than the 1940's.

The most marked secular variations in the Lamb's catalogue of daily weather types occur in the averaged-annual frequencies of the Westerly -type (W). Lamb (1972) has suggested four natural subdivisions of the period 1861 - present: two epochs respectively of marked prevalence of the W-type (from 1861 or earlier to 1874 and from around 1900-1954) and two of blocking (1875 to around 1899 and 1955 to date) [cf. Table 6.6]. Perhaps the most notable trend, has been the decline in the frequency of the W-type since its maximum frequency in the decade 1920-9 (Figure 6.16). This decline has occurred at a mean rate of 5 days per decade (Table 6.6) and has been compensated for primarily by the cyclonic (C) and anticyclonic (A) LWTs, with former type demonstrating a steady increase during the same period and especially since 1960. Over the most recent two decades (1969-1988) there is however, some evidence of a resurgence in the frequency of the W-type. As Figure 6.16 indicates this has **not** arisen from a corresponding reduction in the frequency of either

Period	Mean (mm)	S.D. (mm)	C.V. (%)
1881-1890	673.2	146.4	21.8
1891-1900	624.0	97.4	15.6
1901-1910	651.3	93.5	14.4
1911-1920	745.6	104.8	14.1
1921-1930	744.8	99.6	13.4
1931-1940	700.6	71.8	10.2
1941-1950	685.1	94.8	13.8
1951-1960	720.1	139.3	19.3
1961-1970	699.5	121.9	17.4
1971-1980	693.9	104.7	15.1
1881-1988	695.1	108.2	15.6
1922-1931	765.5 Wettest decade		
1887-1896	586.1 Driest decade		
1981-1988	705.3 Last 8 years		
1976	503.0 Driest year		
1960	963.0 Wettest year		

TABLE 6.5 Summary statistics for Nanpantan rainfall record, Leicestershire (1881-1988).

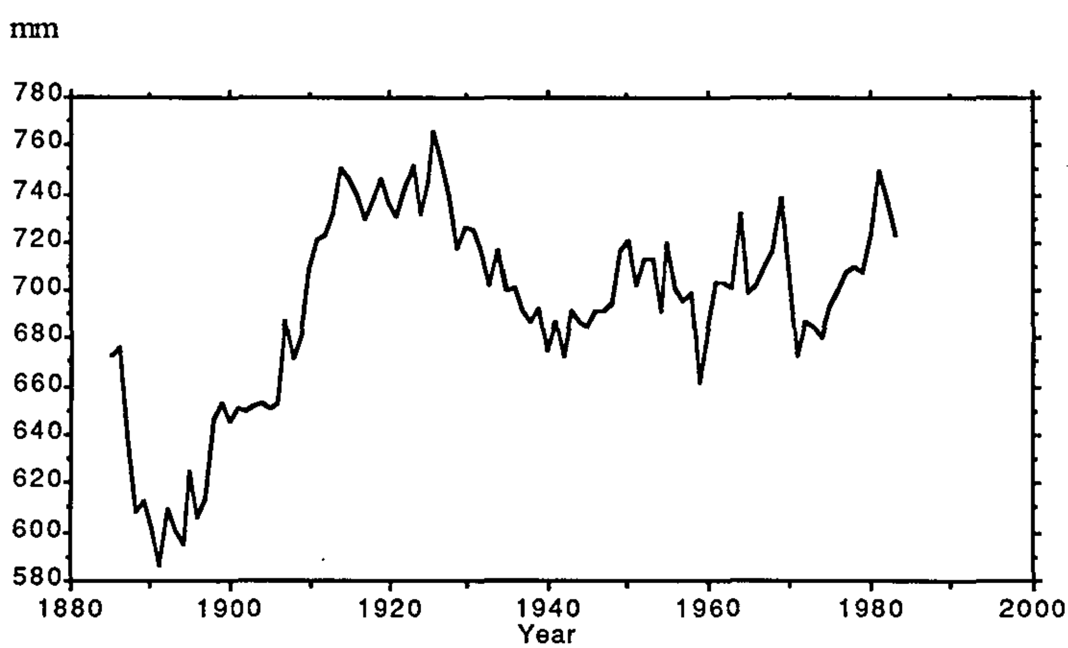


FIG 6.15 10-year running mean of the Nanpantan rainfall record (1881-1988).

Period	W-type	A-type	C-type	Trend* (Days/pa)
1861-1874	71	65	45	-
1875-1899	62	68	44	-
1900-1954	76	65	46	-
1955-1988	57	69	53	-
1861-1988	68	67	47	-0.2
1920-1988	68	67	49	-0.5
1969-1988	54	74	56	+0.9
1920-1929	84	58	47	-
1972-1981	50	69	51	-
1988	73	97	56	-

* W-type only

Best-fit equations

W-type = 68 + 15*sin[π/60(Year-1890)] $r^2 = 19.2\%$ $p = 0.0001$

A-type = 66 + 15*sin[π/25(Year - 1882)] $r^2 = 6.9\%$ $p = 0.0028$

C-type = (Year*0.084) - 114.13 $r^2 = 11.8\%$ $p = 0.0016$

TABLE 6.6 Epochs and trends in the Lamb's register of Daily Weather Types.

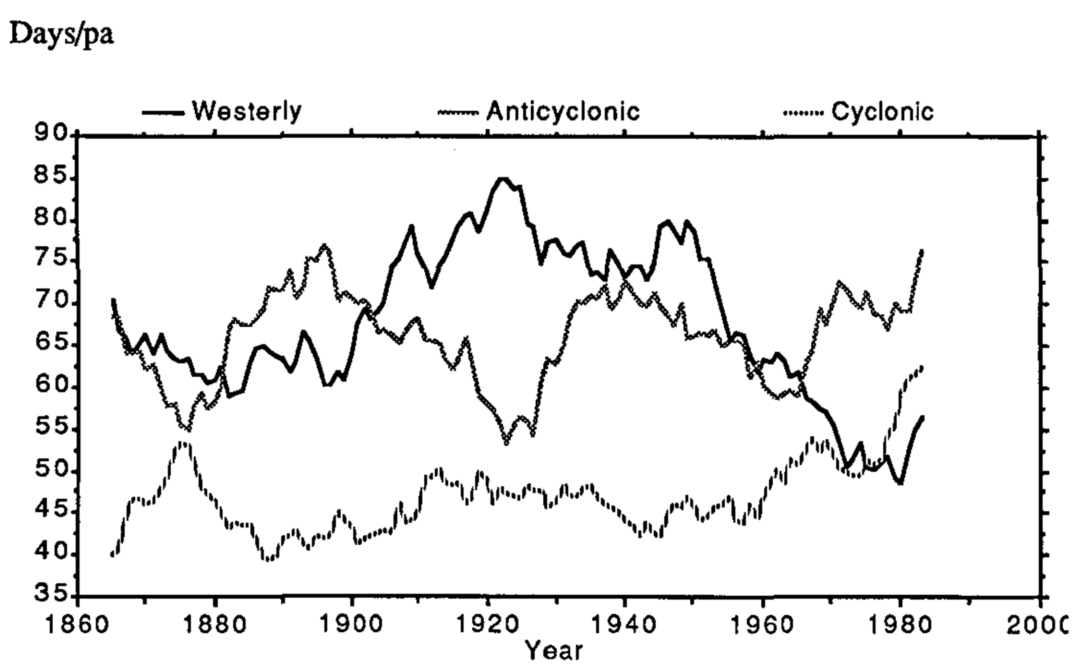


FIG 6.16 10-year running mean of the three dominant LWTs.

the A- or C-type. The year 1988 was also remarkable for the high frequency observed in all three of the main LWTs, out of which the A-type total was particularly noteworthy.

The long-term cyclical behaviour in the annual frequency of the W- (and A-type) is borne out by the significance of the equations given in Table 6.6. The sinusoidal best-fit equation contrasts with the linear relationship derived for the C-type frequencies. Clearly there is some scope for the application of more complex time-series approaches (such as ARIMA) to the prediction of the long-term predominance of each of the key weather-types. For example, Jones and Kelly (1982) have shown using principal components analysis, that 70% of the variance of the annual frequencies in the catalogue (1861-1980) can be accounted for by just six of the 28 weather types (these are the cyclonic, westerly, anticyclonic, northwesterly, northerly and southerly types). Significant correlations found between these components and the annual England and Wales rainfall and Central England Temperature series for the period 1861-1980, further support the assertion that simple indices of synoptic characteristics can yield physically reasonable measures of inter-annual and long-term climatic changes. The most significant relationships were found between the components representing changes in the relative frequency of the anticyclonic, cyclonic and westerly LWT classes, and annual rainfall totals. Thus, years of low rainfall, were associated with enhanced anticyclonicity and/ or decreased westerliness. Such relationships were not, however, as readily derived for central England temperature data where the atmospheric circulation anomalies responsible for temperature extremes vary considerably from season to season (Sowden and Parker, 1981).

At the level of daily precipitation and temperature relation, the situation is reversed. Yarnal et al. (1988) applied a computer-assisted, correlation-based synoptic classification system and found that whilst temperature values tended to be physically reasonable for all synoptic types (such as southerly flows leading to relatively high temperatures), the relationship between daily precipitation and the synoptic types was much more variable. The authors concluded by discouraging the use of correlation-based classification methods in (most) predictive studies.

However, at the super-annual /inter-decadal scale of analysis the three main LWT classes (W-, C- and A-type) are able to account for some of the weather variability associated with circulation fluctuations. This view is supported by the results of a number of correlation tests conducted using the LWT catalogue, Manley CETs and Nanpantan rainfall data (Tables 6.7a and 6.7b). As might be expected, wet-years at Nanpantan, Leics. tended to be associated with increased cyclonicity, and dry-years with elevated anticyclonic activity. Surprisingly, the frequency of the westerlies appears to have little bearing on annual rainfall totals in the East Midlands. Following a similar analysis of regional rainfall variations in

LWT	r	r^2	F-statistic	Confidence
A	- 0.455	0.207	26.906	99.99
C	+0.571	0.326	49.903	99.99
W	+0.044	0.002	00.167	31.63

TABLE 6.7a Relationships between Nanpantan annual rainfall and the frequency of the anticyclonic (A), westerly (W) and cyclonic (C) Lamb's Weather Types (1881-1988).

LWT	r	r^2	F-statistic	Confidence
A	+0.109	0.012	01.505	77.78
C	- 0.132	0.017	02.228	86.20
W	+0.279	0.078	10.633	99.86

TABLE 6.7b Relationship between the mean annual Central England Temperatures and the frequency of the anticyclonic (A), westerly (W) and cyclonic (C) Lamb's Weather Types (1861-1988).

England and Wales (1931-1985) Wigley and Jones (1987) found that the highest positive correlations were found for the cyclonic-type in autumn (r = +0.75, significant at the 1% level). A strong link between precipitation and the westerly-type was found only in the NW region of the U.K..

The correlation between annual Lamb synoptic types and mean annual CETs appears to be more tentative than for rainfall (Table 6.7b). Warmer years tended to be associated with a greater frequency of westerly-types; cooler years with greater cyclonicity. On a monthly basis there is further evidence that, for example, the decline in the frequency of the April westerlies since 1950 has been accompanied by declining CETs (Sowden and Parker, 1981). The pattern of August temperatures since 1900 also clearly reflects the frequency of the August anticyclonic-type. In general, however, it is evident that the resolution and local nature of the LWT classification limits the extent to which the catalogue can be used to account for annual temperature fluctuations (Jones and Kelly, 1982). Furthermore, under a climatic regime tending towards increased cyclonicity and westerly flow any relationship with annual temperatures is likely to become increasingly difficult to detect due to their mutual counter-activity.

6.4 DATA-BASE ASSESSMENT

As discussed in Chapter 4, the value of a data-base (where model calibration and validation are concerned) lies in its length and size as well as in the validity, information content and representativeness of the individual measurements. An assessment of the validity of the techniques was made in 5.4 and where possible error margins and degrees of uncertainty placed upon the data values. An indication of the representativeness of the 16-month observation period has been provided in section 6.2 through comparisons made with long-term means (where available). An evaluation of the data-base in its entirety is now made and general comments about its value and usage are also presented.

With the exception of the very mild winter period, the overall temperature regime complied well with the 30-year mean. The rainfall regime was far from 'normal', and the low aggregate totals resulted in an unusual monthly stream hydrograph. This in turn was reflected in the rapid and extreme changes observed in the surface-water acidity. Where the acid load to the catchment was concerned, this appears to have been highly episodic even when compared with a similar site in the East Midlands. Reference to the Lamb's catalogue indicates that the period exhibited above average frequencies for the anticyclonic weather type in particular: this accounted for the low rainfall and high precipitation acidities.

Therefore, from the point of view of calibrating the SCAM model, the rainfall regime of the calibration data-set represents an obstacle to the derivation of representative parameter values. For example, during the sampling period (12/3/89 - 30/6/89) 206 precipitation events were monitored. As Figure 6.17 indicates, the distribution of event sizes conformed closely to the hypothetical exponential relation assumed in the design of SCAM. However, the total precipitation amount was 90% of the 30-year mean, implying that the sampling period was heavily biased by the extraordinary frequency of the anticyclonic weather-type. As Table 6.3 reveals this was at the expense of the rain-bearing westerly and cyclonic weather-types. By stratifying the total sample of precipitation events into the eight main LWT categories given in Table 6.3, and computing the two parameters (mean rainfall amount and rainfall probability) for each class, the physical basis of the below-average rainfall may be reproduced. It was necessary, however, to assume that the mean rainfall amounts and probabilities derived from the sampling period for each LWT were representative of the long-term condition. The fact that it has been possible to reproduce the rainfall totals for even extreme years using annual LWT proportions only, supports the validity of this assumption (Wilby, 1989).

The effect of the exceptionally mild winter on the suitability of the data-base for model calibration and verification is harder to assess. The fact that there was no significant (and lasting) snowfall during the 16-months requires that this aspect of model performance be verified using less detailed hydrological data collected prior to 1988. Furthermore, because of the high winter temperatures and low rainfall total, the season of zero flow was extended in 1988/1989 by two months. The result being that measurable discharges were limited to approximately 75% of the data-set. However, the 'hydrological variability' contained in the available record may be regarded as highly valuable due to these very same extreme conditions: during March - April 1989 saturated conditions were experienced; juxtaposed against this in May - June 1989 drought conditions; whilst the period March - August 1988 provides a useful indication of 'normal' rates of baseflow recession.

The discussion in section 5.2.3 highlighted some of the difficulties associated with the collection and storage of water samples, and the measurement of pH. These uncertainties applied to both the input (precipitation) and output (discharge) components of the catchment data-base. Although the volume-weighted mean pH of precipitation was found to be lower than many sites in Europe and the U.S.A., the actual distribution of event acidities was in accordance with a comparable site in the East Midlands (Martin and Barber, 1984). If as Mason (1985) suggests, a coefficient of variation of 30-50% for pH measurements is considered the standard level of accuracy between laboratories, then discrepancies of ± 0.2 pH units between sites should not be considered too significant. By utilising the same

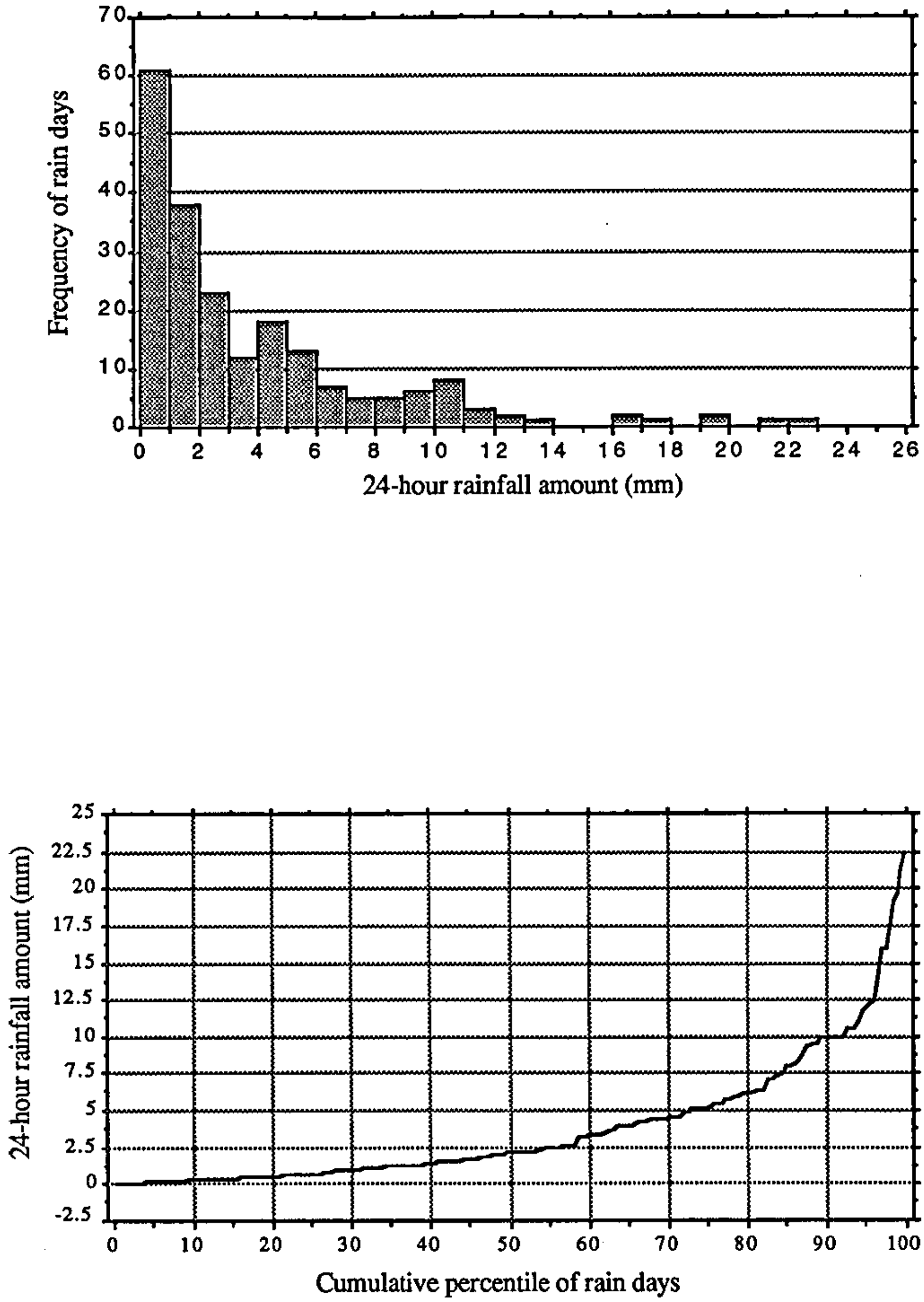


FIGURE 6.17 The exponential distributions of 24-hour rainfall amounts recorded at Loughborough (March 88 to June 89).

instrument for both H-ion inputs and outputs the acidity data should at least be internally consistent. However, the problem of relating the precise results to other sites (both within the U.K. and in Europe) remains a characteristic difficulty of such studies.

The broad 'uncertainty boundaries' which surround individual measurements of precipitation pH also had implications for the accurate categorisation of events and for discriminating between different LWTs. An analysis of the variance of the precipitation event acidities contained in each LWT category (using Scheffes Test), indicated that only three classes could be statistically distinguished from the W-type: namely, the A-, C- and N-types. No other pairs of LWT could be statistically separated on the basis of their inherent rainfall acidity distributions. Furthermore, the LWT classification was only marginally more efficient at accounting for rainfall acidity than the surface wind direction ($r = 0.5$ as opposed to $r = 0.48$).

The implication of these results are as follows. Whilst the Lamb's system of weather-type classification provides a theoretically and physically sound basis for categorising precipitation events and their associated meteorological conditions, in practise, the system's class distinctions are too vague and do not sufficiently discriminate between the various processes of acid deposition. This may in part be attributable to the subjective element involved in the assignment of a given rain-day to the appropriate weather-class using surface pressure maps. The construction of an alternative classification scheme that was 'custom-designed' for acid precipitation processes might facilitate a greater explanation of the observed variance. There is also some scope for the application of multivariate clustering techniques to this problem.

The importance attached to accurately classifying individual precipitation events should not be under-estimated. By relaxing the definition of the main LWT classes it is possible to redistribute these same events into an infinite number of alternative sub-classes. This in turn has direct consequences for the derivation of 'true' weather-type pH, mean rainfall amounts and probability distributions (Table 6.3). These equations and LWT class statistics then determine the stochastic H-ion load generated for different configurations of future LWT frequency proportions.

Therefore to conclude this assessment of the SCAM data-base the following general points are made with regard to its value as a source of empirical calibration data:

1) Although the 16-month observation period contained a number of periods of extreme weather conditions - primarily relating to the mild, dry winter 1988/1989 and the very wet spring of 1989 - it was felt that rather than detracting from the

value of the data, these features actually enhanced its validity. After all, the SCAM model is concerned with simulating some of the impacts of climatic change and of weather conditions which at present could be considered 'unusual' or extreme.

2) By providing additional information regarding processes outside of the immediate temporal- and spatial-scales that concern the SCAM model, the data has enabled model refinement and identified areas which require further development. So for example, information concerning the spatial aspects of surface-water acidity in the Beacon catchment (6.2) offers a partial explanation as to why SCAM does not simulate the streamflow acidity perfectly (cf Chapter 7)! At the same time, temporal studies of the behaviour of the H-ion at various scales of analysis, indicated that relatively simple assumptions could be made concerning its hydrological dependency.

3) The advantages gained from utilising the 1861-1988 Lamb catalogue of daily weather types and the associated classification procedure are partly offset by its subjectivity. In the absence of any formalised and objective system of precipitation events **and** their associated acid deposition meteorology, the class statistics and probability distributions presented in Table 6.3 and Figure 3.4 must suffice. A degree of uncertainty, however, will inevitably be introduced into model parameters and hence model forecasts. This is, of course, also true of the inherent uncertainties associated with rainfall and streamflow measurement - individual daily values upon which the reliability and quality of model predictions ultimately depend.

6.5 SUMMARY

As a means of summarising the main functions of the components of the SCAM data-base, Figure 6.18 illustrates the relational properties of the individual elements within the framework of the modelling objectives. Details concerning long-term climatic fluctuations were provided by the secondary data sources; fluctuations observed in these records are assumed to be symptomatic of the long-term sequence of daily weather types which in turn govern the response of the catchment hydrochemical systems. The 'catchment properties' are represented by parameters derived from a numerical 'fitting' of these observed time-series to sequences of predicted data.

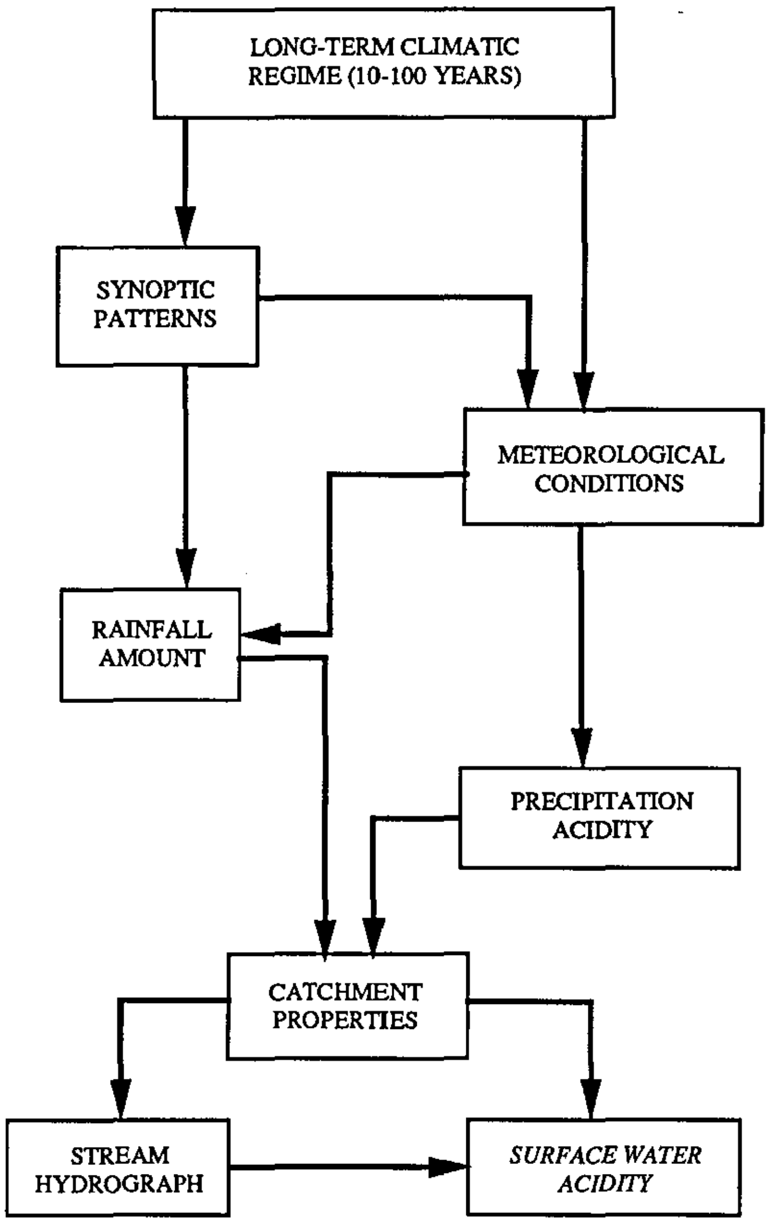


FIGURE 6.18 The relational properties of the SCAM data-base components.

To reiterate, the SCAM data base performs four main functions.

Firstly, the short-term daily data or empirical observations are required in order to **calibrate** the model using contemporary atmospheric inputs and catchment conditions. It is essential that those elements should include representative and accurate measurements of the modelled process(es); any uncertainties incorporated at this stage will have a direct bearing upon the subsequent reliability of the optimised parameters. Whilst it is impossible to eliminate all errors from the calibration data-set, a critique of the methodologies involved in its compilation should be regarded as a necessary precursor to the quantification of model forecast confidence intervals (Rosenblueth,1975).

Secondly, and following on from the demands placed upon a calibration data-set, the data-types (of all temporal and spatial scales) provide an opportunity to **verify** the inherent assumptions of the model design through observations of actual field processes. On-going field experiments have enabled the refinement and modification of the general model structure as its inherent assumptions and conceptualisations have been challenged. This process of theory led observation and subsequent theory modification presupposes the availability of information concerning 'normal' and extreme conditions alike. A data-base that includes a varied set of conditions has a far greater 'information content' than one which describes system stability, and is of particular value to both model calibration and design stages of development.

Thirdly, synthesised versions of the empirical data and secondary data sources provide statistical **inputs** of a different order. An important aspect of the data is to provide realistic boundaries to the parameter values selected by the program operator. For example, records of mean daily temperature taken for a complete year provide actual values for the following parameters: the standard deviation of the daily temperature regime; the mean annual temperature; the seasonal pattern of the temperatures; and the amplitude of these variations.

Finally, by using past climatic data as an **analogue** for future climates the details of characteristic (wet, dry, cold, mild, cyclonic, anticyclonic etc.) phases may be recreated within the computational laboratory of the SCAM model. For example, the climate of the warm phase of 1943-1953 has been employed as an analogue for future global temperatures associated with a doubling of atmospheric carbon dioxide (Lough et al., 1983). Secondary sources such as the Manley Central England Temperature record (Manley, 1973) therefore provide an invaluable source of information regarding the long-term variability, direction and rate of change of annual temperature statistics within the region. Due to the length of the Lamb catalogue it may also be assumed that any atmospheric response to global warming will be an inherent part of the long-term weather type record.

Having now established the basis, theoretical and practical limitations, and comparative representativeness of the data-base, the following chapter in the development of the SCAM model is to provide a formal account of the adopted calibration and verification procedures. This then provides the platform from which the subsequent model forecasts are to be projected in Chapter 8.

CHAPTER 7

SCAM CALIBRATION AND VALIDATION

"*A satisfactory model should characterize the principal chemical processes, account for the changing levels of inputs, and provide good estimates of past, present and future soil and water chemistry. It should also be transferable in the sense that it can be readily applied to a wide range of catchments in differing pollution climates with differing land-use regimes and differing soils and parent geology*" (Mason and Seip, 1990, p 17).

7.1 INTRODUCTION

The previous three chapters have underlined the importance of the calibration process to catchment modelling and have emphasised the need for a reliable and varied data base, a means of stating objectively the standard of the model performance, and a method for optimising the chosen estimation criterion. A theoretical explanation for the difficulties involved in obtaining unique and conceptually realistic parameter sets has also been presented, as were discussions of the practical obstacles encountered during the collection of representative field data. These important issues therefore provide the context within which the actual calibration of the SCAM model must be addressed. In order to preserve a level of continuity the description of the calibration methodology will follow closely the sequence presented in Figure 4.1. The general discussion of the model calibration and validation will be made with reference to the Beacon catchment. An assessment of the model's parsimony is then provided by a similar set of results obtained for the three Llyn Brianne catchments in section 7.7.

7.2 PARAMETER SENSITIVITY ANALYSIS

As was shown earlier a fundamental task of any calibration methodology should be to provide a complete list of the model parameters and their respective levels of sensitivity. This enables attention to be focused upon the most sensitive areas of the model structure by reducing the dimensionality of the parameter space for calibration. Accordingly, a complete inventory of the hydrologic and catchment chemistry parameters are provided in Table 7.1. For convenience the parameter list has been divided into two groups: those which relate to the generation of the streamflow hydrograph only and those which influence the

Rank	Parameter	% Cha..nge HBIAS
1	Rainfall weighting factor	27.2
2	Catchment area	14.3
3	Evaporation weighting factor	13.5
4	Baseflow recession rate	10.8
5	SMD at which baseflow ceases	6.7
6	SMD at which evaporation restricted	5.7
7	SMD at which stormflow ceases	2.9
8	Initial SMD	1.8
9	Stormflow recession rate	1.7

TABLE 7.1a Sensitivity of SCAM hydrological outputs to ±10% change in parameter values.

Rank	Parameter	% Change SFABIAS
1	Minimum soil pH	69.4
2	Maximum soil pH	57.0
3	Mean annual temperature	26.3
4	Rainfall weighting factor	25.8
5	Mean daily storm size	25.6
6	Daily rainfall probability	18.6
7	SMD at which stormflow ceases	18.2
8	Maximum mean monthly temperature	16.0
9	Baseflow recession rate	9.2
10	Evaporation weighting factor	9.1
11	SMD at which baseflow ceases	5.3
12	Stormflow recession rate	5.0
13	Annual frequency of A-type	4.9
14	Annual frequency of W-type	3.5
15	Annual frequency of C-type	3.0
16	Day of maximum temperature	2.8
17	SMD at which evaporation restricted	1.5
18	Daily dry deposition rate	1.1
19	Daily temperature anomalies	1.0
20	Daily weathering rate	0.5

TABLE 7.1b Sensitivity of SCAM hydrochemical outputs to ± 10% change in parameter values.

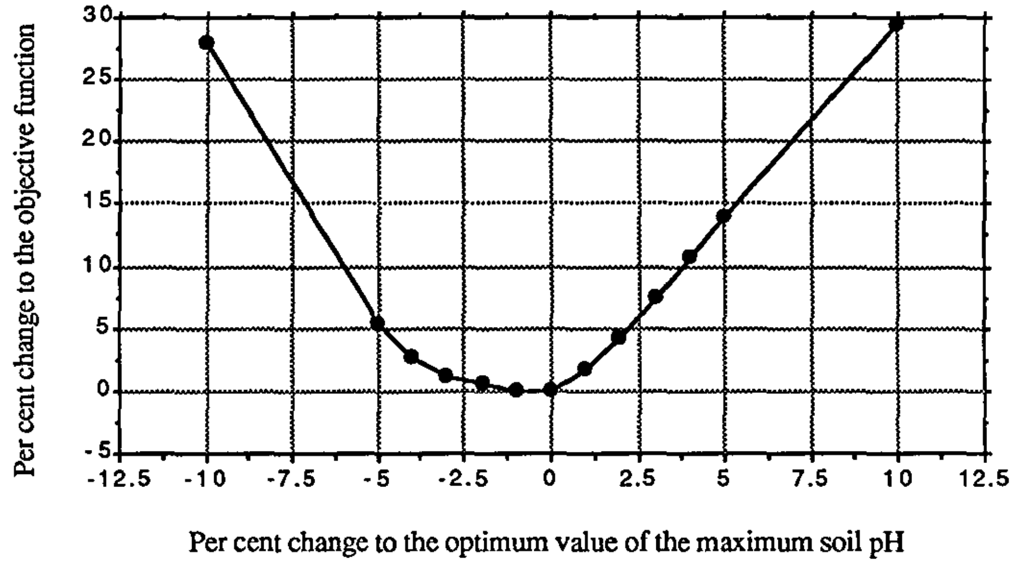
streamflow acidity. This divide was reflected in the choice of the indices of parameter sensitivity: the hydrological parameters were assessed in terms of the HBIAS index and the streamflow acidity parameters in terms of the composite SFABIAS index (both of which are discussed fully in section 7.4).

Commencing with a realistic but arbitrary value, each parameter was adjusted in turn - holding all others constant - by ±10% of its initial value and the mean response to the entire data set was noted in terms of changes to the objective function. Table 7.1 presents the results for the hydrological and hydrochemical parameters in rank order of sensitivity alongside the per centage changes to the HBIAS or SFABIAS objective functions. As might be anticipated, the dominant hydrological parameters relate to the gross inputs and outputs to the catchment area (ie. rainfall totals, catchment area and rates of evapotranspiration). Of secondary importance are the parameters which define the size of the catchment store and the rate at which the baseflow component is released from storage. Finally, the least sensitive parameters pertain to the stormflow response and initial soil moisture status of the catchment.

More specifically where the hydrochemical response of the catchment is of interest, the most sensitive parameters were found to be linked with the maximum and minimum soil profile acidities. Hydrological parameters concerned with the generation of the baseflow proportion and water balance were found to be of secondary importance. The synoptic parameters were found to occupy a position of below average sensitivity and at the lowest end of the spectrum, parameters such as the daily dry deposition and weathering rates (or the size of the store and available supply of cations) were revealed as being highly insensitive to the slight (±10%) changes to their initial values. The contrasting behaviour of these two sets of parameters is demonstrated further in Figure 7.1 through a comparison of the responses of the SCAM model to changes in the maximum pH and the daily dry deposition rate. In the latter case, the maximum departure of the objective function from the base value was slightly over 4%; this was achieved by a 100% reduction of the daily dry deposition rate ! Conversely, for the case of the maximum soil pH parameter, a 10% increase was sufficient to modify the forecast by 30% (as indicated by the objective function). The shapes of the response curves are also not without some significance as the optimum value tends to be more reliably and efficiently located in the symmetrical case (a) than the asymmetrical case (b). Furthermore, in the case of the daily dry deposition parameter (Figure 7.1b) it is clear that the objective function - in this instance, streamflow acidity - is more responsive to reductions in the deposited load than to further increases.

The divide in parameters sensitivities mentioned above - particularly with regard to the model hydrochemistry - was attributed to the respective temporal scales of operation. The

(a)



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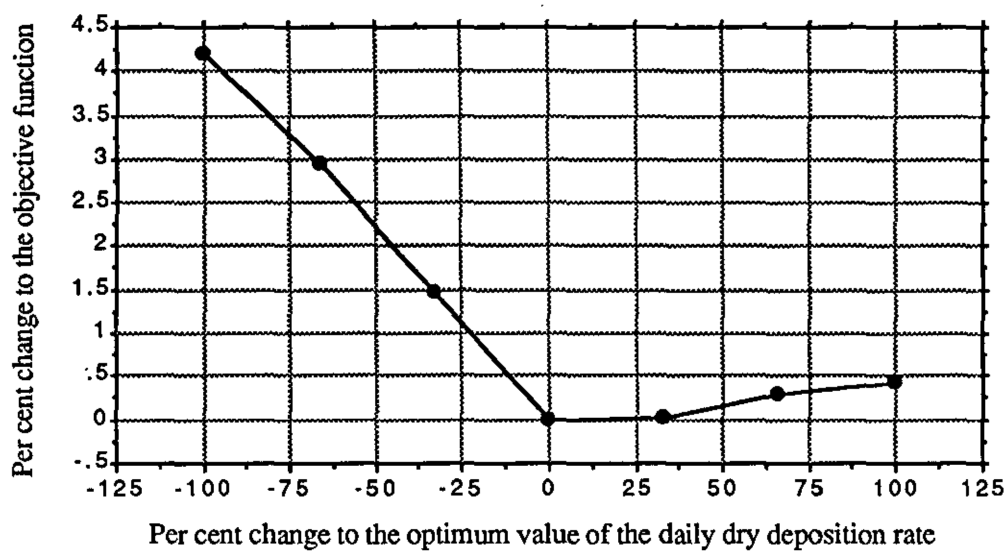


FIGURE 7.1 Comparison of the objective functions for (a) sensitive and (b) insensitive parameters.

most sensitive parameters deal primarily with the short-term (<year) response of the catchment; the least sensitive however, are concerned with long-term alterations to catchment hydrochemical properties operating over scales in excess of 10 years. The intransigence of parameters such as the weathering rate and daily dry deposition rate illustrate the difficulty involved in obtaining reliable parameter estimates derived from short calibration data-sets. For example, the performance of the model over periods of 1-2 years was only moderately affected by the choice of a weathering rate in the range of 10 to 1000 μg/day.

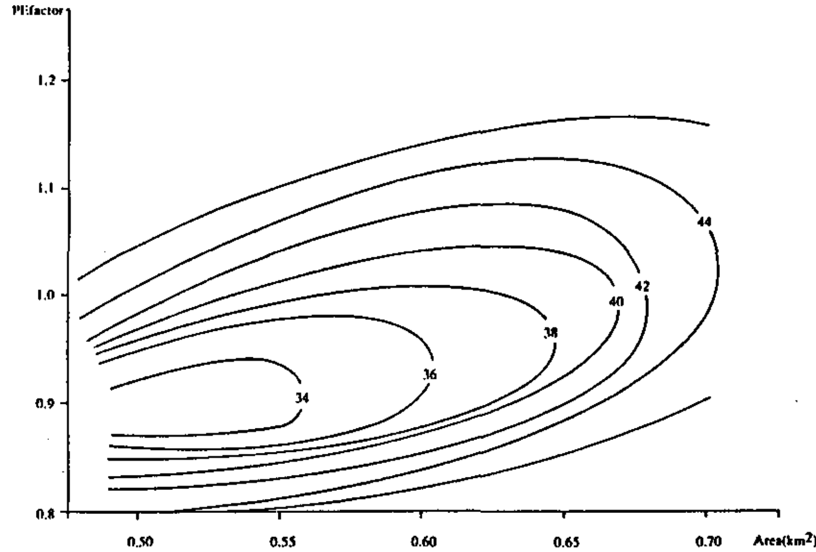
Overall however, the hydrochemical **outputs** of the SCAM model were found to be more sensitive than the hydrology to the assigned parameter values. This underlines the importance of stating which model outputs are of major interest to the simulation exercise, and in turn, which are to be optimised during model calibration. Due to parameter and process interdependency it does not necessarily follow therefore that an optimum set of hydrological parameters will contribute to an optimum hydrochemical description of the calibration data. This observation is examined further with reference to the SCAM model structure.

7.3 ASSESSMENT OF PARAMETER INTERDEPENDENCY

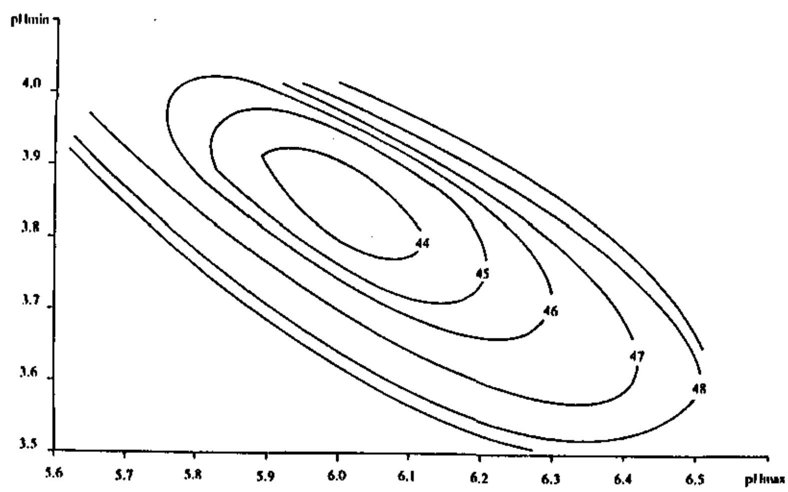
As well as describing some of the properties of individual parameters, a sensitivity analysis conducted simultaneously for two or more parameters may identify structural weaknesses within the model design. In general the ideal shape of the parameter response surface will be a pattern of concentric rings which indicates little or no parameter interdependency. As a means of investigating the level of interdependency between the key SCAM model parameters three sets of parameters were selected.

The first combination of maximum and minimum soil pH values permitted an evaluation of the dominant parameters of the hydrochemical sub-model. The second group - evaporation rate versus catchment area - examined the major components of the catchment water-balance. In either case, multiple model runs were conducted in order to construct a matrix of the model response surface in terms of the objective functions HBIAS and SFABIAS, and the respective parameter values (Figure 7.2). From Figure 7.2a/b and Figure 4.2, it is clear that both parameter couplets exhibited low to moderate interdependency: rather than a clear peak or peaks in the response surface, both sets returned plateau topographies. In terms of searching the parameter space for values, these configurations do not hinder the optimisation algorithm but neither do they return clear global optima. The pattern is not, at least, the valley-shape, being indicative of high parameter interdependency. This was

(a) Potential evaporation weighting factor versus catchment area.



(b) Maximum versus minimum soil pH.



(c) Baseflow recession rate versus maximum soil pH.

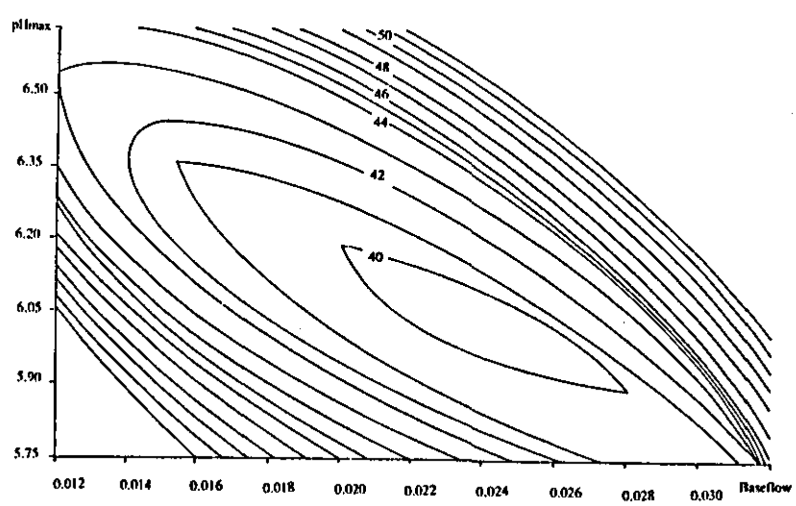


FIGURE 7.2 Three parameter response surfaces.

considered to be an encouraging result in terms of the model structure as these four parameters represent some of the most sensitive elements contained in the model.

As a brief test of the level of interdependency between the hydrological and hydrochemical sub-models the third sensitivity analysis utilised maximum soil pH and baseflow recession rate. As Figure 7.2c indicates, there is again moderate negative interaction between the two parameters and a very steep gradient in the response surface along both axes. In this case the dependency is one-way since the maximum soil acidity is unable to affect the baseflow recession rate, although the converse clearly applies.

As will be shown in the following section this is an example of the need to define specific parameter sets for specific output variables. Due to the interdependency that exists between the two sub-models, no single set of parameter values is able to optimise the output series of both discharge and streamwater acidity consecutively.

7.4 CALIBRATION TECHNIQUES AND THE OBJECTIVE FUNCTION(S)

Having established the individual sensitivities and the nature of the interdependency between some of the key parameters it was then appropriate to implement the calibration methodology and to describe the objective functions.

7.4.1 Methodology

On the basis of the available computational facilities and the detail of the flow record, a semi-automatic calibration technique was devised. This enabled a degree of subjectivity to enter in the choice of an appropriate and realistic parameter set and order in which they are to be optimised. This latter aspect was established on a trial and error basis; the most successful approach being to optimise the parameters in order of their sensitivity commencing with the most sensitive. The exact sequence of manual and computerised actions was as follows (Figure 7.3):

(1) Adopt an initial set of values for the 15 parameters and specify the permissible range over which they are allowed to vary. For example, the rainfall correction factor was allowed to range between ±5% of the initial value, that is to say, the expected error associated with its measurement. An indication of the likely values for each of the main parameters was obtained from the long-term means of the available hydrometric records.

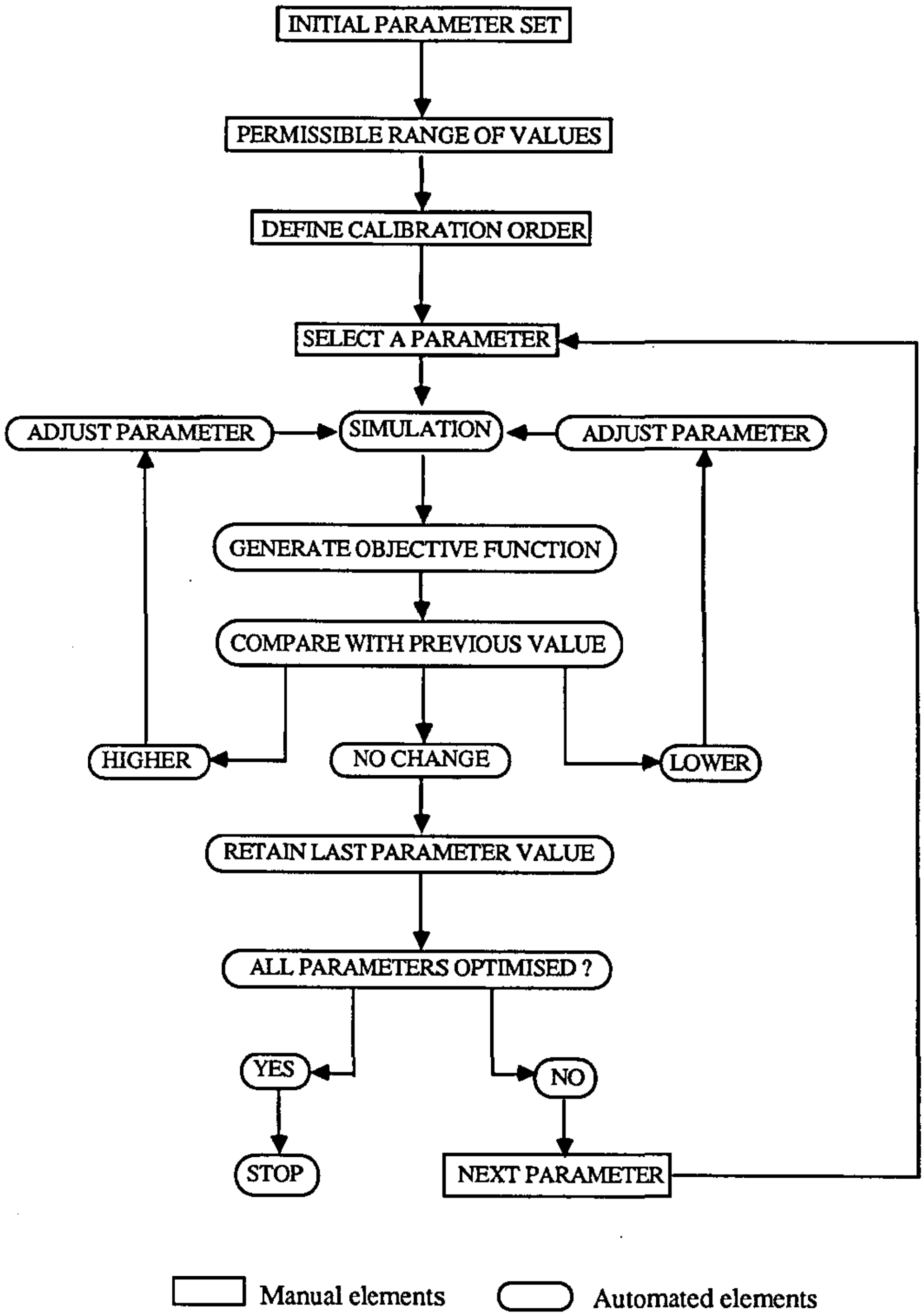


FIGURE 7.3 Algorithm sequence for parameter optimisation.

(2) For each of the parameters in sequence, holding the remaining parameters constant a simulated hydrological and hydrochemical record was produced from the calibration data-base using the daily precipitation amount and acidity, and mean daily temperature.

(3) The model performance was then evaluated using one or a combination of objective functions. The HBIAS statistic was used to detect deficiencies in the reproduction of the streamflow hydrograph and is defined as follows:

$$HBIAS(i) = \Sigma[|Qobs,t - Qsim,t|]/\Sigma Qobs,t$$

where Qsim,t and Qobs,t are the simulated and observed discharges at time t, and (i) is a flow group defined as all the measured flows falling within a predetermined flow range (Sorooshian, 1988). A perfect agreement between observed and simulated flows would result in values of HBIAS consistently close to zero in all flow groups. By examining flow groups (as opposed to the entire discharge record) it is possible to identify inconsistencies in the model forecast performance. The statistic also has the advantage of being unbiased by large discharges unlike the SSR and ABS statistics (cf. 4.5).

The HIONBIAS statistic - used to evaluate the hydrochemical parameter forecasts - simply replaces the observed and simulated discharges of the HBIAS statistic with observed and simulated H-ion concentrations. By utilising the H-ion concentrations rather than the pH units ensures that the emphasis of the simulation was placed upon reproducing periods of elevated acidity.

A third, composite objective function was also used for assessing the quality of the hydrochemical simulations. This SFABIAS index was the mean percentage change to the frequency of flows with pH<4.5, the simulated versus observed total aluminium concentration (ALBIAS) and the HIONBIAS statistic, relative to a predefined reference level or observed concentration time-series. Thus,

$$SFABIAS = 1/3\{(\Sigma|LCD_o - LCD_e|)/\Sigma LCD_e + ALBIAS + HIONBIAS\}$$

where LCD_o and LCD_e are respectively the observed and expected frequency of flows with pH<4.5, HIONBIAS is as described as above, and ALBIAS the same as HIONBIAS but for the total aluminium concentration instead of hydrogen-ion. Of the three components, the LCD fraction was generally found to be the most sensitive to changes in the parameters values. However, by utilising three combined indices the SFABIAS objective function is able to embrace a wider range of factors that corporately describe 'surface water acidity'.

(4) Returning to the calibration procedure (Figure 7.3) the algorithm next compares the current value of the chosen objective function with its previous value. On the first iteration (or if the difference exceeded a predefined limit) the parameter value is then adjusted by 1% and a new time-series is produced by the model. By this means the parameter value is iteratively adjusted either upwards or downwards according to the change in the objective function. If the objective function attains a minimum value, or if each subsequent routine produces a negligible change in its value (<0.01%) the last parameter value is retained.

(5) Provided that the parameter returns a physically reasonable value which falls within the predetermined limits of acceptability, it is then considered to be optimised. The entire sequence (1-4) is then repeated until all of the parameters have been optimised. Note that a split record approach has been adopted in the calibration process which means that 238 days of the total 476 days of available daily data were used; the remainder being reserved for the validation of the parameter values.

7.4.2 Calibration results for the Beacon catchment

Two lists of the resultant optimised parameter values for the Beacon are shown in Table 7.2 as well as the final values of HBIAS and HIONBIAS. The first parameter set (P1) was obtained by attempting to minimise the value of HBIAS without paying attention to HIONBIAS, thereby obtaining the best **hydrological** explanation of the calibration data. It does not necessarily follow therefore, that P1 will produce the best hydrochemical simulation given the same calibration data. For example, Hooper et al. (1988) confronted and overcame a similar problem when calibrating the Birkenes model using the residuals from different signals (daily discharge and ^{18}O concentrations), by normalizing each signal, and then by weighting and combining the individual series to produce an optimum parameter set. However, this technique relies upon the use of a conservative tracer such as ^{18}O to identify and quantify the dominant flow pathways and hydrological processes. As the SCAM model is concerned with the H-ion (which is not conservative) this difficulty was overcome by deriving a second parameter set, P2, for which HIONBIAS was optimised rather than HBIAS. In both cases (P1 and P2) the values obtained for each of the fifteen parameters were derived from 238 days of calibration data (12 March 1988 to 4 November 1988).

Parameter	P1	P2
Catchment area (m^2)	547000	547000
Evaporation weighting factor	0.98	0.98
SMD at which baseflow ceases (mm)	70.0	75.0
SMD at which stormflow ceases (mm)	28.0	28.0
Stormflow recession rate	0.1300	0.1250
Baseflow recession rate	0.0146	0.0170
Initial SMD (mm)	38.0	49.0
Rainfall correction factor	1.085	1.085
SMD at which evaporation restricted (mm)	110.0	110.0
Total soil buffer capacity (μgm^{-2})	$200*10^6$	$200*10^6$
Daily weathering rate (μgm^{-2})	100	100
Maximum soil pH	6.35	6.35
Minimum soil pH	3.70	3.70
Daily dry deposition rate (μgm^{-2})	100	100
Initial soil buffer capacity (μgm^{-2})	$20*10^6$	$20*10^6$

Indices of model performance:

		P1	P2
Calibration:	HBIAS	0.2655	0.3314
	(R-squared)	(88.4)	(80.1)
	HIONBIAS	0.2746	0.1722
	(R-squared)	(87.1)	(96.0)
Validation:	HBIAS	0.3305	0.2904
	(R-squared)	(87.8)	(88.5)
	HIONBIAS	0.4659	0.4647
	(R-squared)	(69.0)	(71.6)

Zero Order Forecasts:

Calibration:	HBIAS	0.28
	(R-squared)	(81.3)
	HIONBIAS	0.46
	(R-squared)	(71.9)
Validation:	HBIAS	0.24
	(R-squared)	(79.3)
	HIONBIAS	0.43
	(R-squared)	(75.4)

TABLE 7.2 Parameter optimisation results for the Beacon catchment with Zero Order Forecasts (ZOF) for comparative purposes.

From Table 7.2 it may be seen that both the calibration sets are remarkably similar - the only differences relate to the moisture retention properties of the catchment. The level of optimisation achieved for HBIAS using P1 was slightly disappointing in comparison with that achieved for HIONBIAS using P2. This is reflected in the quality of the simulation hydrograph where there was a definite underprediction of the magnitude of the storm peaks (Figure 7.4a). This was attributed to a number of contributory factors such as: the brevity of the calibration data-base; uncertainties in the measurement of the areal rainfall inputs and in the stage-discharge relationship; omission by the model of heterogeneous catchment processes such as expanding contributory areas and soil pipe systems; and the accumulation of errors in the calculation of the SMD between storm events.

The success achieved in the optimisation of the HIONBIAS index using P2 was largely due to an increased rate of baseflow release (or shorter period of catchment storage) and via slight adjustments to the initial SMD. The resultant parameter set yielded the closest fit to the observed streamflow acidity data (Figure 7.5a) adding strength to the argument that there exists a very strong correlation between catchment soil moisture status and sources of surface water acidity.

7.5 CALIBRATION OF LONG-TERM CATCHMENT PARAMETERS

In the previous section some comments were made regarding the duration of the calibration period and the reliability of the resultant parameter values. Nowhere are these considerations more crucial than when insensitive parameters which relate to the long-term evolution of the catchment hydro-system must be calibrated against relatively short data sets. Furthermore, these hydrochemical processes are often responding to variable climatic and solute inputs which are themselves notoriously difficult to measure and simulate. Within this context three parameters of the SCAM model were considered to be worthy of special attention. These were the catchment soil buffer capacity, the weathering rate or rapidity with which the former store is replenished, and finally, the dry-deposited H-ion load to the catchment.

7.5.1 Catchment buffer capacity

The catchment base status or base saturation is expressed in terms of the ratio between the total number of cation-exchange sites (or buffer capacity) and the number of these sites which are occupied. The number of exchange sites is in turn a function of soil properties

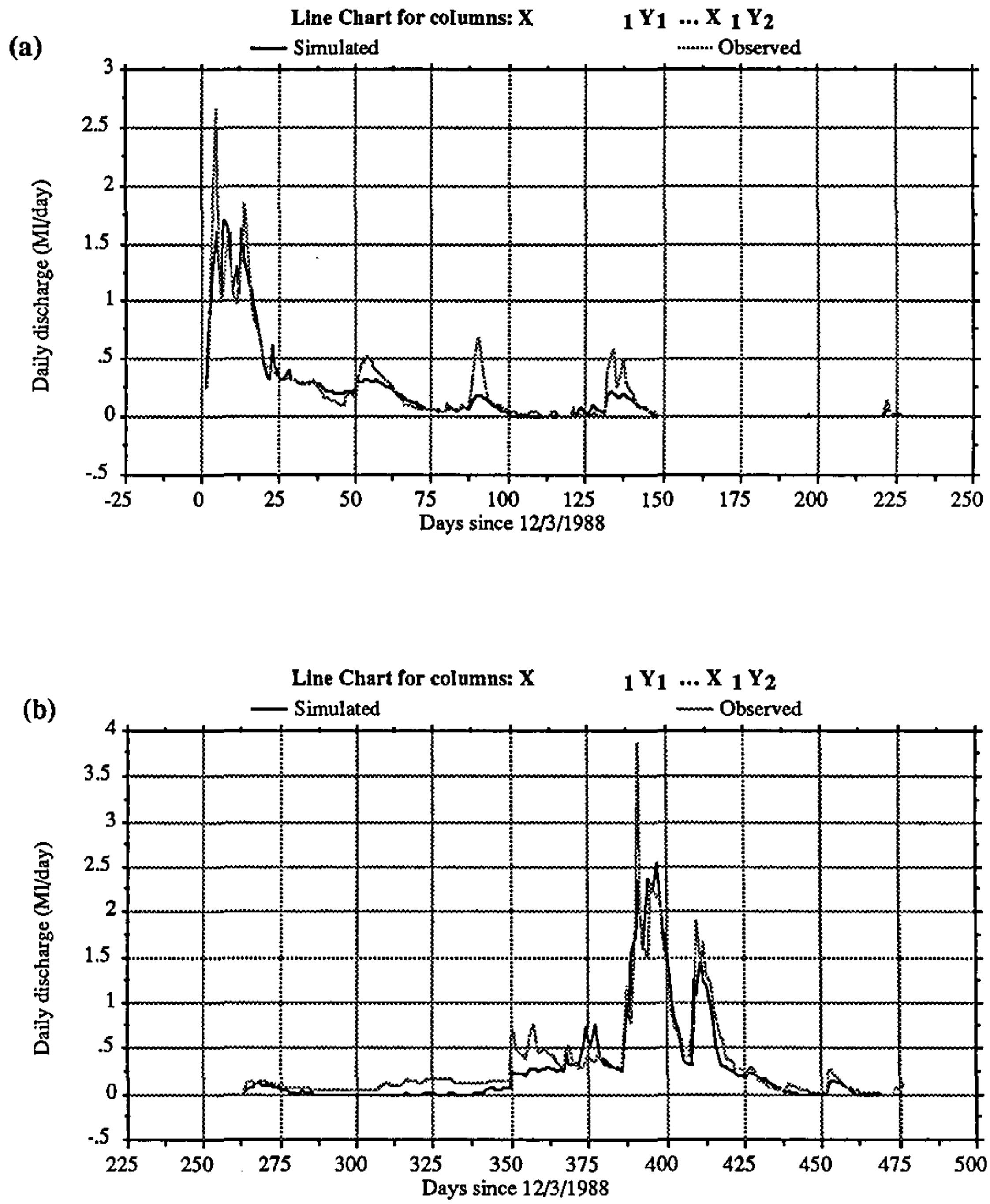


FIGURE 7.4 A comparison of observed and simulated daily discharge for the Beacon catchment during (a) the calibration period [12 Mar 1988 - 4 Nov 1988] and, (b) the validation period [5 Nov 1988 - 30 Jun 1989].

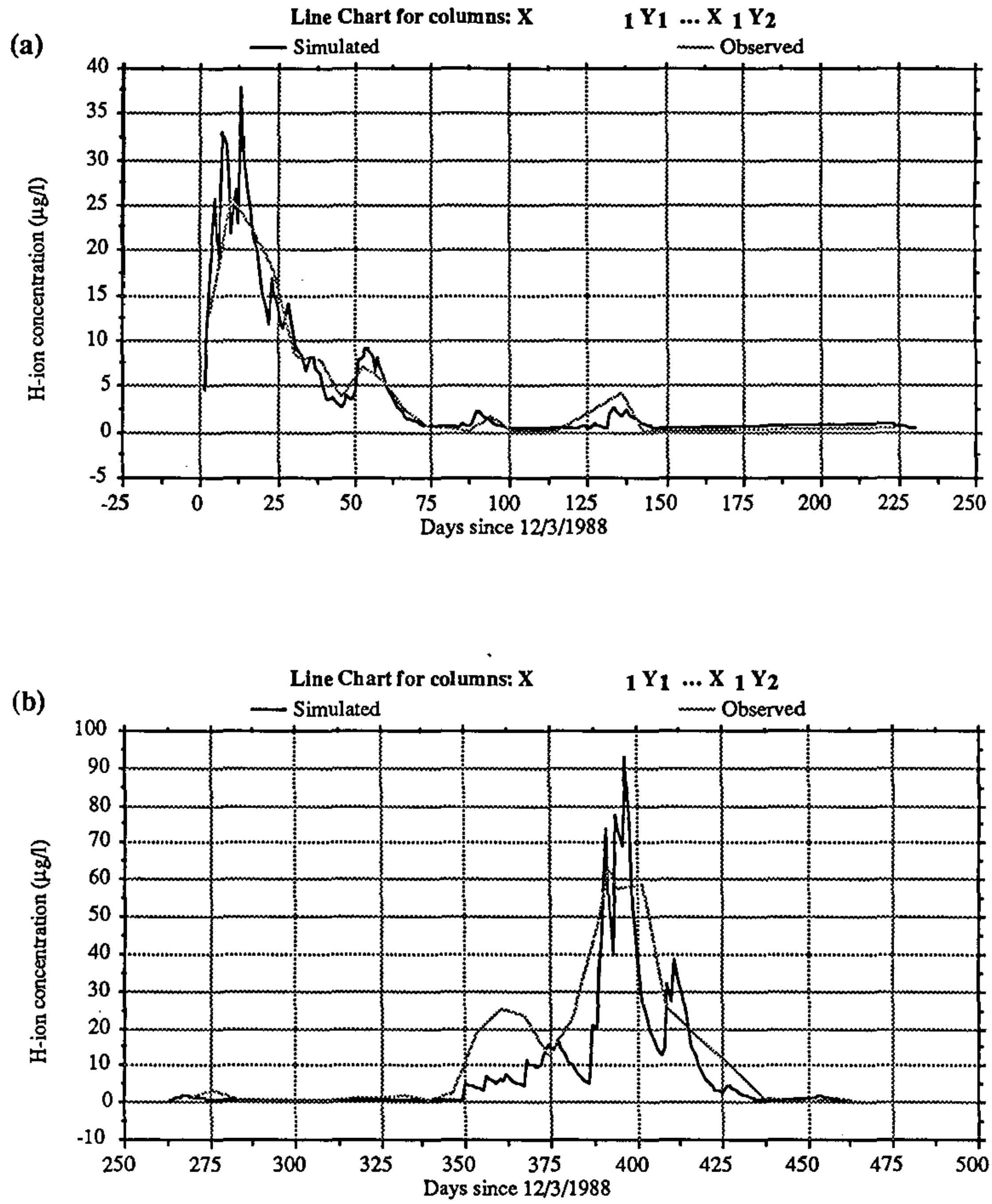


FIGURE 7.5 A comparison of observed and simulated daily discharge acidity for the Beacon catchment during (a) the calibration period [12 Mar 1988 - 4 Nov 1988] and, (b) the validation period [5 Nov 1988 - 30 Jun 1989].

such as the texture. According to Ulrich's (1983) classification of the acid buffering reactions of forest soils, the base saturation for the Beacon catchment lies at an estimated 0.05 - 0.15 (the divide between the cation exchange buffer range and the aluminium buffer range). This assessment was made on the basis of measured soil and streamwater aluminium concentrations issuing from the catchment between 1985-1989 (Greenwood, pers. comm.). The chosen value of 0.10 was further supported by numerous parameter calibrations.

An estimate of the soil profile buffer capacity was obtained from the FAO-UNESCO Soil Map of the World (1974). This source suggests that for an average soil thickness of 50 cm the buffer capacity of the cation-exchange buffer range falls between 125 - $300*10^6$ μeqm^{-2}. Using the base saturation value from above it was then possible to calculate the number of exchange sites occupied as being 125 - $300*10^5$ μeqm^{-2}. These values were therefore assumed during the calibration of the remaining hydrochemical parameters.

7.5.2 Catchment weathering rate

The catchment weathering rate was assumed to provide a **non-variable** source of buffering ions to the overall soil buffer capacity. In this sense the soil acidification process was considered to be reversible provided that the stress rate (or annual H-ion load) was reduced below a threshold which is the value of the weathering rate variable.

Depending upon the silicate status of the parent material the annual weathering rates tend to lie between 20 - $200*10^3$ $\mu eqm^{-2}year^{-1}$, implying a maximum daily weathering rate of 550 μeqm^{-2} and a minimum of 50 $\mu eqm^{-2}day^{-1}$ (Ulrich, 1983; Jacks [in press]; Bain et al. [in press]). Again, these values were confirmed indirectly for the Beacon catchment through multiple calibration runs of the SCAM model. Weathering rates of the same order of magnitude have also been documented elsewhere, for example, van Breemen et al. [1984] provide tables of soil acidification and weathering rates, in terms of the H-ion, for many catchments in the northeastern United States and Western Europe. This survey also showed that ecosystems with low to intermediate rates of soil weathering are characterised by aluminium dissolution as well as strong retention of sulphate. Appreciable amounts of hydrogen and aluminium ion are also exported from these soils to the surface drainage water. This is precisely the situation observed in the Beacon catchment (Lee, pers. comm.), thus supporting the choice of a daily weathering rate in the range of 50 -150 μeqm^{-2} day^{-1}.

7.5.3 Dry-deposition rate for the H-ion

Information concerning the dry-deposition of compounds such as sulphate, oxides of nitrogen and even ammonia are readily available for most areas of the U.K. (DOE, 1988). Much research in this field has focused on sulphur dioxide as in many areas of the U.K. the dry deposition exceeds the wet deposition component. Recent estimates place the dry deposition proportion for the East Midlands at around 30-60% of the total annual acidic deposition which realises a daily dry deposition rate of 50-200 μeqm^{-2} day^{-1} (Cape, pers. comm.).

However, these for the H-ion are derived indirectly from measurements of atmospheric concentrations and laboratory measurements of deposition velocities for SO_2 and NO_2; these in turn are sensitive to type of surface and local topographies. With regard to the SCAM parameters, a value of 100 μeqm^{-2} day^{-1} was selected on the basis of the annual dry-deposition total for sulphate and the mean frequency of rain-days. Since the dry-deposition flux is heavily reliant upon micro-meteorological and -biological processes (Fowler and Cape, 1983; Pruppacher et al.,1983), the use of a single 'precise' value for a catchment as heterogeneous as the Beacon, becomes meaningless. Furthermore, subtle changes to the vegetation cover may also be as significant to the long-term dry deposition rate as changes to the ambient atmospheric concentrations (Whitehead et al., 1988).

7.6 MODEL VALIDATION: THE BEACON CATCHMENT

The validation periods (Figure 7.4b and 7.5b) were an unaltered extension of the ability of the optimised parameter set(s) P1 and P2 to simulate catchment conditions within a forecasting context, being driven solely by input data. A fundamental means of assessing the forecasting proficiency of the model during this period was provided by the Zero Order Forecast (ZOF). From Table 7.2 it may be concluded that the model simulations were more accurate than the ZOF for the hydrochemical as opposed to the hydrological outputs. In general the SCAM model performed better than the ZOF during the calibration period and slightly worse during validation. This was to be expected as during the second half of the data set, the model was subjected to conditions outside of its calibration period, most notably rapid catchment recharge following a prolonged autumn dry-spell. The validation period therefore provided an extremely severe test of the model structure and of its optimised parameter values.

Further analysis of the model's performance was undertaken through an investigation of the normalised residuals of the simulated and observed streamflow acidities and daily discharges. From Figure 7.6 it is clear that the model performed well during the calibration of its hydrological parameters with only a slight tendency to underpredict the magnitude of higher discharge events - the 'noise' shown during the first 25-30 days of the record being attributed to the 'settling period' of the model. During the validation phase the model consistently underpredicted low flows between days 300-375 although the simulated timing and magnitude of high flows between days 375 to 425 was particularly good (Figure 7.4b). This latter aspect was highlighted by the results of an investigation of the model forecasting performance by stage interval (Figure 7.7b). There was a clear pattern of improving forecasts with increasing stage - although it should be underlined that whilst the per centage error was lower for high stages, the absolute magnitude of the residual was considerably larger. The extreme values for the normalised residuals of the flow (days 375-400) were attributed to the mistiming of the peak discharge by 24-hours. This situation arose due to the coarseness of the daily time-step used to compute rainfall inputs and catchment outputs.

A similar pattern was observed for the streamflow acidities with the model performing markedly worse during validation (Figure 7.6), again especially between days 350-400. The 'fit' obtained during calibration was extremely good which served only to emphasize the discrepancies evident in the second half of the record. There was a clear tendency for the model to underpredict the H-ion concentrations for all but the most extreme, high discharge events for which the situation was reversed. As in the case of the daily discharges, the H-ion time-series indicated that the model did not accurately cope with the timing and rate of catchment recharge which occurred around day 350 (Figure 7.6). This in part reflects the fact that the model was calibrated against hydrological data associated with the falling limb of the hydrograph, with very little if any data available for the recharge period; additional reasons for the observed discrepancies will be discussed shortly.

However, the visual comparison of observed and simulated catchment responses whilst commonly undertaken, can be deceptive. Bearing this in mind Figure 7.4b and Figure 7.5b present the respective hydrological and hydrochemical series obtained during the validation phase using the parameter sets P1 and P2. The calibrated regimes (Figure 7.4a and 7.5a) reflected the success or failure of the 'curve-fitting exercise' conducted in 7.4, the quality of the input data and the nature of the model structure itself. These figures indicate that whilst there is in general good agreement between the observed and the simulated discharges there is clear evidence to suggest that the catchment soil moisture store was not depleted to the extent predicted by the model. This then accounts for the delayed return of flow shown in Figure 7.4b at approximately day number 350 during the validation period. When the starting soil moisture deficit for the validation period was reduced from around

(a)

(b)

(c)

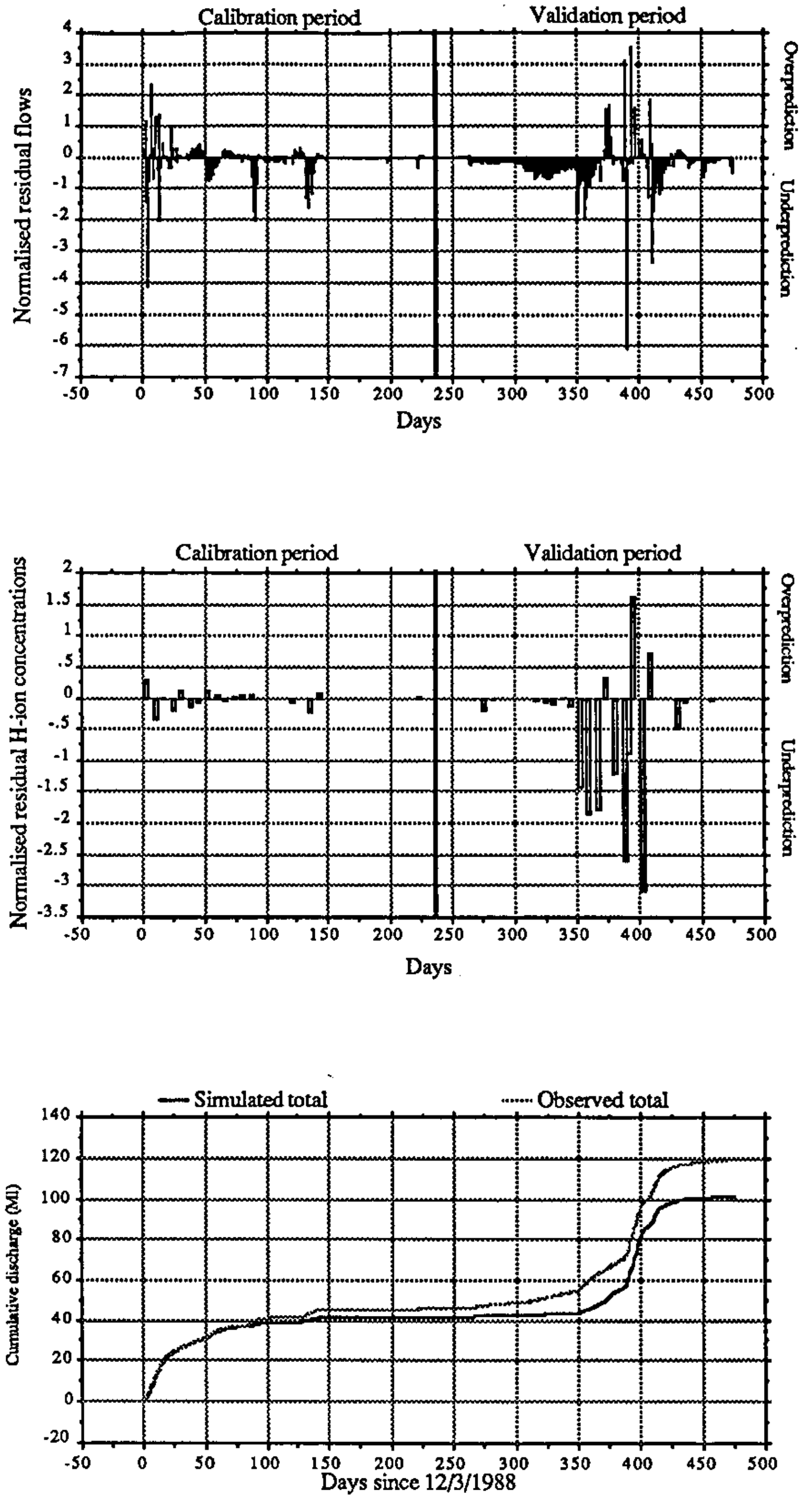


FIGURE 7.6 Analysis of the residuals of the observed and simulated (a) daily flows, (b) weekly H-ion concentration and (c) a comparison of the observed versus simulated cumulative discharge totals.

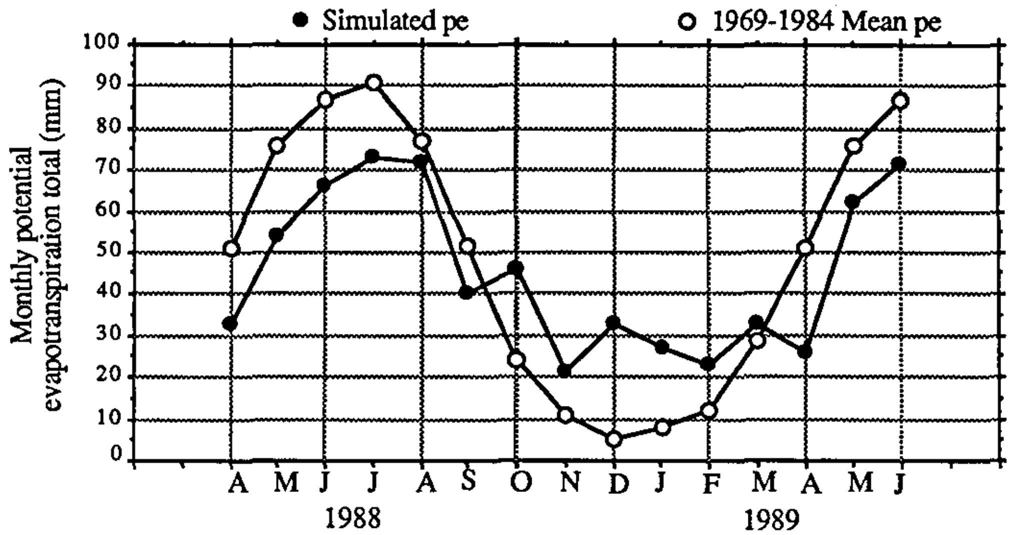


FIGURE 7.7a Comparison of the SCAM simulated monthly evapotranspiration total (1988-1989) with the 1969-1984 mean monthly rate for Sutton Bonington, Nottinghamshire.

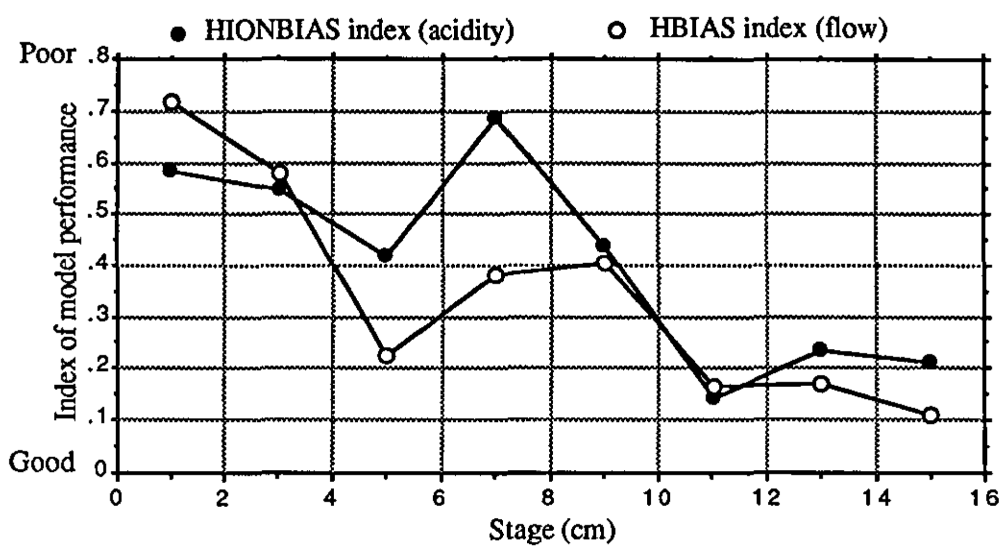


FIGURE 7.7b SCAM simulation performance by stage interval.

90 mm to 60 mm the timing of the recommencing of flow was accurate to within 2-3 days but the overall quality of the model performance was slightly reduced.

Originally the source of the error was thought to be due to the inadequate representation of summer evapotranspiration rates under 'limiting' soil moisture conditions. This possibility was investigated by comparing the simulated monthly potential evaporation with the long-term average rate measured at Sutton Bonington, Nottinghamshire. Even allowing for interannual differences in the weather, Figure 7.7a shows that if anything the model underestimated the summer monthly potential evaporation. Despite this fact, the computed total discharge of the 16-month period was found to be within 15% of the total observed flow over the same period. This implied that the errors were not arising from the computation of the total potential evaporation during the 476-day period, but rather from its seasonal distribution. The period of flow underprediction (approximately December 1988 to March 1989) coincided precisely with the period of maximum overprediction of the monthly potential evaporation by the model (Figure 7.7a). This situation was considered to be the result of the exceptionally mild winter (NERC, 1989; Figure 6.2) and the fact that the evapotranspiration sub-model was driven almost solely by daily mean temperatures. The winter SMD accrued by this overestimation was then later offset to a certain extent by the April-June 1989 underestimation of evaporation. Over these remaining 100 days the hydrological sub-model performed exceptionally well (Figure 7.4b).

7.7 MODEL VALIDATION: THE LLYN BRIANNE CATCHMENTS

As before, the model parameters were optimised using the semi-automatic search routine described in 7.4. However, the selection of appropriate long-term catchment parameters was less problematic since values for the cation exchange capacity, weathering rates and dry/occult deposition rates have all been derived previously for the three Llyn Brianne catchments for the MAGIC model (Whitehead et al., 1988). Summaries of the optimised parameter sets used for each of the catchments, along with their respective calibration and validation performances are presented in Table 7.3a/b. A selection of simulated versus observed stream discharge and acidity time-series are shown in Figures 7.8 and 7.9.

From Table 7.3b it may be seen that, with the exception of catchment CI6, the SCAM model consistently described the daily streamflow acidity more accurately than the daily discharge. At first sight this result appears to be a paradox since the streamflow acidity is in part a function of the predicted discharges. However, there are a number of possible explanations for this occurrence.

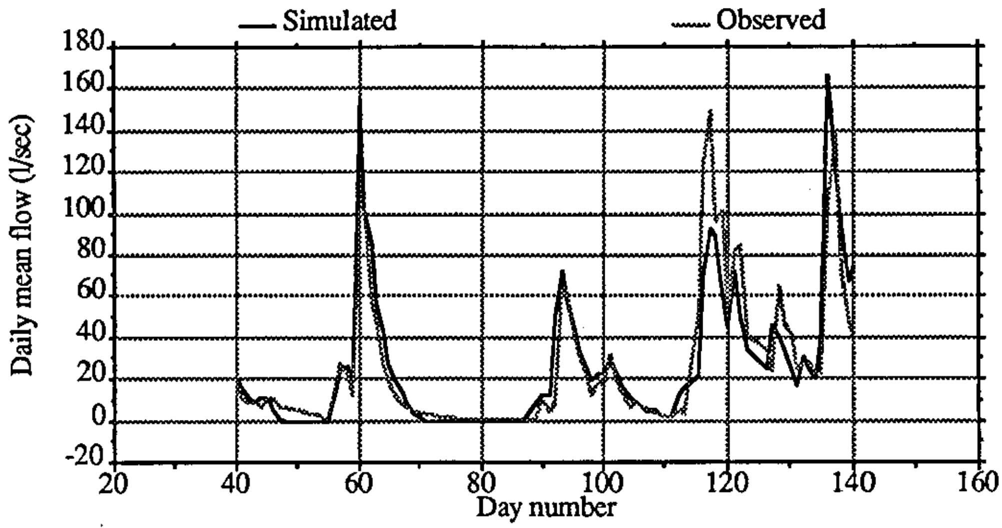
Parameter	LI1	LI6	CI6
Catchment area (m^2)	2000000	2350000	500000
Evaporation weighting factor	0.73	0.73	1.0
SMD at which baseflow ceases (mm)	100.0	77.0	60.0
SMD at which stormflow ceases (mm)	35.0	35.0	35.0
Stormflow recession rate	0.100	0.100	0.105
Baseflow recession rate	0.03	0.03	0.25
Initial SMD (mm)	52.0	52.0	52.0
Rainfall correction factor	1.0	1.0	1.0
SMD at which evaporation restricted (mm)	80.0	80.0	80.0
Total soil buffer capacity (μgm^{-2})	$84*10^6$	$81*10^6$	$81*10^6$
Daily weathering rate (μgm^{-2})	140	950	140
Maximum soil pH	5.84	7.54	6.50
Minimum soil pH	4.88	6.00	4.26
Daily dry deposition rate (μgm^{-2})	275	80	65
Initial soil buffer capacity (μgm^{-2})	$52*10^5$	$11*10^6$	$78*10^5$

TABLE 7.3a Optimised parameter values for the Llyn Brianne catchments

Calibration details	LI1	LI6	CI6
Period	20/6/88 - 24/9/88	13/9/85 - 5/1/86	16/9/85 - 1/1/86
Number of days	96	114	105
Daily flows (R-sq %)	61	43	79
Daily pH (R-sq %)	74	77	68
Validation details			
Period	4/7/85 - 22/12/85	-	11/9/87 - 19/12/87
Number of days	170	-	99
Daily flows (R-sq %)	60	-	70
Daily pH (R-sq %)	67	-	66
Annual statistics (84/85)			
Observed pH	4.80	6.90	5.60
SCAM pH	4.60	6.20	5.20
MAGIC pH	4.60	6.40	-
Observed Al (mg/l)	0.36	0.07	0.10
SCAM Al	0.43	0.06	0.09
MAGIC Al	0.64	0.01	-

TABLE 7.3b Summary of calibration and validation statistics obtained for the three Llyn Brianne catchments LI1, LI6 and CI6.

(a)



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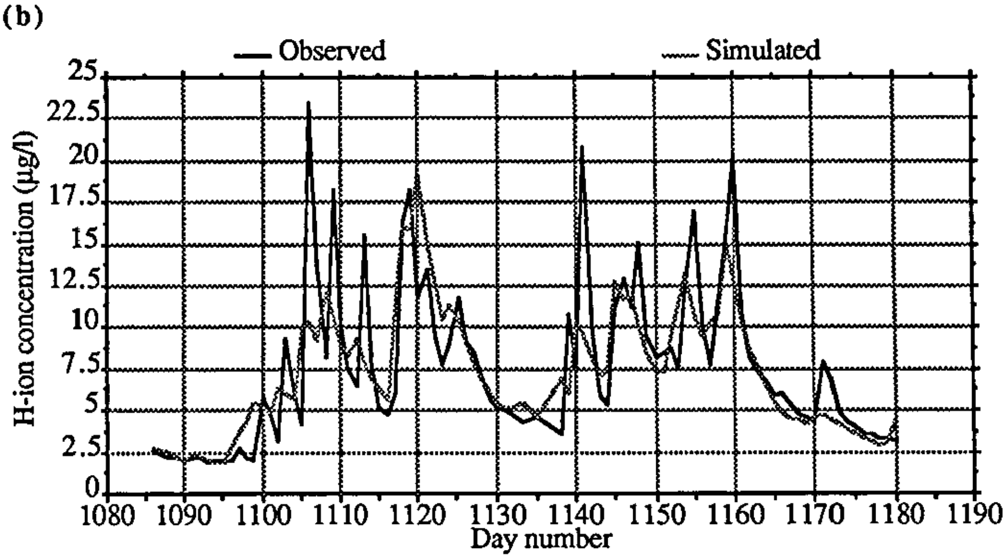
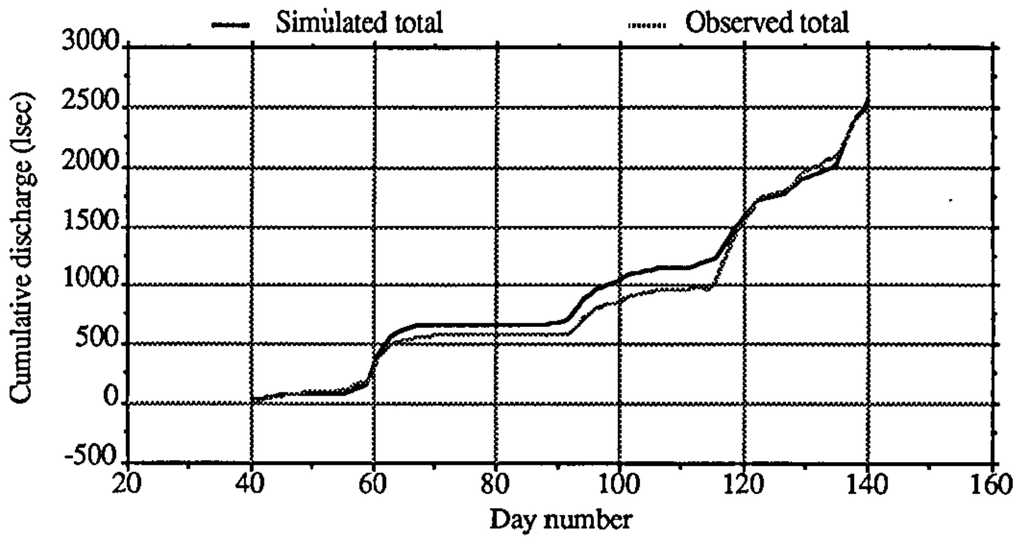


FIGURE 7.8 Comparison of the simulated versus observed (a) daily discharge for catchment CI6 and, (b) streamwater acidity for catchment LI1.

(a)



(b)

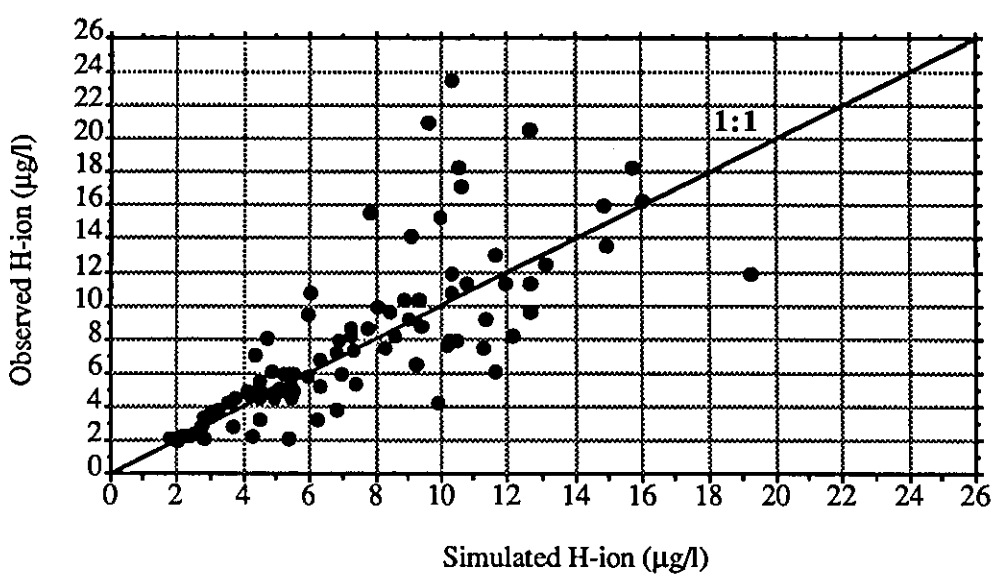


FIGURE 7.9 Comparison of the observed versus simulated (a) cumulative discharge total for catchment CI6 and (b) the daily stream acidity for catchment LI1.

Firstly, whilst the hydrological sub-model was generally only a crude simulator of the daily discharges it was far more effective at describing the long-term water balance. This aspect is critical to the functioning of the soil-moisture dependent hydrochemical sub-model. Thus, the difference between the long-term (>100 days) running total of observed and computed discharge seldom exceeded ± 10%.

Secondly, it should be remembered that even the selected calibration and validation periods were not 100% complete, and that missing data caused discontinuities in the behaviour of the model. This is particularly true of missing rainfall data which still occurred on around 5% of the days. Furthermore, there is also a degree of uncertainty involved in the use of the daily discharge data. In the case of catchment LI6, for example, it was observed that 'bedload movement has resulted in changes in channel cross section following floods' (Welsh Water Authority, 1988, p24). A further limitation that has been cited is the lack of spot gaugings at high flows. These factors will clearly introduce considerable errors to the stage-discharge computations and are perhaps reflected by the poorest performance of the model at this site.

Thirdly, the differences have undoubtedly occurred as a result of the simplicity of the hydrological sub-model. For example, no facility is currently included for the simulation of snow accumulation and melting within the catchment - these mechanisms are clearly of importance when any serious attempt is to be made at describing the hydrology of catchments in central upland Wales. The inclusion of snowmelt processes would probably have improved the description of winter/ spring 'acid pulses' arising from the melting of pollutant laiden snow-pack (Morris, 1988). From Table 7.3 it may be seen that the calibration and validation periods frequently encompassed the winter/ spring snow period, thus providing a very severe test of the SCAM model.

Finally, the model consistently underpredicted the magnitude of stormflows and peak acidities, most notably from the afforested catchment LI1 (Figure 7.8 and 7.9). This fact may reflect the omission by the model of rapid transit routes within the watershed attributed to the presence of drainage ditches. Furthermore, the daily time-step of the model computation is clearly too coarse for the detailed simulation of the storm hydrographs.

A second task involving the Llyn Brianne data-set was the investigation of SCAM's ability to reproduce the gross acidity of the three experimental catchments. This enabled a limited assessment of the model's performance over longer timescales (>year) and was made possible through the comparison of simulated versus observed mean (1984/85) stream pH and total aluminium concentrations (Table 7.3b). As a point of reference the results obtained from the MAGIC model for two of the same catchments are also included. The figures indicate that the SCAM simulations consistently over-estimated the volume-weighted streamflow acidity but that these differences are within the expected boundaries of uncertainty dictated by the methods of pH measurement (Tyree, 1981). The mean error between the simulated and observed time-series for LI1, LI6 and CI6 was found to be ±0.43 pH units. This compares with ±0.35 pH units attained by MAGIC for catchments LI1 and LI6.

The SCAM model's performance with regard to total aluminium concentrations was regarded as being highly satisfactory. In the cases of both LI1 and LI6 the model actually performed better than the MAGIC model. The mean error for the former model was ±17%. These results were seen as a vindication of the model assumptions and have provided an indication of the uncertainty limits which envelope any long-term forecasts of stream water acidity made for these sites.

7.8 SUMMARY

The investigation of the SCAM model's performance during the crucial validation phase of its development has highlighted via practical means its short-comings. In essence the model lacks the necessary temporal and spatial detail required to accurately simulate periods of extreme discharge for a resolution of less than one day.

At the upper extreme, additional parameters and conceptual pathways would be required to accommodate the rapid transfer of water to the catchment outlet via the soil-pipe and tile-drain networks. The rapid routing of storm water through the soil horizon to the channel clearly has implications for the potential buffering of acid precipitation too. The computational time-step is also such that storm inputs and peak flows are truncated and/ or averaged over more than one day. Similarly, daily mean H-ion concentrations will tend to smooth out the extreme fluctuations in the surface water acidity which can undoubtedly occur within the space of several hours (cf. Figure 6.12).

At the lower end of the discharge spectrum, the simulated daily flows are highly sensitive to the cumulative computational error in the catchment SMD resulting from the empirically-based model of daily potential evaporation rates. This sub-model is currently unable to take into account the physiological stresses and feedbacks which operate between the ecosystem, climatic system and moisture supply. Furthermore, it should be noted that under a climatic regime that is responding to elevated carbon-dioxide levels, the plant-stomata-resistance-atmospheric links in particular may be of critical importance to the annual water budget (Lankreyer and Veen, 1989).

In support of the model was its proficiency at reproducing the gross input-output response of the catchment: the errors in the computations of daily potential evaporation, soil moisture status, discharge and H-ion loads all tended to be reduced over timescales in excess of one year. Taking the Beacon as an example, for the 476-day period, the total potential evaporation was within 8% of the mean value for Sutton Bonington, the simulated discharge total was accurate to within 15% of the observed amount, and the total H-ion output from the catchment to within 7-12% depending on the parameter set used.

The results of a brief experimentation with selected aspects of the data from the Llyn Brianne Acid Waters Project (Welsh Water Authority, 1988) have largely supported the value of the SCAM model assumptions given certain premises. In general, the experiment revealed that the model in its current form is difficult to calibrate when the available data base is discontinuous. However, if annual as opposed to daily output statistics are acceptable, then the model is readily modified to accommodate this level of input data. The performance of the model at reproducing the gross discharge amounts and daily streamwater acidities was encouraging given the diversity of the catchment land-use, soil types and simplicity of the model processes (Figure 7.9). It is probable that these results could be surpassed if the model is modified to accommodate the characteristic details of each catchment (such as drainage ditches, canopy interception or snowmelt processes). Inclusion of these processes within the overall SCAM modelling framework would increase the range of its application but would also entail greater parameter dimensionality.

When considering the conceptual simplicity and low parameter dimensionality incorporated by the SCAM model, the overall calibration/ validation responses were surprisingly good. However, some disappointing results were returned during the validation of the daily H-ion component for the Beacon. This was attributed to chemical predictions being made for conditions outside the range of the calibration data and the scope of the model design. This could be overcome to a certain extent by the availability of longer and more hydrologically variable calibration data series. But this would create an even greater demand for data from more diverse sources, with no guarantee of improved performance. On top of this, uncertainties associated with field data (which are introduced to model parameters during calibration), and the calibration procedure itself should not be overlooked.

Not withstanding the acknowledged limitations, particularly at the diurnal time-scale, a brief survey of published results for comparable models was made as an independent check of model performance. This revealed a distinct paucity of data pertaining to the performance of models such as MAGIC and Birkenes during both the calibration and validation stages of their development. However, Hooper et al. (1988) showed using an elaborate, automatic calibration procedure that the Birkenes model was capable of explaining between 74-91%

of the variance in observed daily streamflow over a period of one year. The equivalent figures for the SCAM model were shown in Table 7.2 to be c.88%. With regard to the streamflow acidity, Langan and Whitehead (1987) applied a first order autoregressive moving average model to one month of hourly observations and were able to explain 81-97% of the variance. Again the most comparable figure obtained for SCAM for the Beacon was 96% (Table 7.2).

For an evaluation of the performance of SCAM within the context of medium- to long-term (10-100 years) forecasting, attention should be drawn to the largely successful results of the model validation exercises conducted using the Llyn Brianne data set. Whilst there is undoubtedly a degree of uncertainty involved in the choice of values for long-term parameters (such as the weathering rate) from short calibration data sets, the sensitivity analyses revealed that even over time-scales of up to 25 years such parameters are relatively insensitive. By contrast, parameters which regulate the short- and long-term water balance appear to be of far greater significance to the predictions of surface water acidity.

To summarise the calibration and validation results, it is fair to state that the SCAM model performance was far from perfect, particularly with regard to sub-annual simulations. However, where it has been possible to assess this output against models currently employed elsewhere, the results obtained from SCAM were generally comparable to, if not an improvement upon the alternatives, particularly when considering its relative simplicity. This supports the assertion that the model should be regarded as a semi-quantitative, but objective tool for assessing climate change impacts.

CHAPTER 8

RESULTS OF MODEL SIMULATIONS

"Models and theories are very closely linked......perhaps only differing in the degree of probability with which they predict reality. The terms 'true' and 'false' cannot usefully be applied in the evaluation of models, however, and must be replaced by ones like 'appropriate', 'stimulating', or 'significant'......" (Haggett and Chorley, 1967, p 24).

8.1 INTRODUCTION

On the basis of the validation procedures conducted in the previous chapter it is evident that the SCAM model is no exception to the general observation made by Haggett and Chorley (1967). Indeed the results neither affirmed nor falsified the theoretical basis of the algorithm but rather implied that it may be an 'appropriate' description of the fundamental processes involved. With reference to the objectives stated in 1.3, the following model predictions will reveal the extent to which modified climatic boundary conditions are able to 'stimulate' any 'significant' changes in the catchment hydrogen-ion balance. This will be undertaken in two main sections.

Section A will be concerned with the detailed response of one catchment - the Beacon - to fourteen selected climate and emission scenarios. A brief review of the proposed simulation scenarios will be presented followed by an overview of the instantaneous or equilibrium responses of the model to individual parameter changes. The transient hydrological and hydrochemical responses of the model over a standard period (present - 2055AD) will also be presented. **Section B** deals with the inverse situation, namely, the response of four catchments to a single BASE scenario. Having justified the composition of this scenario the ensuing simulations investigate the modified seasonal, annual and super-annual behaviour of the catchments using the LWT1908 scenario (described below) as the long-term datum. By adopting this twofold approach the first section will cover the relative potency of different hydrometeorological variables (ie the forcing mechanisms) whilst the second will be concerned with the regional variations in the (passive) response to these inputs. These two separate sets of results will then lay the foundations for the discussion in the following chapter on the possible hydrochemical and ecological consequences of climate change for acidic catchments.

SECTION A

8.2 CONSTRUCTION OF THE FOURTEEN CLIMATE SCENARIOS

8.2.1 The scenario concept

The term 'climatic scenario' is used to describe a feasible realisation of an uncertain future climate:- its time evolution and 'vital statistics'. As such it does not equate with a forecast or prediction but only on how a system might reasonably be expected to behave under specified circumstances (Beran, 1989b). However, when constructing a scenario it is generally assumed that: it is internally consistent and does not conflict with known facts; it is sufficiently flexible to allow the incorporation of new facts yet provides an explicit statement of the constituent assumptions; and that it deals with the fundamental processes that are of practical interest (such as mean annual temperature and precipitation statistics). It is also common for a range of alternative scenarios to be applied in areas of broad policy determination or for identifying the sensitivity of resources to environmental changes.

A number of different approaches have been developed by climatologists for the objective and subjective composition of scenarios (Hulme and Jones, 1989). These include:

(a) The use of General Circulation Models to simulate future climate conditions which in turn may be a function of different CO_2-concentration scenarios and rates of increase.

(b) Palaeoclimatic analogues which make use of instrumental records and proxy data sources to describe the natural temporal and spatial variability of the climate under different atmospheric conditions.

(c) Spatial analogues which allow the substitution of climates between sites through the shifting of broad climatic belts .

(d) The arbitrary adjustment of key climatic parameters as a means of assessing the sensitivity of systems to systematic changes in the driving variables.

(e) Hybrid or 'committee' scenarios which represent an amalgam, or concensus of expert opinion based any combination of methods (a) to (d).

None of these methods are entirely satisfactory. For example, whilst spatial analogues provide a relatively straight forward means of transfering the detail of the present climate characteristics from one region to another - such as the substitution of the Southern British Isles climate for one approximating that of current Southern France - there are considerable difficulties involved in the minimisation of locational differences arising from the region's vegetation and land-use. In all cases there also remains the problem of interpreting the expected changes to broad climatic parameters (such as annual rainfall totals) in terms of the terrestrial consequences as they affect man and the environment.

In order to overcome some of the difficulties inherent to the selection of an appropriate climate scenario it is proposed that attention should be focused on the climatic extremes observed within the instrumental record. By investigating the modelled response to a suite of such scenarios, it will be possible to derive the range of - as well as the mean - hydrochemical impact(s).

8.2.2 The climate scenarios

From the infinite number of possibilities just fourteen climate scenarios (Table 8.1) were established for the purpose of assessing the sensitivity to change of the hydrological and hydrochemical properties of the Beacon catchment . The first six scenarios were extracted from the Lamb (1972) register of daily weather types and refer to individual years in which either the westerly, cyclonic or anticyclonic synoptic patterns exhibited an extreme frequency of occurrence. The years 1908/09 represent an exception in that this period provides the closest approximation to the long-term (1861-1988) mean frequencies of each of the three main weather types. This scenario was included for the purpose of establishing a datum against which to compare the other thirteen scenarios. In all of these scenarios the daily weather-type catalogue was used to compile a transformation matrix specific to each year's 'blocking' behaviour (as described in 3.4.1). This enabled the reconstruction of the sequence of weather types and their projection into the future. So for example, the transformation probabilities associated with the eight key classes of weather observed in 1869 were used to simulate a possible future climate in which the frequency of cyclonic activity would be extremely low. [Note that in 1872 the highest frequency of cyclonic-days and the lowest number of anticyclonic days were simultaneously recorded to date]. For each of the first six synoptic scenarios, the mean annual temperature, precipitation and acid loads were held constant at 1988/89 levels.

Four of the remaining scenarios were based upon different interpretations of the Department of the Environment (HMSO, 1988) scenario used in the report on the 'Possible impacts of climate change on the natural environment in the U.K.'. This base scenario envisages a mean temperature rise of 3°C ±1.5°C and a change in mean annual rainfall of ±20% above present by the year 2050. Changes to the annual rainfall total were accomplished by adjusting the mean storm size upwards and downwards by 20% (DOE1 and DOE2). In recognition of the fact that the deposition rate of acidic ions is unlikely to remain constant (ie the 1988/9 rate) over the next 60 years, two complimentary scenarios (DOE3 and DOE4) applied the same climatic scenario as DOE1 and DOE2 but with the H-ion load to the catchment reduced linearly to 50% of present by the year 2050. This value

SCENARIO	DEFINITION
LWT1908/9	1861-1988 mean frequency of W-, A- and C-weather types.
LWT1938	Highest frequency of W-type.
LWT1969	Lowest frequency of W-type.
LWT1872	Highest frequency of C- and lowest A-type.
LWT1971	Highest frequency of A-type.
LWT1869	Lowest frequency of C-type.
DOE1	1908/9 lwt matrix, T +3°C, storm intensity +20%.
DOE2	1908/9 lwt matrix, T +3°C, storm intensity -20%.
DOE3	As DOE1 with deposition rate -50%.
DOE4	As DOE2 with deposition rate -50%.
SEASON1	1908/9 lwt matrix, T + 2°C, wet-winter/ dry summer (+10%).
SEASON2	1908/9 lwt matrix, T +3°C, wet-winter/ dry summer (+20).
SEASON3	As SEASON1 with deposition rate -50%.
SEASON4	As SEASON2 with deposition rate -50%.

TABLE 8.1 Listing of climate scenarios used for the Beacon catchment simulations.

was selected on an arbitrary basis and was included to provide some indication of the effectiveness of emission reductions for surface water acidity relative to broad climatic changes.

The last four scenarios were used to test the significance of changes in climatic seasonality. SEASON1 and SEASON3 assume a mean rise of temperature of +2°C above present and an overall increase in the mean annual precipitation of +10% distributed unevenly across the year. SEASON2 and SEASON4 envisage a temperature change of +3°C and rainfall increase of +20%. In all cases the change in precipitation was distributed such that the winter period (October-April) became wetter and the summer (May-September) drier. In each case the monthly change corresponded approximately to the scheme presented by Arnell and Reynard (1989):

	MONTH											
% CHANGE	J	F	M	A	M	J	J	A	S	O	N	D
PRECIPITATION	20	20	20	20	10	-10	-15	-10	10	20	20	20

As in the case of DOE3 and DOE4, SEASON3 and SEASON4 explore the additional effect of reduced deposition loads to the catchment in addition to the broad climatic changes.

As a means of standardising the results obtained from SEASON1 through SEASON4, and the four DOE scenarios, the mean (1908/9) Lamb's weather type matrix (APPENDIX 1) was applied in all eight cases for the generation of precipitation frequencies, intensities and acidities.

In order to derive each of these fourteen climate scenarios it is clear that it was necessary to make a number of assumptions. Firstly, with any scenario based largely upon individual years extracted from instrumental/ observational records the actual choice of 'representative' or extreme years is arbitrary. There is no scientific reason to suppose that historic conditions will ever be replicated in the future, particularly if boundary conditions are changing. Secondly, when dealing with climatic extremes it must be assumed that the length of the record provides an adequate sample of the long-term extremes and natural variability. The assumption is also made that future extreme conditions will fall within contemporary and historic climatic limits. Thirdly, due to the nature of the Lamb's weather type classification scheme it is impossible to eliminate entirely the subjective element incorporated within the transformation matrices. However, the over-riding advantage of using selected years from the observational record lies in the ability to reconstruct from these matrices detailed hydrometeorological time-series at a spatial and temporal resolution currently surpassing that of current GCMs. Furthermore, the justification for using extreme years as the basis of future climatic scenarios has been coroborated recently by the very mild winter of 1988/89 when the predominance of westerly days was found to be +18.1 more than 'normal' (NERC, 1989).

8.2.3 The simulation methodology

Having established the basis of the fourteen chosen climatic scenarios it was then necessary to define a clear procedure by which to conduct the simulations. The first task was to determine an optimum simulation length so as to yield stable output from the model whilst simultaneously conserving computing time and resources. Through experimentation a simulation period of 10,000 days (log10 = 4.0) was found to provide a reliable response (Figure 8.1). This requirement was placed only upon simulations concerned with the **equilibrium response** of the model; that is, the mean outcome of an instantaneous change to the driving variables. (This form of simulation was essentially a sensitivity analysis of the model parameters). For the sake of consistency, all simulations dealing with the **transient** (or evolutionary) response of the model were conducted over a period of 25,000 days to coincide approximately with the projected date of CO_2-doubling in 2050 (DOE, 1988). In this instance, rather than producing a single (summary) statistic for each variable of interest, the model was used to generate an annual time-series. The results of both the instantaneous/ equilibrium and transient response of the model are presented respectively in the following two sections.

8.3 THE BEACON CATCHMENT EQUILIBRIUM RESPONSES

The basic output statistics for each of the fourteen main scenarios have been summarised in Tables 8.2a/b. As a point of reference, **W**, **C**, and **A** represent the mean annual percentage of days assigned to each of the westerly-, cyclonic- and anticyclonic classes respectively. **Rainfall days** is a count of the number of days during the 10, 000 day simulation period on which precipitation occurred. **T-anomaly** is the temperature anomaly (about the 1980's mean) that may be attributed soley or in part to the prevalence of individual weather types. The **yield** is the total discharge of the simulation period expressed as a percentage of the total incident precipitation to the catchment. **Q>90%** is a count of the number of days on which the computed discharge equalled or exceeded the 1985-1989 90-percentile flow. **Zero flow** is a count of the number of days on which the stream was dry. The **rainfall** and **streamflow pH** are volume-weighted mean acidities for incoming and outgoing precipitation, whilst **H-load** and **H-release** are respectively the total H-ion input and output for the Beacon catchment over the 10, 000 days. **Al-ion** is the volume-weighted mean total-aluminium ion concentration. The **LCD** is a count in days of the frequency with which an arbitrary streamflow pH threshold of - in this case - 4.5 units was equalled or

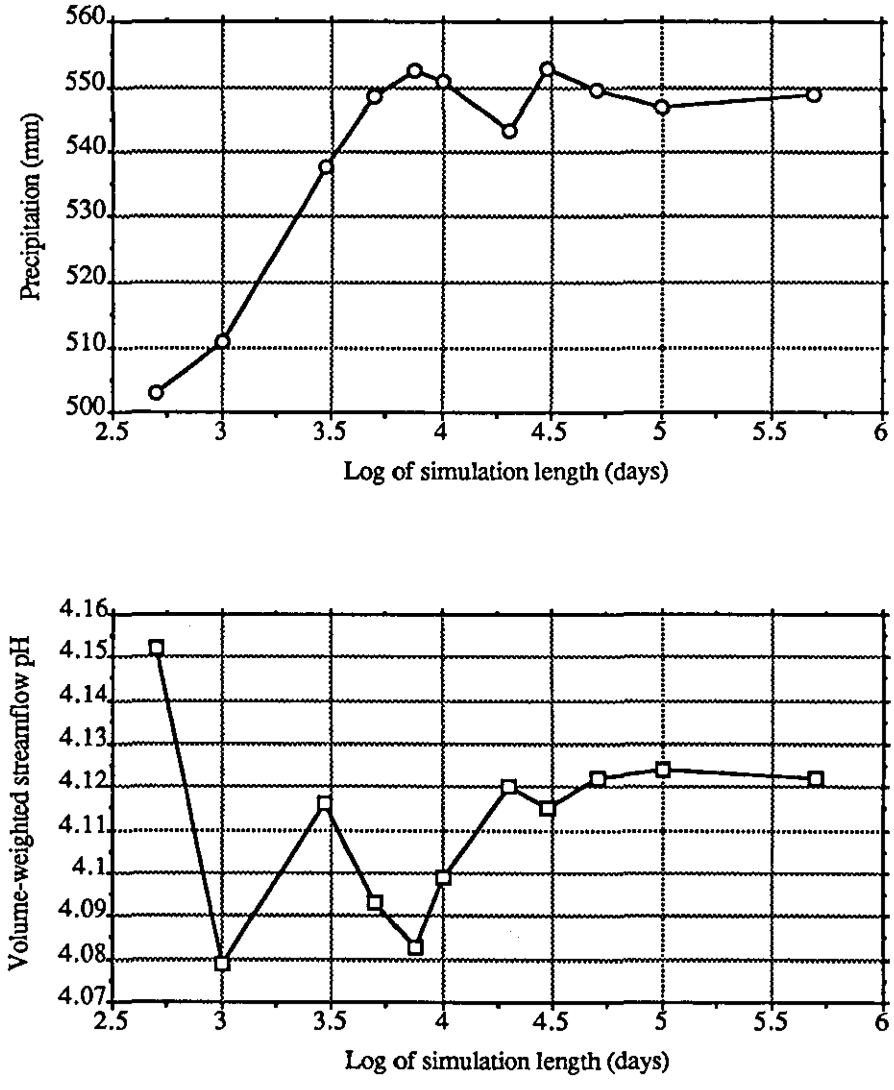


FIGURE 8.1 The sensitivity of SCAM output variables to simulation length

SCENARIO	W (%)	C (%)	A (%)	Rainfall (days)	Rainfall (mm/year)	T-anomaly (C)	Yield (%)	Q>90% (days)	Zero flow (days)
LWT1908/9	18.7	12.2	18.7	4724	720.5	+0.12	29.5	929	2633
LWT1938	30.2	11.7	17.4	4800	712.9	+0.55	26.2	796	3323
LWT1969	9.7	19.0	19.1	4710	745.2	-0.02	32.4	1211	2486
LWT1872	21.5	20.3	6.4	5407	838.1	+0.31	36.5	1688	1446
LWT1971	11.4	17.2	28.0	4366	692.0	+0.07	28.0	809	2988
LWT1869	19.0	6.8	17.7	4560	679.9	+0.11	26.3	715	3277
DOE1	18.7	12.2	18.7	4724	862.8	+3.15	19.2	519	2351
DOE2	18.7	12.2	18.7	4724	578.1	+3.15	2.0	0	8590
DOE3	18.7	12.2	18.7	4724	837.1	+3.15	16.7	377	2851
DOE4	18.7	12.2	18.7	4724	589.0	+3.15	3.0	15	8154
SEASON1/3	18.7	12.2	18.7	4724	793.6	+3.15	22.8	757	3361
SEASON2/4	18.7	12.2	18.7	4724	860.6	+3.15	21.4	803	3368

TABLE 8.2a The hydrological response of the Beacon catchment to fourteen different climate scenarios over a period of 10, 000 days.

SCENARIO	Rainfall pH	Streamflow pH	H-load (tonnes)	H-release (tonnes)	Al-ion (mg/l)	LCD (days)	Base status (%)
LWT1908/9	4.11	4.51	1.119	0.099	1.43	698	9.567
LWT1938	4.17	4.56	1.009	0.077	1.39	576	9.649
LWT1969	4.07	4.47	1.248	0.124	1.52	929	9.472
LWT1872	4.11	4.44	1.236	0.166	1.57	1324	9.523
LWT1971	4.07	4.52	1.186	0.087	1.41	627	9.496
LWT1869	4.18	4.57	0.978	0.072	1.37	511	9.672
DOE1	4.12	4.59	1.279	0.064	1.25	362	9.389
DOE2	4.11	5.46	0.959	0.001	0.50	0	9.624
DOE3	4.42	4.60	0.640	0.062	1.22	321	9.972
DOE4	4.41	5.49	0.479	0.001	0.47	0	10.062
SEASON1	4.12	4.47	1.200	0.092	1.44	567	9.487
SEASON2	4.12	4.42	1.276	0.105	1.48	591	9.430
SEASON3	4.42	4.48	0.600	0.089	1.41	510	10.033
SEASON4	4.42	4.43	0.638	0.102	1.45	538	10.010

TABLE 8.2b The hydrochemical response of the Beacon catchment to fourteen different climate scenarios over a period of 10, 000 days.

exceeded. And finally, the **base status** is the ratio of the number of occupied cation-exchange sites to the total cation exchange capacity of the soil expressed as a percentage (the initial base status being set at 10.0%).

The hydrological responses of the model (Table 8.2a) conformed closely to the anticipated results with the very dry scenarios DOE2 and DOE4 producing by far the greatest number of days with zero flow, the lowest mean catchment yield and the smallest number of flood events. These outcomes contrasted markedly with those arising from the LWT1872 scenario which produced the greatest number of rain days, the highest yield and greatest number of stormflows equalling or exceeding the 1985-1989 90-percentile.

Table 8.2b underlines the importance of defining clearly those dependant variables which most precisely identify the key issues involved. In terms of the base status of the catchment soils, scenario DOE1 resulted in the greatest acidification of the system, whereas in respect to the surface water, the volume-weighted Al-ion concentration and the LCD frequency, identified the 1872 and 1969 LWT scenarios as being the most 'stressful'. Furthermore, had the volume-weighted H-ion concentration been selected the SEASON2 and 4 should be considered the worst-case scenarios. However, reference to Table 8.2b indicates that the factors which were common to all of these scenarios were above average precipitation totals and moderate to high precipitation acidities combining as a high acid load to the catchment soils. Conversely, DOE4 which represented the lowest level of acidity for all parameters was the result of below average precipitation and a low H-ion load.

As a means of investigating these equilibrium responses in greater detail, additional simulations were also conducted using the 1908/9 base-line matrix (Appendix 1). The results of these SCAM forecasts will be dealt with in six parts, namely: the sensitivity of the Beacon catchment to temperature, precipitation, seasonal effects, acidic deposition rates, weathering rates and weather-type variations.

8.3.1 Sensitivity to mean annual temperatures

In section 7.2, the mean annual temperature was found to be one of the most sensitive parameters within the design of the SCAM model. This fact is clearly illustrated by the major changes in the hydrological and hydrochemical variables arising from systematic adjustments made to the temperature about the 1980s mean value (Figures $8.2_{a\text{-}f}$). The mean streamflow H- and Al-ion concentrations, the total H-ion output from the catchment, the frequency of days with streamflow pH less than 4.5 and the number of days with flow in excess of the 1985-1988 90-percentile all demonstrate a significant, non-linear decline with increasing temperatures. This is much as would be expected since the inceases in temperature (which is a surrogate for the evapotranspiration rate) would result in elevated

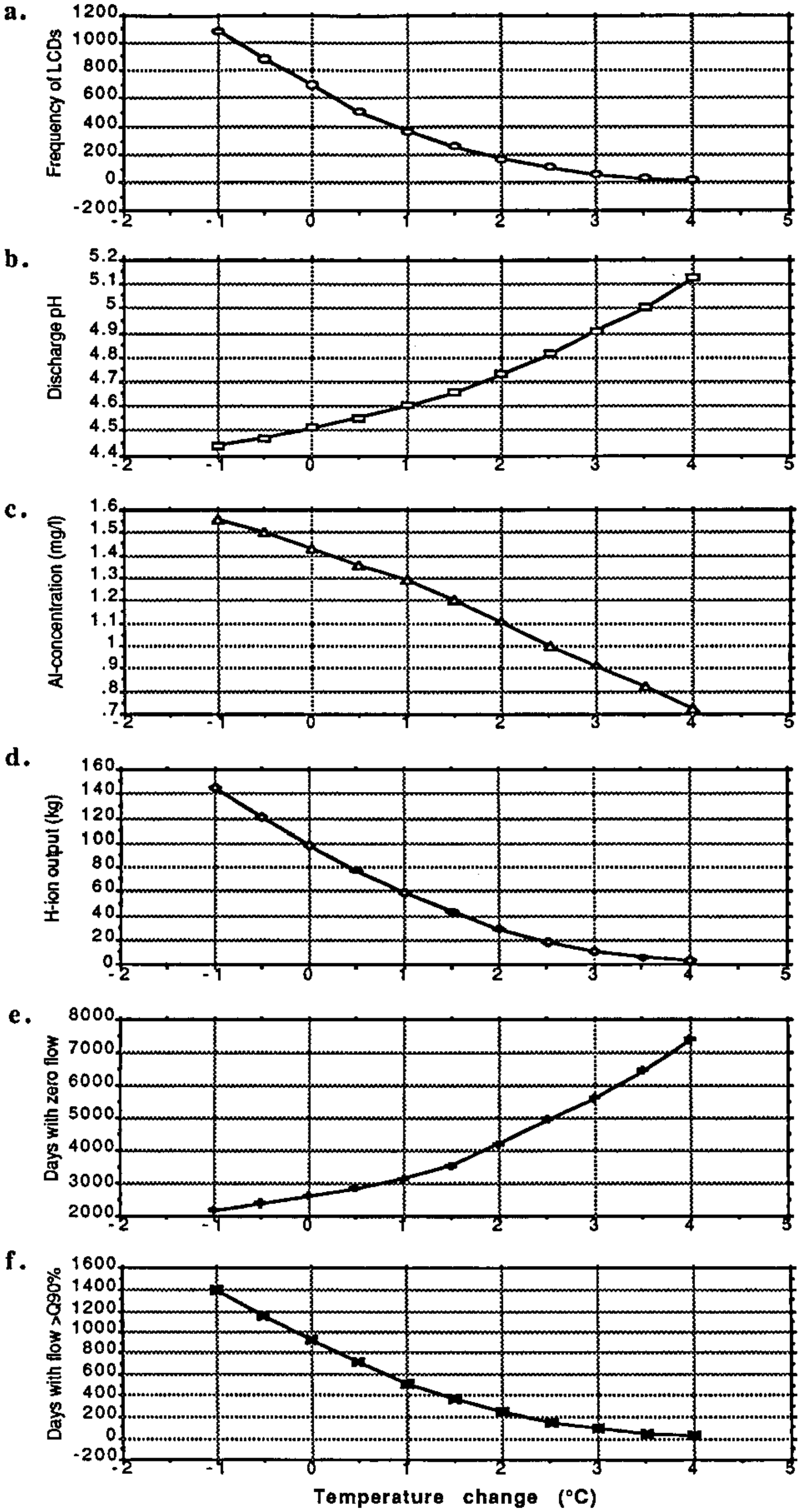


FIGURE 8.2 Simulated equilibrium responses of the Beacon catchment to changes in the mean annual temperature.

mean soil moisture deficits, a shorter period of winter recharge and consequently (on-average) lower stormflow discharges. These in turn ensure that a higher proportion of the total flow is supplied from groundwater sources which tend to exhibit high base-ion concentrations and lower acidities.

However, the fact that all of the relations demonstrated a non-linear trend implies that the hydrochemical system has varying degrees of sensitivity to temperature change. For example, in the case of the LCD, a change of +1°C (above present) would result in a predicted drop in the parameters frequency of 48%, whereas an additional warming of +1°C to +2°C would entail a reduction of only a further 16%. Beyond +3°C the LCD index becomes progressively insensitive to further increases in temperature.

8.3.2 Sensitivity to annual precipitation totals

As might be anticipated increased annual precipitation totals tended to have an opposite effect to that of elevated temperatures. As may be seen from Figures 8.3a-f the modelled response to changing the **mrain** parameter also tended to be non-linear in nature. The frequency of acidic streamflow events (Figure 8.3a), the number of stormflows (Figure 8.3e), the H-ion concentration (Figures 8.3b) and the catchment yield all increased steadily with greater mean storm size and hence annual rainfall totals. Note that the mean response was found to be almost identical regardless as to whether the increased rainfall had arisen from a greater frequency of precipitation events (**prain**) or due to more intense storms (**mrain**). Whilst the volume weighted streamflow acidity demonstrates a progressive increase for a wetter climate it is unclear to what extent this trend might have been affected had the model enabled the increased precipitation total to have occurred due to greater winter snowfalls. By comparison of the parallel outputs of Figures 8.2a-f and Figures 8.3a-f it is possible to suggest that the respective impact of ±1°C change in mean annual temperature equates approximately to a ±10% change in the magnitude of storm sizes. For example, a 10% reduction in the mean storm size had the same impact on the volume-weighted discharge pH as a +1°C rise in the mean annual temperature.

Finally, as Figure 8.3d indicates the hydrological response of the Beacon catchment is highly sensitive to reductions in the mean annual rainfall amount: a 20% reduction in *mrain* is sufficient to increase the proportion of days with zero flow from around 25 to 45% of the year.

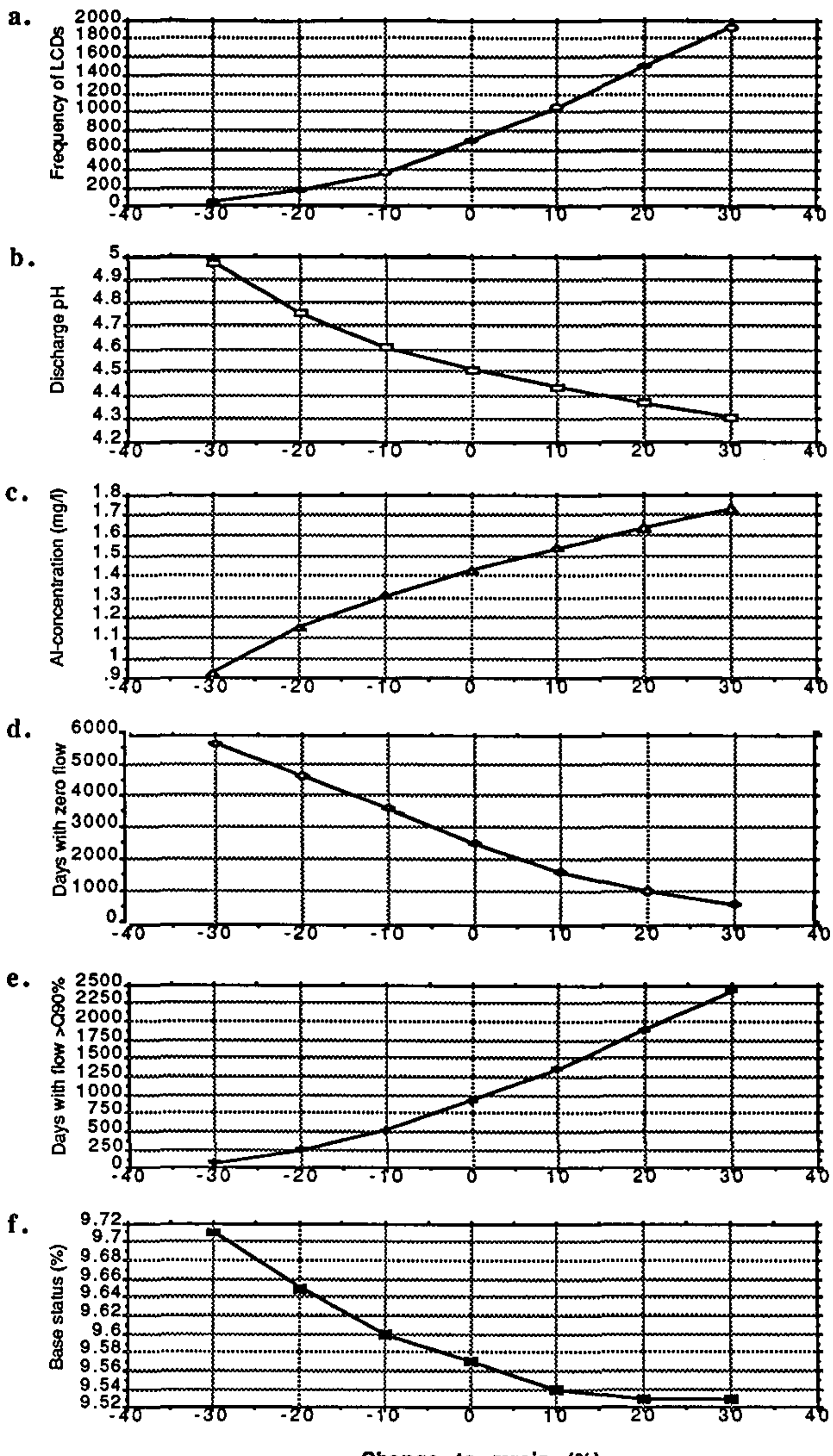


FIGURE 8.3 Simulated equilibrium responses of the Beacon catchment to changes in the mean annual precipitation amount.

8.3.3 Sensitivity to changes in the seasonality of precipitation

With the exceptions of SEASON1 through SEASON4 all of the scenarios distributed the annual precipitation total randomly throughout the year. Whilst the Markov procedure discussed in 3.4.1 is able to reproduce the persistence of certain weather types and hence 'clustering' of rain-days no specific attempt was made to weight the precipitation total by season. A direct comparison of the effect of seasonal rainfall may therefore be made between the results of scenarios SEASON2 and DOE1, with SEASON1 yielding a less extreme seasonal regime. From Table 8.2a it may be seen that the gross rainfall statistics are comparable in all respects as is the temperature regime, yet the responses of the catchment are markedly different. Relative to DOE1, SEASON2 produced a greater number of peak flows and days of zero flow, a higher catchment yield, and major increases in the mean streamflow acidity, total H-ion released, mean Al-ion concentration and frequency of LCDs. The implication of these results are that even in the absence of changes in the mean climatic conditions, a slight change in the annual precipitation regime may have marked hydrochemical consequences.

8.3.4 Sensitivity to acidic deposition rates

In section 8.2.2 emphasis was placed upon the potential consequences for terrestrial hydro-ecological systems of changes in the prevailing climate or weather type regime. However, it is also clear that the loading of acidic ions to the catchment should also be considered dynamic in nature (cf. Figure 3.7). Therefore, as a means of assessing the significance of the 'acid load' to the hydrochemical outputs an analysis was conducted using the 1908/09 transformation matrix (APPENDIX 1) whilst applying various percentages of the 1988/9 H-ion load to the catchment. With the exception of the resulting change to the volume-weighted precipitation acidity, the response to the modified deposition rates (in the range of -100 to +40%) was generally linear. However, even large reductions in the deposited H-ion load brought about relatively minor changes in the surface water acidity of the catchment over the 10,000 day period (Figures 8.4a-d). For example, a 100% reduction in the deposition load was found to have a less significant impact on the frequency of LCDs than a 0.5°C rise in the mean annual temperature over the same 25-year period. This was attributed to a number of factors.

First, the model may not accurately reproduce long-term changes in the soil-acidity profile. Second, the catchment may be insensitive to the acid deposition rate. Or thirdly, the time-scale of the simulation may have been too short. Thus, in its present form the model suggests that an 80% reduction in the deposited acid load would be required to produce a 25% reduction in the frequency of acidic (<pH 4.5) daily streamflows, whilst a 40%

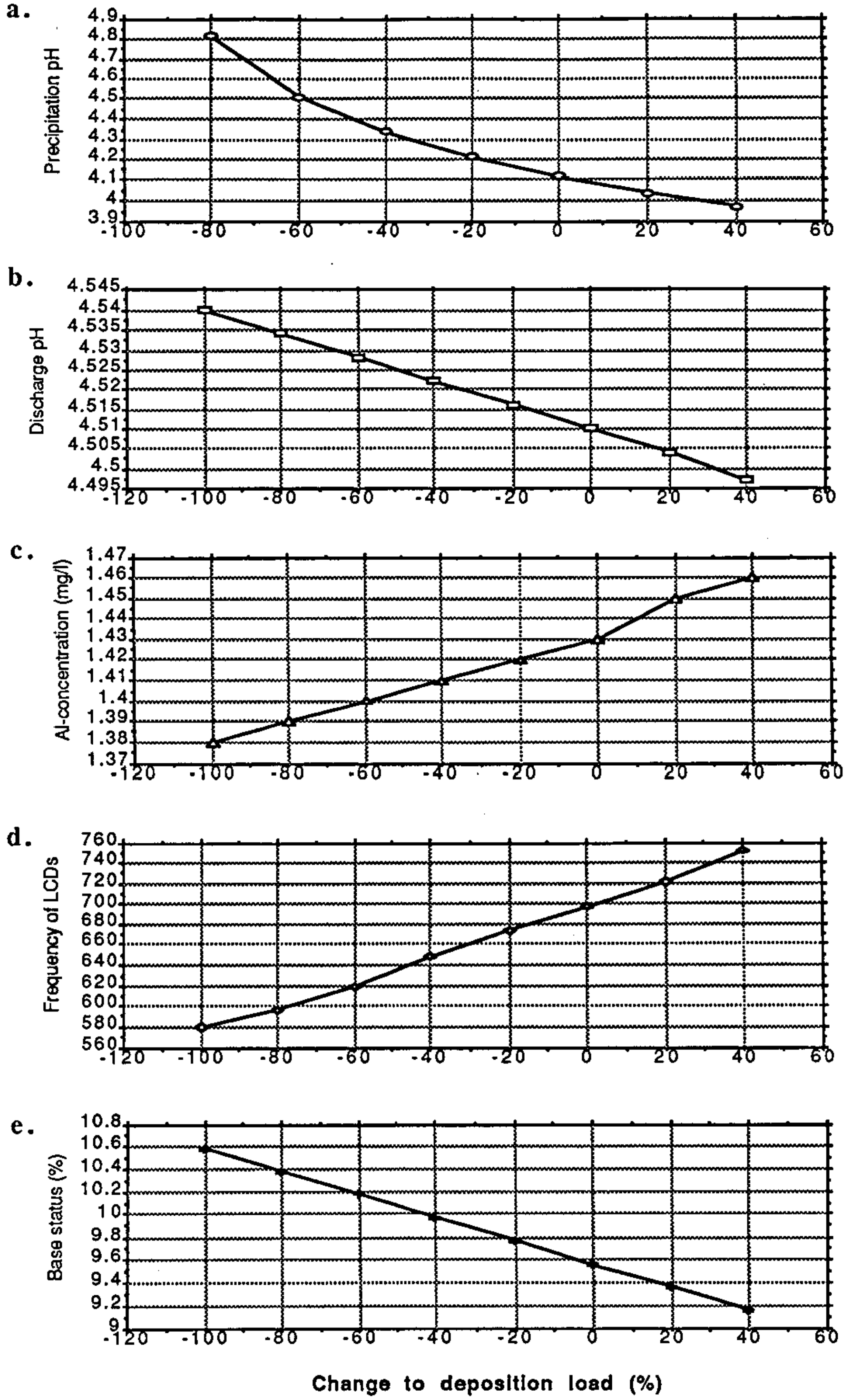


FIGURE 8.4 Simulated equilibrium responses of the Beacon catchment to changes in the annual acid deposition rate.

reduction is required to maintain an equilibrium about the current base status (Figure 8.4e). Although large, this figure is comparable to the value recently suggested by Christophersen et al. (in press) as the required target for re-stocking the Birkenes catchment, Norway, with trout.

8.3.5 Sensitivity to the mean daily weathering rate

Initial sensitivity analyses of the hydrochemistry of the Beacon revealed that the model was also relatively insensitive to the value of the daily weathering rate. This parameter is notoriously difficult to calibrate or measure (Jacks [in press], Bain et al.[in press], Mason and Seip[1990]) and it is therefore important to quantify its effect over a wide range of feasible values. Figures 8.5a-e indicate that the optimised weathering rate of 100 μeqm^{-2} actually falls in the most sensitive region in terms of the modelled outputs. However, a 900% increase in this rate was still required to decrease the LCD frequency from 6.5 to 3.5% of the days each year! These results tend to confirm that the surface water acidity of the Beacon catchment is dominated by antecedent hydrological conditions which govern stormwater pathways and their associated acid buffering processes.

8.3.6 Sensitivity to the prevailing synoptic regime

The sensitivity of Beacon's simulated chemistry to the prevailing synoptic weather conditions - which in turn dictate the precipitation chemistry, its temporal distribution and amount, and the daily temperature anomalies - was investigated using the first six scenarios presented in Table 8.1. The other eight scenarios were not included since they incorporate variable changes in addition to the weather-type matrix.

The SCAM model sensitivity analysis (Table 7.1) showed that (±10%) variations made to the annual frequency of individual weather-types resulted in only minor changes to to the hydrochemical and hydrological outputs of the model. However, from Table 8.2a/b it is clear that there are considerable differences in all parameters arising from the various synoptic matrices. This suggests that it is the composite change made simultaneously to the frequency of all three main classes that has the greater bearing on the simulated responses.

The results obtained from each of the six synoptic scenarios were further analysed to determine the statistical significance of the westerly, cyclonic and anticyclonic weather types as independent determinands of the catchment hydrochemistry. Table 8.3 shows that the cyclonic class is by far the most significant in terms of both the catchment inputs and outputs. It is the cyclonic-type that combines high mean precipitation amounts and frequencies with moderate to high acidities to produce an above average H-ion load.

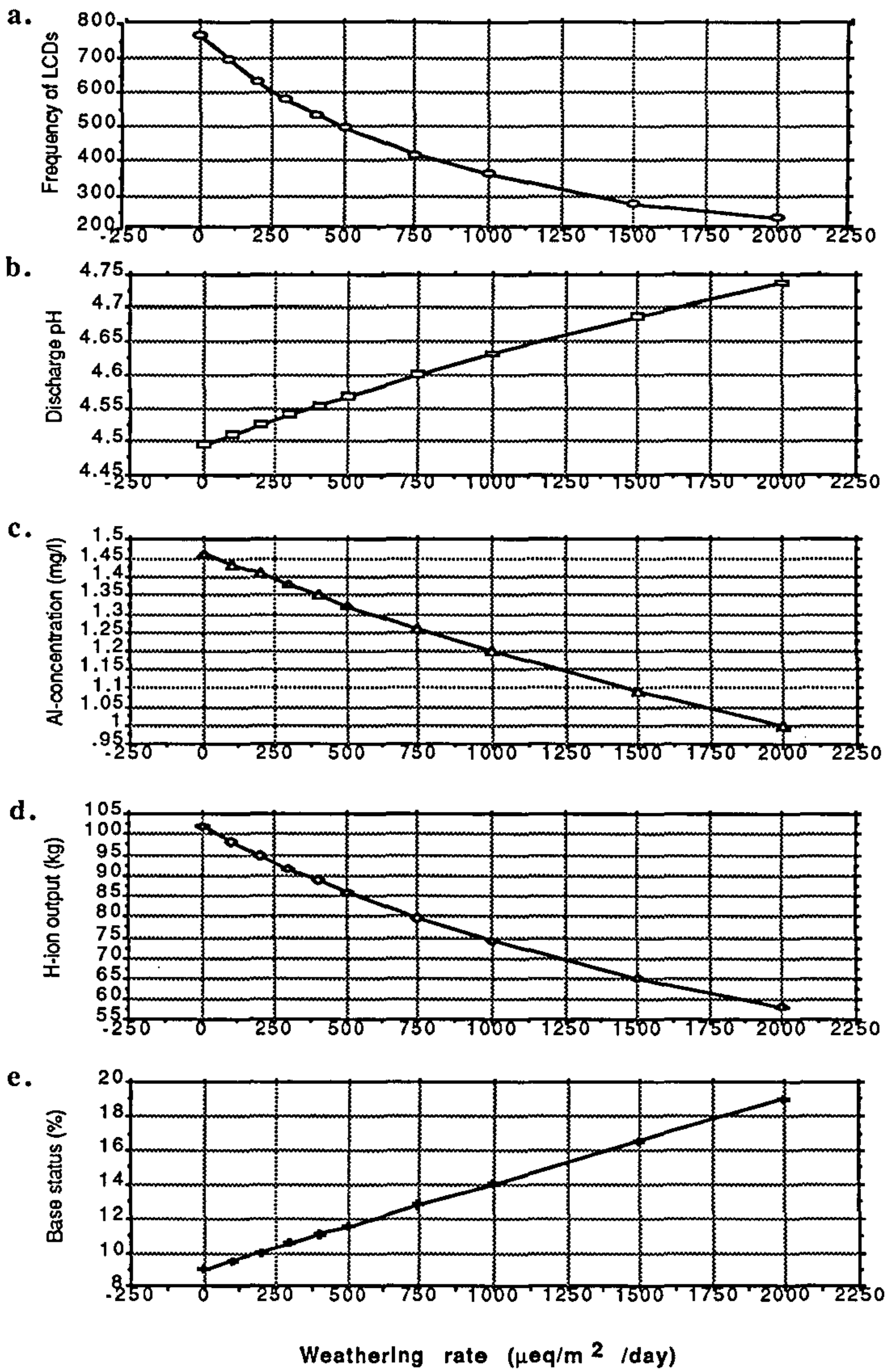


FIGURE 8.5 Simulated equilibrium responses of the Beacon catchment to changes in the mean daily weathering rate.

INDEPENDENT	DEPENDANT	CONFIDENCE	R^2
W-type frequency	Precipitation pH	90%	61.3
"	Final base saturation	90%	53.3
C-type frequency	Catchment yield	95%	65.0
"	Precipitation pH	95%	65.9
"	Streamflow pH	99%	79.6
"	H-ion load	99%	90.7
"	H-ion exported	95%	64.5
"	Frequency of stormflows	90%	59.6
"	Frequency of zero flows	90%	56.1
"	Frequency of LCDs	95%	63.1
"	Al-ion concentration	95%	71.9
"	Final base saturation	90%	81.3
A-type frequency	Number of wet-days	99%	90.1
"	Mean annual precipitation	95%	66.4
"	Frequency of stormflows	90%	56.0
"	Frequency of LCDs	90%	51.9

TABLE 8.3 Relationship between synoptic weather conditions and simulated catchment hydrochemistry.

Perhaps more important, however, is the frequency with which stormflows are generated and baseflow contributions reduced by respectively high and low cyclonic activity. Under conditions of elevated cyclonic activity the catchment may be expected (on average) to exhibit wetter antecedent conditions and as a consequence, more frequent drainage through the acidic upper horizons of the soil column. This in turn results in an increased frequency of LCDs.

By contrast the anticyclonic type has the greatest effect on the frequency of wet-days and mean annual precipitation totals, which in turn is reflected in the frequency of stormflows. Despite having above average precipitation acidities this weather-type tends to promote a counteractive effect of increased baseflow contributions with higher frequencies.

The frequency of the westerly weather-type has a significant bearing primarily on the volume-weighted precipitation acidity by making a major contribution to the dilution of the H-ion levels as has been shown previously by Davies et al. (1986). In terms of activating acidic solute pathways, the annual frequency of this class appears to have little consequence for either the hydrological or hydrochemical responses of the catchment.

8.4 THE BEACON CATCHMENT TRANSIENT RESPONSES

As stated previously the transient response of SCAM provides the output required to investigate the temporal evolution of the modelled catchment hydrochemical system, rather than the mean outcome arising from each of the fourteen different scenarios. The results of the fourteen time-series analyses have been grouped into two broad categories according to selected hydrological responses and their associated hydrochemistry. Because of the number of scenarios involved, the results for each output variable have been further organised by the three generic scenario types: those due to the LWT matrices, the DOE base scenarios and those arising from the seasonally distributed precipitation regimes. Furthermore, it is intended that the following results should provide an indication of the potential **range** of responses, rather than the behaviour of the individual time-series *per se*. This is in line with the confidence that may be placed in the model simulations (cf. 7.8).

8.4.1 The hydrological response

Three main indices were used to assess the long-term hydrological response of the catchment to each of the fourteen scenarios: the cumulative discharge total; the cumulative frequency of days with zero flow; and the cumulative frequency of days with flow exceeding the 1985-1989 90-percentile.

The cumulative discharge total reflects the long-term balance between precipitation inputs and evapo-transpiration losses from the soil (Figure 8.6). If the 1908/9 trend is accepted as the base-line (Figure 8.6a) then just four scenarios resulted in enhanced streamflow relative to the long-term mean condition. These were the cyclonic high and westerly low LWT scenarios of 1872 and 1969 respectively, and the two seasonally adjusted (and increased) precipitation regimes of SEASON1 and 2. The marked non-linear responses of DOE2 indicates a possible exponential decline in the surface water discharged from the catchment with negligible amounts being released annually from 2040 onwards.

From Figure 8.7b it may be seen that the scenario resulting in by far the least number of flood events was also DOE2, whilst the upper limit was attributed to LWT1872 and SEASON2. These reflect respectively the lowest storm intensities and, as before, the highest frequency of the cyclonic weather type, with its characteristically high intensities and probability of precipitation occurrence. SEASON2 (Figure 8.7c) served to exacerbate the frequency of floods by increasing the proportion of the annual rainfall total that fell during the autumn and winter when the groundwater levels were at their highest. With the exceptions of DOE2 and SEASON1/2, all of the scenarios produced cumulative plots that were approximately linear. By contrast, the most marked non-linear case, DOE2, was attributed to an accelerating decline in soil moisture levels as the impact of both temperature (or evapotranspiration) increases and precipitation reductions became increasingly significant with time. This effect was less pronounced in the case of SEASON1 and SEASON2 due to the elevated winter precipitation, although it appears that even with these increases the systematic rise in temperature rapidly assumes the dominant role in determining the mean soil moisture status and hence reduced flood frequencies.

The cumulative frequency of days with zero flow (Figure 8.8) was the inverse situation with scenarios LWT1872 and DOE2 again emerging at opposite ends of the spectrum. From Figure 8.8a it appears that it is the suppressed frequency of cyclonic days as well as the enhanced frequency of relatively dry anticyclonic days that determines the long-term level of aridity. The 1908/9 base-line was found to be one of the least arid scenarios, surpassing only LWT1872 and LWT1969 (both of which exhibited pronounced cyclonic activity). The plots for SEASON1 and SEASON2 (Figure 8.8c) were remarkably similar, thus supporting the assertion that an approximate parity exists between +1°C and -10% mean annual precipitation even if it falls predominantly in winter (cf. 8.3.2).

Finally, Figure 8.8b provides some indication of the range of uncertainty that can arise from extreme interpretations of the published DOE scenarios. The lower boundary equates on average to 115 days per annum of zero flow and the upper to 188 days - a difference of 73 days or 20% of the year! By way of an example, the actual figure for the Beacon catchment during the exceptionally dry year of 1989 was 131 days.

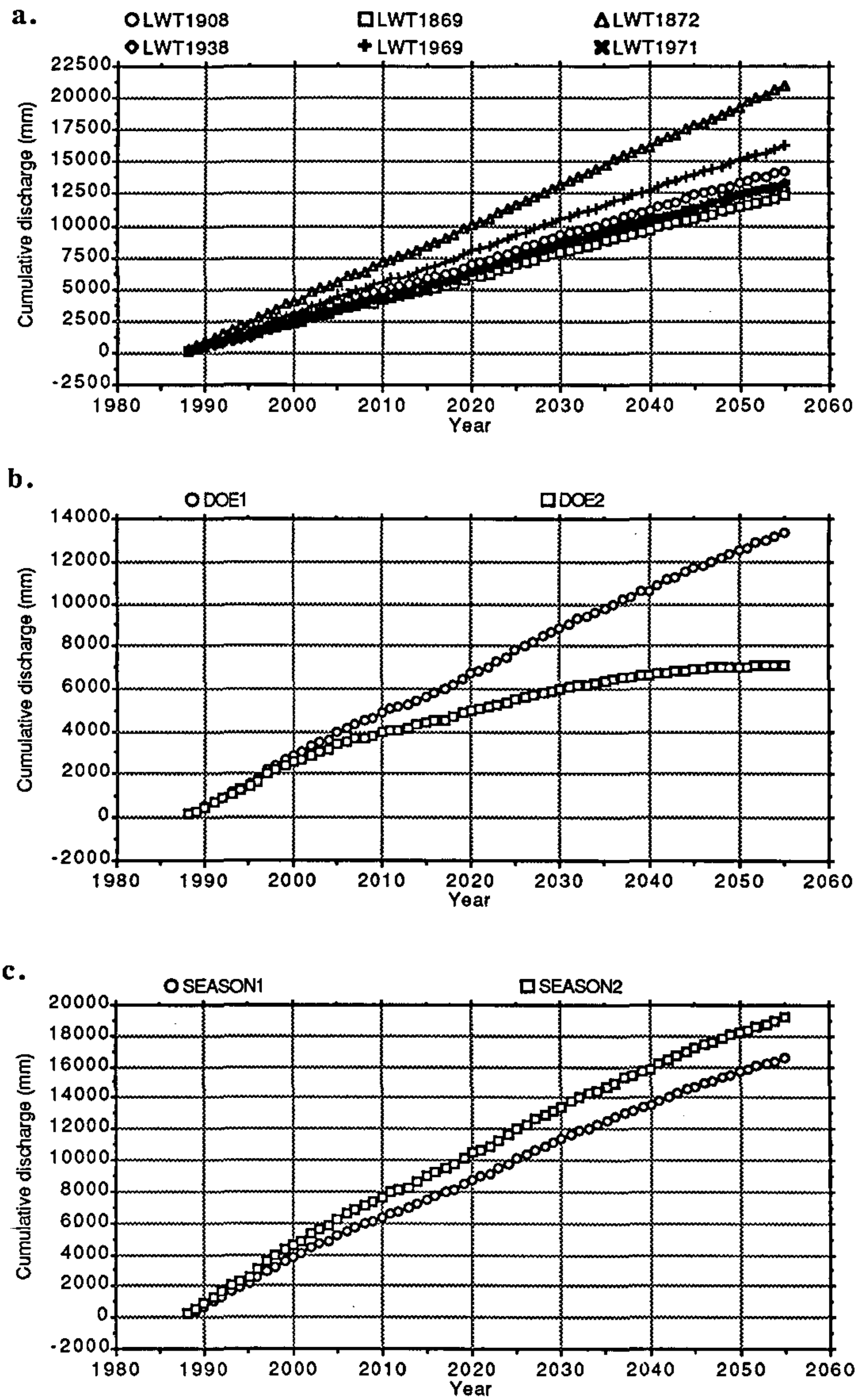


FIGURE 8.6 The cumulative discharge total of the Beacon catchment for various climatic scenarios.

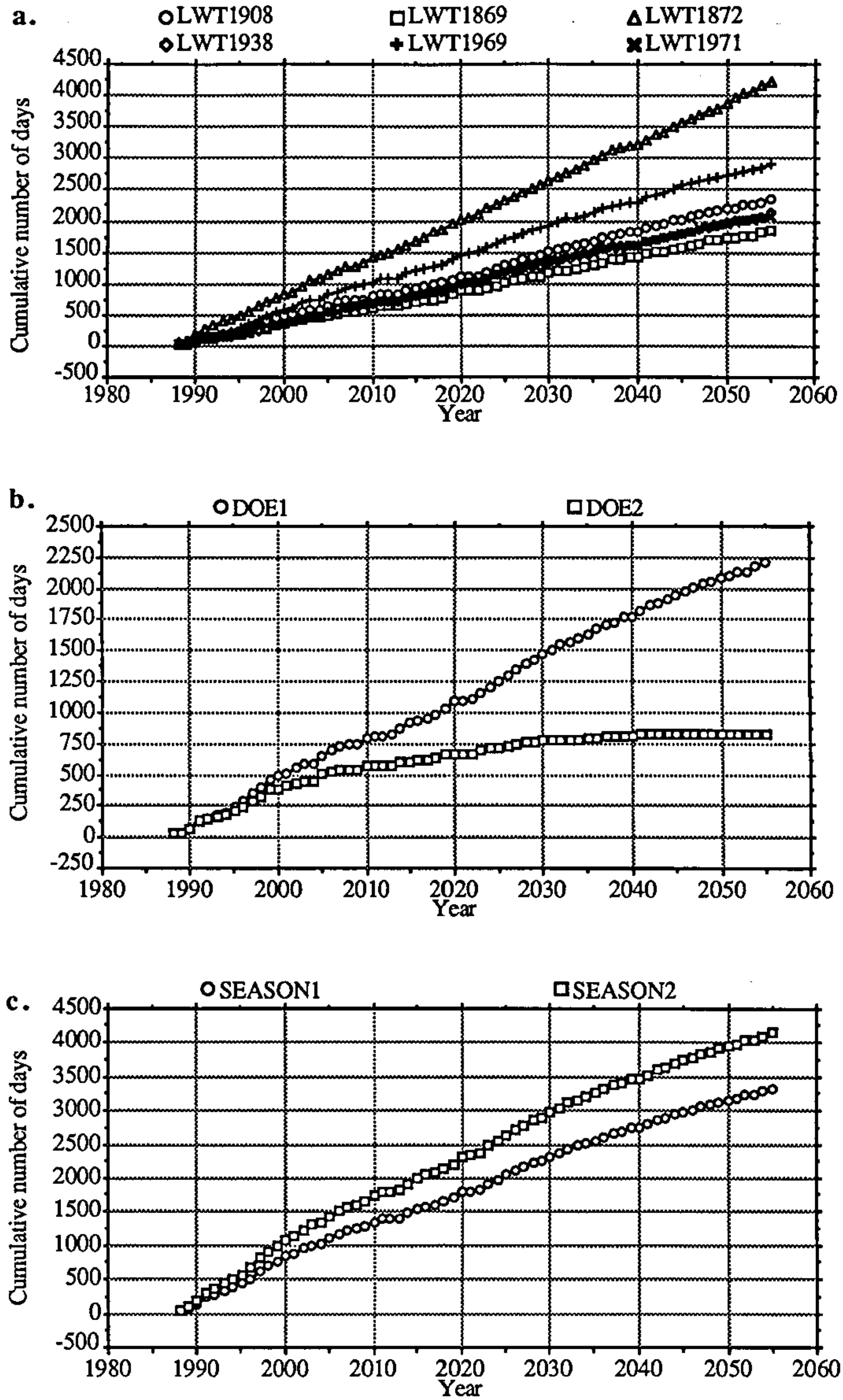


FIGURE 8.7 The cumulative number of days for the Beacon catchment with flow exceeding the 1985-1989 90-percentile under various climate scenarios.

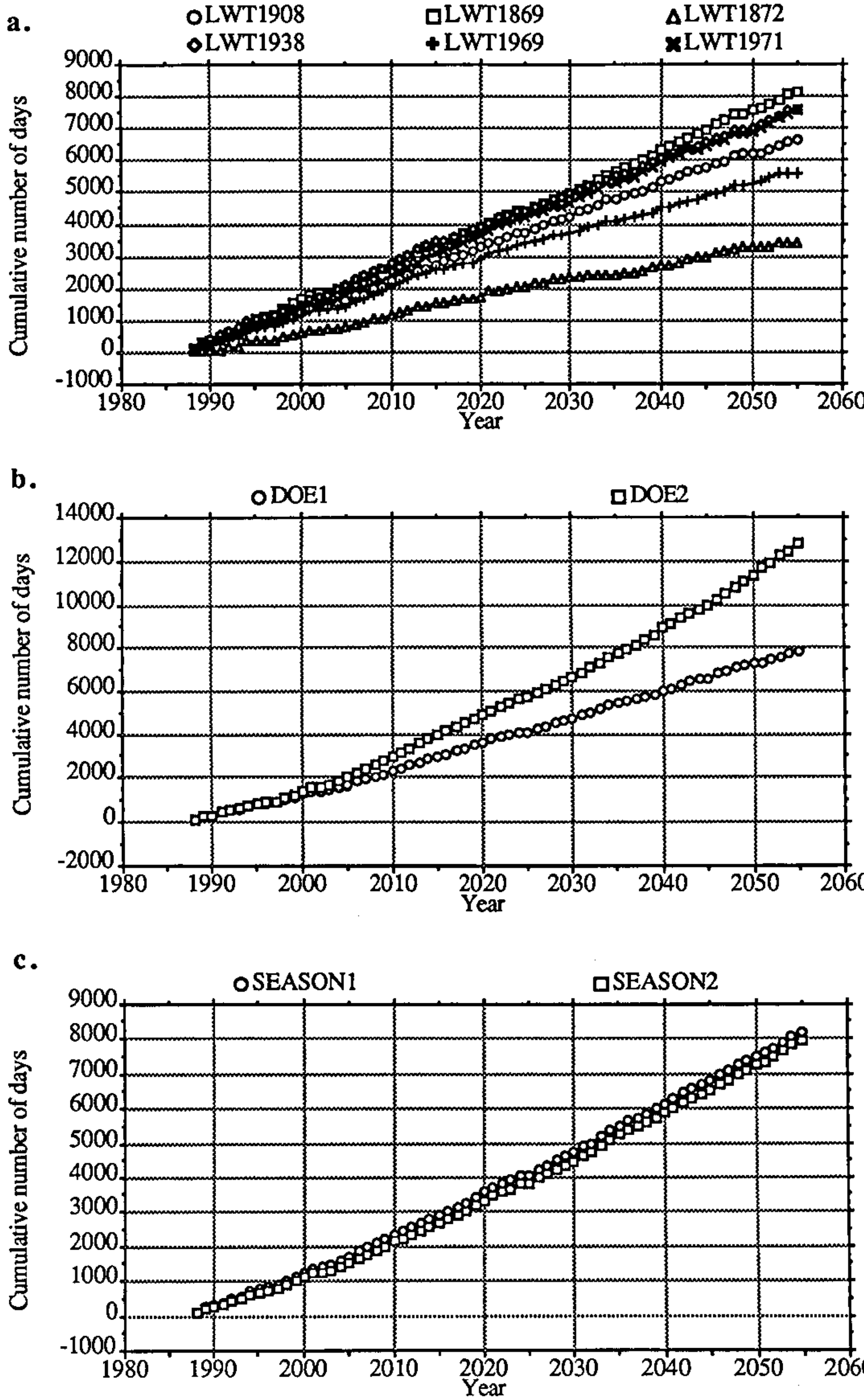


FIGURE 8.8 The cumulative frequency of days for the Beacon catchment with zero flow under various climatic scenarios.

8.4.2 The hydrochemical response

There exists a clear relationship between the hydrological responses described above, the activation and predominance of key solute pathways, and the consequent streamflow acidity. These links are further borne out by the results obtained from the scenarios for the following selected variables:

- the catchment H-ion mass-balance/ base status.
- the volume-weighted streamflow acidities.
- the cumulative frequency of LCDs.

Figure 8.9 presents the simulated long-term base status of the catchment arising from each of the scenarios when the H-ion mass balance between, on the one hand, wet- and dry-deposition inputs and on the other, the sink to weathering products and streamflow outputs was computed. According to this index the most acidifying scenarios were DOE1, LWT1969 and LWT1971 and the least were DOE4, SEASON3 and SEASON4 (all of which incorporated a trend towards a 50% reduction in the deposition load by 2050). It is noteworthy that in the absence of such reductions none of the LWT scenarios (Figure 8.9a) resulted in an increase of the soil base status although there were marked variations in the rates at which acidification was found to proceed. This underlines the significance of the prevailing synoptic weather patterns as a secondary determinand of the long-term acidification process. The fact that none of the LWT scenarios demonstrated soil recovery was believed to be a reflection of the high (1988/9) deposition rates used in each of the simulations.

The impact of the reduced deposition rates on the base status was clearly demonstrated by the curve-linear plots shown in Figure 8.9b/c for the scenarios DOE3, DOE4, SEASON3 and SEASON4. The implications of these results are that with a linear reduction in the deposition rate to 50% of present (1988) by 2050, the soil base status will attain a new equilibrium level by c2030 (in the case of DOE4, SEASON3 and SEASON4) and by c2050+ (for DOE3). The effect of changing the seasonality of the precipitation regime appeared to have a negligable impact on this outcome. A comparison of the trends obtained for DOE3 and DOE4 (Figure 8.9b) suggested that the new equilibrium state would be achieved more rapidly in an increasingly arid (eg DOE4) as opposed to wetter (eg DOE3) climate regime.

The transient response of the volume-weighted streamflow acidity provides an example of the possible implications of the base status changes discussed above. In Figure 8.10 the 5-year moving average of the H-ion concentration (µg/l) has been presented in order to reduce the considerable interannual variations that still arise from the year to year fluctuations in the hydrometeorology. The results obtained for each of the LWT matrices

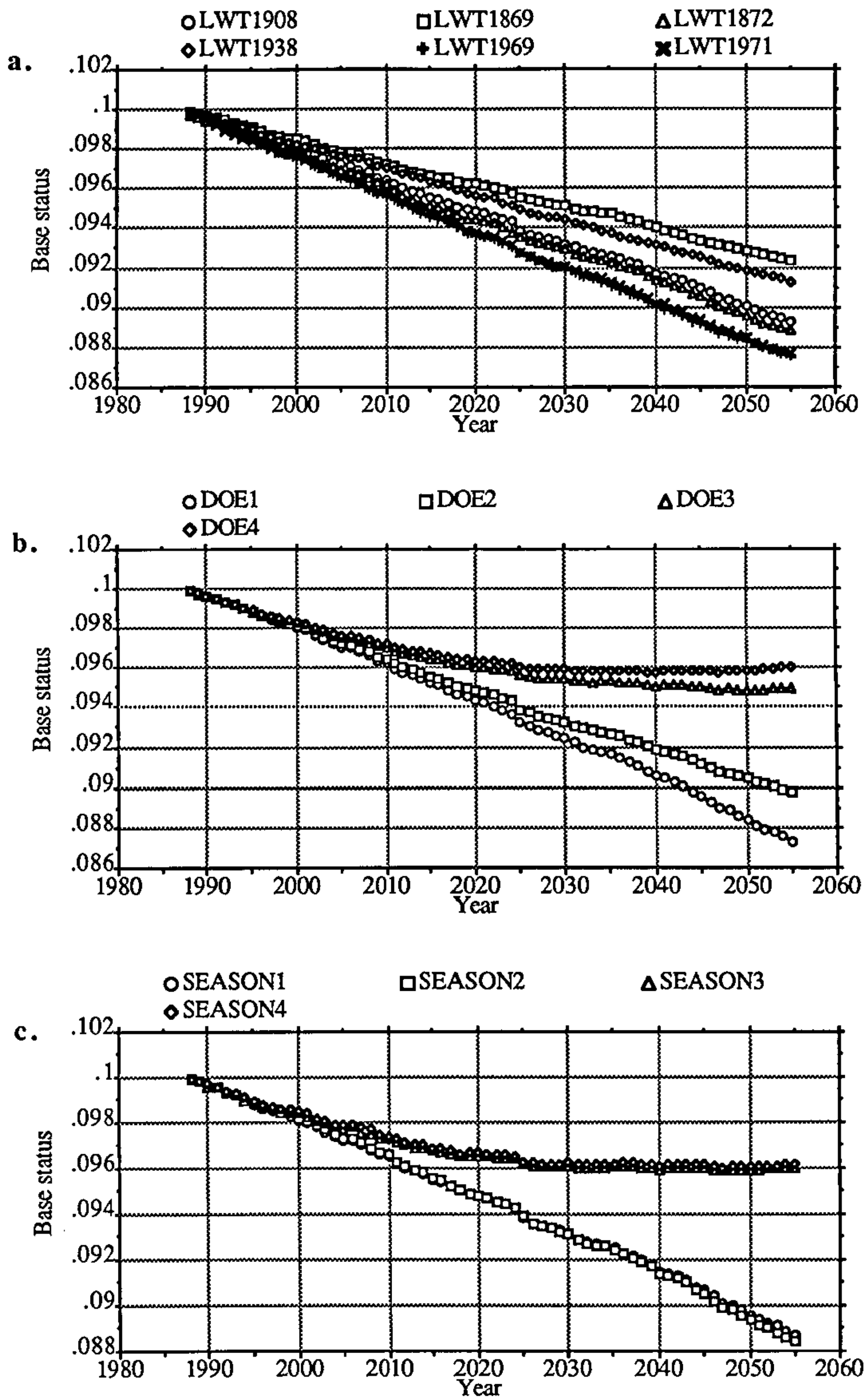


FIGURE 8.9 The transient response of the Beacon catchment base status parameter to various climatic and emission scenarios.

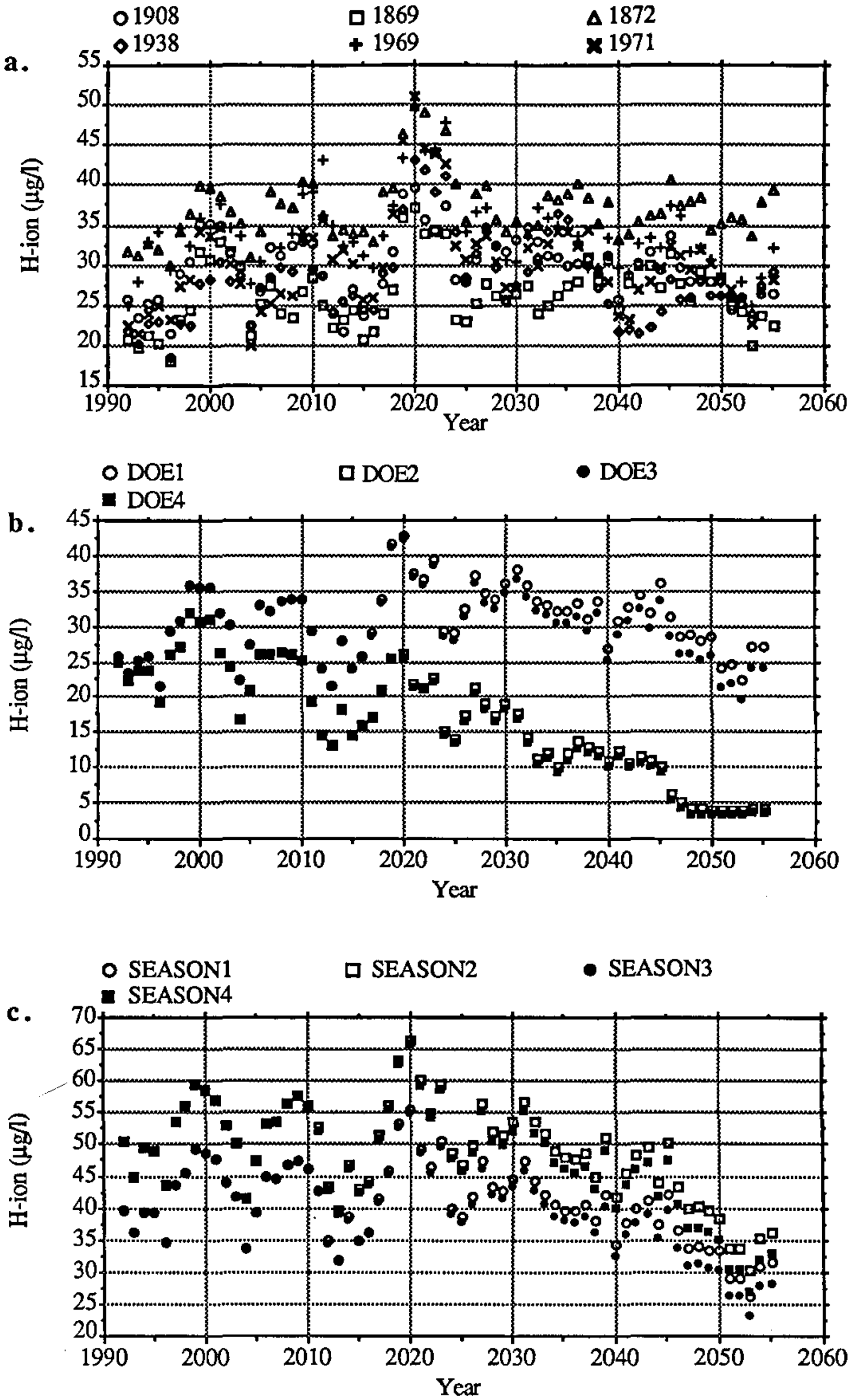


FIGURE 8.10 The transient response of the Beacon catchment discharge volume-weighted H-ion concentration for various climate and emission scenarios.

(Figure 8.10a) indicate that not insignificant variations may occur between the different synoptic scenarios - the mean range being approximately 15 µg/l. This range broadly reflects the difference between the high- and low-cyclonicity scenarios - LWT1872 and LWT1869 respectively. However, no statistically significant trend was detected in the temporal progression of the parameter for any of the six LWT scenarios.

This was not the case for the remaining DOE and SEASON scenarios (Figures 8.10b and 8.10c). SEASON4, DOE2 and DOE4 were each found to produce statistically significant trends at the 99% confidence level, and SEASON3 and SEASON2 at the 95%-level using annual data. The factor common to all of these scenarios was the linear warming by +3°C (above present) by 2050. Note that deposition reductions were applied in only three out of the five scenarios, again implying the secondary importance of this factor relative to those that determine the annual water-balance.

As a means of interpreting these changes more specifically in relation to aquatic biota, the cumulative frequency of days with streamflow acidities exceeding the arbitrary LCD value of pH 4.5 (Figure 8.11) provides a measure of the recurrence interval of the most extreme acidic episodes. Once again the range in the final totals that could be attributed solely to the different synoptic regimes was remarkable (Figure 8.11a), extending from a lower value of 1500 (LWT1869) to in excess of 3700 (LWT1872) days out of 25,000.

Figure 8.11b shows that there was an equally marked divergence in the cumulative totals for DOE1/DOE3 versus DOE2/DOE4, and that this difference was measurable from the outset. However, the effect of deposition reductions appeared to be of minor importance: the 50% reduction resulted in a difference of just 200 LCD events after approximately 65 years in the case of DOE1v DOE3, and only 22 for DOE2v DOE4. The divergent trends are therefore almost entirely attributable to the contrasting mean annual precipitation amounts. A similar pattern also emerged from the SEASON scenarios (Figure 8.11c) for which changes to the meteorological parameters were of greater consequence to the cumulative LCD totals than the deposition reductions. On average however the positive effect of the 50% reduction was marginally greater under a climate of enhanced seasonal differences (ie SEASON) than one of changing mean conditions (ie DOE).

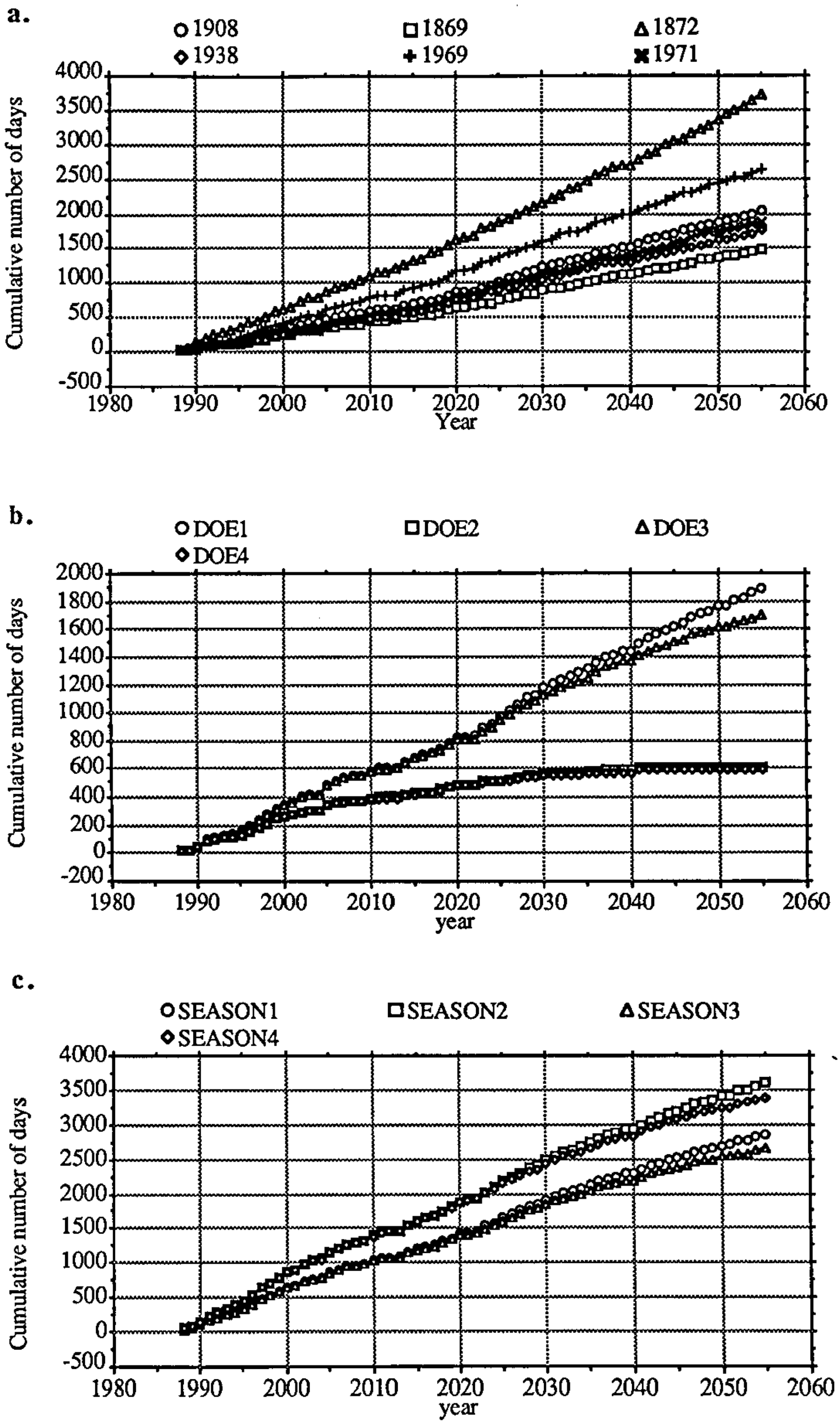


FIGURE 8.11 The cumulative frequency of days with stream flow acidities equalling or exceeding pH 4.5 for various climate and emission scenarios.

SECTION B

8.5 THE BASE SCENARIO

Having conducted the first set of simulations in order to determine the detailed mean annual and transient behaviour of a single catchment to various scenarios, the second stage of investigation was to evaluate the significance of terrestrial influences to the articulation of the dynamic boundary conditions. In order to accomplish this objective, it was once again necessary to construct a single realistic BASE scenario for the future climate and deposition variables. The principal features of the BASE scenario are listed below:

1. Mean annual temperature increased by +2°C.
2. Enhanced frequency of cyclonic weather-types.
3. Mean annual precipitation increased by +20%.
4. Wetter winters (+10%); drier summers (-20%).
5. Deposited acidity reduced by -40% (1988 levels).

Five distinct components were therefore considered: the incremental temperature change; the mean annual and seasonal precipitation regime; the dominant prevailing weather type; the incremental change to the deposited acidity; and the timescale over which the hypothetical changes in these four driving variables are anticipated to occur.

The **timescale** of the simulation was set at 25,000 days from 1st January 1988 onwards. This produces a forecast up until the year 2055 to approximately coincide with the expected date of CO_2 doubling from its pre-industrial level to 540 ppm (DOE, 1988). The fundamental assumption is made that the dominant factor in determining changes in climate over the next 50-100 years will be the greenhouse effect caused by changes in the atmospheric concentrations of CO_2 and other trace gases (Hulme and Jones, 1989). However, it is recognised that the time taken for CO_2 to double is as uncertain as the hypothetical climate impacts that may be its consequence. For example, the date of CO_2 doubling is a function of future emissions, the capacity of the global CO2 sink and the modulating effect of terrestrial ecosystems, and has been variously set between 2050 and 2100+ (SCOPE [1986]).

In response to these changes to the atmospheric composition a linear **temperature** increase of +2°C above present (1980s) by 2050 was postulated. This is compares with an observed Northern Hemisphere warming of approximately +0.5°C between 1880 and 1985 (Jones et al., 1986). The mean global temperature increase predicted for a doubling of CO_2 by twelve different GCMs was recently shown by Bach (1989) to be +2.0°C, although the individual values ranged between +0.2 and +4.2°C. This figure compares favourably with the DOE (1988) forecast for the UK of 3°C ±1.5°C. The chosen value of +2°C for the BASE scenario may therefore be regarded as a realistic, but conservative estimate.

The BASE scenario also envisages an overall increase in the mean annual **precipitation** total as a direct result of the enhanced cyclonicity over the British Isles. A number of recent studies have further suggested that there is likely to be greater inter-annual precipitation variability with a tendency towards increased continental summer dryness and wetter winters and autumns (Hulme and Jones [1989]; Arnell and Reynard [1989]; Bach [1989]; Mitchell [1983];Lough et al. [1983]). This exaggeration of the current seasonal precipitation regime was simulated by SCAM using weighting factors for the mean monthly storm intensities as follows:

J	F	M	A	M	J	J	A	S	O	N	D
1.1	1.1	1.1	1.1	1.1	1.0	.85	.75	.85	1.0	1.1	1.1

The net effect of the imposed regime was to increase the annual total by +1.25%; this is compares with +18% which may be attributed to the increased prevalence of the cyclonic weather type. Note that the latter figure lies within the upper confidence boundary postulated by the DOE (1988).

These precipitation increases were accomplished using the 1872 **Lamb's Weather Type** probability matrix (APPENDIX 1). This transformation matrix was considered to be the most appropriate for inclusion in the BASE scenario for two reasons. Firstly, the results of the sensitivity studies presented in section 8.3.6 and Table 8.4 indicated the overwhelming importance of the cyclonic weather type in determining the long-term response of the Beacon catchment to acidifying ions. Secondly, as Figure 6.16 showed this synoptic class has witnessed a marked increase in its prevalence particularly since 1890 onwards. This trend also contrasts with those of the westerly and anticyclonic classes which are best described by cyclical patterns of mean periodicities 120 and 100 years respectively (Table 6.6).

As well as being sensitive to relative dominance of key weather types, the **deposited acidity** will also depend upon future emissions of acidifying substances. Using 1980 as a base line, the UK is committed to reducing emissions of sulphur dioxide by 20% and oxides of nitrogen by 15% from existing large combustion plants by 1993 as a first stage of the directive 86/609/EC. A further directive requiring the fitting of catalytic converters to most new cars before 1993 is expected to reduce NO_2 emissions by up to 90% (Water Bulletin, 1990). On the basis of these figures an 'optimistic' pollution scenario was constructed in which the total acid deposition is reduced linearly to -40% of the present level by 2050. Whilst it is recognised that some debate surrounds the extent to which reductions in emissions result in a linear change to deposited acidity (eg

Derwent and Nodop, 1986; Shaw, 1984), it was felt that a reduction of 40% to the acid load represents a realistic outcome of recent and future pollution directives. Furthermore, as the simulation results shown in Figure 8.4e have previously indicated, a reduction of 40% was the critical level at which it would be possible to maintain the base status of the Beacon catchment soils at their present level. Local deviations from this reduction figure - due for example to changes in the aerosol scavenging efficiency of different land-use types - may be accommodated using weighting factors as in Whitehead et al. (1988). This approach also overcomes difficulties arising from elevated occult deposition to canopies due to the possibility of more frequent cloud cover, mist and fog (Unsworth, 1984) in the future climate.

The actual **simulation methodology** was identical to that described in section 8.2.3. The four catchments (Beacon, LI1, LI6 and CI6) discussed previously were subjected to both the BASE and LWT1908 scenarios for the period 1988-2055 using their optimum parameter sets; the results obtained from the LWT1908 scenario being used as the long-term mean or control situation. In this way the BASE scenario was applied to four contrasting hydrochemical systems, namely: mixed woodland and bracken (Beacon); coniferous plantation (LI1); unacidified base-rich moorland (LI6); and acidified moorland (CI6). The key model outputs were also unchanged and included hydrological (eg. baseflow and stormflow contributions to total flow, catchment yield, flood frequency and flow cessation measures) as well as hydrochemical parameters (eg. volume-weighted streamflow acidities, total aluminium concentrations, LCD frequency and soil base status). In addition, monthly data for the discharge components and measures of acidity were generated in order to investigate more precisely the seasonal response(s) to climate change of the four catchments. These simulation results form the basis of the discussion below.

8.6 THE SIMULATED HYDROCHEMICAL RESPONSE(S) TO THE BASE SCENARIO

Three temporal scales of the simulated catchment responses were investigated: monthly, annual and superannual. Although there is undoubtedly interaction between each of these scales it is convenient to discuss the results separately.

8.6.1 The seasonal responses

As an effective alternative to the actual simulated monthly baseflow figures, the percentage changes relative to LWT1908 were determined in order to highlight the general pattern of change in flow components arising from the BASE scenario. Figure 8.12a therefore reflects the **net** losses and gains to the baseflow component and Figure 8.12b the **proportional** changes. As Figure 8.12a shows, the results produced for the monthly baseflow totals of each of the catchments were broadly similar. For all catchments the BASE scenario - as might be anticipated - resulted in a net increase of winter baseflow and a net reduction in the summer baseflow relative to the LWT1908 control. However, there were some differences in the timing of these shifts: in the case of the Beacon for example, the switch to higher baseflows occurred in September-October, whereas for LI1, LI6 and CI6, this positive change took place one month earlier. The magnitude of the seasonal anomalies also varied considerably between catchments, with a maximum increase of +61% occuring in November for the Beacon (Figure 8.12a). These differences were thought to reflect the contrasting geological and soil properties, which in turn govern the water retention and drainage characteristics of each of the basins. Thus, in the case of CI6 it is probable that the upland soils are relatively thin (<1m thick) compared with the lower slopes and valley bottoms (eg. LI6) where the drift material is known to be up to 5m in depth (Whitehead et al., 1988). Based on these observations, the baseflow component of catchments with high geological indices (Petts and Foster, 1985) such as chalk, sandstone and clay would therefore be expected to be less sensitive to changes in the prevailing precipitation regime than those consisting of peat, igneous rock and gravel. This is strongly supported by the marked change in the seasonal response of the Beacon catchment which is underlain by impermeable pre-Cambrian geology.

Figure 8.12b shows the monthly baseflow component as a percentage of the total monthly discharge (again expressed as a percentage of the LTW1908 situation). [Note that even where there has been a net increase in the baseflow component (Figure 8.12a), there may still be a decline in relative terms of this fraction of the total flow (Figure 8.12b)]. In all four cases there has been an overall decline in the baseflow fraction (or percentage of total monthly discharge), with the exception of June, July and August which showed an increase of up to +17% in LI1 and LI6. This suggests that the proportion of total flow contributed by the more acidic upper soil horizons has increased between the months of September and May inclusively. These changes clearly reflect the modified precipitation regime resulting in elevated soil moisture contents in winter and lower water-table levels in summer. In this respect the Beacon catchment was found to be the most sensitive, showing an overall reduction of the baseflow proportion of -17%.

Changes to these contributing 'end members' (Christophersen et al. [in press]; Neal et al. [in press]; Reynolds et al. [1986]) of the total discharge were manifested in the monthly streamflow acidities and LCD frequencies (Figure 8.13 and Figure 8.14). Once again, all four examples demonstrated an increased seasonal range of acidities for

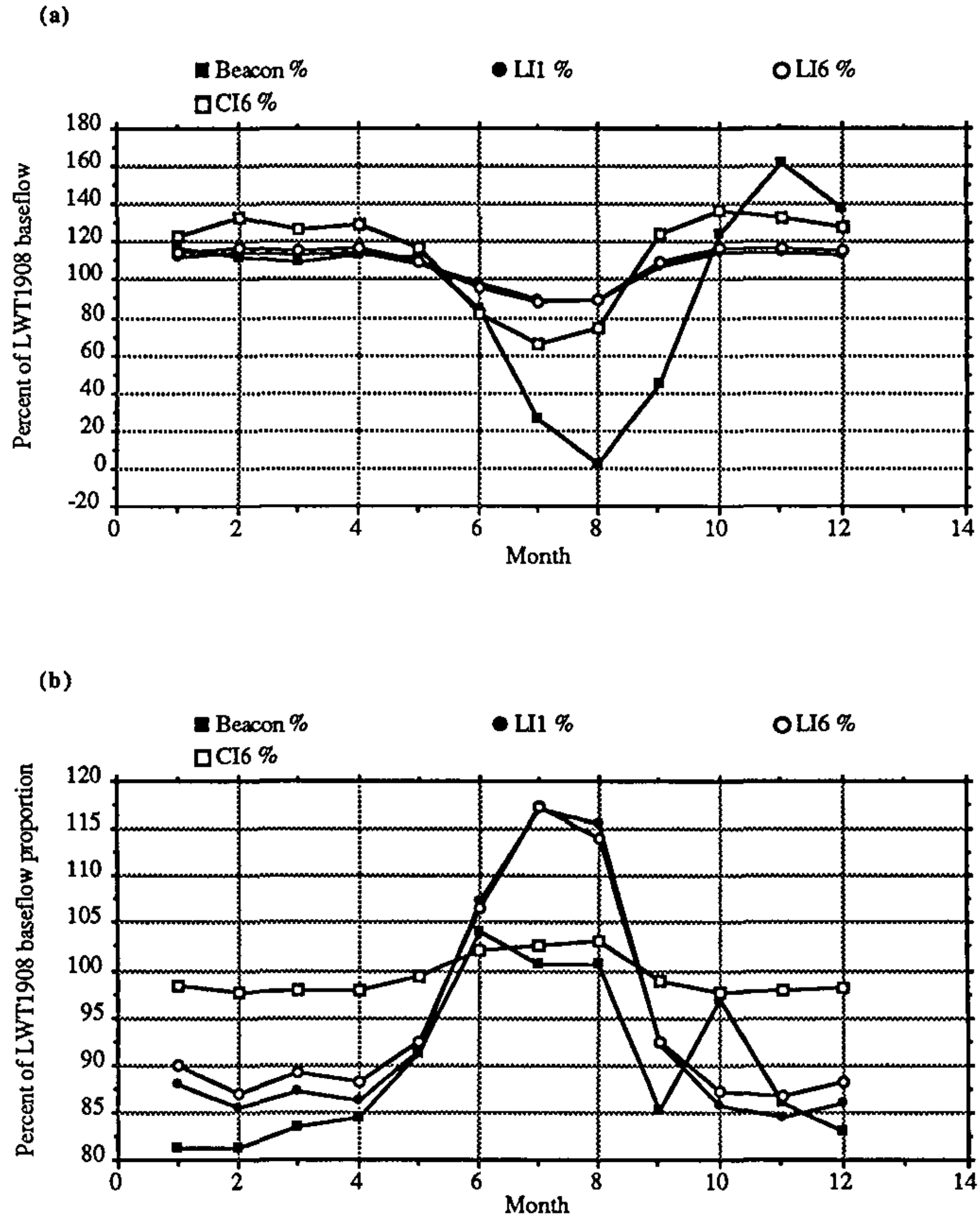


FIGURE 8.12 Changes to the monthly baseflow component arising from the BASE scenario relative to the LWT1908 scenario: (a) net (b) proportional change.

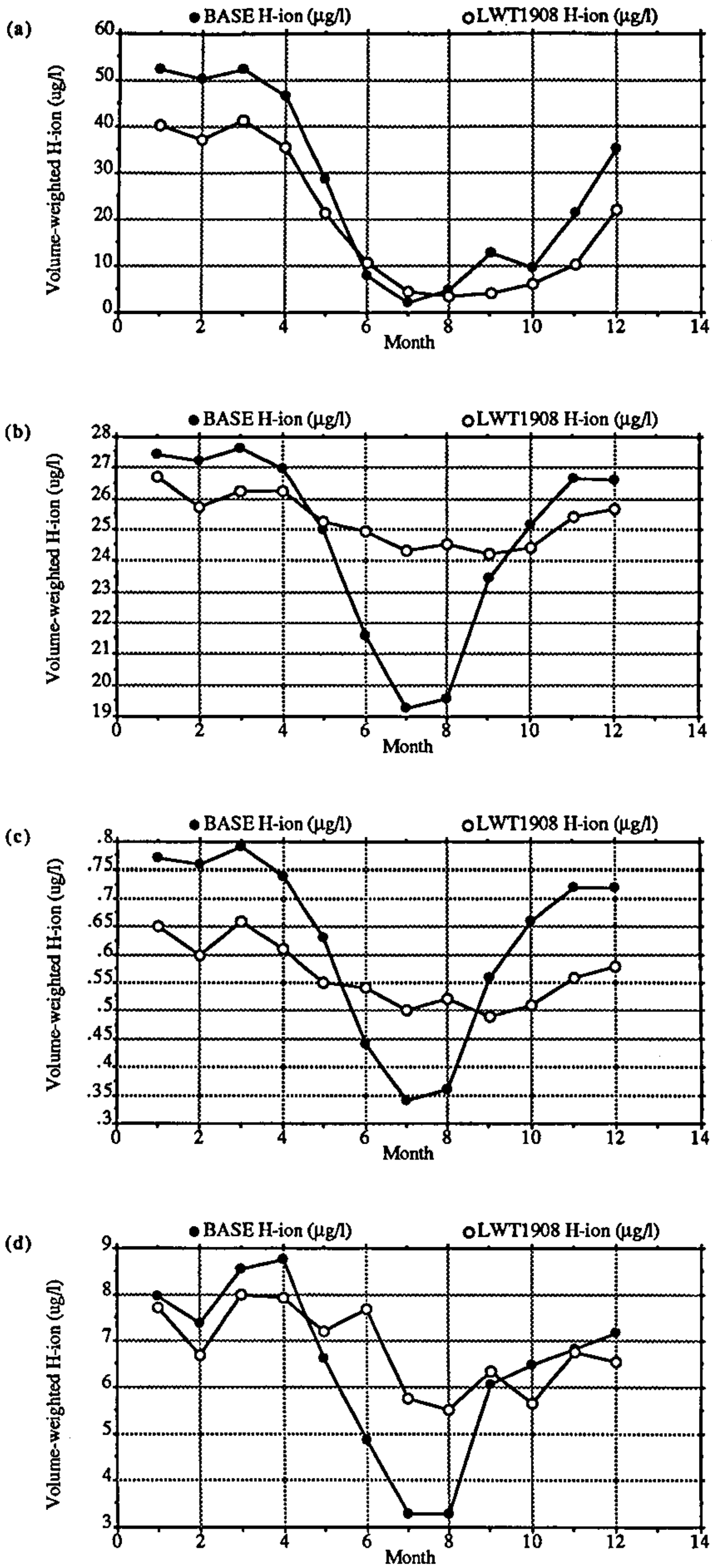


FIGURE 8.13 The mean monthly streamflow acidities (1988-2055) arising from the BASE and LWT1908 scenarios by catchment: (a) Beacon (b) LI1 (c) LI6 (d) CI6

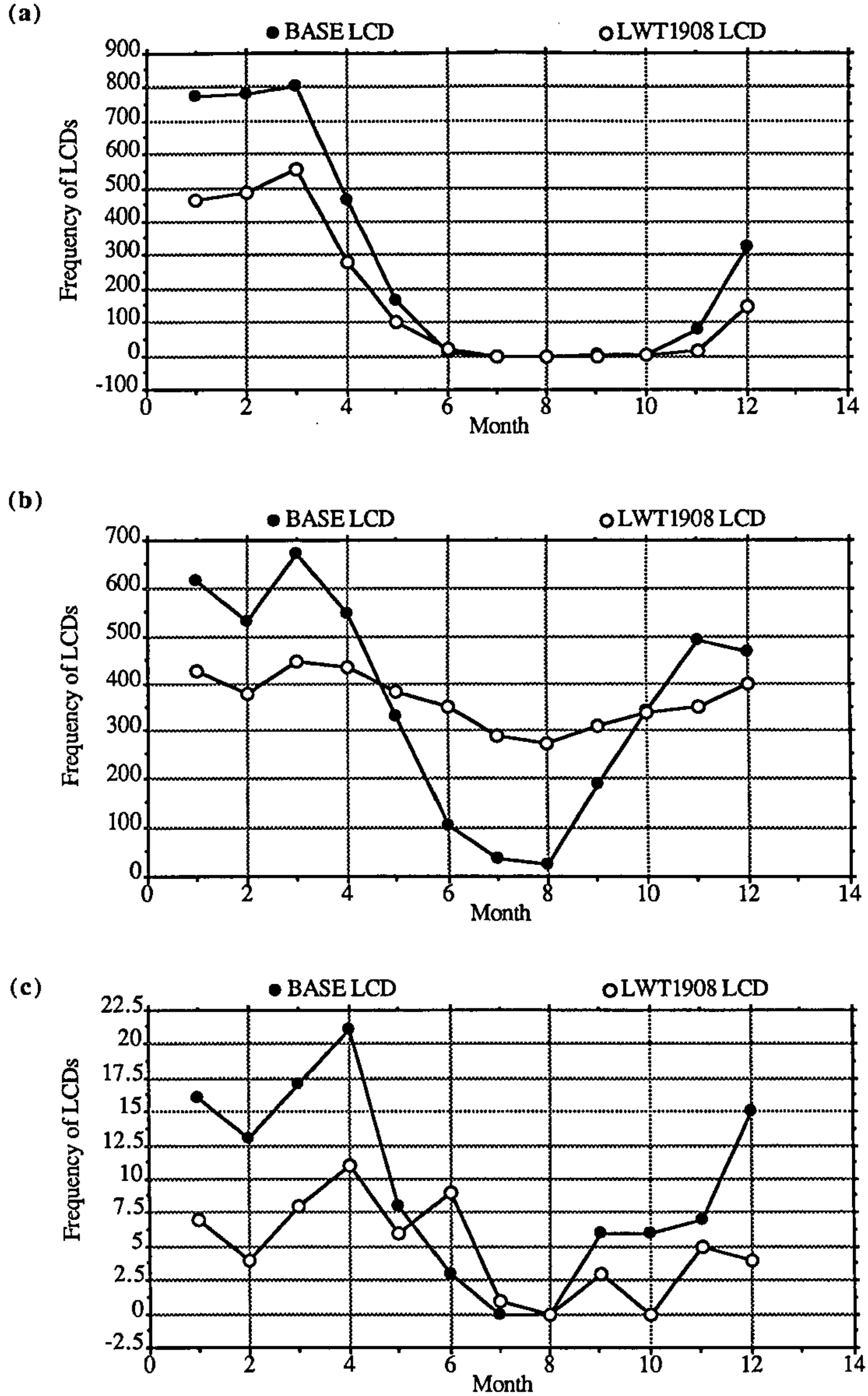


FIGURE 8.14 The monthly frequency of LCDs under the BASE and LWT1908 scenarios: (a) Mixed Beacon (b) Forest LI1 (c) Moorland CI6. NB There were no LCDs for Moorland LI6.

the BASE scenario relative to the LWT1908 datum. Each regime produced by the BASE scenario exhibited increased acidity in the winter (October-April) and lower acidities in the summer months (May-September). For example, the March daily probability of a streamflow exceeding the LCD acidity was increased in the Beacon catchment from 0.265 to 0.386 by the BASE scenario. Conversely, for LI1 in August the daily LCD probability was reduced from 0.139 to 0.012. As Table 8.4 indicates below, despite increases in the frequency of winter LCDs, the lower spring-autumn totals actually resulted in a net reduction in the annual total for LI1.

In general, therefore, the most notable effects of the climate changes at the monthly scale were upon the enhancement of existing seasonal contrasts in catchment hydrochemistry. The increased winter precipitation intensities and storm frequencies lead to a greater proportion of the total flow being supplied from the upper (acidic) soil horizons, which in turn caused the mean streamflow acidities and LCD frequencies to increase. By contrast in summer the dominance of the baseflow fraction was increased relative to the stormflow fraction even though a net decline in the amount of baseflow was experienced. This shift in the composition of the total streamflow was again manifested by reduced streamflow acidities and fewer acidic episodes.

8.6.2 The mean annual responses

The mean annual summary statistics for a selection of hydrological and hydrochemical parameters are presented in Table 8.4. For each of the catchments the simulation results are provided for both the BASE and LWT1908 scenarios. All four catchments demonstrated an increase in the mean annual discharge of between 18-33% in response to a mean annual precipitation increase of approximately +18%. The increase in the yield was greatest for the Beacon suggesting that catchments which currently receive low to moderate rainfall amounts may be more sensitive to increases in the annual precipitation total. This may explain why the three Welsh catchments showed only a proportionate increase in their total annual runoff.

The similarity in the gross hydrological response of catchments LI1 and LI6 is noteworthy bearing in mind their contrasting land-use types (cf. also Figures 8.12a/b). The higher pre-storm baseflow and stormflows of LI6 have been attributed to a combination of high rainfall, low interception losses and a steep, dense channel network, whereas, the high peak discharges of LI1 were explained in terms of the dense network of drainage ditches and root channels within the forest plantation (Whitehead et al., 1988). Due to the lumped nature of the SCAM hydrological model, it is unlikely that these hydrologic differences have been adequately distinguished,

Parameter	CATCHMENT Beacon BASE	Beacon 1908	LI1 BASE	LI1 1908	LI6 BASE	LI6 1908	CI6 BASE	CI6 1908
Days with rainfall (%)	54.2	46.8	54.2	46.8	54.2	46.8	54.2	46.8
Annual rainfall (mm)	847	720	2234	1900	2234	1900	2116	1800
Annual discharge (mm)	280	211	1780	1507	1780	1506	1501	1267
Catchment yield (%)	33.0	29.4	79.7	79.4	79.7	79.3	70.9	70.4
Baseflow (%)	59	71	52	57	41	45	93	94
Frequency of Q90%	4182	2375	2376	1204	2313	1198	1467	971
Days with zero flow	7653	6619	0	0	0	6	3482	3984
Precipitation H (ueq/l)	64.1	76.5	64.4	76.7	61.0	76.5	48.7	64.4
H-ion load (kg/ha/yr)	0.64	0.75	1.70	1.99	1.44	1.61	1.08	1.26
Initial soil base status (%)	10.00	10.00	6.19	6.19	13.58	13.58	9.60	9.60
Final soil base status (%)	9.49	8.93	0.22	0.00	30.83	29.35	5.73	3.98
Discharge H (ueq/l)	43.5	31.6	25.4	25.4	0.7	0.6	7.0	6.9
Discharge Al (ueq/l)	186.8	163.4	47.8	47.3	6.7	6.3	10.3	10.3
LCD frequency	3402	2065	4348	4381	0	0	112	58
Ratio H-out: H-in (%)	19.1	9.0	26.7	19.2	0.8	0.5	9.8	6.9

TABLE 8.4 Summary statistics arising from simulations using the BASE and LWT1908 climate scenarios.

although the model was found to accurately reproduce the mean runoff coefficients of all three of the Welsh catchments.

The values given for the frequency of flows exceeding the respective 90-percentile discharges of each catchment show an expected increase in the incidence of flood events. The greatest net increase arose in the afforested catchment LI1 with the current 90-percentile flow of 210 litres/sec occuring +93% more frequently. This may reflect the importance of rapid or preferential flow paths such as drainage ditches under a future climate of more frequent and intense storms. It is also interesting to note that a high increase in the frequency of peak discharges was also forecasted for the Beacon catchment which is known to be underlain by a network of tile-drains.

The number of days with zero flow demonstrates contrasting behaviour between the catchments. The overall frequency of days with no flow is first and foremost a function of the catchment area (which is a surrogate for the catchment storage potential). However, the Beacon, LI6 and CI6 all have very similar basin areas in the region of $0.7km^2$. The main distinguishing factor (in terms of input-ouput budgeting) then becomes the respective mean annual precipitation amounts (720, 1900 and 1800 mm/year) and their parameterised basin stores (75, 77 and 60 mm equivalent). Thus, the Beacon - which has the lowest precipitation total - and CI6 - the lowest catchment store - are shown to be the most prone to drought.

Such differences are also borne out by the figures for the baseflow expressed as a percentage of the total runoff. As the LWT1908 scenario indicates, the Beacon and CI6 catchments are both highly groundwater dependent. The relatively low percentages for LI1 and LI6 again reflect the influence of rapid flow or preferential pathways via ditching in the first instance and possibly soil piping or root channels in the later. The fact that low flows are maintained within LI6 even under the extreme climatic conditions of the BASE scenario also supports the view that this catchment has a larger groundwater store or that it receives lateral flow from neighbouring watersheds.

All these factors have a bearing upon the mean annual hydrochemical response which showed a lower sensitivity to the meteorological scenario at the annual scale than at the seasonal level. Despite the significant changes to the seasonal flow regimes, the mean annual discharge acidity and aluminium concentrations were largely unchanged in all catchments, excluding the Beacon. But as the final base status parameter suggests, soil acidification has in fact occurred in all catchments (except for LI6 where the weathering rate and base status of the soils are comparatively high). Furthermore, in all instances the rate of acidification was actually greater under the conditions of the LWT1908 as opposed to the BASE scenario. This was thought to reflect the higher mean annual H-ion load to each of the catchments and lower levels of H-ion exported by the surface water network under LWT1908.

Despite the higher final base status of the catchment soils arising from the BASE scenario, there were no significant reductions in the mean streamflow acidities. In the case of the Beacon catchment there was even an increase. This particular result implies that increased streamflow acidity can accompany a higher soil base status if there has been a corresponding shift in the relative contributions made by baseflow and stormflow to the total annual discharge. Conversely, reductions in the mean catchment soil base status may not necessarily result in elevated streamflow acidities if the prevailing climate favours a general increase in the baseflow component of the total discharge. For catchments LI1, LI6 and CI6 it appears that the effect of the lower deposition load merely counterbalanced the increased streamflow acidity that would have been attributed to the prevailing synoptic, meteorological, and precipitation regimes of the BASE scenario. This may be inferred from the response of the Beacon since a 40% reduction in the deposited acidity would - in the absence of climate changes - have maintained the current soil base status (cf. 8.3.4, Figure 8.4e). Even for these catchments the increased frequency of LCDs in CI6 and the unchanged condition of LI1 and LI6 suggest that the deposition reductions only just offset the hydrochemical changes arising from the BASE scenario.

The lack of responsiveness in the mean annual acidities also bring into question the appropriate timescale at which catchment recovery or acidification should be properly assessed. In the case of LI1, for example, it may be argued that over the duration of the simulation period there was no significant change in the mean surface water acidity. However, the seasonal perspective (Figure 8.13 and Figure 8.14) suggests otherwise, and that marked acidification has actually occurred during the winter months and recovery in the summer. As was shown in the previous chapter, the choice of an appropriate 'index of acidification' poses equally difficult questions. For example for CI6, the final soil base status shows that there has been a reduced rate of accumulation of acidity within the catchment under the BASE scenario, whereas the LCD frequency shows a slight increase in the occurrence of acidic episodes.

8.6.3 The transient, long-term responses

As well as highlighting the differing behaviour of each of the four catchments, the transient response also provides a means of forecasting the long-term evolution of the catchments' hydrochemical properties. For the Beacon, LI1 and CI6 the soil base status parameter (Figure 8.15) demonstrates an accelerated curve-linear depletion of soil cations under the long-term average conditions of LWT1908. Although both scenarios

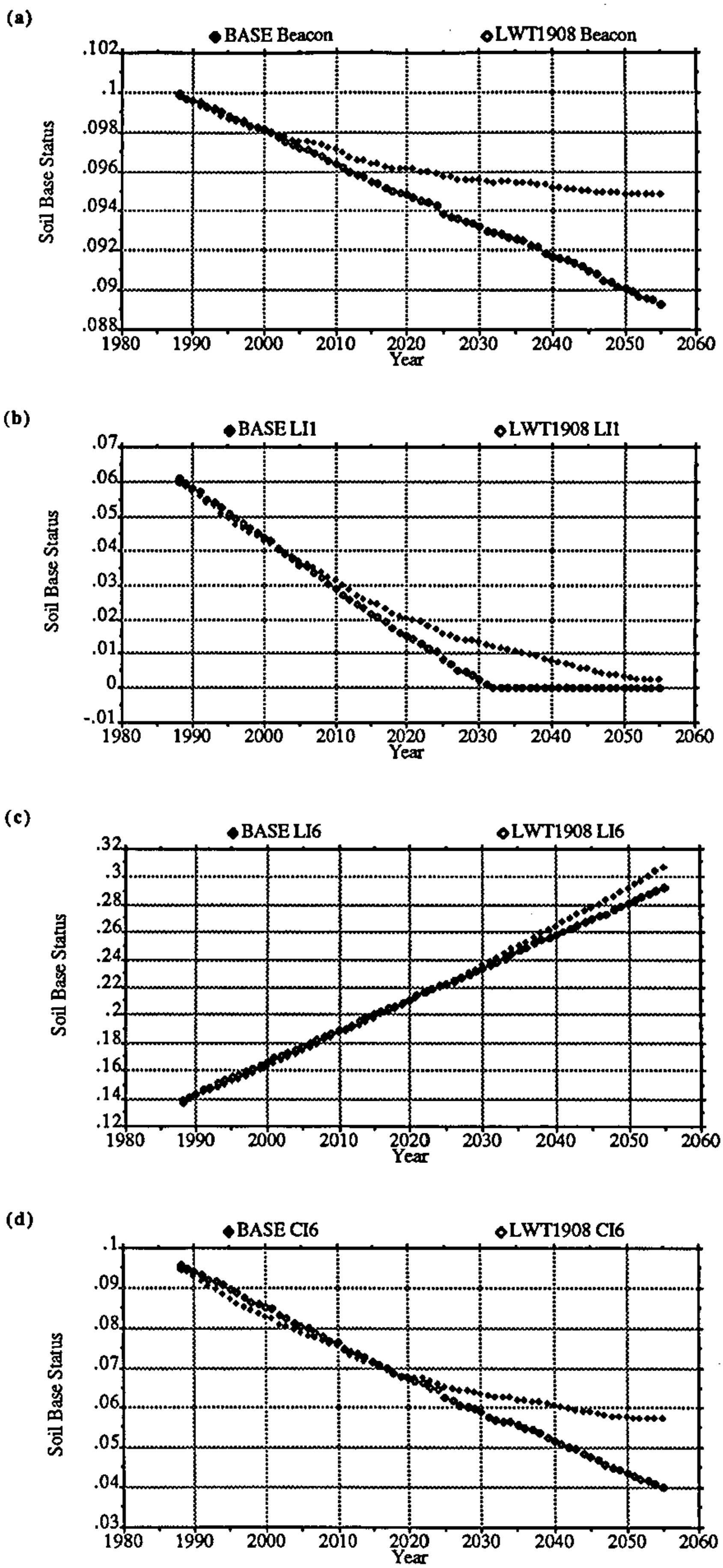


FIGURE 8.15 The simulated soil base status parameter (1988-2055) under the BASE and LWT1908 scenarios by catchment: (a) Beacon (b) LI1 (c) LI6 (d) CI6.

result in soil acidification, the BASE scenario appears to attain a new equilibrium status around 2050 for the Beacon and CI6. The LWT1908 scenario, however, resulted in the continued reduction of the soil base status, and in the case of LI1, even exhausts this reservoir by 2030. Thereafter in this case it is assumed that the soil has attained the aluminium buffer range in which hydrogen-ions are only consumed by the release by weathering of aluminium from clay minerals (Kauppi et al., 1986). Because of its high weathering rate and large store of basic-ions, LI6 was the only exception to the long-term acidification trend. Here the potential to consume incoming acidic ions always exceeded the rate of deposition, and hence the base status of the soil actually increased slightly under both scenarios. Strictly speaking, therefore, soil recovery was not the simulated response in any of the four catchments for either of the scenarios .

The long-term decline in the soil base status of the Beacon, LI1 and CI6 was mirrored by the steady rise in the volume-weighted discharge acidity for each of these catchments (Figure 8.16a-d). The response of the Beacon was unusual in that following an initial increase in streamflow acidities, concentration levels began to decline c2020+. By contrast LI1 and CI6 showed a steady increase throughout the period. The net effects of the BASE scenario are presented in Figure 8.17 which shows the difference between the simulated hydrogen-ion concentrations in each of the catchments for the two separate scenarios. This suggests that for LI1 and CI6 the BASE scenario would result in an initial net increase in the surface water acidity up until 2025-2030, after which levels of acidity are consistently lower than would have been expected for the LWT1908 scenario. At the turning point the deposition reductions have reached a point that presumably is sufficient to offset the acidifying effects of the predominance of the cyclonic weather type (or more specifically, the hydrological changes). In the case of the Beacon, however, the BASE scenario streamflow acidities were consistently higher throughout, reflecting the marked decline in the baseflow fraction experienced by this catchment (Table 8.4).

Figures 8.12a/b suggested that the enhanced winter precipitation and its subsequent effect on stormflow generation ensured that the annual frequencies of LCDs were consistently higher under the BASE scenario. As was shown in 8.6.1, the differences in the final LCD totals (LI6 = 0, Beacon = 3402) reflect the combined and variable effect of flow generation and soil hydrogeochemical processes, as well as the dominant land-use type. Although the annual rate of change of LCD occurrence appeared to be hydrologically determined, there is some evidence in Figure 8.18a that these acidic episodes may be reduced by the progressive decline in both the deposited load and in the frequency of flood events. Figure 8.18b illustrates the extent to which soil buffering processes are also capable of limiting the occurrence of acidic episodes: the discontinuity in the LWT1908 trend occurred at the point at which the available store of basic cations became exhausted. The subsequent rate of LCD generation for the

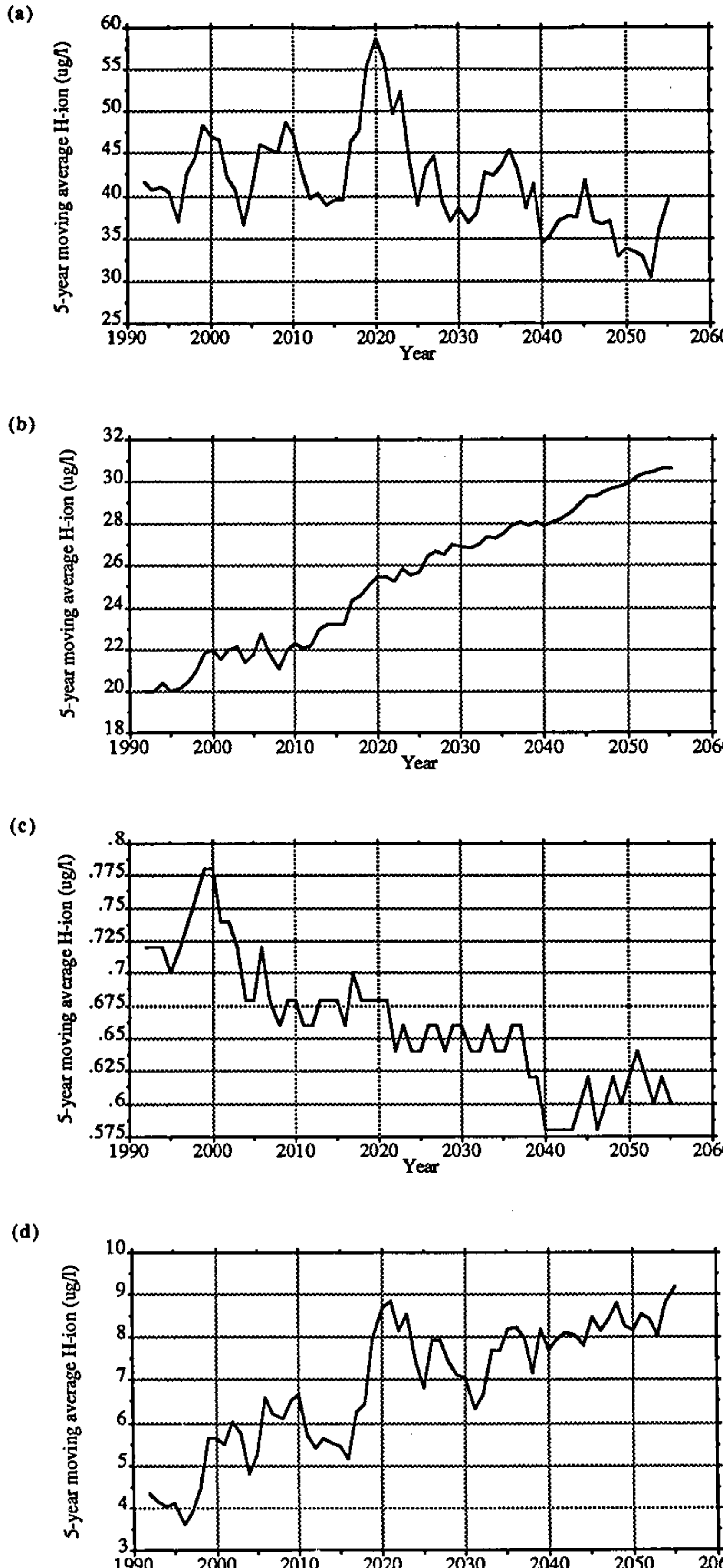


FIGURE 8.16 5-Year moving average of the simulated streamflow acidity under the BASE scenario for: (a) Beacon (b) LI1 (b) LI6 (d) CI6.

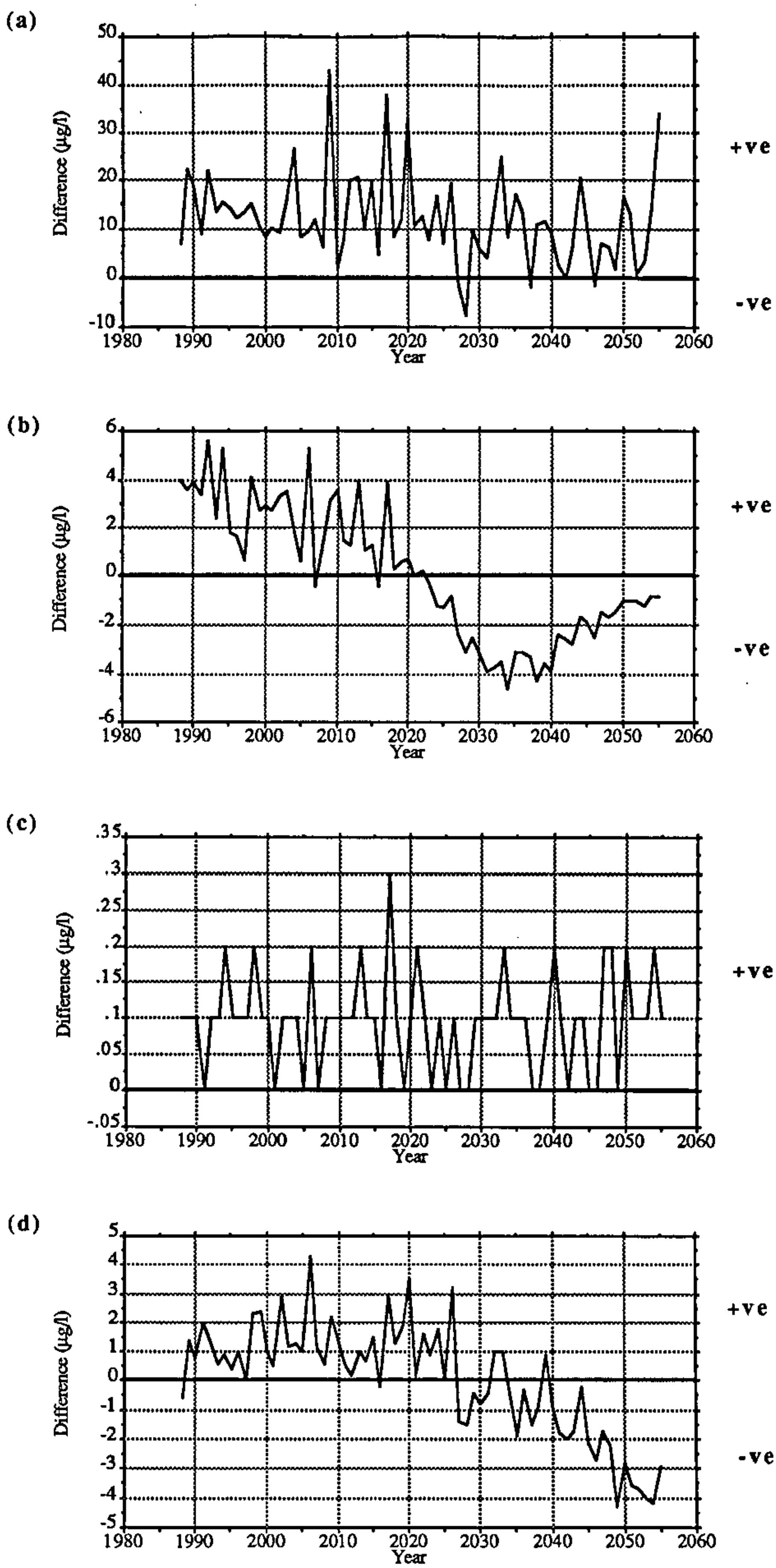
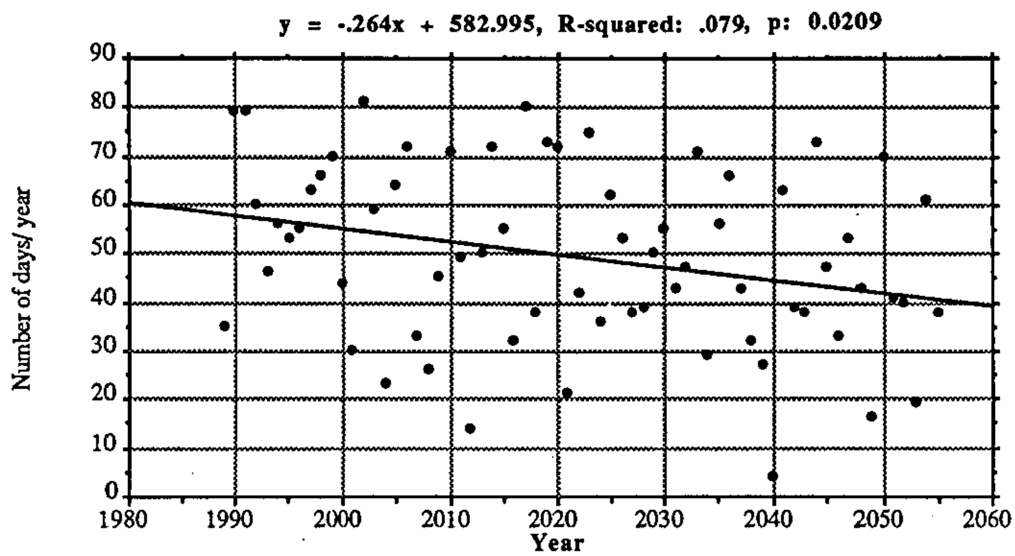


FIGURE 8.17 The difference in the streamflow acidities arising from the BASE minus the LWT1908 scenarios for (a) the Beacon, (b) LI1, (c) LI6 and (d) CI6 catchments.

(a)



(b)

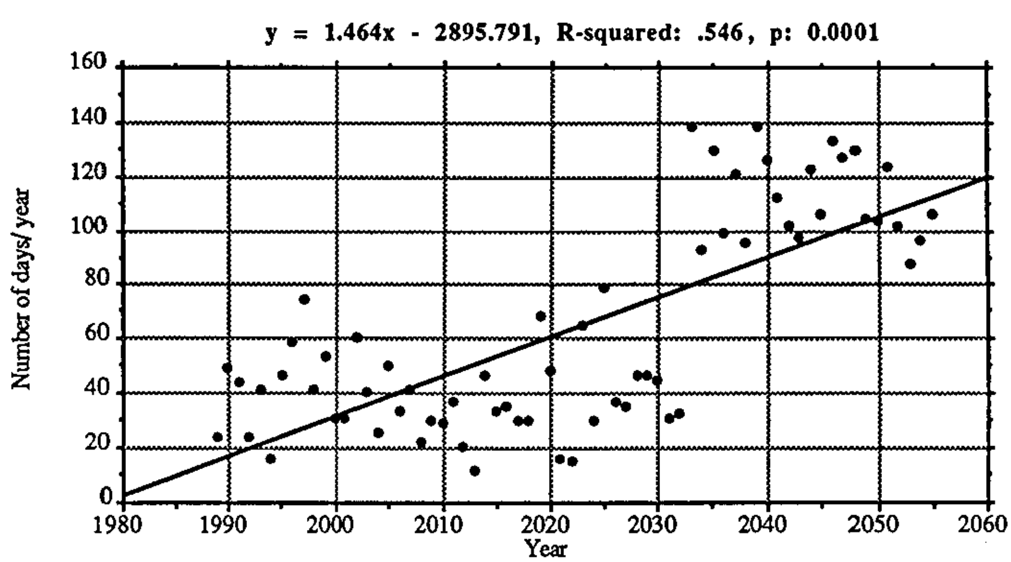


FIGURE 8.18 Linear trends for the annual frequency of LCDs occurring as a result of the BASE scenario in (a) the Beacon, and the LWT1908 scenario in (b) LI1.

unbuffered soil soon exceeds that which may be attributed to the wetter winters of the BASE scenario.

8.7 SUMMARY

The first set of simulations were conducted in order to test the sensitivity of a single acidic catchment to a range of contrasting climate and deposition scenarios. From the results obtained for the Beacon catchment simulations it is possible to assemble a number of summary points:

(1) The arbitrary and largely subjective nature of the chosen scenarios and their respective output parameters should be stressed. A rigorous approach must be applied in the choice of an appropriate and realistic suite of scenarios, recognising that the significance of the impact will be system/problem specific.

(2) For the given hydrological problem - namely that of surface water acidity - meteorological parameters were found to exert the greatest control through their effect on the water balance. Principal amongst these were the temperature and precipitation trends which in turn are a function of the prevalence of key synoptic weather types. The cyclonic weather type in particular was found to combine those attributes such as precipitation frequency, event magnitude and acidities which - by their presence or absence - are able to partially dictate the long-term rate and direction of the surface water and soil acidification/recovery.

(3) Catchment weathering and acid deposition rates, whilst undoubtedly of great significance to the long-term H-ion mass balance, were found to be of secondary importance to the climatic variables in determining the mean annual hydrochemistry. This may reflect the fact that hydrometeorological variables are dominant at the decadal time-scale whereas the parameters which affect the catchment base status operate at much longer time intervals. The extent of this scale difference is likely to be catchment specific.

(4) The precise significance of changes in the seasonality of precipitation and temperature regimes remains uncertain and merits further, more detailed investigation. The provisional analyses conducted in 8.3.3 suggest that a trend towards warmer and drier summers and wetter, milder winters, would increase the overall catchment yield whilst reducing the length of the season with surface flow. The effect on the release of H-ions into the stream network would serve to accentuate the existing levels of acidity.

(5) On the basis of the preceeding results and overview it is possible to present a 'worst case' scenario - that is to say, those factors which if combined would tend to accelerate the soil acidification process:

(a) high(er) deposition rates.
(b) low(er) weathering rates.
(c) low(er) cation exchange capacity and base status.
(d) cyclonic weather type dominant; anticyclonic and westerly types supressed.
(e) low(er) mean annual temperatures/ evapotranspiration rates.
(f) high(er) annual precipitation with enhanced winter rainfall.

Note that factors (a) and (f) are a natural consequence of elevated cyclonic activity.

The second set of simulations investigated the regional articulation of a single BASE scenario relative to the long-term LWT1908 climate response(s). On the basis of the observations made in the preceding discussions it is possible to make two broad generalisations concerning the simulated impact of the BASE scenario on each of the four catchments. Firstly, all catchments - with the exception of LI6 for reasons already discussed - experienced **continued soil and surface water acidification** under both climate scenarios. In terms of the time series plots for the base status parameter, this acidification process progressed at a slower rate under the BASE scenario than under the mean conditions represented by LWT1908. However, the volume-weighted mean-annual streamflow acidities suggested that initially the increased winter precipitation of the BASE scenario would result in a more rapid acidification of the surface waters due to the predominance of acidic flow-pathways. Subsequent reductions in the deposited acidity coupled with the steady rise in the mean annual temperatures (Figure 8.2) and a progressive increase in the dominance of the baseflow fraction brought about a slowing of this trend. Even in the case of Beacon where the BASE scenario acidities were consistently higher than for LWT1908 this deceleration was also observed (Figure 8.17a). Due to the exceptionally high weathering rate in LI6, the hydrochemical response of the catchment was found to be highly insensitive to the prevailing climate and pollution scenario.

The second general observation refers to the sub-annual hydrochemistries of all four catchments. The monthly response of the BASE scenario showed **enhanced seasonal extremes** of both discharge amounts and acidities. These effects corresponded to an increase in the stormflow fraction of the total flow during winter and, by implication, the concentration of more flow through preferential pathways (such as soil pipes and macropores), the near surface soil layers and over the soil surface. The neutralising capacity of these routeways is relatively low or non-existent and may even act as a source of further acidity. By contrast the more arid summer months witnessed an increase in the predominance of baseflow sources contributing to the total flow, and a corresponding reduction in the mean monthly streamflow acidities. The overall mean annual effect of these changes was, however, variable in terms of the incidence of LCDs. For example, the Beacon showed a strong increase in the frequency of LCDs because of the high sensitivity of this catchment's flow regime to the seasonality of precipitation and the winter bias of acidic episodes. Catchment LI1, however, showed little or no effect in the mean annual frequency of LCDs (Table 8.4) over the length of the simulation period, but as Figure 8.15 indicated this condition arose from a rapid increase in the occurrence of acid episodes once the soil base store was exhausted.

These local departures from the general pattern of enhanced seasonality and long-term acidification, underline the significance of the unique land-use, geology, topography, soil properties and flow generation mechanisms of each catchment to the articulation of climate change impacts. As has already been shown the **Beacon** catchment demonstrated a high degree of sensitivity to the precipitation regime of the BASE scenario in terms of the annual discharge total, increased dominance of stormflow over baseflow and the catchment yield. Similarly marked changes to the seasonal timing of moisture retention and release resulted in a major increase in the incidence of winter floods (plus acid episodes) and the extension of summer drought periods (plus base-rich baseflow). This hydrological behaviour was thought to reflect the relatively low storage potential of the basin and the high proportion of precipitation lost to evapotranspiration (approximately 70%). This meant that only minor changes in the amount and timing of precipitation were able to bring about significant changes to the soil moisture status of the catchment and hence to the soil horizons contributing flow.

By contrast the largest catchment **LI1**, appeared (in terms of the net flow changes) to be least sensitive to the inter-annual climate inputs (Figure 8.12a) yet equally showed one of the greatest increases in the proportion of winter discharge contributed by the stormflow component (Figure 8.12b). This enhancement of the acidic 'end member' of the total flow resulted in a marked increase in the occurrence of winter LCDs (Figure 8.13). As in the case of **LI6** the increasing predominance of the stormflow component was attributed to the efficiency of the catchment drainage network. The key difference in the case of LI6 was the availability of a major source of buffering cations to counter this acidifying effect. Furthermore, as Table 8.4 indicates, the forest canopy of LI1 ensured that the occult plus wet-deposited acidity to the catchment was on average +25% higher than to the moorland of LI6. When balanced against the moderate-slow weathering rates this partly accounts for the fact that of the four catchments LI1 experienced the highest rate of soil acidification under both scenarios.

Finally, the behaviour of the acidified moorland control **CI6** was in many ways different from the other three catchments. The net and proportional changes to the baseflow (Figures 8.12a/b) were relatively minor reflecting the continued dominance of the quasi-permanently saturated valley bottom peat as the major source of total flow (WWA, 1987). However, due to the proximity of this contributing area to the basin outlet even slight changes to the flood frequency were reflected in a 93% increase in the frequency of LCDs due to the limited opportunities for buffering within the catchment. The hydrological response was also unusual in that the catchment experienced an increase in the frequency of flows greater than the current 90-percentile in conjunction with a reduced severity of drought. Again this behaviour was attributed to the seasonal dynamics and spatial extent of the main contributing area.

Bearing these regional differences in mind, the following chapter seeks to extrapolate the common features of enhanced seasonality and long-term soil acidification to the key questions concerning catchment recovery potential and ecosystem response to the BASE scenario.

CHAPTER 9

DISCUSSION OF THE SIMULATED HYDROCHEMISTRY AND POTENTIAL IMPACTS TO ACIDIC CATCHMENTS OF CLIMATE CHANGE

9.1 INTRODUCTION

By adopting a modelling strategy that spanned between the detailed hydrochemical simulations of the Birkenes model (Christophersen and Wright, 1981; Christophersen, Seip and Wright, 1982) and the long-term soil-chemistry changes of the MAGIC model (Cosby et al., 1985a), the SCAM model was designed to incorporate the detail required to evaluate the impact of changes to acidic upland catchments arising from adjustments made to both (short-term) meteorological and (long-term) deposition rate variables. The rationale for this design criteria has been the proven significance of broad climate parameters to catchment hydrology, and in turn, the control exerted by hydrological processes on streamflow chemistry (Christophersen et al., in press; Bishop and Grip, in press; Wheater et al., in press; Whitehead et al., 1986; Jenkins, 1989; Bache, 1984; Lawrence et al., 1988; Wolock et al., 1990; Langan and Whitehead, 1987). Furthermore, in order to attempt to evaluate the associated biological impacts it is essential that the model should function at an appropriate temporal resolution. As was shown in 2.5 the diurnal time-step of the SCAM model enables the investigation of cumulative changes to the daily and seasonal variability of streamflow conditions as well as any underlying trends in the mean annual status.

However, a vulnerable point in any model's design and of its consequent simulation results, remains the fact that considerable uncertainty surrounds the long-term input deposition chemistry (Alcamo and Posch, 1985). Hence the keen interest shown in establishing relationships between rates of acidic deposition and long-term trends in synoptic patterns (eg. Bradley, 1986; Davies et al., 1986; Farmer et al., 1989; Wilby, 1989). Any predictions of catchment acidification/ recovery over timescales of 10-200 years are therefore subject to the uncertainty that arises from imperfect knowledge of the future behaviour of pollutant bearing weather-systems. Other factors which may either directly or indirectly influence the spatial and temporal redistribution of acidic inputs include: the equilibrium level and rate of global/regional warming/cooling and its subsequent affect on precipitation patterns; the extent to which seasonal patterns of deposition may be altered; and the future patterns of pollutant sources, their relative significance and the effect of controlling legislation. As if to exacerbate the situation these 'unknowns' are accompanied by uncertainties that pertain to the derivation of reliable parameter estimates for the model itself. As Georgakakos et al. (1989, p1511) observe:

"Input uncertainty together with uncertainty in the form of the mathematical model equations (potential structural model errors) and in the values of the free parameters of the mathematical models (which results from inadequate records for parameter calibration) are major contributors to the total uncertainty of mathematical model predictions."

In short, uncertainties pertaining to issues of structure, parameter values, forcing functions, initial states and operational usage will be inherent to all models used for forecasting, of which SCAM is no exception. Whilst much effort was made to justify the design, it is important that the specific limitations of the model discussed in Chapter 7 should not be overlooked. At the same time it is also recognised that uncertainty in model calculations varied tremendously, depending upon the temporal and spatial scales of interest. Despite the occurrence of significant differences between observed and SCAM simulated time-series at the daily resolution, the aggregated monthly, annual and super-annual H- and Al-ion statistics remained within the limits set by instrumental uncertainty. In this sense, the SCAM model should be seen as more a diagnostic than precise, prognostic tool.

Therefore, having outlined the nature of the constraints placed upon the reliability and sensibility of the SCAM model forecasts, the objective of the following discussion is to utilise the simulation results to speculate on the possible consequences for further soil acidification or recovery, surface water acidification or recovery, and the general implications that climate changes may have for the aquatic ecosystems of acidic catchments.

9.2 THE PROSPECTS FOR REVERSIBILITY OF ACIDIFICATION WITH CLIMATE CHANGE

"*One major problem with designing control strategies for acid deposition is that future deposition patterns must be simulated using past meteorological conditions. We can estimate the emission reductions that would result from the implementation of a given control strategy, but efforts to predict what effect these reductions would have on deposition levels are hampered by uncertainty about future transport and deposition climatology*" (Streets et al., 1985, p 887).

The idea that acidification is in some way reversible is both conceptually appealing and central to all discussions on target loads and goals for future levels of emissions. However, target loads for acidifying compounds have seldom been established within the context of changing climate and hydrological conditions despite the proven significance of atmospheric and catchment processes to the long-term acidification of streams and lakes (Whitehead et al., 1988). Furthermore, some existing models such as MAGIC make no provision for hydrology and so cannot take account of the changing intensity and frequency of acidic episodes and cannot, therefore predict the onset of biological perturbations at this level of resolution (Warren, 1988). In the following paragraphs a number of key concepts and processes concerning the recovery of acidified catchments are therefore discussed from a perspective that acknowledges changing hydrological regimes. The format of the discussion enables a comparison of the most recent empirical and modelling experience with the results obtained from the SCAM model for the BASE scenario and with the sensitivity-to-climate studies of the previous chapter.

The term 'reversibility of acidification' is generally interpreted in terms of declining concentrations of the strong acid anions NO_3 and SO_4, an associated decrease in the concentration of base cations and rising alkalinity of streamflow (Cosby et al, 1985b). Major reductions in the flux of the mobile anions through the soil will in turn lead to changes in the pH and inorganic aluminium in lakes and streams. Input-output budgets may also indicate that the pool of exchangeable base cations in the soil is progressively replenished. As the exclusion of acidity continues, organic acids in streamflow may become increasingly dominant. In addition to these fundamental processes, recent catchment manipulation and simulation exercises have highlighted three additional aspects of recovery.

The first concerns the assumption that a given reduction in acidic loads will yield a desirable response in the hydrochemistry of the target catchment. Henriksen and Brakke (1988) have defined this **critical load** as the highest deposition of strong acid anions to surface waters that will not cause harmful biological effects on populations, such as declines in, or extinctions of fish. The precise value of the critical load required to produce such a response is therefore both impact and regionally specific. This point is readily illustrated by reference to a number of recent modelling and experimental results. Whitehead et al. (1988) and Neal et al. (1988) have proposed - on the basis of MAGIC predictions - that a deposition reduction of 50% over the next 20 years would allow aluminium levels to "*fall significantly*" and the pH to recover to "*reasonable levels*" in the Plynlimon and Dargall Lane moorland catchments. Using the same model Hornberger et al. (1989) have recently shown that: a 5% reduction in deposited sulphate (relative to 1980) would result in the continued acidification of lakes in southernmost Norway; a 30% cut would halt the ongoing acidification of lakes but would result in relatively minor improvements in lake alkalinity; but a 70% cut (applied linearly) between 1986 and 2011 would ensure that only 30% of lakes have negative alkalinity by 2020 (as opposed to 74% in 1986). Similarly Christophersen et al (in press) have shown by means of an ionic balance calculation that a reduction in sulphate deposition of over 80% would be required to re-stock the Birkenes Brook with brown trout. This compares with the 50% reduction predicted by Henriksen's et al. (in press) empirical model of lake acidification as yielding viable conditions for fish in 40% of the 1000 lakes surveyed in Norway in the autumn of 1986. On an international scale, the Regional Acidification INformation and Simulation

(RAINS) model has estimated the 'cost optimal reduction' of -58% of European SO_2 emissions (relative to 1980) would bring about "*large improvements*" of soil acidification in Central Europe and "*improved*" lake-acidification conditions in Southern Finland and Sweden (Alcamo et al., 1987). As some of these examples suggest there are often considerable difficulties involved in actually defining and then quantifying 'recovery' - a problem that is compounded when assumptions about a static climate are no longer valid.

These studies suggest that 'target loads' can and should be evaluated along two quite distinct lines. The first approach establishes the desired consequence of emission reductions and then computes the required deposition rate, whilst the second imposes an arbitrary reduction of acid deposition on the ecosystem and then determines the impact according to selected output variables. The SCAM model may be used to compute the 'load-response' via either of the methods. Thus, using Figure 8.4d it is evident that if a 50% reduction in the frequency of LCDs was desired for the Beacon catchment (from 700 to 350 days in 10,000) then this could not be accomplished by any level of reduced emission over such a short period. However, as Figures 8.2 and 8.3 suggest, such a reduction could result from as little as 1.0-1.5 °C rise in the mean annual temperature - the surrogate for evapotranspiration - or from a 10% reduction in the mean precipitation event magnitude. Such a result reinforces the view that hydrometeorological variables are far more effective at reducing the LCD frequency than cuts in acidic deposition. Furthermore, even in the absence of deposition reductions the climate scenarios generated from the LWT1938 (high westerly-type frequency) and LWT1869 (low cyclonic frequency) probability matrices (APPENDIX 1) brought about 17% and 27% fewer acidic episodes respectively than the long-term mean conditions of LWT1908.

The predominance of broad climatic parameters over the prevailing pollution scenario was also evident from the results obtained using the second approach mentioned above. In the BASE scenario the deposition load was set at -40% (present) in order to maintain the current base status of the Beacon catchment (cf. Figure 8.4e). The corresponding change to the mean annual streamflow acidity - attributable solely to this action - was to nominally increase the pH from 4.51 to 4.52, and to reduce the incidence of streamflows with pH<4.5 by 7%. In purely climatic terms the SCAM model predicts that the same effect would be accomplished by increasing the mean annual temperature by 0.5°C or by reducing the mean storm size by 5% over the same 10,000 day period.

The evidence obtained from the sensitivity studies conducted for the Beacon catchment therefore underline the importance of considering long-term trends in climate variables when establishing target loads. If for example, the positive aspects of a 40% cut in the acidic load equates to 0.5°C increase in mean annual temperatures, then clearly the converse may also apply. Namely, that a 0.5°C drop could offset the desired consequences of a 40% cut in deposited acidity! As well as referring to an emission baseline (such as 1980) pollution directives should also state categorically the assumed climate context of the reductions whilst recognising the complex interplay of the various meteorological parameters involved. As will be shown later the composite effect of the multiple climate and deposition changes represented by the BASE scenario were to promote a trend towards limited soil recovery in the Beacon catchment even though the enhanced predominance of cyclonic weather and of winter precipitation increases would initially favour surface water acidification.

The second aspect of the reversibility of acidified soils and surface water is that marked reductions in acidic anion loads can result in a **rapid recovery** (eg. Dillon et al. [1986]; Neal et al. [1988]; Forsberg et al. [1985]; Wright et al. [1990, 1988]). For example, Dillon et al. (1986) report a rapid recovery in lake SO_4, Al and pH chemistry after the SO_2 emissions of the Sudbury area, Canada were reduced from 1.41 Mt/yr (1973-78) to 0.68 Mt/yr (1979-85). In the same way Forsberg et al. (1985) have suggested that the 35% reduction in sulphate levels in some lakes on the west coast of Sweden since the late seventies may be attributed to a 15-22% reduction in the wet deposited SO_4 concentrations. Similar trends have also been reported for acidified lakes in Galloway, southwestern Scotland. Using diatom and chemical evidence Battarbee et al. (1988a/b) showed that there have been significant changes in both the sulphate concentrations and diatom assemblages since 1978, and that these trends coincided with a 40% decline in national SO_2 emissions since the maximum in 1970. Furthermore, within the space of less than a decade the water chemistry of Loch Enoch showed a rise in the mean pH of 0.22 units from 4.40±0.12 in 1978-79 to 4.62±0.04 in 1984-86. Throughout the study the implicit assumption has been made that the climate regimes of the two decades were comparable.

The recovery of an acidified soil following the reduction of acidic inputs has also been shown at a number of sites to be slower than the rate of acidification (Wright et al. [1990]; Forsberg et al. [1985]; Hauhs [1988]). This behaviour arises from the fact that acidification processes are dominated by the cation exchange and sulphate retention characteristics of the soil whilst deacidification depends primarily upon the silicate weathering rate (Hauhs, 1988). Forsberg et al. (1985) have observed another form of hysterisis in the H-ion and sulphate concentrations of Lake Ramsjon and Lake Stora Halevatten, western Sweden due to elevated hydrogen ion loadings associated with rising emissions of nitrogen oxides. Despite falling acid anion concentrations in the lakes, the acidity of the water is currently higher than it was for similar sulphate concentrations during the acidification phase. The assumed link to increased nitrate loadings has been discounted by Hauhs (1988) who has shown that the highest value of sulphate in both precipitation and lakewater to which the subsequent reductions relate coincided with several hydrological extreme years. Since reductions in emissions of some acidifying substances is a relatively recent phenomenon for much of Western Europe, it may be assumed that more empirical evidence will be collected on the subject of hysterisis in the near future. In the meantime, however, the simulated chemistries obtained from models such as MAGIC in conjunction with the experimental manipulation of whole ecosystems (Wright et al., 1990) strongly support the view that recovery will be slower than acidification. For example, the weathering rate at Sogndal, Norway is believed to be approximately 10 $meqm^{-2}yr^{-1}$ whereas the sulphate flux due to acidic deposition removed base cations from the catchment at the rate of 20-60 $meqm^{-2}yr^{-1}$.

Contrary to the findings of the Galloway study the results derived from SCAM for the BASE scenario - which proposes a comparable reduction in deposited acidity over a similar time-scale - do not show any statistically significant increases in the surface water pH for either the Beacon, LI1 or CI6 catchments (Table 9.1b). The unacidic moorland catchment LI6 being a unique exception due to its high weathering rate. Rather, from all the indices of soil and water acidity in Table 9.1a it is clear that the other three catchments would be expected to acidify further if the mean conditions of the LWT1908 were to prevail until 2055AD. Under the BASE scenario (Table 9.1b) the Beacon catchment did at least provide some evidence of recovery: the differential solution to the soil base saturation trend shows that a minimum turning point will be reached in 2053AD. The corresponding figures for LI1 and CI6 for this new equilibrium level were found to be 2063 and 2057 respectively. Of these three catchments only the Beacon demonstrated an associated reduction in the amount of H-ion exported and in the frequency of the acidic streamflow events. Even with the relatively large (on average 20%) reductions in H-ion input the surface water acidities of catchments LI1 and CI6 still exhibit statistically significant linear increases at least until 2055. The rate of increase of the streamflow acidity was however, lower in the case of the BASE scenario than the LWT1908 scenario. Once again the implication of these findings are that for certain types of catchment, deposition reductions may be inadequate in themselves as a guarantor of catchment recovery. Thus, the BASE climate scenario was capable of postponing the intended consequences of the deposition reductions made to catchments LI1 and CI6.

This spatial or **regional variability** in the rate and direction of the hydrochemical response to a given climate and emission scenario represents the third key characteristic of catchment recovery. The silicate weathering rate is the ultimate source of base cations in soils and this release rate defines the net long-term supply of protons that the system is able to buffer and the rate at which it may recover in the absence of external sources of acidity (Hauhs, 1988). Depending upon the nature of the soil and parent material this rate may lie anywhere between 5-120 $meqm^{-2}yr^{-1}$ (Jacks [in press]; Bain et al [in press]) with the values for individual chemical determinands varying considerably. The response of a catchment to reductions in acidic deposition will also depend upon the sulphate absorption and desorption properties of the soil and the size of the pool of accumulated sulphate. For example, Wright et al. (1990) reported that in the absence of acidic inputs the Risdalsheia catchment, southernmost Norway continued to 'bleed' sulphate at concentrations of 80-100

Variable	Confidence (%)	R^2 (%)	Equation
BEACON			
+ Base saturation	99.9	99.9	0.413 - 1.576E-4T
CATCHMENT LI1			
+ H-ion exported (kg)	99.9	60.2	0.841T - 1624
+ Mean H-ion concentration (µg/l)	99.9	89.4	0.289T - 558.7
+ Base saturation	99.9	91.0	2.857 - 0.001T
+ LCD frequency	99.9	54.6	1.464T - 2896
CATCHMENT LI6			
- H-ion exported (kg)	95.0	10.2	18.616 - 0.008T
- Mean H-ion concentration (µg/l)	99.9	26.3	5.061 - 0.002T
- Base saturation	99.9	99.9	0.002T - 4.418
CATCHMENT CI6			
+ H-ion exported (kg)	99.9	64.3	0.09T - 177.84
+ Mean H-ion concentration (µg/l)	99.9	78.4	0.144T - 284.3
+ Base saturation	99.9	99.8	0.001T - 1.752

TABLE 9.1a Listing of statistically significant trends in annual hydrochemical variables obtained from the LWT1908 scenario 1988-2055.

Variable	Confidence (%)	R^2 (%)	Equation
BEACON			
- H-ion exported (kg)	95.0	7.0	92.6 - 0.043T
- LCD frequency	95.0	7.9	583 - 0.264T
* Base saturation	99.9	99.6	4.775 - 0.005T + 1.11E-6T^2
CATCHMENT LI1			
+ H-ion exported (kg)	99.9	41.9	0.576T - 1073
+ Mean H-ion concentration (µg/l)	99.9	88.3	0.178T - 334.7
* Base saturation	99.9	99.9	44.414 - 0.043T + 1.044-5T^2
CATCHMENT LI6			
- H-ion exported (kg)	99.9	13.7	24.6 - 0.11T
- Mean H-ion concentration (µg/l)	99.9	30.4	5.13 - 0.002T
- Base saturation	99.9	99.7	0.003T - 4.905
CATCHMENT CI6			
+ H-ion exported (kg)	99.9	20.6	0.05T - 94.9
+ Mean H-ion concentration (µg/l)	99.9	36.9	0.073T - 141.26
* Base saturation	99.9	99.9	32.620 - 0.032T + 7.693E-6T^2

TABLE 9.1b Listing of statistically significant trends in annual hydrochemical variables obtained from the BASE scenario 1988-2055.

[Symbols: + catchment acidification; - catchment recovery; * new equilibrium; T = year AD]

μeql^{-1} a year after the exclusion commenced. Such catchments may carry such a high load of previously deposited sulphate that they are not in equilibrium with the acid influx. For practical purposes these catchments may be irreversibly acidified (Warren, 1988). At the other extreme are the sensitive catchments with very thin soils that are in equilibrium with the incoming acidity, which carry a very small reserve of sulphate and which respond relatively rapidly - in terms of the water base cation levels - to any change in the deposition regime. These catchments are typical of large areas of southern Norway and are characterised by barren rock and soils <70 cm in depth (Wright et al., 1990). Localised hydrological processes such as the soil permeability, mean watershed gradient, elevation, biogeochemistry and drainage network density have also been shown to be important in determining the leaching rate of base cations and export of aluminium from hill-slope soil horizons (Wheater et al., in press; Lawrence et al., 1986, 1988). Results obtained from the TOPMODEL have further shown that during high flow periods, both the average stream acidity and the variability of the H-ion concentration are conditioned by the topographic shape of the catchment (Wolock et al., 1990). Thus catchments which generate more surface and near-surface runoff (as indicated by the ln(a/tanß) topographic index) tend to have higher H-ion concentrations.

From the results contained in Tables 8.4 and 9.1 it is clear that considerable differences occurred in the responses of the four catchments to the BASE and LWT1908 scenarios. However, the question arises as to the extent to which these differences were the product of the **susceptibility** of each catchment's hydrochemical pathways to climate change. In order to investigate this problem the composite index of acidification (section 7.4) was applied to each of the four catchments using the LWT1908 scenario results as the baseline. This exercise revealed the following order of sensitivity to climate change(s) (from highest to lowest): Beacon >CI6 >LI6 >LI1. On the basis of this limited sample of catchment types a spectrum of catchment characteristics has been proposed in Figure 9.1 to identify those watersheds that are potentially most sensitive to climate trends. This reveals that it is the catchment of intermediate soil acidity, moderate weathering rates and low catchment yield that is most susceptible to climate-induced water quality changes. Such conditions occur in the Midlands, South-east and South-west of the UK where the high evapotranspiration demands relative to precipitation ensure that the baseflow fraction of the total discharge is highly sensitive to even slight changes in the precipitation and temperature regimes. By contrast the highly acidic Upland regions of much of Wales, Northern England and Scotland may be less sensitive to these subtle changes due to the fact that the incident acid load in many instances already exceeds the buffering due to soil weathering rates. Furthermore the hydrological regimes of these areas of high annual precipitation have been shown to be less sensitive to the vagaries of climate change (Arnell and Reynard, 1989) whilst the basin runoff coefficient has been found to be the major determinant of sensitivity to change (Arnell, 1990).. This view is supported by the fact that of the four catchments

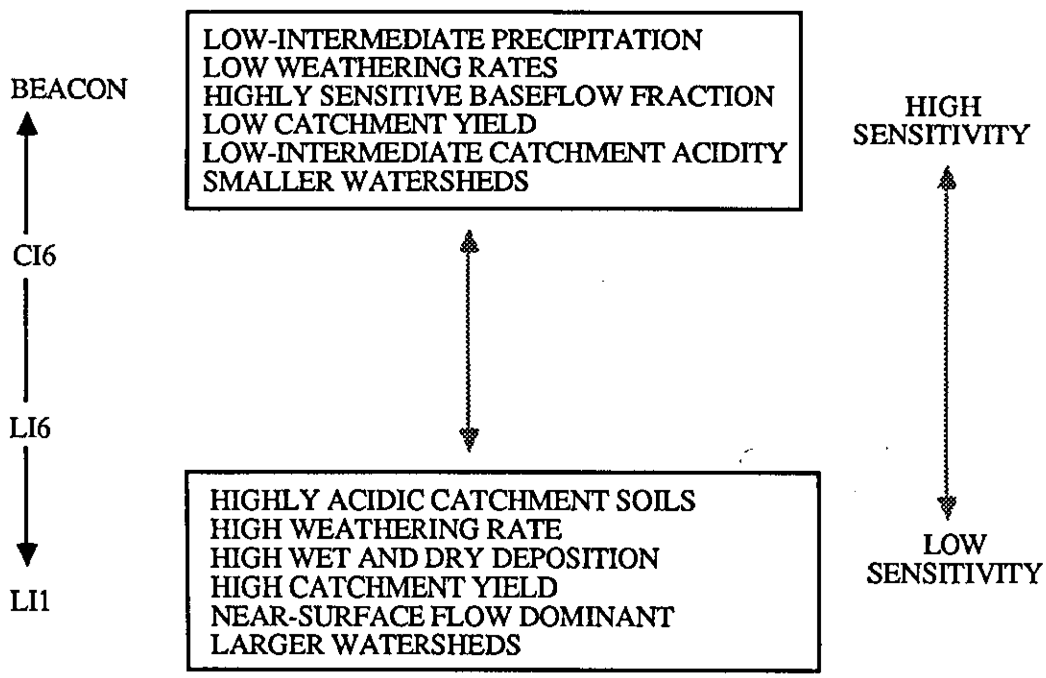


FIGURE 9.1 A spectrum of catchment characteristics favouring high and low sensitivity of the streamflow acidity to climate change.

considered the three upland sites showed on average a 5.1% reduction in the total baseflow fraction due to the BASE scenario compared with 16.9% for the Beacon. Catchments with a high weathering rate or a high base saturation such as LI6 would also be less sensitive to the effects of climate change due to their immense potential to compensate chemically for any shifts in the relative dominance of the hydrochemical pathways.

The implications of these results are that the upland regions of the UK would benefit least from favourable shifts in the climate regime and would be least affected by negative changes. It might be argued that since these areas constitute the dominant proportion of regions classified as susceptible to acidic deposition (UKAWRG, 1986, 1989), that from a UK perspective, climate change poses only a minor threat to the long-term recovery of acidified catchments. By contrast regions such as the East Midlands, Southern Weald and the Hampshire Basin may experience far greater hydrochemical perturbations but in terms of area represent a minority of catchments. On a continental scale, the situation may be reversed with much of Central Europe and North America being potentially vulnerable (Kenttamies amd Merilehto, 1989; Dam, 1988; Cabridenc, 1990).

A source of confirmation or refutation for these observations has been provided by a desk-top study conducted by Whitehead and Jenkins (1989) using the MAGIC model for the Dargall Lane site, Loch Dee, South West Scotland. In this experiment the catchment was subjected to three competing climate and pollution scenarios over a 25 year period from 1990. A scenario of constant climate and deposition showed a continued decline in the stream pH as did the results for a doubling of the deposition of acidic anions and for an increase in soil temperatures of 4°C. The latter two scenarios showed an increased rate of surface water acidification relative to that obtained from a constant climate. The acidifying effect of the temperature rise was attributed to the release of significant quantities of nitrate which acted as a mobile anion, acidifying the stream water. This result in particular conflicted with the predictions of the SCAM model for a similar temperature rise because of two reasons. Firstly, the nitrification process was not included in the SCAM model and secondly, the MAGIC model did not take into account the critical hydrologic changes that would have undoubtedly have arisen from the modified temperature/ evapotranspiration regimes. Rather, the increased mean temperatures were interpreted by the MAGIC model as a mechanism for concentrating the anthropogenic inputs in the soil system through evapotranspiration; whereas, to the SCAM model these losses would have heralded a switch from runoff dominated by flow through the upper acidic and aluminium-rich soil horizons to the base-rich flow of groundwater pathways. Whilst the simulation results obtained from the MAGIC and SCAM models undoubtedly differ for the reasons cited above, they both confirm the significance of climate change to the long-term hydrochemistry of acidic catchments. Since both models are only a partial representation of complex reality neither can be expected to fully account for all processes that may respond to or interact with climate change.

What then would be the general outcome of the BASE scenario (as predicted by the SCAM model) for the selected acidic catchments? Due to their relative insensitivity, catchments LI1 and CI6 do not demonstrate any significant reversal of the surface water acidity for the period 1988-2055 despite major deposition reductions. In effect, the climatic characteristics of the BASE scenario and the consequent hydrological response were sufficient to offset any advantages that may have been anticipated for the 40% deposition reduction. However, the rate of soil acidification was shown to be reduced with the possibility of a new equilibrium base status being achieved after 2060AD. The enhanced winter precipitation ensured that LI1 and CI6 experienced increases in the frequency of acidic episodes. The unacidic moorland catchment LI6 showed the opposite effect due to a major, local supply of basic cations coupled with declining levels of H-ion input to the catchment.

By comparison to LI1, LI6 and CI6 the Beacon catchment would benefit far more from the positive aspects of the BASE scenario (ie deposition reductions and temperature/ evapotranspiration increases). The combined effect of the climate and deposition changes of the BASE scenario was an overall long-term decline in the incidence of acidic episodes despite a net winter increase of these events. However, as the time-series plots of Figure 8.16a indicated, this decline would follow an initial increase in the mean surface water acidity for the simulation period relative to the LWT1908 standard.

These broad trends in 'catchment acidity' are represented in a simplified format in Figure 9.2 and are used as the basis for discussing the potential (indirect) consequences of climate on the aquatic ecosystems of acidic catchments. Of particular concern to the following discussion will be the response of the systems to the combined effect of higher/lower mean streamflow acidities (plus aluminium concentrations) coupled with an elevated/reduced frequency of winter Lethal Concentration Doses (pH<4.5).

9.3 THE IMPLICATIONS OF THE BASE SCENARIO FOR THE AQUATIC ECOSYSTEMS OF ACIDIC CATCHMENTS

"Because biological resources are amongst the most severely affected by acidification, there is a clear need to incorporate biological impacts into studies which model acidification" (Omerod and Tyler, 1989, p178).

For the purpose of discussing the impact of climate change on acidic catchments it is convenient to evaluate these biological affects by trophic level, from primary production, through macro-invertebrates to fishery status. Whilst it is clear that the direct effects of, for example, a temperature rise of 2-4°C would have marked consequences for phytoplankton, zooplankton, macro-invertebrates and fish (Beran, [1989]; DOE, [1988]; NERC, [1989])

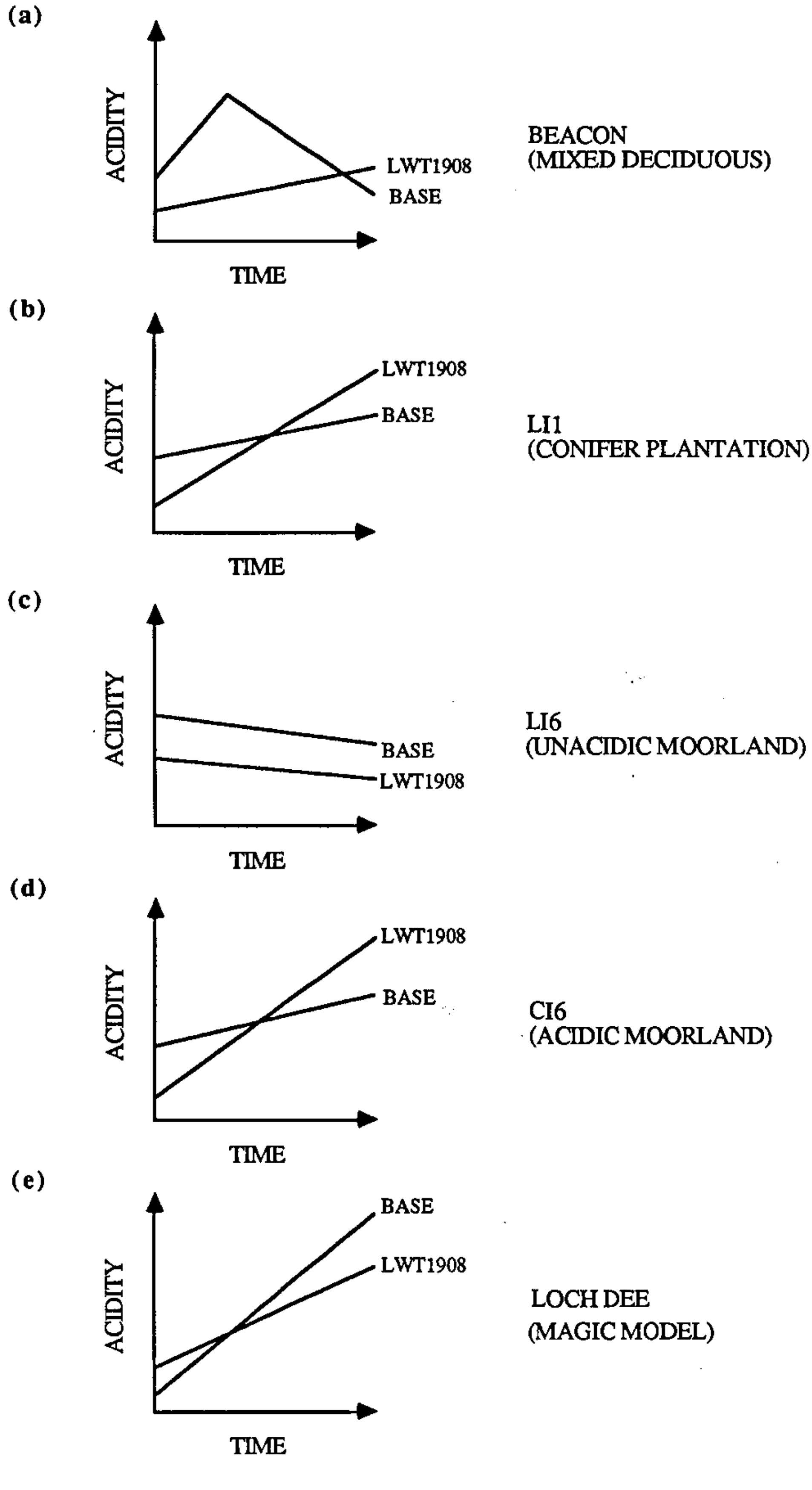


FIGURE 9.2 A simplified representation of 'catchment acidity' for five basins under the BASE and LWT1908 climate scenarios (1988-2050).

the following discussion will focus only upon the indirect impacts arising from changes to the catchment hydrochemistry. However, it is recognised that there is considerable scope for developing biological models which incorporate dynamic environmental controls (such as habitat availability or the thermal-oxygen niche for fish) in conjunction with predicted stream and lake water quality. The availability of limiting nutrients such as nitrogen, phosphorous and carbon would also be a function of the imposed temperature and hydrological regimes, and would no doubt greatly influence the long-term productivity of many aquatic ecosystems.

Preliminary investigations of the primary productivity of streams in the Llyn Brianne region have shown significant spatial differences in the percentage composition of epilithic algae and of mean Chlorophyll 'a' concentrations (WWA, 1987). The afforested catchment LI1 was dominated by *Cyanophyceae* (blue-green); the unacidic moorland LI6 by *Bacillariophyceae* (diatoms) and the acidic moorland CI6 by *Chlorophyceae* (filamentous-green). In acidic lakes, zooplankton diversity is usually reduced and may become largely restricted to the genera *Bosmina* or *Diaptomus* (Hellawell, 1989). Reductions in planktonic biomass combined with an increase in water transparency often permits algal and submerged macrophyte growth to occur at greater depths in acidic lakes.

Strong differences in the bacterial ecology were also apparent between the Llyn Brianne catchments. The acidic streams LI1 and CI6 had a significantly higher number of bacteria than the circumneutral streams (LI6). The volume and activity of the bacterial cells of LI6 favour invertebrates such as ephemeropteran nymphs which graze the epilithon and which dominate the fauna of this stream (WWA, 1987). Due to the selective elimination of certain kinds of bacteria and fungi, acidification commonly results in the depression of the normal decomposition of organic matter which in turn can favour an increase in the algal biomass of lakes (Hellawell, 1989). Furthermore, mosses and fungus mats may develop which modify the exchange of nutrients between sediments and lake water whilst acting as a reservoir for mobile aluminium (Mason and Seip, 1990). The affects of enhanced acidity may therefore have significant consequences for the entire food-chain by reducing the overall productivity and modifying the community structure and species diversity of the lower trophic levels.

Acidification of surface waters affects invertebrates and mollusc fauna through both food-chain and/or physiological effects. For example, grazing herbivores and filter feeders tend to be scarce in acidic streams whereas shredders of coarse detritus such as leaf litter, tend to dominate the fauna as an indirect consequence of the reduced microbial activity (UKAWRG, 1989). Physiologically an invertebrate may be harmed by direct acidity effects (which cause a net loss of sodium ions from the animal) or by the increased toxicity of certain metals (Herrmann, [in press]). For example, experimental toxicity tests performed in the Nant Mynydd Trawsnant stream, mid Wales using sulphuric acid and aluminium sulphate resulted in a 25% mortality rate in *Ecdyonurus venosus*, *Baetis rhodani* and *Gammarus pulex* when the pH fell from 7.0 to 4.28 and the aluminium concentration rose to 0.052-0.347 $gAlm^{-3}$ (Omerod et al., 1987). For the same experiment *Chironomus riparius*, *Hydropsyche angustipennis* and *Dinocras cephalotes* suffered no mortality, whilst the drift of *Baetis rhodani* increased by a factor of 8.4 during the acid episode. The depth distribution of invertebrates in the substratum were found to differ between the stream zones following the treatment, with more individuals present at the surface of the unacidified reference zone than for the acidified sections. Significant differences in the drift density (but not the relative abundance of single taxa) have also been shown for invertebrates in the Fyllean stream-lake system of Halland County, south-west Sweden (Kullberg and Petersen, 1987). Further effects observed for invertebrates include the bioaccumulation and transfer of metals such as cadmium to terrestrial food chains via stone-, caddis- and may-flies to riverine birds (Herrmann, [in press]).

Modelling studies conducted with the procedures TWINSPAN and DECORANA showed that the invertebrate faunas of selected Welsh streams were highly correlated with water quality and are most strongly discriminated by pH, total hardness, aluminium, stream gradient and flow (Wade et al., 1989; WWA, 1987). Invertebrate densities were generally lower in the acidic moorland (CI6) streams than in the circumneutral (LI6) and forest streams (LI1). The circumneutral streams were also found to have the greatest number of may-fly nymphs and caddis larvae, whilst acidic streams were dominated by stone-flies (WWA, 1987). Using aluminium and streamflow acidity data provided by the MAGIC model in conjunction with Multiple Discriminant Analaysis of current ecological data, it has been possible to reconstruct the invertebrate ecology of two Welsh streams for 1844 (Omerod et al., 1988). The results demonstrated that the invertebrate assemblages of the nineteenth century differed from those that now exist in circumneutral moorland streams. The most impoverished invertebrate assemblages occurred in the simulated forest site which did not show any sign of recovery despite reduced deposition.

Observations from field studies and well-designed laboratory experiments have confirmed that the concentrations of calcium and monomeric inorganic aluminium together with pH are the most important chemical factors that determine the fishery status of lakes and streams (Mason [1985]; Mason and Seip [1990]; Harrimann et al. [in press]; Morris and Reader [in press]; Potts [in press]). Other metals which have been shown to be toxic to fish at low pH (<4.5) include cadmium, copper, lead, zinc, and to a lesser extent iron, manganese and nickel (Everall et al. [1989]; Reader et al. [1989]). The principal mechanisms of toxicity appear to be the failure of ionoregulation leading to large losses of ions such as sodium, potassium and calcium during the rising limb of acidic pulses, leading to respiratory difficulties. Long term exposure to acidic waters and trace metals also affects the growth, development and calcium metabolism of yolk-sac fry (Reader et al., 1989). Experiments in continous-flow chambers with juvenile trout - in which the chemistry, duration and frequency of acidic episodes may be closely controlled - have provided a number of quantitative results concerning fish mortality (Morris and Reader, [in press]):

i) If yoke is present mortality is minimal even at pH 4.0.
ii) Juvenile mortalities are proportional to the length of the plateau stage of the episode.
iii) Most mortality occurs on the falling limb of the episode.
iv) Mortality declines as the interval between successive acidic episodes is increased.
v) Exposure to multiple episodes decreases the equivalent mortality rate that would have occurred from the sum of individual episodes.

Thus, the survival and recovery of fish is dependant upon the species, size and maturity of individuals, as well as the antecedent conditions and precise characteristics of each acidic episode. In general, salmonid populations fail to survive if the pH remains below 5.2, the concentration of inorganic aluminium exceeds 60 μeq/l and the calcium concentrations are less than 50 μeq/l. Large kills of juveniles (1-2 year) tend to occur when episodes of pH<4.5, Ca<40 μeq/l and $Ca/Al_i<2$ last for more than 48 hours (Mason and Seip, 1990). Preference and avoidance studies conducted using treated water from the Alt a Mharcaidh site in Scotland have shown the importance of considering the water quality of interstatial flow and the composition of the substrate (Harrimann et al, [in press]). For example, trout density was found to approach zero when the pH of this water was less than 5.5 for 30% of the time. All of these studies have therefore shown the need for chemical models which function at a high temporal and spatial resolution if the response of aquatic fauna is to be accurately simulated.

Although the presence or absence of individual fish species may indicate the critical water chemistry limits to fish survival and mortality, the age structure dynamics of a population provides an informative means of predicting its future evolution given certain environmental conditions. Data from a selection of limed and unmanaged lakes in Norway indicates two characteristic responses to changing the physical and chemical composition of the water (Bravington et al., [in press]). The first, senescence occurs when partial or complete recruitment failures lead to the progressive aging of the population. The second, juvenilization, reflects increased post-spawning mortality and leads to a large proportion of immature fish with marked inter-year variability. Matrix models indicate that the median times to extinction of senescent populations of trout are less than 10 years, and for juvenilized populations, 20-40 years given similar water chemistry.

As was shown earlier, the MAGIC model has enabled the reconstruction of historical changes to the ecology of acidic catchments as well as the prediction of future impacts. This was accomplished by predicting stream biology based upon empirically derived relationships with present day water chemistry (Omerod et al., 1988). Using simple linear and multiple variate analyses it has been possible to determine the densities and survival times of brown trout from simulated aluminium concentrations, total hardness and stream size. The results indicate that trout survival times and densities have both declined markedly between 1844 and 1984 in the studied Welsh streams. The most severe decline occurred under the simulated forest, where high aluminium concentrations resulted in the virtual elimination of trout. Only when the sulphate deposition was reduced to 50% of the 1984 levels was further decline in the population prevented, although there was no significant recovery of the trout density under any of the scenarios considered. This decline in the trout population has direct implications for other animals in the food-chain. For example, it has been demonstrated that the restoration of the Dipper (*Cinclus cinclus*) habitat in Wales would require not only European-wide action on air pollution, but also a land-use strategy which removes or ameliorates the negative impacts of forestry (Omerod and Tyler, 1989).

The importance of considering anthropogenic effects on whole ecosystems rather than on individual species has been confirmed by recent field evidence. During an 8-year experiment in which a small lake was artificially acidified from pH 6.8 to 5.0, Schindler et al. (1985) observed that key organisms in the food chain of lake trout (*Mysis relicta* and *Pimephales*) were eliminated at pH values as high as 5.8. This was regarded as an indication that irreversible stresses on aquatic ecosystems had occurred earlier in the acidification process than was previously thought possible. Similarly, Schindler et al. (1989) predicted the loss of 40-70% of acid sensitive taxa (such as leeches, molluscs, insects, cyprinids and salmonids) in the Adirondacks, mid-west US when the median pH of lakes declined by 70%. It was concluded that while most of the species eliminated are not of direct value to man, they nonetheless maintain the integrity of vital foodchains, biogeochemical cycles, and genetic stocks.

Such empirical and modelling studies provide the general backdrop to the potential ecological impacts arising specifically from the BASE scenario. Although the ecological effects of surface water acidification have been extensively reviewed elsewhere (eg Haines, 1981), Figure 9.3 provides an indication of the possible changes in each of the four simulated catchments. As a point of reference the estimated level of acidity for 24 species of North American and European fish that is not directly lethal lies broadly between pH 5 and pH 9 (Hellawell, 1989). However, the toxicities of metals such as aluminium and zinc vary enormously over such a range (Reader et al. [1989]; Everall et al. [1989]) whilst high acidity alone is seldom sufficient to bring about high mortality in the absence of trace metals.

Bearing these factors in mind, it is apparent from Figure 9.3 that the most significant change to occur as a result of either of the scenarios is the predicted acidification of the moorland stream CI6. Although brown trout (*Salmo trutta*) were present in this stream during the two surveys conducted in October 1984 and 1985 (WWA, 1987) the density was already low (0.1 to 0.3 m^{-2}) as was the invertebrate abundance. This implies that the

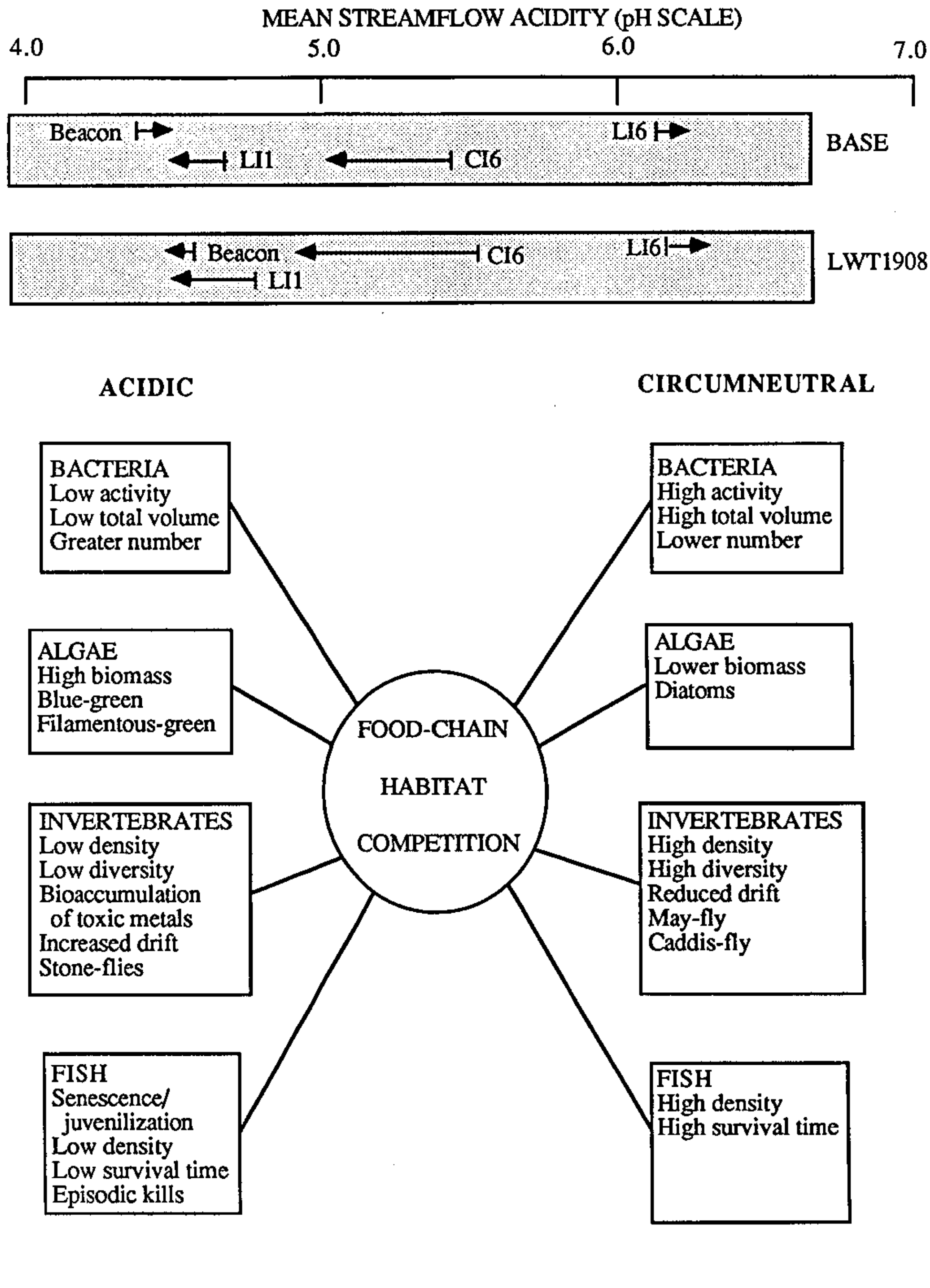


FIGURE 9.3 A summary of some of the ecological characteristics of acidic and circumneutral streams as mediated by local food-chain, habitat and competition factors. The arrows mark the magnitude and direction of the changes to stream pH predicted by SCAM for the two scenarios.

present condition of the stream's water quality may be approaching the limits of the brown trout. Whilst the simulated long-term mean aluminium concentration of around 100 μg/l (cf. Table 8.4) is not excessively high, maximum concentrations of 200+ μg/l have been recorded for winter snow melts (WWA, 1987). Furthermore, this site also experienced a 93% increase of daily flows with pH<4.5 under the BASE scenario. Given that the mean calcium concentration is of the order of 1.0 mg/l it is highly probable that fish kills would occur under these extreme storm runoff situations. For example, the LC_{50} for adult brown trout, alevins, egg development and hatching is between pH 4.5 and pH 4.6 (Mason, 1985). Although in the long run the BASE scenario yields lower streamflow acidities than LWT1908 (Figure 9.2) this site will probably experience an increased drift frequency and impoverishment of its invertebrate fauna over coming decades.

The water quality responses for the streams of LI6 and LI1 do not exhibit any major differences between the two scenarios in terms of their implications for the ecology. The water of LI6 remains circumneutral with mean aluminium concentrations of 60 μg/l but maximum values of 450+ μg/l during snowmelt. However, unlike CI6, the high mean calcium concentrations (2.75 mg/l) ensure that the stream pH never falls below pH 4.5 for either of the scenarios. The fauna are therefore unlikely to demonstrate any major changes in terms of diversity or composition for the foreseeable future. Conditions will remain favourable for brown trout and the current density levels of 1.2 nm^{-2} sustained.

LI1 by contrast exhibits continued surface water acidification under both scenarios although for the BASE scenario the trend is not as marked (Figure 9.2). As Table 8.4 indicates the simulated aluminium concentration is also very high with a mean value of 430 μg/l for both scenarios, with a maximum observed concentration of 800 μg/l attained during snowmelt episodes (WWA, 1987). Although there was a slight decline in the mean annual frequency of LCDs under the BASE scenario, the datum provided by LWT1908 of 64 days/year is already very high. This acidic environment is presently characterised by the complete absence of brown trout and by an impoverished invertebrate taxonomy (WWA, 1987). The predicted tendency towards further long-term acidification offers little hope of a reversal of this ecological response but the continued dominance of Plecopteran taxa over Ephemeropteran. Therefore, under the conditions of BASE and LWT1908, the ecology will reflect the continued acidification of the stream despite major deposition reductions under the former scenario. Even with sulphate deposition reduced to 50% of 1984 levels it is unlikely that the trout density or invertebrate assemblages would recover (Omerod et al., 1988).

The water quality of the Beacon catchment is unusual in that it is relatively sensitive to the prevailing climate and pollution scenario (Figure 9.1). As was shown in 9.2, the surface water declines from a higher starting value under the BASE scenario. Despite some evidence for a long-term reversal in the mean annual streamflow acidity and aluminium concentrations (Figure 8.16a and Figure 8.18a) fundamental obstacles to the recovery of the invertebrate and fish populations remain the very high mean- aluminium and hydrogen-ion concentrations plus the high incidence of spring flows with pH<4.5. However, a survey of the invertebrate community of the Beacon conducted between 1985 and 1986 (Greenwood et al., 1986) revealed considerable spatial variability in habitat conditions within the catchment. Of the three principle sites investigated, the Frying Pan Pond (site 7, Figure 5.2) had the greatest species diversity (22 species of Insecta) whilst Birches Pond (site 6, Figure 5.2) and the channel network (site 1, Figure 5.2) each had 18 species. The dominant fauna for each of the sites were respectively _Cloeon dipterum_, Chironomidae and Plecoptera. It was concluded from the water quality information in Table 9.2 that the macroinvertebrate fauna of each of the sites reflects an integrated response to both long-term changes in the prevailing environmental conditions and short-term responses to the ranges of concentrations of the key ions (pH, aluminium and calcium). Therefore, any transition in the water quality across taxonomic thresholds would be reflected by changes in the community structure at each site.

It has been suggested that the presence or absence of Ephemeroptera (and in particular _Cloeon dipterum_) provides a useful indicator of environmental stress (Wade et al., 1989). The optimum water quality of the species lies between pH 6.6-8.8 although they have been recorded in conditions of pH 4.35-6.70 in the case of the Beacon (site 7). Whilst the forecasted water quality of the SCAM model refers to the mean conditions at the catchment outlet, it is probable that the long-term improvement of conditions under the BASE scenario would eventually result in the expansion of the may-fly habitat into sites currently occupied by the stonefly. This response would be expected to occur first in site 6 and then (after 2055AD) within the stream itself. An overall improvement in the species diversity and reduced drift-intensity would also be anticipated as a result of the declining frequency of acidic episodes. A reduced likelihood of exposure to flows of very low pH and high Al would favour the resident amphibian species which may experience embryonic mortality, delayed hatching, reduced size at metamorphosis, behavioural and morphological abnormalities when the pH is less than 4.5 (UKAWRG, 1989). This may be good news for the Beacon's crested newt population!

However, it must be emphasised that many of these ecologically significant changes are unlikely to occur prior to 2055 due to the initial acidification phase attributed to the expected enhanced cyclonicity (cf. Figure 8.16a and 8.17a). Even by the year 2050, SCAM predicts that acidic episodes of pH<4.5 will occur on average 40 days/year. As the simulated frequency of the cyclonic weather type represents one of the most severe synoptic situations on record to date, it is probable that the BASE scenario projects one of the 'worst case' scenario in terms of the consequences for the Beacon's taxa.

		Mean	Min	Max
SITE 7 (Frying Pan Pond)	Conductivity ($\mu S\ cm^{-1}$)	149	106	190
	pH	5.05	4.35	6.70
	Total Aluminium ($mg\ l^{-1}$)	0.157	0	0.545
	Sodium ($mg\ l$-^{1})	8.84	2.39	26.88
	Calcium ($mg\ l^{-1}$)	5.43	3.33	8.00
SITE 6 (Birches Pond)	Conductivity ($\mu S\ cm^{-1}$)	307	200	447
	pH	4.72	4.05	6.34
	Total Aluminium ($mg\ l^{-1}$)	0.72	0	2.28
	Sodium ($mg\ l^{-1}$)	25.3	16.52	60.0
	Calcium ($mg\ l^{-1}$)	9.74	2.38	25.8
SITE 2 (Stream network)	Conductivity ($\mu S\ cm^{-1}$)	296	178	447
	pH	4.70	3.90	7.87
	Total Aluminium ($mg\ l^{-1}$)	0.856	0.004	3.69
	Sodium ($mg\ l^{-1}$)	21.83	10.67	33.8
	Calcium ($mg\ l^{-1}$)	8.56	4.83	16.88

TABLE 9.2 A synopsis of the prevailing freshwater chemistry for three sites within the Beacon catchment for the year March 1985 to February 1986 (based on Greenwood et al., 1986)

Figure 9.3 therefore presents a selective summary of some of the extremes in the ecologies of acidic and circumneutral streams, and of the relative shifts in the position of each of the catchments within this spectrum arising from the BASE and LWT1908 scenarios. It is accepted that the depicted changes in the faunal composition and density would arise from both the direct physiological impacts described above and indirectly from altered food resources or predator-prey relationships. Further, it must be assumed that no land-use changes have occurred during the simulation period since numerous field studies have identified this as a major determinand of the fishery status of upland streams and lakes (eg. WWA, 1987). There is inevitably immense difficulty in distinguishing between the relative significance of land-use, deposition rates and climate changes to the community structure and diversity. However, one factor remains common to all of these components, namely the potential to modify fundamental aspects of the surface water quality. The simulated hydrochemistry provided by models such as MAGIC and SCAM therefore facilitates an assessment of the dynamic nature of these broad thresholds to survival. The presence of multiple colinearity between many of the variables involved remains both undisputed and unavoidable.

9.4 SUMMARY

The multiple scenario simulations conducted in previous chapters have indicated that the prospects for reversibility of acidification given the assumed climate changes of the BASE scenario, are catchment specific. This spatial variability arises from the manner in which different hydrological, geochemical, land-use management practises and vegetation types translate climate change into the terrestrial, water quality response. Acidic catchments which are hydrologically most sensitive to changing inputs (in terms of the total water balance and the ratio of near-surface to deep water) are also the most responsive in terms of the concomitant water quality. Such basins would stand to gain the most from the favourable attributes of the BASE scenario (such as enhanced evapotranspiration and lower summer precipitation amounts) and by its antithesis, greater negative effects due to greater precipitation acidities, enhanced cyclonicity and higher winter precipitation. The Beacon catchment provides one such example of a highly sensitive watershed type.

The implications for the corresponding aquatic ecosystems are a further step removed from the climate, depending upon the extent of the potential water quality changes in relation to the individual (or corporate) preference thresholds of the taxa. The indirect effects of climate on the food-chain, competition and habitat availability may be of equal importance to the viability of communities in acidic environments. Fish and invertebrate populations that currently occupy marginal sites (as in the case of CI6) may be particularly vulnerable to water quality changes arising from climate shifts. Even more so if contemporary extremes in the range of acidities experienced are exacerbated at critical stages of an animal's development. There appears to be considerable scope for the use of sensitive indicator species such as the mayfly for detecting subtle changes in community structure due to changing environmental conditions. However, outside of the controlled conditions of model simulations there would be considerable difficulty involved in linking climate cause- and ecological-effect, particularly over such long periods of time.

CHAPTER 10

CONCLUSIONS

"If predictions of future climatic change are substantiated, there will be a need to re-assess the response of acid and acid-sensitive waters......under different climatic regimes" (UKAWRG, 1989, p 48).

Accelerated surface water acidification or recovery are just two possibilities of the potential consequences of climate change for upland catchments. Other sensitive aspects of water quality that have been identified for the uplands in recent years include: increased nitrate concentrations; increased erosion and sedimentation; increased phosphate concentrations and algal blooms; increased water colour; and increased bacterial contamination (Whitehead and Jenkins, 1989; NERC, 1989; DOE, 1988). Since the uplands have been traditionally viewed as a major source of potable water for the UK's urban centres all these issues may have serious consequences for water supply if exacerbated by unfavourable shifts in the climate. In the past, however, there has been a tendency to focus upon the quantitative impacts of climate on water resources rather than qualitative effects. For example, a recent survey of published work on the theme of Climate and Water (Lemmela et al., 1990) revealed that out of 200 papers less than 5% dealt with quality issues as opposed to 60% with aspects of the water balance. Nonetheless recent experiences of extreme climate have highlighted the sensitivity of water quality systems and demonstrated the need for a comprehensive framework within which to assess the relative significance of climate, land-use change and hydrological processes to surface water chemistry (Webster et al., 1990; NERC, 1989; DOE, 1988).

Regardless of whether or not it is practised as a science or a technology, hydrology is uniquely placed for the investigation of these interactive processes. The movement of water from the atmosphere to the vegetation surface, to the soil and substrata, the stream network and thence returning to the atmosphere provides a unifying theme to the whole debate of climate and water quality. Furthermore, the historical development of the hydrological discipline reveals a long-standing tradition of problem-solving juxtaposed with pure and strategic research. Hydrologists have therefore cultivated a range of tools necessary for the investigation of the multiplicity of climate change impacts on aquatic systems.

Since the 1950s and 1960s increasing trust and reliance has been placed in the prognostic and explanatory powers of mathematical models. These tools have provided a complimentary yet alternative option to lengthy and costly field monitoring whilst offering a heuristic capability that is particularly appealing to catchment managers. As well as enabling the prediction of hydrological events, models have also contributed to the advance of understanding, rationalised data collection and above all yielded a coherent means of expressing a complex and ever-changing reality. Given that future boundary conditions are unlikely to remain constant (Georgakakos et al., 1989) mathematical models facilitate the manipulation of 'conceptualised catchments' over an infinite number of possible climate and pollution scenarios without incurring the financial costs or protracted field work of actual field experiments (eg RAINS [Wright et al., 1990]). This is not to say that models are without there critics; considerable debate still surrounds the mathematical articulation of basin-scale processes, the optimum use of distributed data sets and the parameterisation of key soil processes (Beven, 1988). Furthermore, it is important to recognise that the detail and reliability of model forecasts are inseparable from the gathering of detailed and reliable data-sets. Indeed, some model types - such as the physically-based distributed models - have even created demands for new types of data that may only be collected by costly field sampling or remote sensing techniques. Elsewhere it has been necessary to resort to the use of proxy data sets as a means of verifying the long-term simulations of hydrochemical models (Jenkins et al., 1990). At all levels of complexity, models are therefore unable to escape from a reliance upon data-sets for their design, calibration and most importantly, verification.

Data considerations were a major factor influencing the ultimate design of the Shifting Climate and Catchment Acidification Model. The minimal input data (of daily temperature, precipitation amount and acidity) required to drive the model facilitated the construction of a highly robust and versatile system in exchange for a moderate level of conceptual realism. These criteria were used to justify the use of the analogue method for the derivation of the climatic parameters, and the lumped conceptual approach for the catchment hydrological modelling. The daily time-step was established as an appropriate temporal resolution at which to compute catchment inputs, storage changes, hydrochemical outputs and hence the qualitative ecological impact(s). Not only did this scale enable the description of individual flood/ acidic episodes but also the simulation of long-term (10-100 year) shifts in mean water quality parameters. Balanced against the ease with which the model may be calibrated and transferred to other catchments, the main shortcomings of its design were thought to be as follows:

[1] The representation of vegetation by the present model version is inadequate.

Two main objections are thought to exist. The first refers to the impact on the water balance of the direct and indirect effects of carbon dioxide on canopy transpiration. In its current form the model sums daily transpiration and evaporation as determined by Linacre's (1977) equation. Differences between catchments of the dominant vegetation or land-use must be accommodated by a simple weighting factor set against this daily total. However, to improve the sensitivity of the model to canopy type and to meteorological controls of the evaporation rate would require a significant increase in the data input. For example, the forest evapotranspiration model of Lankreyer and Vean (1989) cited in 3.5 requires the following data to compute soil moisture status on a daily basis: precipitation, temperature, solar radiation, air humidity, and wind speed. If indeed the transpiration process may be regarded as conservative (Roberts, 1983; Andersson, 1989) there would be little advantage gained from applying such complex models to long-term simulations of catchment water-balances.

The second area acknowledges that for simulation periods of 10-100 years it is unreasonable to expect the land-use characteristics of a watershed to remain static. Changes in the spatial and temporal patterns of vegetation will have consequences for the canopy scavenging efficiency of dry/occult deposition, the uptake of cations by trees during the early stages of growth, and the ratio of near-surface runoff to baseflow, as well as the catchment yield. Some of these differences arising from land-use and management practises were reflected in the contrasting behaviour of the four catchments to the same BASE scenario. Nonetheless, it would not require too many modifications of the model to incorporate, for example, a dry deposition factor to simulate the transition of a catchment from moorland to forest. In general, however, the role of vegetation in regulating the water and chemical balance of catchments has been understated by the SCAM model.

[2] The simulation mechanisms representing the long-term variations in soil and surface water acidity require further detailed field validation.

Whilst it is possible to demonstrate that the soil acidity profile is catchment specific (eg Figs 3.8 and 6.10) there is a clear need to relate this property more generally to key soil parameters such as the base status or cation exchange capacity. Although this link was successfully established through parameterisation, the precise value of the k-factor (in Table 3.4a) will largely determine the long-term response of the catchment to acidic inputs.

Furthermore, at present the streamflow pH vs soil moisture deficit relationship is assumed to be linear, and is therefore only likely to occur in relatively homogeneous soils. This may account for the varying levels of performance of the hydrochemical model in each of the four studied catchments. In complex soil systems the assumption of linearity would be a gross oversimplification of the profile characteristics and would justify the use of a composite relationship determined by the major horizons of the soil column. However, the fundamental assumption of a 'wave-front' of acidification progressing down the soil horizons is supported by empirical evidence (Hallbacken and Tamm, 1986; Tamm and Hallbacken, 1988).

Whilst the present version of SCAM is only capable of simulating daily stream H- and Al-concentrations, the ecological interpretations would benefit from information concerning other major cations and anions such as NO_3, SO_4 and Mg+Ca. This could only be achieved by increasing the data input and complexity of the model. However, it is reasonable to assume that some of this data could be generated synthetically - perhaps the sulphate concentrations in precipitation - using probability distributions that are specific to individual LWTs.

[3] The brevity of the model calibration and validation periods dictate that the long-term simulations should be viewed with caution.

This fundamental obstacle to model usage and interpretation is common to all such studies and inevitably places a strong onus on the ability of the model to accurately describe the present behaviour of the catchment. In this respect the overall performance of the SCAM model was considered to be satisfactory given the standard set by counterparts such as the MAGIC or Birkenes algorithms. SCAM consistently exceeded the levels set for daily discharges by the Zero Order Forecasts; reproduced the timing but not always the magnitude of major acidic events and discharges; and simulated the observed long-term volume-weighted averages for the H- and Al-ion concentrations to within the limits of instrumental uncertainty. However, the fact remains that the long-term reliability of the model (over periods >10 years) is untested and could only be evaluated by the use of a proxy data set such as water quality inferred from diatom assemblages (Batterbee et al., 1988a). Despite the limited data requirements of the SCAM model, the absence of a lengthy, continuous and accurate data-base placed a high degree of reliance upon published data for setting the likely ranges and initial values of catchment parameters such as the soil weathering rate.

The most severe test of the model assumptions was the transfer of the model from the site of its conception (Beacon) to the untested domain of the three Llyn Brianne catchments (LI1, LI6 and CI6). The results of this exercise assert that the model tends to underpredict extreme episodes but is good at reproducing the mean hydrochemical situation at each site. This suggests that the long-term simulations obtained for the BASE scenario are conservative. It may also be argued that the sensitivity analysis of the model was just as informative (if not more so) than the predicted time-series. For example, under these controlled conditions it was revealed that in the long-term factors which affect the water balance such as the mean annual precipitation are more significant to the stream acidities than changes in precipitation acidity arising from emission reductions. Furthermore, the spatial analysis facilitated by the use of four catchments has provided further insights into the relative significance of catchment characteristics versus climate, to surface water acidity.

Having outlined some of the most significant sources of uncertainty associated with the model design and calibration, it is an appropriate point at which to present the key contributions of the study. Three areas in which it is felt that positive advances have been made are set out below:

[1] The field monitoring and modelling experiments have revealed the extent to which meteorological and synoptic conditions affect the deposition of acidic ions to, and their subsequent export from catchments at various temporal scales.

Two factors relating to synoptic climatology and meteorology are identified here: the regional redistribution of acidic loads, and the regulation/ activation of contrasting hydrological pathways. In either case, the Lamb's (1972) register of daily Weather Types (LWTs) and classification system were shown to be invaluable to the synthesis and generation of a coherent data set for long-term simulation of water hydrochemistry. Thus on a diurnal scale it was possible to relate much of the variability in precipitation acidity to basic meteorological variables such as rainfall amount, mean wind speed and direction of surface air-flows. By means of ANOVA testing it was also demonstrated that the eight chosen classes of LWTs could account for 25% of this variability. Only three LWT classes (C, N and A-types) could be statistically distinguished from the W-type. This suggests that the classification procedure still requires significant refinement. Nonetheless, on a monthly basis the frequency of individual LWTs (such as the westerly, cyclonic and anticyclonic types) figured prominently in the determination of the H-ion concentrations and loads.

Simulations using only the climate module of SCAM (Wilby, 1989) have revealed that even in the absence of emission reductions, super-annual trends in the frequency of the three key LWTs (W-, C- and A-types) have the potential to significantly alter the deposited acidity in both space and time. For example, the results obtained from the scenarios LWT1869 and LWT1969 indicate that variations in the predominance of these LWTs alone are sufficient to incur up to ±12% in the total deposited acidity between extreme years. If only wet-deposited acidity is taken into consideration, this figure increases to ±20%. Major differences were also found between individual years for the relative contributions of wet- and dry-deposited acidity: the highest percentage of dry-deposition occuring under LWT1869, and the greatest wet-only deposition under LWT1872. These were respectively the years of lowest and highest cyclonic activity. (By way of a comparison, Alcamo and Posch (1985) used the RAINS model to demonstrate that interannual meteorological variability could potentially cause a ±13% mean relative deviation in deposited sulphur).

As well as possessing characteristic precipitation acidity probability distributions, each LWT exhibits distinct probabilities of precipitation occurrence, magnitude of events and temperature anomalies. Because hydrological processes are central to the manifestation of surface water acidity, subtle shifts in the frequency of major LWTs will therefore have significance for the relative dominance of contrasting hydrochemical pathways. This was clearly evident from the sensitivity studies conducted on the Beacon model formulation using the 14 selected synoptic scenarios. For example, the highly cyclonic LWT1872 scenario resulted in the highest frequency of wet-days, the greatest catchment yield, number of very high discharges and the least number of days with zero flow. Since these conditions favour the predominance of near-surface flow it follows that the LWT1872 scenario also produced the most acidic streamflow, highest mean total Al-concentrations, and the greatest frequency of days with flows of pH<4.5. The increase to the frequency of LCDs of +90% (relative to LWT1908) was particularly noteworthy. By contrast the highly anticyclonic and westerly scenarios (LWT1971, LWT1869 and LWT1938) produced below average acidity by favouring an elevated contribution of the baseflow component. In the case of LWT1869, the changes to the LCD index, mean H- and Al-ion concentrations were respectively: -27%, -13% and -4% relative to LWT1908. Meteorological variability may therefore significantly affect both the atmospheric (deposition) and terrestrial (buffering) of acidic compounds. The former impact will be even more marked in remote areas where acidic deposition is highly sensitive to the frequency of winds from critical sectors (Fowler and Cape, 1984).

[2] The sensitivities of acidic watersheds to given climate change(s) are spatially variable, depending upon the complex interaction of lithology, hydrology and land-use.

This conclusion is based upon the results obtained from the application of a single BASE scenario to all four study catchments. In general the model predicted that the scenario would yield a reduced rate of surface water acidification relative to the LWT1908 datum. Whilst there were similarities in the seasonal behaviour of the catchments (such as a universal increase in winter/spring acidity and lower summer/autumn acidity) there were major differences in the magnitude of the mean-annual and transient behaviour that can only be attributed to spatial factors. For example, the Beacon was the only catchment to produce any evidence for the reversal of acidity before 2055 as a direct result of the BASE scenario. This contrasted with LI1 and CI6 which showed a quantitatively smaller effect but continued acidification despite linear reductions in the acid load of up to 40%. This led to the conclusion that the least sensitive sites will be large, upland, highly acidic watersheds currently receiving high annual precipitation and acidic loads. Conversely, the most sensitive sites are likely to have lower annual precipitation totals, smaller basin areas, and relatively low catchment yields due to the high importance of evapotranspiration losses to the annual water balance. The results also support the assertion that the surface water acidity of the four catchments is more sensitive to variations in spatial factors (eg. soil pH, topography and vegetation) than climate (eg temperature, precipitation amount, weather types) , and to climate than to precipitation acidities.

[3] A review of the literature in conjunction with the model results indicated that the concept and application of 'critical loads' should be based upon meaningful ecological parameters and within the context of probable land-use and/or climate change(s).

Throughout the discussion on the potential consequences for aquatic biota it was clear that the ecological communities of acidic upland areas are particularly sensitive to changes in the frequency, magnitude and duration of acidic episodes. The effect of such events occur at all trophic levels and may be experienced both directly (through the chemical toxicity of H-, Al- and trace metals) or indirectly (through food-chain effects, competition and recruitment)[Henriksen and Brakke, 1988; Keller et al, 1990; Schindler et al, 1985, 1989]. Therefore models of long-term acidification should generate information on the physiochemical properties of the water, and at a scale appropriate to the ecological response. If the recovery of damaged ecosystems (such as the return of a trout population to a formerly acidified lake or stream) is to constitute the rationale for emission reductions, there is a clear need to reassess the design criteria of future generations of acidification model. It will no longer be acceptable to simply reproduce mean-annual statistics of water quality. The pioneering work of Wade et al. (1989), Omerod et al. (1988) and Schindler et al (1989) has provided some indication of the potential benefits of linking empirically derived biological relationships to statistical and conceptual models of water chemistry. However, there still remains considerable scope for the development of ecological models that incorporate different measures of water quality such as the rate of change of acidity, the antecedent conditions in relation to the peak concentrations, and the duration and frequency of major episodes in relation to sensitive stages of the life-cycle of individual biota. These developments would presuppose the parallel existence of detailed biological and water quality data of the type presented in Greenwood et al. (1986).

Whilst it is accepted that the recovery of acidified waters may occur rapidly under favourable conditions there are also instances in which this process will be hysteretic, occurring over centuries rather than decades (eg Whitehead et al., 1988; Neal et al., 1986). This introduces the possibility that boundary conditions that might formerly have been considered stable for shorter periods of time are in fact far from constant. Land-use and climate change provide two such examples of dynamic boundary conditions. The SCAM model indicated that the ecosystems of catchments of intermediate acidity (pH 5.0-6.0) are potentially the most vulnerable to adverse changes in the climate. An example of this type of watershed was provided by the acidic moorland site CI6 in which the present brown trout population is already close to the limit of its range. Under these circumstances, where the major goal is the restoration or protection of a fishery, liming may be a suitable strategy (Omerod et al., 1990). By contrast it is unlikely that the highly acidic catchments of the Beacon and LI1 will experience major community changes as the direct result of climate-induced water quality changes. The community structure and diversity at each of these sites is impoverished to the extent that any minor shifts in the water quality will have little effect. However, as the Beacon survey (Greenwood et al., 1986) revealed, there may be localised sites (such as Frying Pan Pond) within these catchments in which the current Al- and H-ion concentrations are not as extreme or where greater buffering by calcium enables organisms to withstand more acidic conditions. Such sites offer considerable potential for linking the simulated hydrochemistry to the known thresholds to survival of sensitive macroinvertebrates like the mayfly *Cloeon dipterum*. It is at these points in the catchment that the first biological indication of adverse water quality changes would be anticipated. The future, sustained presence or absence of sensitive organisms at these marginal sites would, therefore, be a true 'acid test' for the success or failure of proposed 'critical loads'.

With reference to the stated aims at the outset of this work, the SCAM model has enabled the quantification of climate change impacts on selected aspects of the water quality of acidic catchments over timescales of <1day to >60 years. The results obtained from sensitivity analyses, transient and equilibrium forecasts have justified the inclusion of climate on the agenda when 'critical loads' are discussed. The study has also demonstrated the value of synoptic classification schemes as a source of synthetic data for driving robust hydrochemical models. Furthermore, the technique offers the possibility for the reconstruction and bridging of both water quality and flows at ungauged sites, and as a 'front-end' source of regional climate data for more complex chemical models such as MAGIC. In the past considerable emphasis has been placed upon the quantitative significance of climate change on water resources, but as competition increases for finite supplies it is inevitable that quality issues will assume greater importance. Whenever the boundary conditions are uncertain there will always be a need for robust models of intermediate complexity for predicting the properties of the real world. It is intended that the Shifting Climate and Catchment Acidification Model should be one such versatile tool, and that it will find potential applications amongst contemporary issues of environmental change and ecological response.

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APPENDIX 1

PROBABILITY MATRIX FOR 1869

VARIABLE INPUT PARAMETERS

No.days: 10000 Start date: 1 1 1988

maxc: 15.6 maxdc: 205 meanc: 9.808 trendc(pa): 0.00

seed1: 60 seed2: 180 seed3: 120 dddrate: 100.0

LWT PROBABILITY MATRIX

A	W	C	N	NW	S	SW	OT	MRAIN	PRAIN	TANOM
0.485	0.103	0.015	0.015	0.015	0.044	0.000	0.323	3.413	0.110	0.150
0.044	0.544	0.044	0.000	0.044	0.015	0.088	0.221	3.346	0.593	1.830
0.000	0.120	0.160	0.240	0.000	0.000	0.000	0.480	4.539	0.750	-0.540
0.105	0.000	0.000	0.421	0.000	0.000	0.000	0.474	3.511	0.692	-3.300
0.000	0.167	0.056	0.167	0.389	0.000	0.000	0.221	4.042	0.400	-0.100
0.000	0.000	0.000	0.000	0.000	0.167	0.167	0.666	4.100	0.556	2.640
0.000	0.286	0.000	0.000	0.000	0.143	0.143	0.428	3.103	0.500	2.920
0.200	0.100	0.107	0.020	0.047	0.000	0.000	0.526	3.819	0.456	-0.160
0.104	0.152	0.048	0.108	0.062	0.046	0.050	0.417	3.762	0.439	0.523

CATCHMENT PARAMETER SET

r(1):	547000.0000	r(2):	0.9800
r(3):	75.0000	r(4):	28.0000
r(5):	0.1250	r(6):	0.0170
r(7):	49.0000	r(8):	1.0850
r(9):	110.0000	r(10):	200000000.0
r(11):	100.0000	r(12):	6.3500
r(13):	3.7000	r(14):	100.0000
r(15):	20000000.0	r(16):	476.0000

SIMULATION OUTPUT STATISTICS

Total rain (mm): 18614.7 Total discharge (mm): 4902.8

Mean annual rain (mm): 679.9 Mean annual discharge (mm): 179.1

Mean daily temperature: 9.91 Number of westerly days: 1899

Number of cyclonic days: 679 Number of anticyclonic days: 1774

Number of wet-days: 4560 Discharge-rainfall(%): 26.34

Total H-ion input (kg): 978.494 Total H-ion output (kg): 72.3239

Mean rain pH is: 4.175 Mean discharge pH is: 4.569

Initial base saturation: 0.100000 Final base saturation: 0.096717

Total Al-ion output (kg): 3666.8 Al-ion concentration (mg/l): 1.37

The frequency of LCDs: 511 Ratio of H-ion out-in(%): 7.39

The frequency of Q90%: 715 Days with zero flow: 3277

APPENDIX 1

PROBABILITY MATRIX FOR 1872

VARIABLE INPUT PARAMETERS

No.days: 10000 Start date: 1 1 1988

maxc: 15.6 maxdc: 205 meanc: 9.808 trendc(pa): 0.00

seed1: 60 seed2: 180 seed3: 120 dddrate: 100.0

LWT PROBABILITY MATRIX

A	W	C	N	NW	S	SW	OT	MRAIN	PRAIN	TANOM
0.292	0.250	0.042	0.000	0.000	0.042	0.000	0.374	3.413	0.110	0.150
0.027	0.521	0.096	0.014	0.027	0.014	0.068	0.233	3.346	0.593	1.830
0.000	0.133	0.440	0.040	0.013	0.027	0.040	0.307	4.539	0.750	-0.540
0.238	0.048	0.095	0.333	0.095	0.000	0.000	0.191	3.511	0.692	-3.300
0.222	0.111	0.000	0.111	0.000	0.000	0.000	0.556	4.042	0.400	-0.100
0.000	0.000	0.217	0.000	0.000	0.348	0.043	0.392	4.100	0.556	2.640
0.000	0.167	0.167	0.000	0.000	0.222	0.222	0.222	3.103	0.500	2.920
0.066	0.132	0.190	0.074	0.033	0.058	0.033	0.414	3.819	0.456	-0.160
0.106	0.170	0.156	0.072	0.021	0.089	0.051	0.336	3.762	0.439	0.523

CATCHMENT PARAMETER SET

r(1):	547000.0000	r(2):	0.9800
r(3):	75.0000	r(4):	28.0000
r(5):	0.1250	r(6):	0.0170
r(7):	49.0000	r(8):	1.0850
r(9):	110.0000	r(10):	200000000.0
r(11):	100.0000	r(12):	6.3500
r(13):	3.7000	r(14):	100.0000
r(15):	20000000.0	r(16):	476.0000

SIMULATION OUTPUT STATISTICS

Total rain (mm): 22946.1

Total discharge (mm): 8366.2

Mean annual rain (mm): 838.1

Mean annual discharge (mm): 305.6

Mean daily temperature: 10.11

Number of westerly days: 2154

Number of cyclonic days: 2029

Number of anticyclonic days: 639

Number of wet-days: 5407

Discharge-rainfall(%): 36.46

Total H-ion input (kg): 1235.700

Total H-ion output (kg): 166.6183

Mean rain pH is: 4.105

Mean discharge pH is: 4.439

Initial base saturation: 0.100000

Final base saturation: 0.095228

Total Al-ion output (kg): 7162.7

Al-ion concentration (mg/l): 1.57

The frequency of LCDs: 1324

Ratio of H-ion out-in(%): 13.48

The frequency of Q90%: 1688

Days with zero flow: 1446

APPENDIX 1

PROBABILITY MATRIX FOR 1908/09

VARIABLE INPUT PARAMETERS

No.days: 10000 Start date: 1 1 1988

maxc: 15.6 maxdc: 205 meanc: 9.808 trendc(pa): 0.00

seed1: 60 seed2: 180 seed3: 120 dddrate: 100.0

LWT PROBABILITY MATRIX

A	W	C	N	NW	S	SW	OT	MRAIN	PRAIN	TANOM
0.534	0.060	0.015	0.008	0.023	0.045	0.008	0.307	3.413	0.110	0.150
0.022	0.511	0.080	0.029	0.036	0.029	0.022	0.271	3.346	0.593	1.830
0.056	0.111	0.444	0.067	0.033	0.000	0.022	0.267	4.539	0.750	-0.540
0.151	0.000	0.038	0.321	0.094	0.000	0.000	0.396	3.511	0.692	-3.300
0.150	0.300	0.050	0.200	0.100	0.000	0.000	0.200	4.042	0.400	-0.100
0.172	0.138	0.138	0.000	0.000	0.310	0.103	0.139	4.100	0.556	2.640
0.000	0.313	0.063	0.000	0.000	0.125	0.188	0.311	3.103	0.500	2.920
0.163	0.127	0.112	0.084	0.012	0.032	0.016	0.454	3.819	0.456	-0.160
0.156	0.195	0.118	0.089	0.037	0.068	0.045	0.293	3.762	0.439	0.523

CATCHMENT PARAMETER SET

r(1):	547000.0000	r(2):	0.9800
r(3):	75.0000	r(4):	28.0000
r(5):	0.1250	r(6):	0.0170
r(7):	49.0000	r(8):	1.0850
r(9):	110.0000	r(10):	200000000.0
r(11):	100.0000	r(12):	6.3500
r(13):	3.7000	r(14):	100.0000
r(15):	20000000.0	r(16):	476.0000

SIMULATION OUTPUT STATISTICS

Total rain (mm): 19725.8	Total discharge (mm): 5811.4
Mean annual rain (mm): 720.5	Mean annual discharge (mm): 212.3
Mean daily temperature: 9.92	Number of westerly days: 1869
Number of cyclonic days: 1217	Number of anticyclonic days: 1874
Number of wet-days: 4724	Discharge-rainfall(%): 29.46
Total H-ion input (kg): 1119.127	Total H-ion output (kg): 98.2718
Mean rain pH is: 4.114	Mean discharge pH is: 4.510
Initial base saturation: 0.100000	Final base saturation: 0.095668
Total Al-ion output (kg): 4560.7	Al-ion concentration (mg/l): 1.43
The frequency of LCDs: 698	Ratio of H-ion out-in(%): 8.78
The frequency of Q90%: 929	Days with zero flow: 2633

APPENDIX 1

PROBABILITY MATRIX FOR 1938

VARIABLE INPUT PARAMETERS

No.days: 10000 Start date: 1 1 1988

maxc: 15.6 maxdc: 205 meanc: 9.808 trendc(pa): 0.00

seed1: 60 seed2: 180 seed3: 120 dddrate: 100.0

LWT PROBABILITY MATRIX

A	W	C	N	NW	S	SW	OT	MRAIN	PRAIN	TANOM
0.548	0.113	0.016	0.032	0.016	0.048	0.016	0.211	3.413	0.110	0.150
0.037	0.617	0.065	0.019	0.093	0.009	0.028	0.132	3.346	0.593	1.830
0.000	0.167	0.548	0.000	0.024	0.024	0.024	0.213	4.539	0.750	-0.540
0.308	0.000	0.000	0.385	0.077	0.000	0.000	0.230	3.511	0.692	-3.300
0.136	0.364	0.000	0.000	0.273	0.000	0.000	0.227	4.042	0.400	-0.100
0.053	0.053	0.053	0.000	0.000	0.474	0.211	0.156	4.100	0.556	2.640
0.000	0.333	0.167	0.000	0.000	0.083	0.167	0.250	3.103	0.500	2.920
0.184	0.161	0.103	0.046	0.034	0.057	0.011	0.404	3.819	0.456	-0.160
0.158	0.226	0.119	0.060	0.065	0.087	0.057	0.228	3.762	0.439	0.523

CATCHMENT PARAMETER SET

r(1):	547000.0000	r(2):	0.9800
r(3):	75.0000	r(4):	28.0000
r(5):	0.1250	r(6):	0.0170
r(7):	49.0000	r(8):	1.0850
r(9):	110.0000	r(10):	200000000.0
r(11):	100.0000	r(12):	6.3500
r(13):	3.7000	r(14):	100.0000
r(15):	20000000.0	r(16):	476.0000

SIMULATION OUTPUT STATISTICS

Total rain (mm): 19518.0	Total discharge (mm): 5122.3
Mean annual rain (mm): 712.9	Mean annual discharge (mm): 187.1
Mean daily temperature: 10.35	Number of westerly days: 3022
Number of cyclonic days: 1170	Number of anticyclonic days: 1741
Number of wet-days: 4800	Discharge-rainfall(%): 26.24
Total H-ion input (kg): 1008.561	Total H-ion output (kg): 77.4003
Mean rain pH is: 4.169	Mean discharge pH is: 4.559
Initial base saturation: 0.100000	Final base saturation: 0.096488
Total Al-ion output (kg): 3895.2	Al-ion concentration (mg/l): 1.39
The frequency of LCDs: 576	Ratio of H-ion out-in(%): 7.67
The frequency of Q90%: 796	Days with zero flow: 3323

APPENDIX 1

PROBABILITY MATRIX FOR 1969

VARIABLE INPUT PARAMETERS

No.days: 10000 Start date: 1 1 1988

maxc: 15.6 maxdc: 205 meanc: 9.808 trendc(pa): 0.00

seed1: 60 seed2: 180 seed3: 120 dddrate: 100.0

LWT PROBABILITY MATRIX

A	W	C	N	NW	S	SW	OT	MRAIN	PRAIN	TANOM
0.521	0.085	0.000	0.014	0.014	0.028	0.000	0.338	3.413	0.110	0.150
0.054	0.297	0.162	0.027	0.108	0.000	0.000	0.352	3.346	0.593	1.830
0.000	0.058	0.493	0.072	0.058	0.029	0.014	0.276	4.539	0.750	-0.540
0.105	0.000	0.053	0.263	0.158	0.000	0.000	0.421	3.511	0.692	-3.300
0.048	0.190	0.095	0.190	0.333	0.000	0.000	0.144	4.042	0.400	-0.100
0.000	0.000	0.154	0.000	0.000	0.154	0.231	0.461	4.100	0.556	2.640
0.125	0.000	0.125	0.000	0.000	0.125	0.375	0.250	3.103	0.500	2.920
0.212	0.088	0.168	0.035	0.027	0.044	0.018	0.408	3.819	0.456	-0.160
0.133	0.089	0.156	0.075	0.087	0.048	0.080	0.331	3.762	0.439	0.523

CATCHMENT PARAMETER SET

r(1):	547000.0000	r(2):	0.9800
r(3):	75.0000	r(4):	28.0000
r(5):	0.1250	r(6):	0.0170
r(7):	49.0000	r(8):	1.0850
r(9):	110.0000	r(10):	200000000.0
r(11):	100.0000	r(12):	6.3500
r(13):	3.7000	r(14):	100.0000
r(15):	20000000.0	r(16):	476.0000

SIMULATION OUTPUT STATISTICS

Total rain (mm): 20401.7 Total discharge (mm): 6611.5

Mean annual rain (mm): 745.2 Mean annual discharge (mm): 241.5

Mean daily temperature: 9.78 Number of westerly days: 966

Number of cyclonic days: 1897 Number of anticyclonic days: 1906

Number of wet-days: 4710 Discharge-rainfall(%): 32.41

Total H-ion input (kg): 1248.197 Total H-ion output (kg): 123.9388

Mean rain pH is: 4.066 Mean discharge pH is: 4.465

Initial base saturation: 0.100000 Final base saturation: 0.094723

Total Al-ion output (kg): 5503.4 Al-ion concentration (mg/l): 1.52

The frequency of LCDs: 929 Ratio of H-ion out-in(%): 9.93

The frequency of Q90%: 1211 Days with zero flow: 2486

APPENDIX 1

PROBABILITY MATRIX FOR 1971

VARIABLE INPUT PARAMETERS

No.days: 10000 Start date: 1 1 1988

maxc: 15.6 maxdc: 205 meanc: 9.808 trendc(pa): 0.00

seed1: 60 seed2: 180 seed3: 120 dddrate: 100.0

LWT PROBABILITY MATRIX

A	W	C	N	NW	S	SW	OT	MRAIN	PRAIN	TANOM
0.624	0.010	0.040	0.020	0.010	0.000	0.010	0.286	3.413	0.110	0.150
0.073	0.512	0.049	0.000	0.024	0.024	0.024	0.294	3.346	0.593	1.830
0.034	0.103	0.586	0.069	0.000	0.000	0.000	0.207	4.539	0.750	-0.540
0.231	0.077	0.077	0.154	0.154	0.000	0.000	0.307	3.511	0.692	-3.300
0.400	0.000	0.200	0.400	0.000	0.000	0.000	0.000	4.042	0.400	-0.100
0.000	0.125	0.000	0.000	0.000	0.250	0.250	0.375	4.100	0.556	2.640
0.083	0.167	0.000	0.000	0.000	0.167	0.250	0.333	3.103	0.500	2.920
0.220	0.071	0.134	0.024	0.008	0.024	0.039	0.480	3.819	0.456	-0.160
0.208	0.133	0.136	0.083	0.025	0.058	0.072	0.285	3.762	0.439	0.523

CATCHMENT PARAMETER SET

r(1):	547000.0000	r(2):	0.9800
r(3):	75.0000	r(4):	28.0000
r(5):	0.1250	r(6):	0.0170
r(7):	49.0000	r(8):	1.0850
r(9):	110.0000	r(10):	200000000.0
r(11):	100.0000	r(12):	6.3500
r(13):	3.7000	r(14):	100.0000
r(15):	20000000.0	r(16):	476.0000

SIMULATION OUTPUT STATISTICS

Total rain (mm): 18945.0	Total discharge (mm): 5298.3
Mean annual rain (mm): 692.0	Mean annual discharge (mm): 193.5
Mean daily temperature: 9.87	Number of westerly days: 1140
Number of cyclonic days: 1723	Number of anticyclonic days: 2804
Number of wet-days: 4366	Discharge-rainfall(%): 27.97
Total H-ion input (kg): 1185.555	Total H-ion output (kg): 87.1681
Mean rain pH is: 4.072	Mean discharge pH is: 4.522
Initial base saturation: 0.100000	Final base saturation: 0.094960
Total Al-ion output (kg): 4096.1	Al-ion concentration (mg/l): 1.41
The frequency of LCDs: 627	Ratio of H-ion out-in(%): 7.35
The frequency of Q90%: 809	Days with zero flow: 2988

APPENDIX 2

SCAM MODEL PROGRAM
FORTRAN 77 VERSION

```
      program scam

      real r(16),s(12),m(9,11),q(24),t(24),tempc,rain,rop,tfp,mrain,
     1     totrain,meansr,actprob,rainconc,pHrain,Hin,Hout,mod,randX4,
     1     Hratio,chemer,westerly,acyclon,cyclonic,other,south,
     1     north,nw,sw,randX2,randX3,loadtot,qtot,vwrain,vwHload,
     1     Hint,Houtt,tqout,totraint,avloadin,deltac,prain,tanom,
     1     temptren,maxc,meanc,sumgrad,wingrad,pHiontot,pHthresh,
     1     coef,CEC,CECtot,wr,pHmax,pHmin,bs,obspH,meant,mtemp,
     1     Alout,Almean,chemtot,hbias,pH,SMD,qat,qa,qt,ersum,dep

      integer opt,dbase,day,month,year,dstart,mstart,ystart,aindex,
     2     seed,maxdc,totrday,seed2,seed3,seed4,colmn,row,col,
     2     fday,fmonth,fyear,nday,windex,trendc,nexceed,cindex,
     2     oldyear,wat,cat,aat,qexceed,dry

C Greeting and mode options

      print*,'Welcome to SCCAM....Shifting Climate and Catchment'
      print*,'        Acidification Model....'
      print*
    5 print*,'Select simulation option please:'
      print*,'  1 = Hydrological simulation only'
      print*,'  2 = SSAM catchment model'
      read*,opt
      if (opt.gt.2.or.opt.lt.1) goto 5
      print*
   15 print*,'Select form of data base to be used:'
      print*,'  1 = Met. Station data base'
      print*,'  2 = Synthetic data set'
      read*,dbase
      if (dbase.gt.2.or.dbase.lt.1) goto 15

      if (dbase.eq.2) then
       print*
       print*,'Which of the following parameters do you'
       print*,'wish to adjust?'
       print*,'   1 = temperature regime only'
       print*,'   2 = catchment parameters only'
       print*,'   3 = synoptic patterns only'
       print*,'   4 = all of the above'
       print*,'   5 = none'
       read*,dfault
       print*
      end if

C Opening files

      open (22,file = 'RESULTS',status = 'old')
      open (20,file = 'LOADS',status = 'old')
      open (2,file='DATASHEET',status='old')
      open (4,file = 'R',status = 'old')
       read (4,*) r
      open (3,file = 'S',status = 'old')
       read (3,*) s
```

```
      open (12,file = 'LWT190809',status = 'old')
       do 50 row = 1,9
        read (12,*) (m(row,col),col = 1,11)
 60     format (11(f6.3,1x))
 50    continue
       open (14,file = 'LWT',status = 'old')

      if (dbase.eq.1) then
       open (8,file = 'DATA',status = 'old')
      end if

C Calibration mode set-up.

      if (dbase.eq.1) then
       print*
        print*,'Enter first day of callibration period:'
        read*,fday
        print*
        print*,'Enter first month of callibration period:'
        read*,fmonth
        print*
        print*,'Enter first year of callibration period:'
        read*,fyear
        print*
  40   print*,'Enter length of simulation period'
       print*,'    (This must be less than or equal to ', r(16),' days)'
       read*,nday
        if (nday.gt.r(16)) goto 40
      end if

C Initialising variables

      SMD = r(7)
      pHmin = r(13)
      pHmax = r(12)
      dddinp = r(14)
      CEC = r(15)
      wr = r(11)
      CECtot = r(10)
      bs = r(15)/r(10)
      coef = (pHmax - pHmin)/(r(3)*bs)
      Alout = 0.0
      vwpH = 0.0
      Hint = 0.0
      Houtt = 0.0
      chemer = 0.0
      chemtot = 0.0
      qat = 0.0
      ersum = 0.0

      ystart = s(1)
      mstart = s(2)
      dstart = s(3)
      day = dstart - 1
      month = mstart
      year = ystart
      oldyear = ystart

      totrday = 0.0
      nexceed = 0.0
      qexceed = 0.0
      dry = 0.0
      temptren = 0.0
```

```
      if (dbase.eq.2) then
      nday = s(4)
      end if
      seed = s(5)
      seed2 = s(6)
      seed3 = s(7)
      seed4 = seed3 + seed2 + seed
      pHthresh = s(8)

      maxc = s(9)
      maxdc = s(10)
      meanc = s(11)
      trendc = 1.0
      meant = 0.0
      deltac = 0.0

      syntrend = 1
      season = 2
      loadtot = 3
      totrain = 0.0
      windex = 0.0
      cindex = 0.0
      aindex = 0.0
      wat = 0.0
      cat = 0.0
      aat = 0.0
      qtot = 0.0
      vwHload = 0.0
      vwrain = 0.0
      tqout = 0.0
      totraint = 0.01
      pHiontot = 0.0

      if (dbase.eq.1) goto 1999

      if (dfault.eq.5) goto 1999

      if (dfault.eq.1.or.dfault.eq.2.or.dfault.eq.3.or.
     1      dfault.eq.4) goto 35

C Interactive parameter set-up

       print*
       print*,'You are now able to generate a synthetic data set,'
       print*,'to your own specifications.....'
       print*

       print*,'***** AUTOMATIC CLOCK *****'
       print*
       print*,'Enter first year of sequence:'
       read*,ystart
       print*
       print*,'Enter first month of sequence:'
       read*,mstart
       print*
       print*,'Enter first day of sequence:'
       read*,dstart
       print*
       print*,'Enter (in days) the desired data set length:'
       read*,nday
       print*
       print*
```

```
 35  if (dfault.eq.2.or.dfault.eq.3) goto 85
     print*,'***** MONTHLY TEMPERATURE GENERATOR *****'
     print*
     print*,'(All temperatures should be in degrees Celsius...'
     print*
     print*,'Enter mean maximum monthly temperature:'
     read*,maxc
     print*
     print*,'Enter day of mean maximum temperature:'
     read*,maxdc
     print*
     print*,'Enter mean annual temperature:'
     read*,meanc
     print*
     print*,'Select the appropriate temperature trend:'
     print*,'     1 = no change'
     print*,'     2 = annual incremental change'
     print*,'     3 = seasonally adjusted change'
     read*,trendc
     if (trendc.lt.2.or.trendc.gt.3)  then
      deltac = 0.0
      goto 85
     end if
     if (trendc.eq.2) then
      print*
      print*,'Enter the annual rate of change (in Celsius)....'
      print*,'.......1945-1988 average = -0.007'
      read*,deltac
     end if
     if (trendc.eq.3) then
      print*,'Enter the SUMMER gradient.......'
      print*,'.....1969-1988 value = -0.026 C/pa'
      read*,sumgrad
      print*
      print*,'Enter the WINTER gradient.......'
      print*,'.....1969-1988 value = -0.057 C/pa'
      read*,wingrad
      print*
     end if
85   print*
     print*
     print*
     if (dfault.ne.4) goto 78
     print*,'***** LETHAL CONCENTRATION DOSE *****'
     print*
     print*,'Enter a "lethal" pH value............'
     print*,'....the frequency of occurence will be counted.'
     read*,pHthresh
     print*
     print*
     print*,'***** RANDOM NUMBER GENERATOR *****'
     print*
     print*,'Enter a positive integer:'
     read*,seed
     print*
78  if (dfault.eq.2.or.dfault.eq.4) then
     print*
     print*,'***** CATCHMENT PARAMETERS *****'
     print*
     print*
     print*,'Enter maximum soil water pH:'
     print*,'(...suggested value = ',r(12),' )'
     read*,pHmax
```

```
      print*
      print*,'Enter the minimum soil water pH:'
      print*,'(...suggested value = ',r(13),' )'
      read*,pHmin
      print*
      print*,'Enter the daily weathering rate in micrograms'
      print*,'per square metre per day:'
      print*,'(...suggested range is 50 to 550 )'
      read*,wr
      print*
      print*,'Enter the base saturation :'
      print*,'(...suggested value = ',r(15)/r(10),' )'
      read*,bs
      coef = (pHmax - pHmin)/(r(3)*bs)
      print*
      print*,'Enter the initial number of cation sites:'
      print*,'(...suggested value = ',r(15),' )'
      read*,CEC
      CECtot = CEC/bs
      print*
     end if
     if (dfault.lt.3) goto 1999

C ******************** SYNOPTIC WEATHER GENERATOR ******************

      print*,'***** SYNOPTIC WEATHER PROPORTIONS *****'
      print*
      print*,'You are now able to modify the Lambs Weather'
      print*,'Type statistics to the desired specifications.'
   90 print*
      print 100
  100 format (4x,'A',6x,'W',6x,'C',6x,'N',6x,'NW',5x,
     1  'S',5x,'SW',5x,'OT',4x,'MRAIN',2x,'PRAIN',2x,'TANOM')
      print*
      do 75 row = 1,9
       print 120, (m(row,col),col = 1,11)
  120  format (11(1x,f6.3))
   75 continue
      print*
      print*,'Select COLUMN number (press 0 to quit):'
      read*,colmn
      if (colmn.gt.11.or.colmn.lt.1) goto 125
      print*
      print*,'Enter change to column values:'
      read*,mod
      if (colmn.le.8.and.colmn.ge.1) then
      if (mod.gt.1.0.or.mod.lt.-1.0) then
       print*
       print*,'ERROR: value given outside accepted range !'
       print*,'..........please try again....'
       print*
       goto 90
      end if
      end if
      do 150 row = 1,9
       m(row,colmn) = m(row,colmn) + mod
       if (colmn.le.8.and.colmn.ge.1) then
       if (m(row,colmn).gt.1.0) then
        print*
        print*,'ERROR: value given too large....try again !'
        print*
        goto 90
       end if
```

```
       end if
       write (14,122) (m(row,col),col = 1,11)
122    format (11(1x,f6.3))
 150  continue
      close (14)
      goto 90
125   continue
      close (14)
      print*
      print*
      print*,'Please select the desired results format from:'
      print*,'     1 = event loads and totals'
      print*,'     2 = monthly loads and totals'
      print*,'     3 = annual loads and totals'
      read*,loadtot
      print*
      if (loadtot.gt.1) then
       vwrain = 0.0
       vwHload = 0.0
       qtot = 0.0
       oldmonth = mstart
       oldyear = ystart
       windex = 0.0
       cindex = 0.0
      end if

 520  if (dfault.ne.5) goto 1999
      print*,'Please enter the desired daily dry deposition rate:'
      print*,'....this is in MICROGRAMS per square metre per day'
      print*,'(optimum value >200.0 and <700.0)'
      read*,dddinp
      print*

      print*,'Please enter a positive integer.....'
      read*,seed3
      print*

      print*,'Please enter another positive integer....'
      read*,seed2
1999  print*
      print*,'Please wait a moment whilst I think..........'
      print*

C Summary file: "datasheet".

       if (dbase.eq.2) then
      write (2,548)
548   format (1h0,1x,'VARIABLE INPUT PARAMETERS')
      write (2,550) nday,dstart,mstart,ystart
550   format (1h0,1x,'No.days: ',i6,t24,'Start date: ',i2,1x,i2,1x,i4)
      write (2,552)maxc,maxdc,meanc,deltac
552   format (1h0,1x,'maxc:',f5.1,t20,'maxdc:',i4,t35,'meanc:',f6.3,
     1          t50,'trendc(pa): ',f6.3)
      write (2,556) seed,seed3,seed2,dddinp*s(12)
556   format (1h0,1x,'seed1: ',i7,t20,'seed2: ',i7,t40,
     1    'seed3: ',i7,t60,'dddrate: ',f6.1)

      write (2,558)
558   format (1h0,1x,'LWT PROBABILITY MATRIX')
      write (2,560)
560   format (1h0,4x,'A',6x,'W',6x,'C',6x,'N',5x,'NW',6x,
     1    'S',5x,'SW',5x,'OT',3x,'MRAIN',2x,'PRAIN',2x,'TANOM')
      do 70 row = 1,9
```

```
      write (2,562) (m(row,col),col = 1,11)
562   format (11(1x,f6.3))
70   continue
     row = 1

     end if
     write (2,566)
566  format (1h0,1x,'CATCHMENT PARAMETER SET')

     write (2,450) r(1),r(2)
450  format(1h0,1x,'r(1):',f12.4,20x,'r(2):',f12.4)
     write (2,452) r(3),r(4)
452  format(2x,'r(3):',f12.4,20x,'r(4):',f12.4)
     write (2,454) r(5),r(6)
454  format(2x,'r(5):',f12.4,20x,'r(6):',f12.4)
     write (2,456) r(7),r(8)
456  format(2x,'r(7):',f12.4,20x,'r(8):',f12.4)
     write (2,458) r(9),r(10)
458  format(2x,'r(9):',f12.4,20x,'r(10):',f13.1)
     write (2,460) r(11),r(12)
460  format(2x,'r(11):',f12.4,19x,'r(12):',f12.4)
     write (2,462) r(13), r(14)
462  format(2x,'r(13):',f12.4,19x,'r(14):',f12.4)
     write (2,464) r(15),r(16)
464  format (2x,'r(15):',f13.1,18x,'r(16):',f12.4)
     write (2,580)
580  format (1h0,1x,'SIMULATION OUTPUT STATISTICS')


C ******************** HYDRO-GEOCHEMICAL MODEL ********************

2000 do 1000 i=1,nday

C Calibration option.

      if (dbase.eq.1) then
25     read (8,26) day,month,year,tempc,rain,stage,pHrain,obspH
26     format (3(i2,1x),1x,f4.1,1x,f5.2,1x,f6.4,1x,2(f4.2,1x))

       rain = rain*r(8)

       if (rain.eq.0.0) then
        rainconc = 10.0**(6.0 - pHrain)
        dddinp = (0.025*rainconc) - 0.05024
        dddinp = dddinp/0.0491
       else
        rainconc = 10.0**(6.0 - pHrain)
        dddinp = 0.0
       end if

       if (year.lt.fyear) goto 25
       if (year.eq.fyear.and.month.lt.fmonth) goto 25
       if (year.eq.fyear.and.month.eq.fmonth.and.day.lt.fday) goto 25
       if (stage.gt.0.03) then
       stage = stage - 0.03
       qa = 1.3*1.38*24*3600*1000*(stage)**2.5
       elseif (stage.lt.0.0) then
        qa = -1
       elseif (stage.eq.0.03) then
        qa = 0.0
       end if
      end if
```

```
C Synthetic data-base option.

       if (dbase.eq.2) then
        day = day + 1
        if (month.eq.1.and.day.eq.32.or.month.eq.3.and.day.eq.32.or.
     3     month.eq.5.and.day.eq.32.or.month.eq.7.and.day.eq.32.or.
     4     month.eq.8.and.day.eq.32.or.month.eq.10.and.day.eq.32) then
         day = 1
         month = month + 1
        elseif (month.eq.4.and.day.eq.31.or.month.eq.6.and.day.eq.31.
     5     or.month.eq.9.and.day.eq.31.or.month.eq.11.and.day.eq.31)
     6     then
         day = 1
         month = month + 1
        elseif (month.eq.2.and.day.eq.29) then
          day = 1
          month = 3
        elseif (month.eq.12.and.day.eq.32) then
          day = 1
          month = 1
          year = year + 1
        end if


C Synthetic input-output H-ion loads.

        if (loadtot.eq.2.and.month.ne.oldmonth) then
         if (totrain.gt.0.0) then
         vwrain = vwrain/totrain
         end if
         vwHload = vwHload/(qtot*r(1))
         Hin = Hin/1.0E09
         Hout = Hout/1.0E9
         write (20,600) oldmonth,year,totrain,qtot,Hin,Hout,
     1           vwrain,vwHload,windex,cindex
 600     format (2(2x,i2),2x,6(2x,f7.3),2(2x,i2))
           Hin = 0.0
           Hout = 0.0
           totrain = 0.0
           vwrain = 0.0
           vwHload = 0.0
           qtot = 0.0
        elseif (loadtot.eq.3.and.year.ne.oldyear) then
         vwrain = vwrain/totrain
         if (qtot.gt.0.0) then
         vwHload = vwHload/(qtot*r(1))
         end if
         Hin = Hin/1.0E09
         Hout = Hout/1.0E09
         if (nday.le.100000) then
         write (20,620) oldyear,totrain,qtot,Hin,Hout,vwrain,vwHload,
     1                 CEC/CECtot,nexceed,dry,qexceed
         end if
 620     format (i4,2x,2(f6.1,2x),4(f5.1,2x),f8.4,2x,i5,2x,i5,2x,i5)
           Hin = 0.0
           Hout = 0.0
           totrain = 0.0
           qtot = 0.0
           vwrain = 0.0
           vwHload = 0.0
           windex = 0.0
           cindex = 0.0
```

```
          aindex = 0.0
        end if

C Synoptic sequence generator.

       westerly = m(row,2)
       cyclonic = westerly + m(row,3)
       acyclon = cyclonic + m(row,1)
       north = acyclon + m(row,4)
       nw = north + m(row,5)
       south = nw + m(row,6)
       sw = south + m(row,7)
       other = 1.0

        seed2 = seed2*2045 + 1
        seed2 = seed2 - (seed2/1048576)*1048576
        randX2 = real (seed2 + 1)/1048577.0

        seed3 = seed3*2045 + 1
        seed3 = seed3 - (seed3/1048576)*1048576
        randX3 = real (seed3 + 1)/1048577.0

        if (randX2.ge.0.0.and.randX2.le.westerly) then
         rainconc = 3.449 + (8.714*randX3) - (14.929*(randX3**2))
     1               + (9.682*(randX3**3))
         windex = windex + 1
         wat = wat + 1
         mrain = m(2,9)
         prain = m(2,10)
         tanom = m(2,11)
         row = 2
        elseif (randX2.gt.westerly.and.randX2.le.cyclonic) then
         rainconc = 3.039 + (6.037*randX3) - (13.738*(randX3**2))
     1               + (11.029*(randX3**3))
         cindex = cindex + 1
         cat = cat + 1
         mrain = m(3,9)
         prain = m(3,10)
         tanom = m(3,11)
         row = 3
        elseif (randX2.gt.cyclonic.and.randX2.le.acyclon) then
         rainconc = 3.15 + (1.804*randX3)
         aindex = aindex + 1
         aat = aat + 1
         mrain = m(1,9)
         prain = m(1,10)
         tanom = m(1,11)
         row = 1
        elseif (randX2.gt.acyclon.and.randX2.le.north) then
         rainconc = 3.128 + (2.88*randX3) - (5.942*(randX3**2)) +
     1              (5.093*(randX3**3))
         mrain = m(4,9)
         prain = m(4,10)
         tanom = m(4,11)
         row = 4
        elseif (randX2.gt.north.and.randX2.le.nw) then
         rainconc = 3.815 - (3.223*randX3) + (14.426*(randX3**2)) -
     1              (8.715*(randX3**3))
        mrain = m(5,9)
        prain = m(5,10)
        tanom = m(5,11)
        row = 5
        elseif (randX2.gt.nw.and.randX2.le.south) then
```

```
         rainconc = 3.976 + (0.003*randX3) + (2.852*(randX3**2))
         mrain = m(6,9)
         prain = m(6,10)
         tanom = m(6,11)
         row = 6
        elseif (randX2.gt.south.and.randX2.le.sw) then
         rainconc = 3.698 + (2.498*randX3) - (0.079*(randX3**2))
         mrain = m(7,9)
         prain = m(7,10)
         tanom = m(7,11)
         row = 7
       elseif (randX2.gt.sw.and.randX2.le.1.0) then
         rainconc = 3.662 + (2.836*randX3)
         mrain = m(8,9)
         prain = m(8,10)
         tanom = m(8,11)
         row = 8
        end if

C Stochastic rainfall generation.

 750  seed = seed*2045 + 1
      seed = seed - (seed/1048576)*1048576
      randX = real(seed + 1)/1048577.0

      seed4 = seed4*2045 + 1
      seed4 = seed4 - (seed4/1048576)*1048576
      randX4 = real(seed4 + 1)/1048577.0

      mrain = mrain + ((year-1988)*0.0)
      dep = s(12)-((year-1988)*0.00)

      if (randX.le.prain) then
       rain = -mrain*r(8)*log(randX4)
      else
       rain = 0.0
      end if

C Temperature generation.

 920    if (oldyear.ne.year.and.trendc.eq.2) then
         temptren = temptren + deltac
        end if
        if (trendc.eq.1) then
         temptren = 0.0
        end if

        tempc = meanc + (maxc - meanc)*cos(-(i-maxdc)*0.017214)

        if (trendc.eq.2) then
         tempc = tempc + temptren
        end if
        if (trendc.eq.3) then
         if (month.ge.5.and.month.le.9) then
          tempc = tempc + (real(year - ystart)*sumgrad)
         elseif (month.ge.11.or.month.le.3) then
          tempc = tempc + (real(year - ystart)*wingrad)
         end if
        end if

        tempc = tempc + tanom
        meant = meant + tempc
        mtemp = real(meant)/nday
```

```
      end if

C Rainfall totals.

      totrain = totrain + rain
      if (rain.gt.0.0) then
       totrday = totrday + 1
      end if

C Hydrological model.

       if (tempc.gt.0.6) then
        pe = r(2)*(10.64*tempc - 5.90)/(80 - tempc)
       else
        pe = 0.0
       end if
       if (SMD.ge.r(9)) then
        pe = 0.0
       end if

       SMD = SMD - rain
       if (SMD.lt.r(4)) then
        rop = (r(4) - SMD)*r(5)
        SMD = SMD + rop
       else
        rop = 0.0
       end if
       if (SMD.lt.r(3)) then
        tfp = (r(3) - SMD)*r(6)
        SMD = SMD + tfp
       else
        tfp = 0.0
       end if

       SMD = SMD + pe

C Monthly averaging and totalling of outputs

       do 400 l=1,12
        if (month.eq.l) then
         q(l)=q(l)+tfp+rop
         q(l+12)=q(l+12)+tfp
         goto 410
        end if
  400  continue

  410  qt = (rop + tfp)*r(1)

       if (qt.ge.856271.0) then
        qexceed = qexceed + 1
       end if

       if (qt.eq.0.0) then
       dry = dry + 1
       end if

       if (dbase.eq.1.and.obspH.ne.0.0) then
        print 365,day,month,year,SMD,obspH
 365    format (3(2x,i2),2x,f5.1,2x,f4.2)
       end if
```

```
C Catchment acidification model(s).

       if (opt.eq.2) then
         if (rain.gt.0.0) then
          rainconc = 10.0**(6.0-rainconc)
        CEC = CEC - (dep*rainconc*rain) + wr
         elseif (rain.eq.0.0) then
         CEC = CEC - (dep*dddinp) + wr
        end if
        if (CEC.lt.0.0) then
         CEC = 0.0
        end if
        bs = CEC/CECtot

        if (SMD.lt.0.0) then
         pH = pHmin
        elseif (SMD.lt.r(3).and.qt.gt.0.0) then
         pH = pHmin + (coef*bs*SMD)
        elseif (qt.eq.0.0) then
         pH = 0.0
        else
         pH = pHmax
        end if

        elseif (opt.eq.1) then
         stage = (qt/(1.3*1.38*24*3600*1000))**0.4
         if (stage.le.14.0) then
         pH = 7.157 - (0.374*stage*100.0) + (0.013*(stage*100.0)**2.0)
         else
         pH = 4.46
         end if
        end if

         if (pH.lt.7.0.and.pH.ne.0.0) then
          Al = 13.997 - (pH*4.073) + (0.297*(pH**2.0))
         else
          Al = 0.0
         end if
         Alout = (Alout + (Al*qt))

        if (qt.gt.0.0) then
         CEC = CEC + ((10.0**(6.0-pH))*(qt/r(1)))
        end if


C Stream input-output budget for H-ion.

       if (rain.gt.0.0) then
        Hin = Hin + ((rain*rainconc)*r(1)*dep)
       else
        Hin = Hin + (dddinp*r(1)*dep)
       end if
       if (pH.ne.0.0) then
       Hout = Hout + ((10.0**(6.0 - pH))*qt)
       end if
       if (Hin.gt.0.0) then
       Hratio = Hout*100.0/Hin
       else
       Hratio = 0.0
       end if
```

```
C Hydrological model performance evaluator.

       if (dbase.eq.1.and.qa.ge.0.0) then
       ersum = ersum + ((qa - qt)**2)**0.5
       qat = qat + qa
       if (qat.gt.0.0) then
       fit = ersum*100.0/qat
       end if
       end if

C Chemical model performance evaluator.

      if (obspH.gt.0.0.and.pH.gt.0.0.and.dbase.eq.1) then
       chemer = chemer + (((10**-pH)-(10**-obspH))**2.0)**0.5
       chemtot = chemtot + (10**-obspH)
       hbias = chemer/chemtot
      end if

C Threshold acidity exceedence counter.

        if (pH.le.pHthresh.and.pH.ne.0.0) then
         nexceed = nexceed + 1
        end if

C Total catchment outputs for "datasheet" file.

      if (pH.gt.0.0) then
       pHion = (10.0**-pH)*qt
      end if
      tqout = tqout + rop + tfp
      if (tqout.gt.0.0) then
      Almean = Alout/(tqout*r(1))
      end if
      pHiontot = pHiontot + pHion
      if (tqout.gt.0.0.or.tfp.gt.0.0) then
       vwpH = pHiontot/(tqout*r(1))
      end if
      if (pHiontot.gt.0.0.and.vwpH.gt.0.0) then
       pHmean = -log10(vwpH)
      end if
      Houtt = Houtt + (pHion*0.001)

C Total precipitation inputs for "datasheet" file.

      totraint = totraint + rain
      flowprop = tqout*100.0/totraint
      if (rain.gt.0.0) then
       Hint = Hint + ((rain*rainconc)*r(1)*dep*1.0E-09)
      elseif (rain.eq.0.0) then
       Hint = Hint + (dddinp*r(1)*dep*1.0E-09)
      end if

      if (Hint.gt.0.0) then
      Hratiot = Houtt*100.0/Hint
      else
      Hratiot = 0.0
      end if

C Seasonal distribution of streamflow acidity.

        do 445 k=1,12
         if (month.eq.k) then
```

```
          t(k)=t(k)+(pHion*1.0E06)
          if (pH.le.s(8).and.pH.gt.0.0) then
           t(k+12)=t(k+12)+1
          end if
         end if
  445   continue

C H-ion subtotal for 'loads' file.

        if (loadtot.gt.1) then
         vwrain = vwrain + (rainconc*rain*dep)
         vwHload = vwHload + (pHion*1.0E06)
         qtot = qtot + (rop + tfp)
        end if

C Writing to destination file: results

        if (nday.le.1000) then
         write (22,86) i,rain,tempc,qt,qa,pH,obspH,Al
  86     format (i3,2x,2(2x,f4.1),2x,2(2x,f10.0),2x,3(2x,f5.2))
        end if

         oldyear = year
         oldmonth = month

 1000   continue


C Simulation summary values (screen).

       if (dbase.eq.1) then
        print*
        print*,'***** SUMMARY OF CALIBRATION RUN *****'
        print*
       print 180,fit
  180 format (1x,'Simulation error of the actual flow is:',f6.2,' %')
        print*
        print 200,hbias*100.0
  200   format (1x,'Total error in simulated pH is:',f8.2,' %')
        print*
        print*,'The simulation length was ',i-1,' days'

        write (6,260) i-1
 260    format (1h0,1x,'Simulation length (days): ',i4)
        write (6,205) fit,hbias*100.0
 205    format (1h0,1x,'Discharge error(%): ',f6.2,t39,
     1      'H-ion error(%): ',f6.2)
       end if

       if (dbase.eq.2) then
        meansr = totraint/totrday
        actprob = real (totrday )/nday
        print*
        print*,'***** SUMMARY OF SYNTHETIC RAINFALL GENERATION *****'
        print*
        print*,'The mean daily temperature = ',mtemp
        print*,'The number of days = ',nday
        print*,'The generated wet-day probability = ',actprob
        print*,'The number of rain days generated = ',totrday
        print*,'The total rainfall generated was = ',totraint
        print*,'The mean daily rainfall (generated) = ',meansr
        print*,'The total discharge generated (mm) = ',tqout
        print*,'The discharge-rainfall ratio (%) = ',flowprop
```

```
      print*,'The mean volume-weighted pH = ',pHmean
      print*,'The number of days < input LCD value = ',nexceed
      print*,'The number of days with flow > Q90% = ',qexceed
      print*,'The number of days with zero flow = ',dry
      print*
      print*
      print*,'Discharge seasonal distribution:'
      print*
      do 420 l=1,12
       print 415,l,q(l),q(l+12),t(l)/(q(l)*r(l)),t(l+12)
 415   format (i2,2x,f7.0,2x,f7.0,2x,f6.2,2x,i5)
 420  continue
      print*
      print*

      end if

C Catchment total input-output budget for DATASHEET file.

      write (2,220) totraint,tqout
 220  format (1h0,1x,'Total rain (mm): ',f8.1,t39,
     1     'Total discharge (mm): ',f8.1)

      if (dbase.eq.2) then
      write (2,222) totraint*real(365.25)/nday,tqout*real(365.25)/nday
 222  format (1h0,1x,'Mean annual rain (mm): ',f5.1,t39,
     1     'Mean annual discharge (mm): ',f5.1)

      write (2,855) mtemp,wat
 855  format (1h0,1x,'Mean daily temperature: ',f5.2,t39,
     1    'Number of westerly days: ',i6)

      write (2,860) cat,aat
 860  format (1h0,1x,'Number of cyclonic days: ',i6,t39,
     1     'Number of anticyclonic days: ',i6)
      end if

      write (2,224) totrday,flowprop
 224  format(1h0,1x,'Number of wet-days: ',i5,t39,
     1     'Discharge-rainfall(%): ',f5.2)


      write (2,210) Hint,Houtt
 210  format(1h0,1x,'Total H-ion input (kg): ',f9.3,t39,
     1     'Total H-ion output (kg): ',f8.4)

      avloadin = Hint - (dddinp*dep*r(1)*1.0E-09*
     1              (nday - totrday))
      avloadin =avloadin/(totraint*r(1)*0.001)
      if (avloadin.gt.0.0) then
      avloadin = -1.0*log10(avloadin)
      else
      avloadin = 0.0
      end if

      write (2,230) avloadin,pHmean
 230  format (1h0,1x,'Mean rain pH is: ',f5.3,t39,
     1     'Mean discharge pH is: ',f5.3)

      write (2,240) r(15)/r(10),bs
 240  format (1h0,1x,'Initial base saturation: ',f9.6,t39,
     1     'Final base saturation:',f9.6)
```

```
      write (2,245) Alout*1.0E-06,Almean
 245  format (1h0,1x,'Total Al-ion output (kg): ',f8.1,t39,
    1    'Al-ion concentration (mg/l): ',f5.2)

      write (2,250) nexceed,Hratiot
 250  format (1h0,1x,'The frequency of LCDs: ',i5,t39,
    1    'Ratio of H-ion out-in(%): ',f6.2)

      write (2,255) qexceed,dry
 255  format (1h0,1x,'The frequency of Q90%: ',i5,t39,
    1    'Days with zero flow: ',i5)

      write (2,270)
 270  format (1h0,1x,'NOTES:')
      close(6)

 5000 stop
      end
```

EXTERNAL FILE NAMES

DATA	calibration data-base
DATASHEET	simulation summary statistics
LOADS	monthly/annual simulation statistics
LWT	weather type probability matrix (generated)
LWT1908	weather type probability matrix (input)
M	weather type probability matrix (array)
R	catchment parameter values
RESULTS	daily hydrochemical simulation results
S	parameter default values

APPENDIX 3
SCAM DEMONSTRATION PROGRAM LISTING
BASICA VERSION 1.1

```
10 REM
20 REM*****************************************************
30 REM** SCAM.BAS to demonstrate SCAM model capabilities **
40 REM*****************************************************
50 REM*****************************************************
60 REM
70 REM
80 REM
90 REM
100 REM+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
110 REM+ Active files  Description                                +
120 REM+ DEFAULT.REF   default parameter values file              +
130 REM+ HEADERS.REF   parameter headings and abrreviations       +
140 REM+ LWTyyyy.REF   Lamb's Weather Type matrix for year yyyy   +
150 REM+ CAT$.REF      default parameters for catchment CAT$      +
160 REM+ RESULTS.REF   default results file                       +
170 REM+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
180 REM
190 FOR I=440 TO 880 STEP 440
200 SOUND I,.5
210 NEXT
220 RANDOMIZE TIMER
230 COLOR 15,1,1
240 KEY OFF
250 REM**************************
260 REM* INITIALISING VARIABLES *
270 REM**************************
280 DIM P(100)
290 DIM DESC$(100)
300 DIM LWT(8,8)
310 DIM RES(200,20)
320 DIM MON(12,20)
330 DIM HD$(20)
340 DIM FORM$(20)
350 DIM UNT$(20)
360 DIM ST(20,7)
370 GREET=0
380 DEFT$="DEFAULT.DEF"
390 CLS
400 DEFT$="A:\"+DEFT$
410 OPEN "I",#1,DEFT$
420 IF GREET=1 THEN COLOR 13: LOCATE 5,1:
    PRINT"LOADING NEW PARAMETERS....":    GOTO 540
430 REM********************
440 REM* GREETINGS SCREEN *
450 REM********************
460 LOCATE 5,10
```

```
470 PRINT"THE SHIFTING CLIMATE AND CATCHMENT ACIDIFICATION MODEL
480 PRINT:PRINT TAB(25);"DEMONSTRATION SOFTWARE
490 PRINT:PRINT TAB(35);"BY
500 PRINT:PRINT TAB(30);"ROBERT WILBY
510 LOCATE 20,29
520 PRINT"(C) VERSION 1.1
530 PRINT:PRINT TAB(35);"1990
540 FOR I=1 TO 200
550 INPUT #1,R$
560 IF MID$(R$,1,2)="99" THEN CLOSE #1:GOTO 610
570 CODE=VAL(MID$(R$,1,2))
580 P(CODE)=VAL(MID$(R$,5,8))
590 DESC$(CODE)=MID$(R$,23,56)
600 NEXT I
610 IF GREET=1 THEN GOTO 2040
620 OPEN "I",#1,"a:\HEADERS.REF
630 FOR I=1 TO 15
640 LINE INPUT #1,H$
650 HD$(I)=MID$(H$,1,8)
660 FORM$(I)=MID$(H$,9,7)
670 UNT$(I)=MID$(H$,18,5)
680 NEXT I
690 CLOSE #1
700 CLS
710 COLOR 15,1,1
720 REM****************
730 REM* PRIMARY MENU *
740 REM****************
750 X$=STRING$(10,45)
760 LOCATE 5,20
770 PRINT X$;" MASTER MENU ";X$
780 LOCATE 7,20
790 COLOR 14:PRINT"A";TAB(24):COLOR 7:
    PRINT"View/modify default parameters
800 PRINT
810 COLOR 14:PRINT TAB(20);"B";TAB(24):COLOR 7:
    PRINT"Model simulation options
820 PRINT
830 COLOR 14:PRINT TAB(20);"C";TAB(24): COLOR 7:
    PRINT"Produce statistical summary
840 PRINT
850 COLOR 14:PRINT TAB(20);"D";TAB(24):COLOR 7:
    PRINT"Time-series plot
860 PRINT
870 COLOR 14:PRINT TAB(20);"E";TAB(24):COLOR 7:
    PRINT"Scattergraph/trend plot
880 PRINT
890 PRINT TAB(20);"-----";X$;X$;X$
900 PRINT:PRINT:PRINT
910 COLOR 14
920 PRINT TAB(20);"Enter choice and press <RETURN> ";
930 COLOR 15
940 LINE INPUT CHOICE$
950 IF CHOICE$="A" OR CHOICE$="a" THEN GOTO 1040
960 IF CHOICE$="B" OR CHOICE$="b" THEN GOTO 1880
```

```
970 IF CHOICE$="C" OR CHOICE$="c" THEN GOTO 4050
980 IF CHOICE$="D" OR CHOICE$="d" THEN GOTO 4960
990 IF CHOICE$="E" OR CHOICE$="e" THEN GOTO 5060
1000 BEEP: GOTO 700
1010 REM***********************
1020 REM* DEFAULT MENU OPTIONS *
1030 REM***********************
1040 CLS
1050 LOCATE 5,20
1060 COLOR 15,1,1
1070 PRINT X$;" DEFAULT MENU ";X$
1080 LOCATE 7,20
1090 COLOR 14
1100 PRINT "A";TAB(24);
1110 COLOR 7:PRINT "Simulation period
1120 COLOR 14:PRINT TAB(20);"B";TAB(24);
1130 COLOR 7:PRINT "Catchment hydrology
1140 COLOR 14:PRINT TAB(20);"C";TAB(24);
1150 COLOR 7:PRINT "Catchment hydrochemistry
1160 COLOR 14:PRINT TAB(20);"D";TAB(24);
1170 COLOR 7:PRINT "Annual temperature regime
1180 COLOR 14:PRINT TAB(20);"E";TAB(24);
1190 COLOR 7:PRINT "Seasonal temperature regime
1200 COLOR 14:PRINT TAB(20);"F";TAB(24);
1210 COLOR 7:PRINT "LWT temperature anomalies
1220 COLOR 14:PRINT TAB(20);"G";TAB(24);
1230 COLOR 7:PRINT "Precipitation event magnitudes
1240 COLOR 14:PRINT TAB(20);"H";TAB(24);
1250 COLOR 7:PRINT "Precipitation event probabilities
1260 COLOR 14:PRINT TAB(20);"I";TAB(24);
1270 COLOR 7:PRINT "Seasonal precipitation regime
1280 COLOR 14:PRINT TAB(20);"J";TAB(24);
1290 COLOR 7:PRINT "LWT precipitation acidities
1300 PRINT
1310 PRINT TAB(20);X$;X$;X$;"-----"
1320 PRINT
1330 COLOR 14:PRINT TAB(24);"Enter option and press <RETURN> ";
1340 COLOR 15,1,1
1350 LINE INPUT A$
1360 IF A$="" THEN GOSUB 6730:GOTO 700
1370 IF A$="A" OR A$="a" THEN FIRST=1: LAST=4: GOTO 1520
1380 IF A$="B" OR A$="b" THEN FIRST=5: LAST=13: GOTO 1520
1390 IF A$="C" OR A$="c" THEN FIRST=14: LAST=23: GOTO 1520
1400 IF A$="D" OR A$="d" THEN FIRST=24: LAST=27: GOTO 1520
1410 IF A$="E" OR A$="e" THEN FIRST=28: LAST=39: GOTO 1520
1420 IF A$="F" OR A$="f" THEN FIRST=40: LAST=47: GOTO 1520
1430 IF A$="G" OR A$="g" THEN FIRST=48: LAST=56: GOTO 1520
1440 IF A$="H" OR A$="h" THEN FIRST=57: LAST=65: GOTO 1520
1450 IF A$="I" OR A$="i" THEN FIRST=66: LAST=77: GOTO 1520
1460 IF A$="J" OR A$="j" THEN FIRST=78: LAST=85: GOTO 1520
1470 BEEP
1480 GOTO 1040
1490 REM**********************************
1500 REM* DEFAULT PARAMETER MANIPULATION *
1510 REM**********************************
```

```
1520 COLOR 14,0,0:CLS
1530 LOCATE 4,10
1540 IF A$="a" OR A$="A" THEN PRINT X$;"SIMULATION LENGTH";X$
1550 IF A$="b" OR A$="B" THEN PRINT X$;"HYDROLOGICAL
     PARAMETERS";X$
1560 IF A$="c" OR A$="C" THEN PRINT X$;"HYDROCHEMICAL
     PARAMETERS";X$
1570 IF A$="d" OR A$="D" THEN PRINT X$;"ANNUAL TEMPERATURE
     REGIME";X$
1580 IF A$="e" OR A$="E" THEN PRINT X$;"MONTHLY TEMPERATURE
     REGIME";X$
1590 IF A$="f" OR A$="F" THEN PRINT X$;"TEMPERATURE ANOMALIES";X$
1600 IF A$="g" OR A$="G" THEN PRINT X$;"PRECIPITATION EVENT
     SIZES";X$
1610 IF A$="h" OR A$="H" THEN PRINT X$;"PRECIPITATION EVENT
     PROBABILITIES";X$
1620 IF A$="i" OR A$="I" THEN PRINT X$;"MONTHLY PRECIPITATION
     REGIME";X$
1630 IF A$="j" OR A$="J" THEN PRINT X$;"PRECIPITATION
     ACIDITIES";X$
1640 PRINT
1650 COLOR 2,0
1660 PRINT "Default";TAB(12);"New value";TAB(24);"Parameter
     description"
1670 COLOR 7
1680 PRINT
1690 FOR J=FIRST TO LAST
1700 PRINT P(J);TAB(22);DESC$(J)
1710 NEXT J
1720 COLOR 13
1730 LOCATE 22,20
1740 PRINT "Press ";
1750 COLOR 15
1760 PRINT"<RETURN> ";
1770 COLOR 13
1780 PRINT"to keep default values"
1790 COLOR 15
1800 FOR K=1 TO LAST+1-FIRST
1810 LOCATE 7+K,13
1820 LINE INPUT V$
1830 IF V$="Q" OR V$="q" THEN COLOR 15,1,1:GOTO 1040
1840 IF V$<>"" THEN P(K+FIRST-1)=VAL(V$): ELSE LOCATE 7+K,12:
     PRINT P(K+FIRST-1)
1850 NEXT K
1860 COLOR 15,1,1
1870 GOTO 1040
1880 REM**********************
1890 REM* SIMULATION OPTIONS *
1900 REM**********************
1910 CLS
1920 COLOR 15,1,1
1930 LOCATE 5,20
1940 PRINT X$;" DEFAULT OPTIONS ";X$
1950 PRINT
1960 COLOR 7
```

```
1970 FILES"A:\*.DEF
1980 PRINT:PRINT
1990 PRINT TAB(20);"Select parameter default file: ";
2000 COLOR 15
2010 LINE INPUT DEFT$
2020 IF DEFT$="" THEN DEFT$="DEFAULT.DEF"
2030 GREET=1:GOTO 390
2040 CLS
2050 COLOR 15,1,1
2060 LOCATE 5,20
2070 PRINT X$;" SIMULATION OPTIONS ";X$
2080 PRINT
2090 COLOR 7
2100 PRINT TAB(20);"Available climate scenarios
2110 PRINT
2120 PRINT TAB(20);"1869";TAB(26);"C-type at minimum frequency
2130 PRINT TAB(20);"1969";TAB(26);"W-type at minimum frequency
2140 PRINT TAB(20);"1872";TAB(26);"C-type at maximum frequency
2150 PRINT TAB(20);"1938";TAB(26);"W-type at maximum frequency
2160 PRINT TAB(20);"1971";TAB(26);"A-type at maximum frequency
2170 PRINT TAB(20);"1908";TAB(26);"Long-term mean condition
2180 PRINT
2190 PRINT TAB(20);X$;X$;X$;X$
2200 COLOR 15
2210 PRINT:PRINT
2220 PRINT TAB(20);"Enter year of choice and press <RETURN> ";
2230 COLOR 7
2240 LINE INPUT F$
2250 IF F$="" THEN GOTO 700
2260 F$="A:\LWT"+F$+".REF"
2270 OPEN "I",#3,F$
2280 FOR I=1 TO 9
2290 LINE INPUT #3,LWT$
2300 FOR J=1 TO 8
2310 LWT(I-1,J)=VAL(MID$(LWT$,(1+((J-1)*7)),7))
2320 NEXT J
2330 NEXT I
2340 CLOSE #3
2350 CLS
2360 COLOR 15
2370 LOCATE 5,15
2380 PRINT X$;"---- CATCHMENT SELECTION ----";X$
2390 COLOR 7
2400 LOCATE 7,15
2410 PRINT "Available calibrated catchments
2420 PRINT
2430 PRINT TAB(15);"BEACON";TAB(24);"Mixed bracken and woodland,
     East Midlands
2440 PRINT TAB(15);"LI1";TAB(24);"Coniferous plantation, Lynn
     Brianne, Wales
2450 PRINT TAB(15);"LI6";TAB(24);"Unacidic moorland, Lynn Brianne,
     Wales
2460 PRINT TAB(15);"CI6";TAB(24);"Acidic moorland, Lynn Brianne,
     Wales
2470 PRINT
```

```
2480 PRINT TAB(15);X$;X$;X$;X$;X$
2490 PRINT:PRINT
2500 COLOR 15
2510 PRINT TAB(15);"Enter name of catchment and press <RETURN> ";
2520 COLOR 7
2530 LINE INPUT CAT$
2540 IF CAT$="" THEN COLOR 15,1,1:GOTO 700
2550 IF CAT$="Beacon" OR CAT$="BEACON" OR CAT$="beacon"
     THEN GOTO 2630
2560 IF CAT$="CI6" OR CAT$="ci6" OR CAT$="LI6" OR CAT$="li6" OR
     CAT$="LI1" OR CAT$="li1" THEN GOTO 2570 ELSE BEEP:GOTO 2350
2570 CAT$="A:\"+CAT$+".REF"
2580 OPEN "I",#3,CAT$
2590 FOR I=1 TO 19
2600 LINE INPUT #3,R$
2610 P(I+4)=VAL(R$)
2620 NEXT I
2630 CLOSE #3
2640 REM*****************************************************
2650 REM*   SCAM MODEL ALGORITHM - INITIALISING VARIABLES    *
2660 REM*****************************************************
2670 CLS
2680 COLOR 11
2690 LOCATE 5,20
2700 PRINT"LOADING PARAMETER VALUES
2710 DEFT$="A:\"+"DEFAULT.REF"
2720 OPEN "O",#3,DEFT$
2730 FOR I=1 TO 85
2740 PRINT #3,TAB(5);"P";I;TAB(10);P(I);TAB(20);DESC$(I)
2750 NEXT I
2760 CLOSE #3
2770 LOCATE 7,20
2780 PRINT"INITIALISING VARIABLES
2790 DAY=CINT((P(3)-1)*30.5)+P(2)-1
2800 SMD=P(8)
2810 K=(P(17)-P(18))/(P(9)*P(14))
2820 N=1
2830 CEC=P(14)*P(16)
2840 YEAR=P(4)
2850 ROW=1
2860 FOR I=1 TO P(1)
2870 LOCATE 9,20
2880 COLOR 11:PRINT"PROCESSING DAY NUMBER "
2890 COLOR 14
2900 LOCATE 9,42
2910 IF DAY<10  THEN PRINT "      "
2920 LOCATE 9,42
2930 PRINT DAY
2940 COLOR 11
2950 LOCATE 9,50
2960 PRINT"OF"
2970 COLOR 14
2980 LOCATE 9,53
2990 PRINT YEAR
3000 DAY=DAY+1
```

```
3010 IF DAY>366 THEN RES(N,1)=YEAR:RES(N,14)=BS:YEAR=YEAR+1:
     N=YEAR-P(4)+1:DAY=1
3020 RN1=RND
3030 FOR J=1 TO 8
3040 LWTSUM=LWTSUM+LWT(ROW,J)
3050 IF LWTSUM>RN1 THEN ROW=J:LWTSUM=0:GOTO 3070
3060 NEXT J
3070 PROB=P(57+ROW)*(1+(N*P(57)))
3080 IF RND>PROB THEN RAIN=0:HIN=P(21)*(1+(N*P(22)*P(23))):
     GOTO 3130
3090 MRAIN=P(65+CINT(.5+((DAY-1)/30.5)))*P(ROW+48)
3100 RAIN=-MRAIN*P(7)*LOG(RND)*(1+(P(48)*N))
3110 HIN=RAIN*(1+(P(22)*N))*P(77+ROW)
3120 REM*************************
3130 REM* TEMPERATURE GENERATION *
3140 REM*************************
3150 MTEMP=P(27+CINT(.5+((DAY-1)/30.5)))
3160 ATEMP=P(24)+(N*P(27))
3170 TEMP=ATEMP+MTEMP+P(ROW+39)+((P(25)-P(24))*COS(-(DAY-P(26))*
     .017214))
3180 REM****************
3190 REM* PE GENERATION *
3200 REM****************
3210 IF TEMP>.6 THEN PE=P(6)*((10.64*TEMP)-5.9)/(80!-TEMP)
     ELSE PE=0
3220 REM*********************
3230 REM* HYDROLOGICAL MODEL *
3240 REM*********************
3250 IF SMD>=P(11) THEN PE=0
3260 SMD=SMD-RAIN
3270 IF SMD<P(10) THEN ROP=(P(10)-SMD)*P(12):SMD=SMD+ROP
     ELSE ROP=0
3280 IF SMD<P(9) THEN TFP=(P(9)-SMD)*P(13):SMD=SMD+TFP
     ELSE TFP=0
3290 SMD=SMD+PE
3300 QT=ROP+TFP
3310 REM***************************
3320 REM* SOIL ACIDIFICATION MODEL *
3330 REM***************************
3340 CEC=CEC-HIN+P(15)
3350 IF CEC<0 THEN CEC=0
3360 BS=CEC/P(16)
3370 IF SMD<0 THEN PH=P(18):GOTO 3410
3380 IF SMD<P(9) AND QT>0 THEN PH=P(18)+(K*BS*SMD):GOTO 3410
3390 IF QT=0 THEN HOUT=0:GOTO 3460
3400 PH=P(17)
3410 HOUT=QT*(10^(6-PH))
3420 CEC=CEC+HOUT
3430 REM****************
3440 REM* TOTAL RESULTS *
3450 REM****************
3460 RES(N,2)=RES(N,2)+RAIN
3470 RES(N,3)=RES(N,3)+QT
3480 RES(N,4)=RES(N,4)+HIN
3490 RES(N,5)=RES(N,5)+HOUT
```

```
3500 RES(N,6)=RES(N,6)+TEMP
3510 IF PH<P(19) AND QT>0 THEN RES(N,7)=RES(N,7)+1
3520 IF QT>1.5 THEN RES(N,8)=RES(N,8)+1
3530 IF QT=0 THEN RES(N,9)=RES(N,9)+1
3540 IF ROW=1 THEN RES(N,10)=RES(N,10)+1:GOTO 3570
3550 IF ROW=2 THEN RES(N,11)=RES(N,11)+1:GOTO 3570
3560 IF ROW=3 THEN RES(N,12)=RES(N,12)+1
3570 IF RAIN>0 THEN RES(N,13)=RES(N,13)+1
3580 NEXT I
3590 REM*************************************
3600 REM* SIMULATION COMPLETED - SAVING RESULTS *
3610 REM*************************************
3620 BEEP
3630 COLOR 13
3640 LOCATE 13,20
3650 PRINT"SIMULATION COMPLETED
3660 COLOR 11
3670 LOCATE 17,20
3680 PRINT"ENTER NAME FOR RESULTS FILE (<8 CHARACTERS)
3690 COLOR 14
3700 LOCATE 19,20
3710 PRINT"FILE NAME : ";
3720 LINE INPUT RES$
3730 IF RES$="" THEN RES$="RESULTS"
3740 RES$="A:\"+RES$+".DAT"
3750 OPEN "O",#3,RES$
3760 PRINT #3,"SUMMARY OF ANNUAL RESULTS FROM SCAM SIMULATION
3770 PRINT #3," "
3780 PRINT #3,"Date of simulation : ";DATE$;TAB(35);"Time :
     ";TIME$
3790 PRINT #3,"Simulation length : ";P(1);" days"
3800 PRINT #3,"Climate scenario : ";MID$(F$,4,7)
3810 PRINT #3,"Catchment : ";CAT$
3820 PRINT #3,"  "
3830 PRINT #3," "
3840 OPEN "I",#1,"a:\HEADERS.REF
3850 FOR I=1 TO 14
3860 LINE INPUT #1,H$
3870 HD$(I)=MID$(H$,1,8)
3880 FORM$(I)=MID$(H$,9,7)
3890 PRINT #3,TAB(1+((I-1)*10));HD$(I);
3900 NEXT I
3910 PRINT #3," "
3920 FOR I=1 TO N-1
3930 FOR J=1 TO 14
3940 IF J=6 THEN RES(I,J)=RES(I,J)/366
3950 IF J=14 THEN RES(I,J)=RES(I,J)*100
3960 PRINT #3, USING FORM$(J);RES(I,J);
3970 PRINT #3,TAB(J*10);
3980 RES(I,J)=0
3990 NEXT J
4000 PRINT #3," "
4010 NEXT I
4020 COLOR 15,1,1
4030 PRINT #3,"*"
```

```
4040 CLOSE #3:GOTO 700
4050 REM****************************
4060 REM* STATISTICAL SUMMARY MENU *
4070 REM****************************
4080 CLS
4090 COLOR 15,1,1
4100 LOCATE 5,20
4110 PRINT X$;" STATISTICAL SUMMARY ";X$
4120 PRINT
4130 GOSUB 5800
4140 REM
4150 REM****************************
4160 REM* STATISTICAL CALCULATIONS *
4170 REM****************************
4180 REM
4190 CLS
4200 COLOR 15,1,1
4210 LOCATE 3,10
4220 PRINT X$;" STATISTICAL SUMMARY OF ";STAF$;" ";X$
4230 COLOR 13
4240 V=0
4250 PRINT
4260 PRINT "VARIABLE";
4270 PRINT TAB(10);"MAXIMUM";
4280 PRINT TAB(20);"MINIMUM";
4290 PRINT TAB(32);"MEAN";
4300 PRINT TAB(42);"SDEV";
4310 PRINT TAB(52);"TREND";
4320 PRINT TAB(60);"R-SQUARED";
4330 PRINT TAB(70);"CONFIDENCE
4340 PRINT
4350 YAXIS=2:XAXIS=1
4360 FOR I=YAXIS TO 15
4370 FOR J=1 TO S
4380 IF I=15 THEN RES(J,I)=RES(J,5)/RES(J,2)
4390 IF RES(J,I)>ST(I,1) THEN ST(I,1)=RES(J,I)
4400 IF J=1 THEN ST(I,2)=RES(J,I)
4410 IF RES(J,I)<ST(I,2) THEN ST(I,2)=RES(J,I)
4420 ST(I,3)=ST(I,3)+RES(J,I)
4430 ST(I,4)=ST(I,4)+RES(J,XAXIS)
4440 ST(I,5)=ST(I,5)+(RES(J,I)*RES(J,XAXIS))
4450 ST(I,6)=ST(I,6)+(RES(J,XAXIS)^2)
4460 ST(I,7)=ST(I,7)+(RES(J,I)^2)
4470 NEXT J
4480 MEAN=ST(I,3)/S
4490 IF S<3 THEN GOTO 4620
4500 GRAD=((S*ST(I,5))-(ST(I,4)*ST(I,3)))/((S*ST(I,6))-
     (ST(I,4)^2))
4510 SDEV=0
4520 FOR J=1 TO S
4530 SDEV=SDEV+((RES(J,I)-MEAN)^2)
4540 NEXT J
4550 SDEV=(SDEV/(S-1))^.5
4560 R=(ST(I,5)-(ST(I,4)*ST(I,3)/S))/SQR((ST(I,6)-
     (ST(I,4)*ST(I,4)/S))*(ST(I,7)-(ST(I,3)*ST(I,3)/S)))
```

```
4570 IF R^2<1 THEN TSTAT=ABS((R*SQR(S-2))/SQR(1-R^2))
4580 IF S*(LOG((TSTAT^2)+S)-LOG(S))>10 THEN PF=99.99:GOTO 4610
4590 PF=((1+(TSTAT^2/(S-2)))^(-.5*(S-1)))*(.5*(S-1))/
     SQR(3.1416*(S-2)*.5*(S-2))
4600 PF=(1-PF)*100
4610 RSQ=(R^2)*100
4620 IF V=1 THEN GOTO 6650
4630 REM*****************************
4640 REM* STATISTICAL RESULTS TABLE *
4650 REM*****************************
4660 COLOR 11:PRINT HD$(I);
4670 COLOR 10
4680 PRINT TAB(10);
4690 PRINT USING FORM$(I);ST(I,1);
4700 PRINT TAB(20);
4710 PRINT USING FORM$(I);ST(I,2);
4720 PRINT TAB(30);
4730 PRINT USING FORM$(I);MEAN;
4740 IF S<3 THEN PRINT :GOTO 4830
4750 PRINT TAB(40);
4760 PRINT USING FORM$(I);SDEV;
4770 PRINT TAB(50);
4780 PRINT USING "###.####";GRAD;
4790 PRINT TAB(60);
4800 PRINT USING "###.## %";RSQ;
4810 PRINT TAB(71);
4820 PRINT USING "###.## %";PF
4830 ST(I,1)=0:ST(I,2)=0:ST(I,3)=0:ST(I,4)=0:ST(I,5)=0:
     ST(I,6)=0:ST(I,7)=0
4840 NEXT I
4850 PRINT
4860 COLOR 15
4870 PRINT TAB(10);X$;X$;X$;X$;X$;X$
4880 PRINT
4890 COLOR 14
4900 PRINT TAB(30);"Press <ENTER> to continue ";
4910 LINE INPUT ANY$
4920 GOTO 700
4930 REM************************
4940 REM* TIME SERIES ANALYSIS *
4950 REM************************
4960 CLS
4970 COLOR 15,1,1
4980 LOCATE 5,20
4990 PRINT X$;" TIME-SERIES PLOTS ";X$
5000 PRINT
5010 GOSUB 5800
5020 GOSUB 6140
5030 V=0
5040 GOSUB 5210
5050 GOTO 5020
5060 REM*********************
5070 REM* SCATTERGRAPH PLOT *
5080 REM*********************
5090 SCREEN 0:COLOR 15,1,1:CLS
```

```
5100 COLOR 15,1,1
5110 LOCATE 5,20
5120 PRINT X$;" SCATTERGRAPH PLOTS ";X$
5130 PRINT
5140 GOSUB 5800
5150 V=0
5160 GOSUB 6140
5170 V=1
5180 GOSUB 6140
5190 GOSUB 5210
5200 GOTO 5150
5210 REM
5220 REM*****************************************
5230 REM* SUBROUTINE FOR GRAPHICAL PRESENTATION *
5240 REM*****************************************
5250 REM
5260 SCREEN 2,,0,0
5270 CLS
5280 DRAW "bm 100,150"
5290 DRAW "r480 m-480,0 u100 M100,150"
5300 FOR I=1 TO S
5310 Y=150-(CINT(((RES(I,YAXIS)-MINY)/(MAXY-MINY))*100))
5320 X=100+(CINT(((RES(I,XAXIS)-MINX)/(MAXX-MINX))*480))
5330 IF V=1 THEN PSET(X,Y):GOTO 5350
5340 LINE -(X,Y)
5350 NEXT I
5360 IF V=1 THEN GOSUB 6600:GOTO 5390
5370 Y=150-CINT(((MEANY-MINY)/(MAXY-MINY))*100)
5380 LINE (X,Y)-(100,Y),,,&HAAAA
5390 REM
5400 REM PRINT X-AXES VALUES
5410 REM
5420 LOCATE 20,10
5430 PRINT MINX;
5440 FOR I=1 TO 4
5450 PRINT TAB(10+I*15);
5460 PRINT USING FORM$(XAXIS);(MINX+(I*(MAXX-MINX)/4));
5470 NEXT I
5480 PRINT
5490 LOCATE 22,38
5500 PRINT HD$(XAXIS);UNT$(XAXIS)
5510 REM
5520 REM PRINT Y-AXIS VALUES
5530 REM
5540 LOCATE 7,1
5550 PRINT USING FORM$(YAXIS);MAXY
5560 A=7
5570 FOR I=1 TO 3
5580 A=A+4
5590 LOCATE A,1
5600 YINT=(MAXY-(I*(MAXY-MINY)/3))
5610 PRINT USING FORM$(YAXIS);YINT
5620 NEXT I
5630 LOCATE 5,3
5640 PRINT HD$(YAXIS);" ";UNT$(YAXIS)
```

```
5650 LOCATE 3,30
5660 IF V=1 THEN PRINT" R-sq =";RSQ;TAB(50);"Conf =";PF:GOTO 5680
5670 PRINT "Time-Series For ";HD$(YAXIS);
5680 LOCATE 24,28
5690 PRINT"Press <ENTER> to continue";
5700 LINE INPUT ANY$
5710 SUMY=0
5720 SUMX=0
5730 MAXY=0
5740 MINY=0
5750 MAXX=0
5760 MINX=0
5770 V=0
5780 RETURN
5790 REM
5800 REM***************************************
5810 REM* SUBROUTINE TO LOAD RESULTS FILES *
5820 REM***************************************
5830 REM
5840 COLOR 11
5850 PRINT "Available files
5860 PRINT
5870 COLOR 14
5880 FILES"a:\*.dat
5890 PRINT
5900 COLOR 15:PRINT TAB(10);X$;X$;X$;X$;X$;X$
5910 COLOR 14
5920 PRINT:PRINT
5930 PRINT TAB(20);"Enter filename ";
5940 COLOR 15
5950 LINE INPUT STAF$
5960 IF STAF$="" THEN GOTO 700
5970 STAF$="A:\"+STAF$
5980 OPEN "I",#3,STAF$
5990 S=0
6000 COLOR 13
6010 PRINT:PRINT
6020 PRINT"LOADING DATA...."
6030 LINE INPUT #3,R$
6040 IF MID$(R$,1,1)="*" THEN GOTO 6110
6050 IF VAL(MID$(R$,1,7))<P(4) THEN GOTO 6030
6060 S=S+1
6070 FOR K=1 TO 14
6080 IF K>1 THEN RES(S,K)=VAL(MID$(R$,((K-1)*10),7)) ELSE
     RES(S,K)=VAL(MID$(R$,1,7))
6090 NEXT K
6100 GOTO 6030
6110 CLOSE #3
6120 RETURN
6130 REM
6140 REM*******************************
6150 REM* CALCULATE GRAPH DIMENSIONS *
6160 REM*******************************
6170 SCREEN 0 : COLOR 15,1,1
6180 CLS
```

```
6190 COLOR 15,1,1
6200 LOCATE 3,16
6210 PRINT X$;
6220 IF V=0 THEN PRINT" Y-AXIS";
6230 IF V=1 THEN PRINT" X-AXIS";
6240 PRINT " VARIABLE SELECTION ";X$
6250 XAXIS=1
6260 PRINT
6270 FOR I=1 TO 15
6280 COLOR 14:PRINT TAB(30);I;
6290 COLOR 7:PRINT TAB(40);HD$(I);UNT$(I)
6300 NEXT I
6310 PRINT
6320 PRINT TAB(16);X$;X$;X$;X$;"-------"
6330 PRINT
6340 COLOR 14
6350 PRINT TAB(20);"Select variable number and press <ENTER> ";
6360 LINE INPUT ANY$
6370 IF ANY$="" THEN FOR I=1 TO S: FOR J=1 TO 15: RES(I,J)=0:
     NEXT J: NEXT I:  V=0: GOTO 700
6380 IF V=0 THEN YAXIS=VAL(ANY$):XAXIS=1
6390 IF V=1 THEN XAXIS=VAL(ANY$):MAXX=0
6400 IF YAXIS<1 OR YAXIS>15 THEN BEEP:GOTO 6140
6410 SUMY=0
6420 FOR I=1 TO S
6430 IF V=1 THEN GOTO 6500
6440 IF YAXIS=15 THEN RES(I,YAXIS)=RES(I,5)/RES(I,2)
6450 IF RES(I,YAXIS)>MAXY THEN MAXY=RES(I,YAXIS)
6460 IF I=1 THEN MINY=RES(I,YAXIS):MINX=RES(I,1)
6470 IF RES(I,YAXIS)<MINY THEN MINY=RES(I,YAXIS)
6480 SUMY=SUMY+RES(I,YAXIS)
6490 IF V=0 THEN GOTO 6550
6500 IF XAXIS=15 THEN RES(I,XAXIS)=RES(I,5)/RES(I,2)
6510 IF RES(I,XAXIS)>MAXX THEN MAXX=RES(I,XAXIS)
6520 IF I=1 THEN MINX=RES(I,XAXIS)
6530 IF RES(I,XAXIS)<MINX THEN MINX=RES(I,XAXIS)
6540 SUMX=SUMX+RES(I,XAXIS)
6550 NEXT I
6560 MEANY=SUMY/S
6570 IF V=0 THEN MAXX=RES(S,XAXIS)
6580 RETURN
6590 REM
6600 REM*********************************************
6610 REM* SUBROUTINE TO COMPUTE/PLOT REGRESSION LINE *
6620 REM*********************************************
6630 REM
6640 GOTO 4360
6650 C=MEAN-(ST(YAXIS,4)*GRAD/S)
6660 FOR I=1 TO 7:ST(YAXIS,I)=0:NEXT I
6670 Y1=(GRAD*MINX)+C
6680 Y2=(GRAD*MAXX)+C
6690 Y1=150-(CINT(((Y1-MINY)/(MAXY-MINY))*100))
6700 Y2=150-(CINT(((Y2-MINY)/(MAXY-MINY))*100))
6710 LINE(100,Y1)-(580,Y2),,,&HAAAA
6720 RETURN
```

```
6730 REM
6740 REM*******************************************
6750 REM* SUBROUTINE TO SAVE MODIFIED PARAMETER SET *
6760 REM*******************************************
6770 REM
6780 LOCATE 22
6790 COLOR 14:PRINT TAB(24);"Enter (<8 characters) filename";
6800 COLOR 15,1,1
6810 LINE INPUT PARAF$
6820 IF PARAF$="" THEN GOTO 6910
6830 IF LEN(PARAF$)>8 THEN BEEP:GOTO 6780
6840 PARAF$="A:\"+PARAF$+".DEF"
6850 OPEN "O",#1,PARAF$
6860 FOR I=1 TO 85
6870 PRINT #1,I;TAB(6);P(I);TAB(23);DESC$
6880 NEXT I
6890 PRINT #1,"999"
6900 CLOSE #1
6910 RETURN
```

PLATES: THE BEACON CATCHMENT, CHARNWOOD

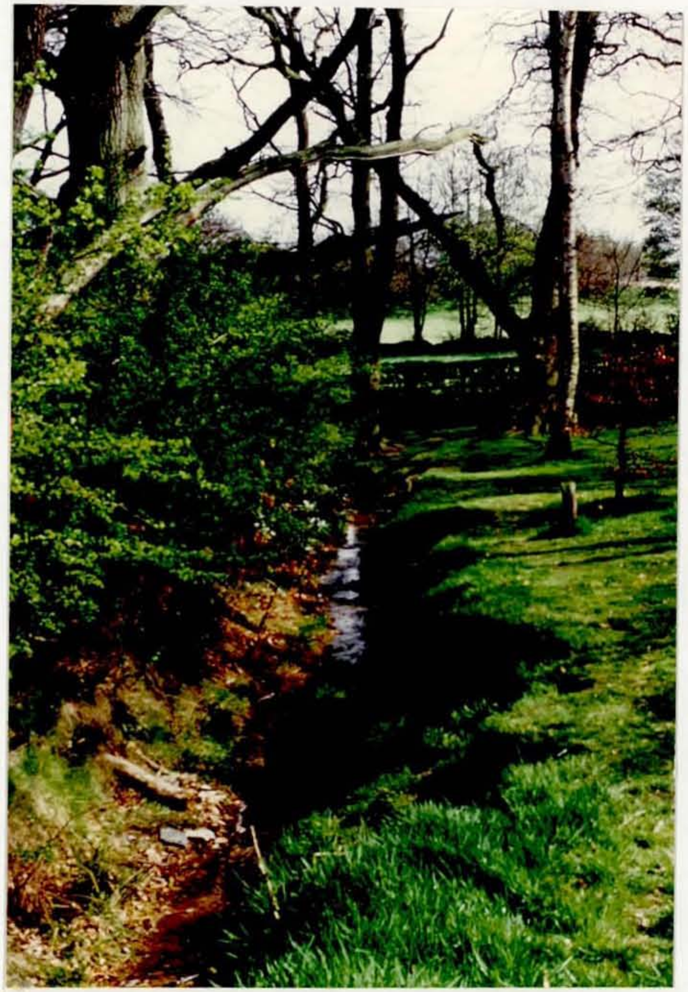

Plate 1: The main channel and catchment outlet

Plate 2: The outlet of a tile-drain

Plate 3: Birches Pond

Plate 4: Upslope of Birches Pond

Plate 5: View of the mixed woodland zone

Plate 6: The summit of the Beacon catchment