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Abstract

Accurate analysis of heat transfer with phase change is important for many natural phenomena and engineering applications. Modelling of this phenomenon is a challenging mathematical problem due to the multi-physical nature of the processes involved. The phase transition introduces strong non-linearity caused by rapid variations of thermo-physical properties of the material and release of latent heat of solidification or evaporation. We present a non-local approach for modelling heat diffusion with phase change (solidification) by developing a bond-based Peridynamic formulation that considers the enthalpy form of the heat transfer equation. The material domain is categorised into three regions - liquid, mushy and solid - separated by temperature-dependent boundaries. We present results obtained by the proposed model and compare them with the 1D analytical solution of a test problem. The comparison demonstrates that the model can predict accurately the position of the phase change front and the temperature distribution. Our approach can be used for coupled modelling of materials' behaviour at various temperatures and phase states.

Key words: *Peridynamics; heat transfer; phase change; Stephan problem*

1 Introduction

A wide range of problems in natural and engineered materials involve heat transfer with phase change between solid and liquid. Examples are the seasonal and artificial freezing of soil; metal, polymer and ceramic casting and thermal energy storage systems based on latent heat. Such problems are associated with evolving inter-phases, i.e. strong discontinuities in the mathematical description of the problem, rendering local (differential) formulations inappropriate and calling for non-local approaches. One approach is Peridynamics (PD), where the partial differential equations of a local theory are replaced by a set of integral-differential equations. This results in a mathematically consistent formulation, even in the presence and evolution of strong discontinuities. The first application of the classical bond-based PD formulation for thermal diffusion problems was described in [5, 6]. However, PD formulations for problems with phase change have not been developed to date. We present for the first time a bond-based PD model for the problem of heat diffusion with phase change. Our model is based on the enthalpy form of the heat transfer equation, presented firstly in the local form in Section 2 and then in PD form in Section 3. A verification exercise is presented in Section 4, by which the PD results are compared against the 1D analytical solution to the problem [1].

2 Local formulation for heat diffusion with phase change

The heat diffusion is governed by Fourier's law:

$$\mathbf{q}(\mathbf{x},t) = -K(\mathbf{x},T)\nabla T(\mathbf{x},t) \tag{1}$$

where $\mathbf{q}(\mathbf{x},t)$ is the heat flux, $K(\mathbf{x},T)$ is the thermal conductivity, and $T(\mathbf{x},t)$ is the temperature - all at spatial position $\mathbf{x}$ and time t.
The energy conservation in the enthalpy form reads [1]:

$$\frac{\partial \rho(\mathbf{x},T)H(T,\mathbf{x},t)}{\partial t} = \nabla \cdot K(\mathbf{x},T)\nabla T(\mathbf{x},t) \tag{2}$$

where $\rho(\mathbf{x},T)$ is the material density, and $H(T,\mathbf{x},t)$ is the enthalpy at position $\mathbf{x}$.

Analytical solution to Eq. (2) exists for the 1D heat transfer problems for which $\rho(\mathbf{x},T)=const$ and the average thermal properties of the material are only depending on the phase state [1]. We consider the thermal properties in the same way to facilitate comparison.
The domain is divided to three regions: (i) solid region, with temperature $T<T_s$, where T_s is the temperature below which all material is in solid state; (ii) mushy region with temperature $T_s\leq T\leq T_l$, where T_l is the temperature above which all material is in liquid state; and (iii) liquid region, with $T_l<T$.
For the enthalpy function $H(T,\mathbf{x},t)$ we assume that the latent heat of solidification is linearly dependent on temperature, so that:

$$H(T,\mathbf{x},t)=\begin{cases} C_sT(\mathbf{x},t) & \text{for} \quad T(\mathbf{x},t)\leq T_s \quad \text{solid} \\ C_sT_s+\left(T(\mathbf{x},t)-T_s\right)\bar{C}_m+\frac{T(\mathbf{x},t)-T_s}{T_l-T_s}L & \text{for} \quad T_s<T(\mathbf{x},t)<T_l \quad \text{mushy} \\ C_sT_s+\left(T_l-T_s\right)\bar{C}_m+L+C_l\left(T(\mathbf{x},t)-T_l\right) & \text{for} \quad T_l\leq T(\mathbf{x},t) \quad \text{liquid} \end{cases} \tag{3}$$

where C_s, $\bar{C}_m=\left(C_l-C_s\right)/2$ and C_l are the heat capacity of solid, mushy and liquid regions and L is the latent heat of solidification. Solving Eq. (3) for temperature $T(H,\mathbf{x},t)$ gives:

$$T(H,\mathbf{x},t)=\begin{cases} H(\mathbf{x},t)/C_s & \text{for} \quad H(\mathbf{x},t)\leq H_s \quad \text{solid} \\ \frac{\left(H(\mathbf{x},t)-C_sT_s\right)\left(T_l-T_s\right)}{L+\left(T_l-T_s\right)\bar{C}_m}+T_s & \text{for} \quad H_s<H(\mathbf{x},t)<H_l \quad \text{mushy} \\ \frac{H(\mathbf{x},t)-C_sT_s-\left(T_l-T_s\right)\bar{C}_m-L+C_lT_l}{C_l} & \text{for} \quad H_l\leq H(\mathbf{x},t) \quad \text{liquid} \end{cases} \tag{4}$$

We also assume that the thermal properties of the material vary linearly with temperature within the mushy region. Therefore the heat conductivity and the specific heat capacity are given by:

$$K(T)=\begin{cases} K_s & \text{for} \quad T(\mathbf{x},t)\leq T_s \quad \text{solid} \\ K_s+\frac{T(\mathbf{x},t)-T_s}{T_l-T_s}\left(K_l-K_s\right) & \text{for} \quad T_s<T(\mathbf{x},t)<T_l \quad \text{mushy} \\ K_l & \text{for} \quad T_l\leq T(\mathbf{x},t) \quad \text{liquid} \end{cases} \tag{5}$$

$$C(T)=\begin{cases} C_s & \text{for} \quad T(\mathbf{x},t)\leq T_s \quad \text{solid} \\ C_s+\frac{T(\mathbf{x},t)-T_s}{T_l-T_s}\left(C_l-C_s\right) & \text{for} \quad T_s<T(\mathbf{x},t)<T_l \quad \text{mushy} \\ C_l & \text{for} \quad T_l\leq T(\mathbf{x},t) \quad \text{liquid} \end{cases} \tag{6}$$

The lower indexes s and l in all equations refer to properties of the solid and the liquid states of the material, respectively.

3 Bond-based PD model and numerical implementation

In peridynamics, a body occupying a region $\mathbf{R}$ is considered to be a collection of arbitrary many, but distinct particles, as illustrated in Fig. 1. A particle at a position $\mathbf{x}$ interacts with (is connected to) all particles at positions $\mathbf{x}'$ within a certain finite region $\mathbf{H_x}$, referred to as the horizon of $\mathbf{x}$. The horizon radius is denoted by δ. In the bond-based PD, the term 'bond' refers to the interaction between two particles at positions $\mathbf{x}$ and $\mathbf{x}'$ [7]. A bond for the heat transfer problem is referred to as the 't-bond'. The peridynamic heat flux per unit volume along a 't-bond' depends on the distance between $\mathbf{x}$ and $\mathbf{x}'$. For the heat transfer problem with phase change we consider three bond types: solid-solid, interfacial, and liquid-liquid bonds.
Following [5, 6], the energy conservation equation in the enthalpy form in a single 't-bond' between particles at positions $\mathbf{x}$ and $\mathbf{x}'$ is

$$\rho\frac{\partial\bar{H}(T,\mathbf{x}',\mathbf{x},t)}{\partial t}=K(\mathbf{x},\mathbf{x}',t)\frac{T\left(\mathbf{x}',t\right)-T\left(\mathbf{x},t\right)}{\left\|\mathbf{x}-\mathbf{x}'\right\|^2}\cdot\frac{\mathbf{x}-\mathbf{x}'}{\left\|\mathbf{x}-\mathbf{x}'\right\|} \tag{7}$$

where $K(\mathbf{x},\mathbf{x}',t)=[K(\mathbf{x},t)+K(\mathbf{x}',t)]/2$ is the thermal conductivity of the 't-bond', calculated from the conductivities $K(\mathbf{x},t)$ and $K(\mathbf{x}',t)$ at positions $\mathbf{x}$ and $\mathbf{x}'$, respectively.

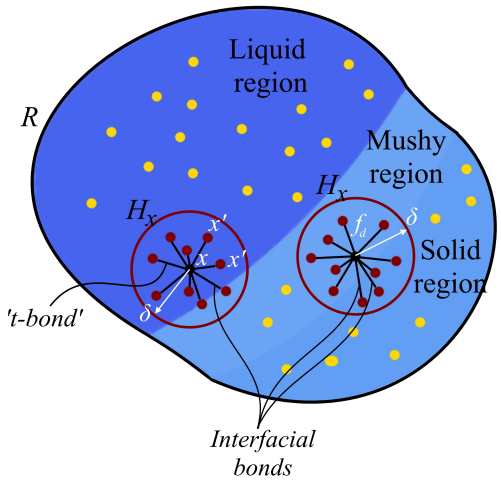

Figure 1: Peridynamic horizon and thermal bonds ('t-bonds')

The energy conservation at point $\mathbf{x}$ involves the heat fluxes from all adjacent bonds and is obtained by integrating Eq. (7) over the horizon $\mathbf{H_x}$. Following [5], the equation describing the enthalpy evolution in a particle at position $\mathbf{x}$ is:

$$\rho\frac{\partial H(T,\mathbf{x},t)}{\partial t} = \int_{\mathbf{H_x}} k(\mathbf{x},\mathbf{x}',t)\frac{T\left(\mathbf{x}',t\right)-T\left(\mathbf{x},t\right)}{\left\|\mathbf{x}-\mathbf{x}'\right\|^2}\mathbf{dV}_{\mathbf{x}'} \tag{8}$$

where $\mathbf{V}_{\mathbf{x}'}$ is the volume of the t-bond between particles at $\mathbf{x}$ and $\mathbf{x}'$, and $k(\mathbf{x},\mathbf{x}',t)$ is the peridynamics microscopic thermal diffusivity. For the 1D case, this is related to the macroscopic thermal diffusivity by $k(\mathbf{x},\mathbf{x}',t) = K(\mathbf{x},\mathbf{x}',t)/\delta$ [5].
The time integration of Eq. (8) is performed by the forward Euler finite difference method. The discretised form of this equation is:

$$H(T,\mathbf{x},t^{n+1}) = H(T,\mathbf{x},t^n) + \frac{\Delta t}{\rho}\sum_p \frac{K(x_p,t^n)+K(x_i,t^n))}{2\delta}\frac{T\left(\mathbf{x}_p,t^n\right)-T\left(\mathbf{x}_i,t^n\right)}{\left\|\mathbf{x}_p-\mathbf{x}_i\right\|^2}V_{ip} \tag{9}$$

4 Model verification

Considering the one-dimensional heat transfer problem with phase change, we analyse a semi-infinite region, $x \geq 0$. The spacing between peridynamic particles is $0.002m$ and the horizon size is $\delta = 0.006m$.
The average thermal properties of the material are: $K_l = 0.6$ W m^{-1} K^{-1}, $K_s = 2.14$ W m^{-1} K^{-1}, $C_s = 2060$ J kg^{-1} K^{-1}, $C_l = 4182$ J kg^{-1} K^{-1}, $\rho = 1000$ kg m^{-3}, $L = 334000$ J kg^{-1}.
The initial condition for the problem is $T\left(x,0\right) = 12°\text{C}$, and the boundary conditions are $T\left(0,t\right) = -30°\text{C}$ and $T\left(\infty,t\right) = 12°\text{C}$. The phase change temperatures are $T_l = -4°\text{C}$ and $T_s = -5°\text{C}$. The step for time integration is $\Delta t = 2s$.
The results from the PD simulation are compared with the analytical solution for this problem [1]. The phase front evolution and the temperature distribution, obtained by the analytical and the PD models are shown in Fig. 2. It can be seen that the proposed PD formulation reproduces the analytical solution with high accuracy, lending strong support for the model physical realism and its numerical implementation.

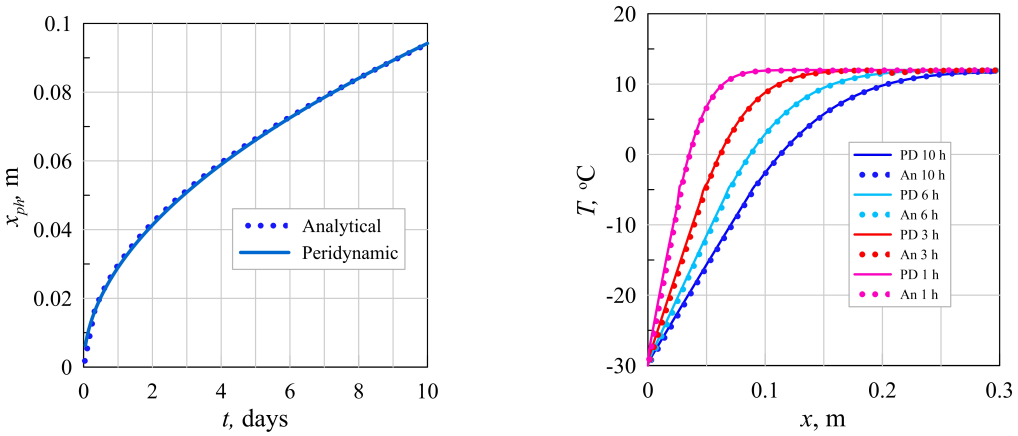

Figure 2: One-dimentional heat transfer with phase change according to the proposed PD model and analytical solution: Left figure shows the dynamic of phase front propagation; Right figure shows the temperature distribution at different time instances.

5 Conclusions

We presented a non-local approach for modelling heat diffusion with phase change by developing a bond-based Peridynamic formulation where the enthalpy form of the heat transfer equation is considered. The results obtained with the developed model were shown to be in excellent agreement with the 1D analytical solution, providing confidence in the theoretical and the implementation parts of the work. In particular, it was demonstrated that the proposed model could predict accurately the position of the inter-phase front and the temperature distribution. Our approach provides an advanced capability for couple modelling of thermal behaviour with phase change, specifically where discontinuities exists.

Acknowledgments

The financial support received by Petr Nikolaev in the form of a President doctoral scholarship award (PDS award) by the University of Manchester is gratefully acknowledged.

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