A Lattice Monte Carlo Approach for the Analysis of Transient Heat Transfer in Phase Change Materials

T. Fiedler1,*, I.V. Belova1, A. Öchsner1,2, G.E. Murch1

1University Centre for Mass and Thermal Transport in Engineering Materials
Priority Research Centre for Geotechnical and Materials Modelling
School of Engineering, The University of Newcastle
Callaghan, NSW 2308
AUSTRALIA

2Department of Applied Mechanics, Faculty of Mechanical Engineering
Technical University of Malaysia
81310 UTM Skudai, Johor
MALAYSIA

*Thomas.Fiedler@newcastle.edu.au http://livesite.newcastle.edu.au/cgmm

Abstract: - Heat sinks are used for the thermal management of electrical devices under cyclic temperature variation or the storage of thermal energy. To this end, phase change materials can store thermal energy in the form of latent heat at constant phase transition temperatures. The aim of this work is the numerical analysis of the transient heat transfer in composite structures containing phase change materials. A recently formulated Lattice Monte Carlo Method is applied to determine temperature distributions and the amount of energy transferred versus time.

Key-Words: - Heat Sinks, Phase Change Material, Transient Heat Transfer, Lattice Monte Carlo

1 Introduction

As passive thermal management systems for cyclic thermal loading heat sinks are continuously gaining importance, e.g. due to rapid developments in the electronic industry [1-3]. Alternative applications comprise solar energy storage where heat sinks decrease maximum temperatures during the daytime and provide heat at low temperatures [4,5] or are used for the heating of water [6,7]. In principle, every material can be used as a heat sink. However, engineering problems often put constraints on weight or volume and compact lightweight solutions are required. To this end, phase change materials (PCM) allow additional storage of thermal energy in the latent heat of the material [8]. Figure 1 schematically shows the interdependence of temperature $T$ and stored thermal energy per mass unit $Q / m$. At the phase transition temperature $T_\Delta$, the latent heat $L$ must be transferred before the temperature further increases. Essential requirements for PCMs are a high value of the heat of fusion $L$ and specific heat $C$, a suitable phase change temperature $T_\Delta$ with respect to operation temperatures, chemical stability and non-corrosiveness, a small volume change during the phase change and low cost. In addition, a high thermal conductivity is required.

An excellent material with respect to most of these requirements is paraffin. However, paraffin exhibits a low thermal conductivity. Recent approaches aim for the increase of its effective thermal conductivity by creating paraffin-metal [9] or paraffin-graphite [10] composite structures. Hong and Herling conducted experiments on open-cell aluminium foams filled with paraffin [11]. A distinct increase of cooling and heating times could be observed, potentially decreasing the thermal stress of a device.
under cyclic thermal loading. Analytical solutions for the transient heat transfer including phase change are limited to a few special cases [12] and are merely useful for validation purposes. A finite-difference method using an enthalpy-based model was presented in [13]. However, this interesting approach is restricted to relatively simple geometries and boundary conditions. The current work proposes the use of a recently formulated Lattice Monte Carlo (LMC) method [14]. A major advantage of the LMC method is the ability to address complex geometries, e.g. obtained by computed tomography [15]. In addition, further non-linearities such as temperature-dependent material properties [16] can readily be included in the calculation.

2 Methodology

In the following, a simple load case is considered where a constant temperature boundary condition \( T_c \) is defined at the edge of the geometry while the structure is initially at temperature \( T_i \) (cf. Fig. 2). Two cases can be distinguished: for \( T_i > T_\Delta \) the initial phase is liquid and \( T_c < T_\Delta \) must be valid in order to observe solidification. Analogously, \( T_i < T_\Delta \) imposes a solid PCM that melts starting from the boundary for \( T_c > T_\Delta \).

![Fig. 2. Temperature boundary conditions.](image)

Heat transfer is brought about by three different mechanisms: thermal radiation, thermal convection and thermal conduction. Inside solids and most liquids, the effect of thermal radiation has no significance. Also as a good approximation convective heat transfer can be disregarded because of the high viscosity of paraffin oil (approx. 1 Pa · sec). As a consequence, the heat transfer in the PCM or the copper ribs can be entirely characterized by thermal conduction.

### 2.1 Analytical Solution

Assuming incompressible material behavior, the maximum storable/available energy per unit mass of each material \( Q_j / m \) can be calculated by integration of

\[
\frac{Q_j}{m} = \int_{T_i}^{T_c} C(T) \, dT.
\]

In the case of composite materials, the arithmetic mean needs to be determined in order to obtain the effective thermal energy \( Q_{\text{eff}} \)

\[
\frac{Q_{\text{eff}}}{m} = \frac{1}{m} \sum_j \frac{Q_j \cdot m_j}{m} = \frac{\sum_j Q_j \cdot m_j}{m^2},
\]

where \( m \) is the total mass of the heat sink and \( m_j \) the mass of each material \( j \). This energy maximum is reached for steady state \( T \rightarrow T_c \).

For special cases, an analytical solution of the temperature distribution inside a phase change material exists. If the PCM is initially at temperature \( T_i > T_\Delta \) and \( T_c = 0 \) K then the following relations are valid [12]

\[
u_s(x,t) = \frac{T_\Delta}{\text{erf}(\lambda)} \text{erf} \left( \frac{x}{2 \sqrt{\kappa_t t}} \right),
\]

\[
u_l(x,t) = T_i - \frac{T_i - T_\Delta}{\text{erfc}(\lambda \sqrt{\kappa_s / \kappa_l})} \text{erfc} \left( \frac{x}{2 \sqrt{\kappa_l t}} \right),
\]

where \( \nu_s \) is the temperature inside the solid, \( \nu_l \) is the temperature inside the liquid phase and coordinate \( x \) describes the distance from the 0 K boundary condition. The variable \( t \) is the lapsed time and \( \kappa = K_l / (\rho \cdot C_l) \) is the thermal diffusivity of phase \( k \). For each phase, a constant density \( \rho \) needs to be presumed whereas the thermal conductivity \( K_l \) may vary. Finally, \( \lambda \) is a numerical parameter which can be determined by the solution of [12]

\[
e^{-\frac{x^2}{\kappa_t}} \frac{k_s \sqrt{\kappa_s} (T_i - T_\Delta) e^{-\frac{x^2}{\kappa_l}}}{k_s \sqrt{\kappa_s} \sqrt{T_i \text{erfc} \left( \frac{\kappa_s}{\sqrt{\kappa_l}} \right) \sqrt{C_s T_\Delta}}} = \frac{\lambda L \sqrt{\pi}}{C_s T_\Delta}.
\]
2.2 Lattice Monte Carlo Method

The LMC method is based on the fact that thermal diffusion is a random process that can be represented by random walks of particles on a discrete lattice. A comprehensive description and applications of the LMC method can be found in [14]. In a thermal LMC analysis, the random walks are performed by virtual thermal energy particles. The constant energy $E_p$ assigned to particles is defined by:

$$E_p = s^3 \left( \rho \cdot C(T) \right)_{\min} \frac{T_c}{n}$$

(5)

where $s$ is the length of a random jump from one lattice node to its nearest neighbour, $T_c$ is the constant temperature prescribed in the boundary condition and $n$ is the number of particles. $C(T)$ and $\rho$ denote the specific heat and density, respectively. If multiple phases or materials exist, the particular combination of phase and temperature resulting in the minimum product $\rho \cdot C(T)$ must be identified and used for the calculation of the particle energy. The number of particles $n$ can be selected freely; higher numbers of particles yield more accurate results, but of course longer computation times.

The random walks of the particles are directed by two parameters: the jump probability $p_{j,i}(T)$ (the scaled thermal conductivity $K$) and the selection probability $p_{s,i}(T)$ (the scaled inverse product $\rho \cdot C_i(T)$). Both jump and selection probabilities depend on the material parameters of the region $i$ and on the temperature $T$. The jump and selection probabilities $p_{j,i}(T)$ and $p_{s,i}(T)$ are required to have values between zero (the event never occurs) and unity (the event always occurs). Then the jump probability in a phase must be scaled with respect to the highest thermal conductivity to make:

$$p_{j,i}(T) = \frac{K_i(T)}{K(T)_{\max}}$$

(6)

The selection probability $p_{s,i}(T)$ is scaled with respect to the lowest $\left( \rho \cdot C(T) \right)_{\min}$ already used in Eq. (5):

$$p_{s,i}(T) = \frac{\left( \rho \cdot C(T) \right)_{\min}}{\rho_i \cdot C_i(T)}$$

(7)

According to Eq. (7), materials with a high specific heat and density possess a low selection probability. The increased number of unsuccessful jump attempts due to low values of $p_{s,i}(T)$ in effect simulates an accumulation of thermal energy in that phase.

Prior to LMC analysis, initial and boundary conditions need to be implemented (cf. Fig. 2). To this end, a global reference temperature $T_{\text{ref}}$ is introduced. This temperature corresponds to zero thermal energy particles present at a lattice node and is therefore the minimum temperature any node can exhibit. Next, virtual thermal particles are added to each node until the initial temperature $T_{\text{init}}$ is reached. For obvious reasons $T_{\text{ref}} \leq T_{\text{init}}$ is required. The number of virtual particles required depends on the local density $\rho$ and specific heat $C_i(T_{\text{init}})$ and can be obtained using Eq. (8). In addition, at one of the free surfaces of the lattice model, a constant temperature boundary condition $T_c \equiv T_{\text{ref}}$ is prescribed. To this end, additional particles are added or removed until the condition $T = T_c$ is fulfilled. The temperature $T$ at a node with coordinates $(x,y,z)$ and time $t$ can be obtained from the relation:

$$T(x,y,z,t) = \frac{n(x,y,z,t) \cdot E_p}{s^3 \cdot \rho \cdot C_{p,i}(T)} + T_{\text{ref}}$$

(8)

where $n(x,y,z,t)$ is the number of energy particles present at the node and the constant particle energy $E_p$ is defined according to Eq. (5). It is important to note that Equation (8) is only valid for temperatures $T \neq T_{\lambda}$. For example, a solid that exceeds the phase change temperature enters the two-phase area represented by the constant temperature line in Fig. 1. During the phase change, additional particles that enter the site are ‘destroyed’ and do not increase $n(x,y,z,t)$. Instead, the latent heat $L$ of the node is incrementally increased by $E_p$ until the phase change is completed for $L_n > L$.

In LMC analysis, time is modelled as discrete and represented by the variable $t_{\text{LMC}}$. At the beginning of the simulation the LMC time is equal to zero and incremented for each jump attempt by $1 / N_{\text{tot}}$. The variable $N_{\text{tot}}$ is the total number of virtual energy particles currently present in the system and may change during the calculation due to a change of the internal energy of the system due to heat transfer. The derivation of the conversion of $t_{\text{LMC}}$ to real time $t$ has been shown elsewhere [14]:

$$t = \frac{t_{\text{LMC}} \cdot s^2 (\rho \cdot C(T))_{\min}}{6 \cdot \lambda(T)_{\max}}$$

(9)

At the beginning of each time-step, a particle is randomly selected. Next, a random number between
0 and 1 is generated and compared to the selection probability corresponding to the phase at that lattice site. If this random number is higher than the selection probability, the attempt is unsuccessful; the Monte Carlo time $t_{LMC}$ is increased and another particle is randomly chosen. Otherwise, a jump direction for the particle is randomly selected and, depending on the phases of the starting and target lattice sites, the jump probability $p_j$ is now determined. In the case that the jump attempt is successful, the coordinates of the particle are updated before $t_{LMC}$ is increased and a new particle is selected. In order to sustain the constant temperature boundary condition $T_c$, as soon as a particle leaves the boundary plane a new one is generated. Analogously, particles entering the starting plane are destroyed. Accordingly, the number of particles (or internal system energy) will increase over time for $T_c > T_i$ and decrease for $T_c < T_i$. The change of number of energy particles can be related to the total amount of thermal energy $Q(t)$ conducted into the structure at particular times $t$ ($N_i$ is the number of particles at the beginning of the simulation).

Within the LMC analysis, two different geometries are considered: homogeneous paraffin and a paraffin-copper composite (cf. Fig. 3 a) and b) respectively). The composite is assembled by alternating layers of paraffin and copper where the copper occupies 10% of the total volume. At the boundaries in $y$ and $z$ direction, periodic symmetry conditions are defined. According to the thermal boundary conditions shown in Fig. 2 a constant temperature $T_c$ is prescribed at the left side of the structures whereas the right side is thermally insulated ($\dot{Q} = 0$). The width of all structures in $x$-direction is 0.002 m.

![Fig. 3. Geometries and boundary conditions of the LMC analysis.](image)

## 3 Results

In the following, the results of the LMC analysis are presented. First, the temperature distributions are validated by comparison with the analytical solution given by Eq. (3). Next, the heating and cooling of

The PCM paraffin with and without copper ribs are considered.

### 3.1 Verification

Figure 4 shows the results of the analytical solution Eq. (3) and LMC simulations. The chosen temperature boundary conditions are $T_i = 350$ K and $T_c = 0$ K, the material properties of the solid and liquid phases of paraffin are: $K_s = 0.24$ W / (m·K), $C_s = 2200$ J / (kg·K) and $K_l = 0.15$ W / (m·K), $C_l = 2790$ J / (kg·K), respectively. The analytical solution (3) requires a constant density of both phases which is assumed to be $\rho = 800$ kg / m$^3$. In addition to the temperature profiles at times $t = 0.1$, 0.2 and 0.4 seconds the position of the phase boundary $X(t)$ is indicated in the graph. An excellent agreement between the analytical and numerical solutions is found.

![Fig. 4. Comparison of analytical and LMC solutions.](image)

### 3.2 Heating of Paraffin

The material parameters of the PCM paraffin are defined in section 3.1. However, in order to improve the accuracy of the numerical model the density of the solid phase is now defined as 891.2 kg / m$^3$. Using Eqs. (1) and (2) the maximum amounts of storable energy per unit mass $Q_{eff} / m$ for $T_i = 290$ K and $T_c = 500$ K can be calculated. The results are 717 kJ / kg for pure paraffin and 364 kJ / kg for a composite material where a copper matrix occupies 10% of the total volume. The material properties of copper are defined as $K_c = 386$ W / (m·K), $C_c = 385$ J / (kg·K) and $\rho_c = 8960$ kg / m$^3$ [17]. The values indicate that the copper distinctly decreases the maximum amount of $Q_{eff} / m$ since the metal has no phase transition within the considered temperature range and a low specific heat capacity in comparison to paraffin.

Figure 5 shows the transferred thermal energy per unit mass plotted versus time. In the case of pure
paraffin, energy is only slowly transferred. In the composite structure, periodic copper ribs increase the surface area of the PCM (cf. Fig. 3a) and, due to their high thermal conductivity, accelerate energy transport: at \( t = 1 \) sec approximately 1/3 more energy is transferred into the composite structure in comparison to pure paraffin. The results indicate that by varying the composition of paraffin-metal composites, heat sinks can be optimized between the requirements of maximum energy storage capacity and fast dynamic response. Increase of the fraction of metal accelerates energy transport but simultaneously decreases the maximum energy storage capacity.

Fig. 6. Two dimensional temperature maps: a) pure paraffin, b) copper-paraffin composite.

Two dimensional temperature maps are shown in Fig. 6 for the time \( t = 1 \) sec. Fig. 6 a) represents the case of pure paraffin. The temperature increases in proximity of the temperature boundary condition and the distribution in \( x \) direction can be approximated by a modified error function (cf. Eq. (3) or Fig. 4). A different picture emerges in Fig. 6 b) where high thermally conducting copper ribs protrude into the PCM. The temperature in the copper ribs rises rapidly, thereby storing a fraction of the thermal energy. Originating from the copper ribs, thermal energy is now transferred into the heat sinks resulting into a two dimensional temperature field. The temperature distribution is symmetrical with regard to the centerline of the copper rib.

### 3.3 Cooling of Paraffin

In the following, the inverse process of the heating process considered in section 3.2 is addressed. The initial temperature of the liquid paraffin is now \( T_c = 500 \) K and the constant temperature boundary condition is prescribed as \( T_i = 290 \) K. The specific internal energy is plotted versus time in Figure 7. Analogous to the heating, the composite structure releases energy faster than pure paraffin. Again, the explanation is the high thermal conductivity of the copper ribs. At \( t = 1 \) sec the composite structure reaches 90% of the analytical maximum. In comparison, the pure paraffin only releases 30% of the maximum amount of energy possible.
For the pure paraffin, the released energy after 1 second is approximately 8% lower than the energy stored in an inverse heating process (cf. Section 3.2). The reason is that in the case of heating, initially only solid paraffin exists whereas the cooling process starts with a superheated fluid. In addition, the thermal conductivity of solid paraffin exceeds the one of paraffin oil: \( K_s = 0.24 \text{ W} / (\text{m} \cdot \text{K}) > K_l = 0.15 \text{ W} / (\text{m} \cdot \text{K}) \). The deviation between stored and released energy of the composite is smaller (5 %), since the initial material properties of the copper ribs are independent of the load case. Accordingly, for both heat sinks energy is stored faster than it can be released.

4 Conclusion

The aim of this work was the LMC analysis of transient heat transfer in composite structures containing phase change materials. The validity of the numerical method was shown by comparison with an analytical solution for a simple case where excellent agreement was obtained. In addition, pure paraffin and a paraffin-copper composite structure where subjected to heating and cooling processes with phase change of the PCM. The composite structure allowed for faster energy transfer. In contrast, the pure PCM exhibits a higher maximum thermal energy storage capacity. Both heat sinks stored energy slightly faster than could be released to the environment.

References: