**Supplementary Material**

**Hydrothermal carbonisation of mixed agri-food waste: Process optimisation and mechanistic evaluation of hydrochar inorganic chemistry**

**Authors**

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Table S1. Analysis of variance (ANOVA) of the regression model for prediction of hydrochar yield

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Source** | **Sum of squares** | **Degree of freedom** | **Mean square** | **F Value** | **p-value (Prob > F)** |
| **Model** | 1445.6985 | 9 | 160.633 | 146.4959 | <0.0001 |
| T | 377.43627 | 1 | 377.4363 | 344.2184 | <0.0001 |
| **t** | 12.56785 | 1 | 12.5679 | 11.3706 | 0.0014 |
| SL | 736.16440 | 1 | 736.1644 | 671.3751 | <0.0001 |
| T × t | 51.53870 | 1 | 51.5387 | 47.0028 | <0.0001 |
| T × SL | 34.92094 | 1 | 34.9209 | 31.8476 | <0.0001 |
| t × SL | 11.05684 | 1 | 11.0568 | 10.0837 | 0.0026 |
| T2 | 72.00227 | 1 | 72.0023 | 65.6654 | <0.0001 |
| t2 | 0.61979 | 1 | 0.6198 | 0.5652 | 0.4557 |
| SL2 | 18.17455 | 1 | 18.1745 | 16.5750 | 0.0002 |
| **Residual** | 54.8251 | 50 | 1.097 |  |  |
| **Lack of Fit** | 23.401228 | 5 | 4.68025 | 6.7023 | <0.0001 |
| **Pure Error** | 31.423894 | 45 | 0.69831 |  |  |
| **Cor Total** | 1500.5236 | 59 |  |  |  |

Table S2. Analysis of variance (ANOVA) of the regression model for prediction of higher heating value

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Source** | **Sum of squares** | **Degree of freedom** | **Mean square** | **F Value** | **p-value (Prob > F)** |
| **Model** | 148.45082 | 9 | 16.4945 | 105.3811 | <0.0001 |
| T | 126.25957 | 1 | 126.2596 | 806.6536 | <0.0001 |
| **t** | 16.83003 | 1 | 16.8300 | 107.5246 | <0.0001 |
| SL | 0.15038 | 1 | 0.1504 | 0.9608 | 0.3317 |
| T × t | 0.13157 | 1 | 0.1316 | 0.8406 | 0.3636 |
| T × SL | 0.01274 | 1 | 0.0127 | 0.0814 | 0.7766 |
| t × SL | 1.19662 | 1 | 1.1966 | 7.6450 | 0.0080 |
| T2 | 3.19599 | 1 | 3.1960 | 20.4187 | <0.0001 |
| t2 | 0.11505 | 1 | 0.1151 | 0.7350 | 0.3953 |
| SL2 | 0.10304 | 1 | 0.1030 | 0.6583 | 0.4210 |
| **Residual** | 7.82613 | 50 | 0.1565 |  |  |
| **Lack of Fit** | 2.0317900 | 5 | 0.406358 | 3.1559 | 0.0159 |
| **Pure Error** | 5.7943431 | 45 | 0.128763 |  |  |
| **Cor Total** | 156.27695 | 59 |  |  |  |

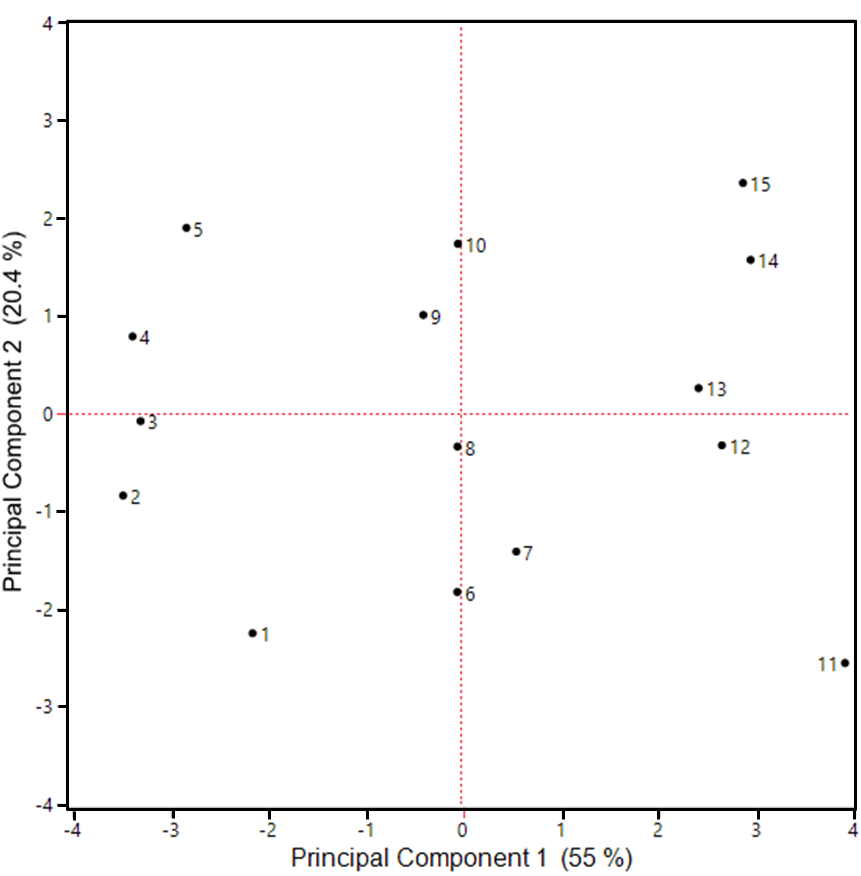
[[Table S3](https://lunet-my.sharepoint.com/personal/cvfok_lunet_lboro_ac_uk/Documents/PROGRESSION/R3/MANUSCRIPT%201/Supplementary%20data.docx?web=1)](https://lunet-my.sharepoint.com/personal/cvfok_lunet_lboro_ac_uk/Documents/PROGRESSION/TOWARDS%20R1/MANUSCRIPT/JBAB-S-21-00256_word.docx?web=1). Analysis of variance (ANOVA) of the regression model for prediction of ash content

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Source** | **Sum of squares** | **Degree of freedom** | **Mean square** | **F Value** | **p-value (Prob > F)** |
| **Model** | 75.536712 | 9 | 8.39297 | 27.8725 | <0.0001 |
| T | 0.241203 | 1 | 0.24120 | 0.8010 | 0.3751 |
| **t** | 1.256653 | 1 | 1.25665 | 4.1733 | 0.0464 |
| SL | 59.473920 | 1 | 59.47392 | 197.5092 | <0.0001 |
| T × t | 2.419350 | 1 | 2.41935 | 8.0345 | 0.0066 |
| T × SL | 4.216817 | 1 | 4.21682 | 14.0038 | 0.0005 |
| t × SL | 0.470400 | 1 | 0.47040 | 1.5622 | 0.2172 |
| T2 | 5.282000 | 1 | 5.28200 | 17.5412 | 0.0001 |
| t2 | 2.952027 | 1 | 2.95203 | 9.8035 | 0.0029 |
| SL2 | 1.442727 | 1 | 1.44273 | 4.7912 | 0.0333 |
| **Residual** | 15.055986 | 50 | 0.30112 |  |  |
| **Lack of Fit** | 9.440875 | 5 | 1.88817 | 15.1320 | <0.0001 |
| **Pure Error** | 5.615111 | 45 | 0.12478 |  |  |
| **Cor Total** | 90.592698 | 59 |  |  |  |

Table S4. Inorganic elemental composition of the hydrochar at different HTC operating conditions

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | mg/kg (dry basis) | | | | | | | |
| Sample\* | Al | Ca | Fe | K | Mg | P | S | Si |
| 190-1-5 | 491 | 2835 | 303 | 898 | 116 | 171 | 627 | 62 |
| 190-5-5 | 397 | 2263 | 229 | 762 | 108 | 136 | 541 | 21 |
| 210-3-5 | 455 | 1223 | 299 | 754 | 117 | 135 | 523 | 30 |
| 230-1-5 | 487 | 589 | 337 | 658 | 160 | 245 | 519 | 30 |
| 230-5-5 | 450 | 1295 | 369 | 900 | 175 | 613 | 631 | 35 |
| 190-3-12.5 | 395 | 2865 | 228 | 2518 | 239 | 325 | 633 | 29 |
| 210-1-12.5 | 512 | 2520 | 327 | 2308 | 233 | 332 | 602 | 39 |
| 210-3-12.5 | 428 | 2208 | 289 | 2278 | 257 | 434 | 651 | 37 |
| 210-5-12.5 | 375 | 1795 | 286 | 2040 | 256 | 611 | 661 | 27 |
| 230-3-12.5 | 468 | 1465 | 394 | 2638 | 314 | 793 | 712 | 36 |
| 190-1-20 | 494 | 3225 | 270 | 4813 | 478 | 708 | 946 | 52 |
| 190-5-20 | 371 | 3115 | 272 | 4730 | 397 | 585 | 773 | 21 |
| 210-3-20 | 424 | 2315 | 294 | 3898 | 405 | 745 | 746 | 32 |
| 230-1-20 | 376 | 2195 | 346 | 5585 | 531 | 893 | 801 | 31 |
| 230-5-20 | 378 | 2375 | 380 | 5613 | 553 | 1101 | 854 | 55 |

\*Samples are denoted as “Temperature (℃)-time (hr)-solid loading (%)” sequence.

(a) 

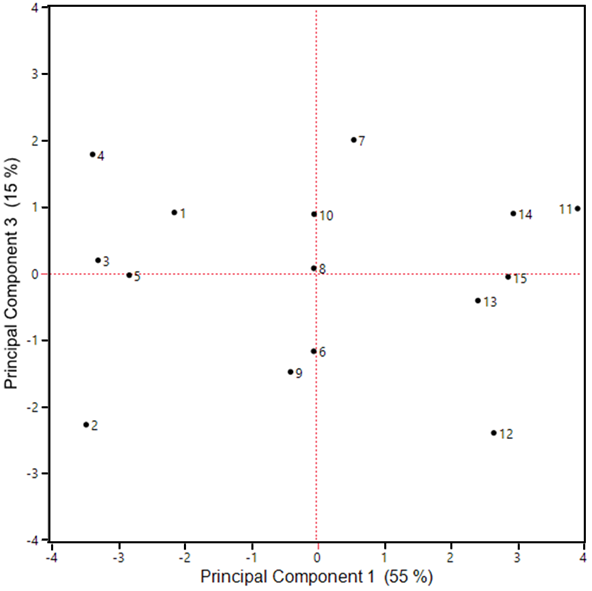
(b)

Fig. S1. Score plot showing relationship between experimental runs (a) based on principal component 1 and 2 (b) based on principal component 1 and 3.

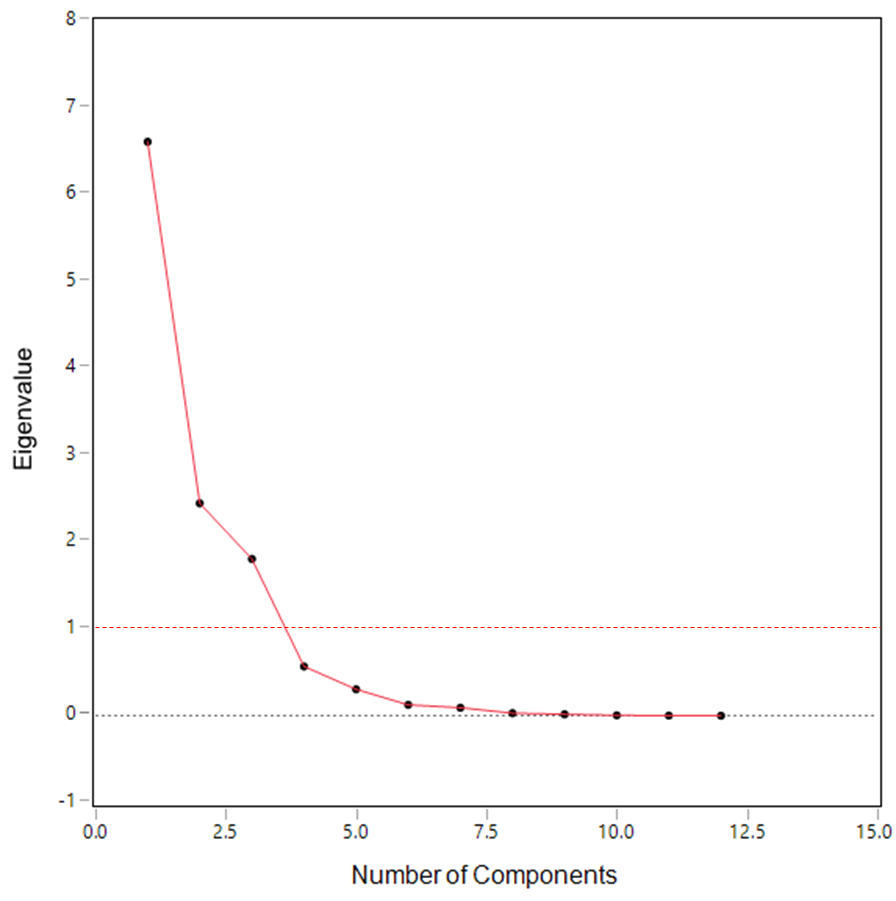


Fig. S2. Scree plot of eigen values of each principal component for selection of relevant principal component. Principal component with eigen value greater than 1 was the selection criterion [1].

A group of graphs showing different types of data

Description automatically generated with medium confidence

Figure S3 Analysis of the effect of operating parameter on fouling and slagging tendency using main effect plot. A main effect plot shows the mean of the responses across the level of each factor.

# **References**

[1] Abdi H, Williams LJ. Principal component analysis. Wiley Interdiscip Rev Comput Stat 2010;2:433–59. https://doi.org/10.1002/WICS.101.