Lattice Boltzmann simulations to assess heating and cooling strategies of phase-change materials based on second-law analysis

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Abstract:

Phase change materials (PCMs), as storage means of latent heat, have recently become widely invested as alternative materials able to reduce energy consumption in buildings. However, for a proper integration in buildings thermal systems, the industry needs to optimize their performance. One of the key parameters in the assessment of these materials is the characterization of heating and cooling cycles. To achieve this, we propose, in this work, an optimization method based on the analysis of the second law of thermodynamics, namely, we intend to minimize the entransy dissipation. The simulations are performed using a thermal lattice Boltzmann model (TLBM), which is a mesoscopic method suitable for multi-phase problems in fluid and heat transfer. Moreover, the optimization is attained for the cases of pure conduction and conduction plus convection regimes. Theoretical solutions of the optimization problem are derived and then compared to the numerical results. Consequently, the achieved compatibility between analytical and numerical results proves the adequacy of the procedure. For the case of pure conduction, the optimal heating is via a hyperbolic function of exponent *(n = 0.33)*. On the other hand, for the mixed conduction plus convection regime, the optimal path is via a hyperbolic function of *(n = 0.5).* In the light of the obtained results, we can propose an optimal thermal path for the external fluid temperature surrounding (PCMs) within a latent heat storage system.

Keywords:

Lattice Boltzmann method, Phase-change materials, Entransy concept, Convection, Conduction, Heating, Cooling.

1. Introduction

Phase change materials (PCMs), as storage means of latent heat, have recently become widely invested as alternative materials able to reduce energy consumption in buildings. The number of studies concerning the integration of PCMs in buildings to improve their energy efficiency has been increasing during the last decade [1-6]. This shows the keen interest of researchers towards developing latent heat thermal energy systems (LHTES) to decrease the overall energy demand in buildings. However, for a proper integration, there is a vital need to optimize the performance of (PCMs). One of the key parameters in the assessment of these materials is the characterization of heating and cooling loads and cycles. The temperature response of (PCMs) depends upon the nature of the thermal loads applied to them. These solicitations are usually due to the modification of the external environment. Thus, it is reasonable to raise the question on how would the change in the external temperature affect the behavior of (PCMs). The examination of such an effect is important, however, this should be provoked by an optimization of the up-mentioned load. The analysis of the second law of thermodynamics is adequate to address issues related to storage (or

release) time duration and the temperature of the surroundings [5]. Hence, this work proposes the optimization of heating and cooling strategies based on the second law of thermodynamics. To do so, we choose the minimization of entransy dissipation as an objective.

Since the 70s, the analysis of the second law of thermodynamics has started entering into the design of thermal and chemical processes. These processes are usually considered in terms of either exergy (available energy) or irreversibility (entropy generation). Nevertheless, in this work, we will use the entransy concept to optimize the performance of (PCMs). This concept was brought by Guo et al. [7], where the entransy dissipation extremum approach was presented as an optimization criterion for heat transfer processes [8]. Recently, Xia et al. [9] extended the entransy theory to the optimization of solid-liquid phase-change (PC) processes taking the entransy dissipation minimization as the optimization objective. This choice is mostly suitable since phase-change processes are independent of the heat-work conversion [10].

The major aim of this work is to analytically derive the optimal heating and cooling strategies and compare them with the numerical simulation results. The used procedure is inspired from the work of [9] for one-dimensional conduction (PC) problem. However, we extend the method to handle 2D convective (PC), as an enhancement. The numerical simulations are performed using a single relaxation time lattice Boltzmann model (SRT-LBM) with the BGK-approximation [11,12]. This approach is a discrete-particles-based method that numerically solves the Boltzmann equation unlike the conventional methods that are based on the Navier-Stokes (NS) equations.

The paper is organized as follows: in section 2 we present the concept of the problem and methodology of handling it. Section 3 is dedicated for the minimization of entransy dissipation for pure conduction, while in section 4; we extend the procedure for convective regime. In section 5, we present how to can benefit from the optimal heating/cooling strategies in practical PCM applications. We then draw some conclusions in the last section.

2. Concept and methodology

Due to the presence of irreversibility, all transport processes contain two different types of physical quantities, the conserved ones and the non-conserved ones. The loss or dissipation in the non-conserved quantities can then be used as a measurement of the irreversibility in the transport process [13]. Based on this, Guo et al. [7,14] introduced the concept of entransy and defined it as the heat transfer ability of an object. This is equivalent to the heat transport potential capacity in analogy with electrical and heat conductions [14]. Entransy possesses both the nature of "energy" and the transfer ability. Subsequently, if an object is put in contact with an infinite number of heat sinks that have infinitesimally lower temperatures, the total quantity of "potential energy" of heat that can be output is the entransy and derived as [7,14],

$$G = \frac{1}{2}UT = \frac{1}{2}mc_vT^2, \qquad (1)$$

where c_v is the constant volume specific heat capacity, T is the temperature, m is the mass, U is the internal energy of an object and G is the entransy. Dividing the entransy by the volume gives the entransy density G' [7,14,15],

$$G' = \frac{1}{2}\rho c_vT^2, \qquad (2)$$

where ρ is the density.

Similarly to the electric charge, the fluid mass is also non-dissipative and conserved during fluid flow, while the mechanical energy is dissipated due to fluid friction. The dissipation of mechanical energy is a measure of the fluid friction induced-irreversibility of the fluid flow that is not involved in a thermodynamic cycle [15]. Consequently, the entransy dissipation caused by heat conduction and convection, can be defined as a measure of irreversibility during these processes.

To benefit from this concept, which is based on the second law of thermodynamics, we intend employ it for optimizing the time paths of the external temperature in phase-change materials (PCMs). As mentioned previously, one of the key parameters in the assessment of these materials is the characterization of heating and cooling loads and cycles. The temperature response of (PCMs) depends upon the nature of the thermal loads applied to them. These solicitations are usually due to the modification of the external environment. Thus, the type and rate of change in the external temperature affects the behavior of (PCMs). To investigate this effect, we analyze the entransy dissipation due to different external temperature loading. We then propose a method to optimize the strategy of loading through minimization of the entransy dissipation. This will be done analytically and then tested numerically for melting and solidification with conduction and convection. So, briefly the methodology is the following:

- Analytical derivation of the entransy dissipation;
- Optimization of the heating/cooling strategy by minimizing the entransy dissipation;
- Verify that the analytical and numerical results are equivalent.

3. Thermal lattice Boltzmann model (TLBM)

The TLBM [16,17] consists of simulating the statistical behaviour of a set of particles on a lattice with finite velocities. It stems from the discrete Boltzmann equation and allows providing macroscopic fluid properties such as density, velocity, pressure, etc. through weighted averages, or moments, of the particle distribution for all discrete lattice velocities. The SRT-LBM (also called the Bhatnagar-Gross-Krook (BGK) model [11]) for incompressible thermal flows builds on two distribution functions (DFs), f_i and g_i, and their corresponding evolution equations [18,19]. However, its extension to flows with heat transfer is not straightforward due to numerical instabilities engendered. In the thermal lattice Boltzmann method (TLBM), a separate DF is used to solve for the temperature. In other words, two sets of distribution functions are defined, one for the velocity field and the other for the temperature. Thereby, such an approach can easily handle arbitrary Prandtl numbers. This double distribution function (DDF) scheme has been successfully used to solve thermal problems in two dimensions. Nevertheless, it only applies when the fluid density depends weakly on the temperature. This is the approach we have adopted here to conduct this work, with the below defined evolution equations [16-19],

$$f_i\left(x+e_i,t+1\right)=f_i\left(x,t\right)-t_f^{-1}\left(f_i\left(x,t\right)-f_i^{eq}\left(x,t\right)\right)+F_b, \quad (3)$$

$$g_i\left(x+e_i,t+1\right)=g_i\left(x,t\right)-t_h^{-1}\left(g_i\left(x,t\right)-g_i^{eq}\left(x,t\right)\right)+S_h, \quad (4)$$

where e_i is the microscopic particle velocity in the i-direction, τ_f and τ_h are the dimensionless relaxation times, and f_i^{eq} and g_i^{eq} are local equilibrium distributions functions that can be computed from:

$$f_i^{eq}=\rho\omega_i\left[1+\frac{3(e_i.\vec{u})}{c_s^2}+\frac{9(e_i.\vec{u})^2}{2c_s^4}-\frac{3(\vec{u}.\vec{u})}{2c_s^2}\right], \quad (5)$$

and

$$g_i^{eq} = T\omega_i\left[1+\frac{e_i.\vec{u}}{c_s^2}\right], \qquad (6)$$

where $w_i = \begin{cases} 4/9 & for \quad i=0 \\ 1/9 & for \quad i=2,4,6,8 \\ 1/36 & for \quad i=0,3,5,9 \end{cases}$ and $e_i = \begin{cases} (0,0) & for \quad i=0 \\ (0,\pm1) & for \quad i=2,4 \\ (\pm1,0) & for \quad i=1,3 \\ (\pm1,\pm1) & for \quad i=5,6,7,8 \end{cases}$, (7)

are, respectively, the weight coefficient and the velocity vector of the *D2Q9* model; with, *u* and *v* representing velocities in the *x*- and *y*-directions, respectively. Note that the relaxation times τ_f and τ_h can be determined via $\nu = c_s^2\Delta t(\tau_f - 0.5)$ and $\alpha = c_s^2\Delta t(\tau_h - 0.5)$, c_s being the lattice sound speed. Likewise, additional terms $F_b = -\beta g_r(T-T_0)/(T_h-T_c)$ and $S_h = \pm Ste^{-1}(\partial\varepsilon/\partial t)$ are Boussinesq force which simulates natural convection and the source (or sink) term that handles the phase-change. The liquid fraction ε is computed from [20] as,

$$e = \begin{cases} 0 & h < h_s = c_p T_m \\ \dfrac{h - h_s}{h_l - h_s} & h_s \le h \le h_l = h_s + L_f, \\ 1 & h > h_l \end{cases} \qquad (8)$$

where *h* is the local enthalpy and T_m is the fusion temperature. It is useful to address that in the current model, the solid and liquid phases are defined according to the liquid fraction value. Therefore, the solid state is assigned when the value of ε is less than 0.5 (by convention). In this case, the velocity field is fully bounce-backed and the macroscopic velocity of the solid phase is set to zero.

Note that, to implement BCs in the current method, we are led to convert them, at mesoscopic level, in terms of distribution functions f_i and g_i. For the velocity field, the non-slip boundary conditions realised by the on-grid bounce-back (BB) on boundaries. On the other hand, to specify a constant temperature, we use the method proposed by Inamuro et al. [21]. As for the adiabatic BCs, the Neumann BCs are achieved using the BB boundary conditions for the distribution g_i, as prescribed for f_i.

Finally, the basic thermo-hydrodynamic properties, such as density, ρ, momentum density, ρu, and temperature, T, are defined as moments of the DFs, f_i and g_i, as follows,

$$r = \sum_{i=0}^{N=8} f_i, \quad ru = \sum_{i=0}^{N=8} e_i f_i, \text{ and } T = \sum_{i=0}^{N=8} g_i. \qquad (9)$$

3. Conduction and phase-change

3.1. Problem description

For the investigation of entransy dissipation concept in 1D conduction problem with phase-change, we adopt the same configuration depicted in [9]. Figure 1 shows a one-dimensional slab of

thickness *l*, which is perfectly insulated except where cooling or heating external temperature $T_s(t)$ is applied. The slab is initially all liquid (for freezing) or all solid (for melting) at the fusion temperature T_m. As a constraint for optimization, the freezing or melting process is fixed to occur in a given time denoted by t_0. Position along the slab is denoted by variable *x*, with and $x = \delta$ denoting the position of the phase boundary between liquid and solid during the freezing or melting process.

The aim here is to reproduce the analytical derivation of the optimized external temperature $T_s(t)$ time path, and test whether the numerical investigation will result in confounded results. And later extend the proposed procedure to handle the convective melting.

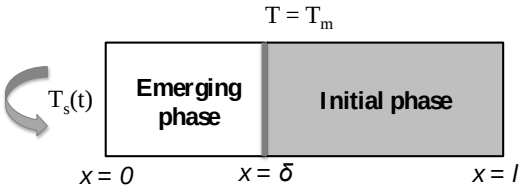

Fig. 1. 1D conduction solid-liquid phase-change schema.

3.2. Entransy dissipation calculation

The entransy dissipation rate per unit area of the slab is obtained as [9],

$$E = k\int_0^d \left(\frac{\partial T}{\partial x}\right)^2 dx, \qquad (10)$$

where *k* is the conductivity and δ is the position of the phase front. Hence, the entransy dissipation over the entire process from $t = 0$ to $t = t_0$ is,

$$DE = \int_0^{t_0} E\,dt. \qquad (11)$$

The Stefan condition for the time evolution of the phase boundary is given by,

$$r L d' = \pm k\left(\frac{\partial T}{\partial x}\right)_{x=d}, \qquad (12)$$

where *L* is the latent heat of fusion and δ' is the rate of the phase boundary propagation. By applying the adequate quasi-stationary approximation in the vicinity of small Stefan numbers [22,23], and as proved in [9], the optimisation of the time-dependent external temperature is the same as optimizing $\delta(t)$. The solution of the slab temperature is then given by,

$$T(x,t) = T_m \pm (r L / k) d'(x - d). \qquad (13)$$

By combining (10), (11), and (13), the entransy dissipation for the phase-change process is obtained as follows,

$$DE = \frac{r^2 L^2}{k} \int_0^{t_0} dd'^2 \, dt. \qquad (14)$$

3.3. Optimization procedure

The optimization problem is based on the calculation of the expression of the external temperature $T_s(t)$ corresponding to the minimum entransy dissipation of the phase-change process with a constraint of a fixed time t_0. To do so we follow the procedure proposed in [9], where the modified Lagrange is given by,

$$y = \frac{r^2 L^2}{k} dd'^2. \qquad (15)$$

The Euler-Lagrange equation to determine the optimal solution is then,

$$\frac{\partial y}{\partial d} - \frac{d}{dt}\left(\frac{\partial y}{\partial d'}\right) = 0. \qquad (16)$$

This yields to the below condition:

$$d'^2 + 2dd'' = 0, \qquad (17)$$

where $\delta'' = d^2\delta/dt^2$. By applying the known boundary conditions presented in Fig. 1, we obtain,

$$\frac{d}{l} = \left(\frac{t}{t_0}\right)^{2/3}, \qquad (18)$$

which gives the optimal dimensionless front phase position $\theta = \delta/l$ versus the dimensionless time $\zeta = t/t_0$ corresponding to the optimal heat exchange strategy that results in minimum entransy dissipation. Substituting (18) with its derivative in (13) and setting $x = 0$, we obtain:

$$T_s(t) = T_m \pm \frac{2 r L l^2}{3 k t_0}\left(\frac{t}{t_0}\right)^{1/3}. \qquad (19)$$

Therefore, to obtain an optimum response of this configuration based on the criterion of entransy dissipation the external temperature $T_s(t)$ should increase or decrease as per (19). So practically, as an application on (PCMs), how can this be employed? This is discussed thoroughly in section 5.

3.4. Numerical results

The numerical simulation of the conduction phase-change problem proposed in Fig. 1 implied the same results expected by the theoretical equations. The optimum thermal loading coincides with (19). In the light of these results, the numerical model is verified and the straightforward implementation of the lattice Boltzmann model proves the adequacy of this numerical method to handle such problems. The total entransy dissipation is plotted in Fig. 2 versus the exponent n in the general form (20), which reads as,

$$T_s(t) = T_m \pm B\left(\frac{t}{t_0}\right)^n . \qquad (20)$$

where $B = 2\rho Ll^2/3kt_0$ in lattice units, and n is an exponent varied from 0 till 0.5 to explore to what exponent the minimum entransy dissipation corresponds numerically. The simulations are performed on a phase-change material (PCM) namely Octadecane, whose Prandtl number is $Pr = 50$, and for a Stefan number $Ste(t) = 0.0084(T_s(t) - T_m)$. As deduced from Fig. 2, the minimum entransy dissipation, calculated by (14), is obtained for (20) at $n = 0.33 = 1/3$, and this conforms to the theoretical solution in (19).

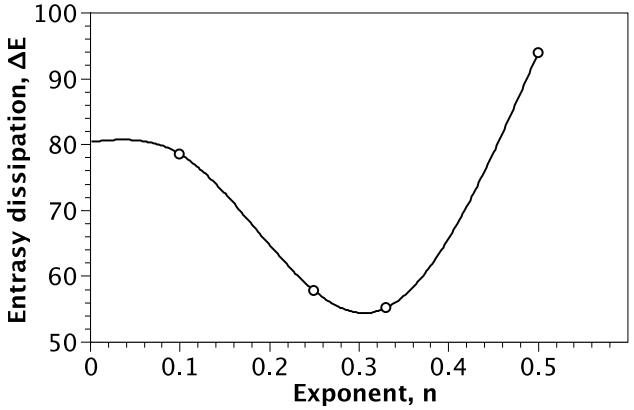

Fig. 2. Pure conduction: Entransy dissipation of phase-change versus the exponent n of (20).

4. Convection dominated phase-change

4.1. Problem description

The natural convection problem with phase-change studied by many researchers [22-30] is a complicated problem with no unified theoretical treatment [25], due to the strong coupling between the natural circulation of the liquid phase and the melting rate of the solid. It is this coupling that determines the instantaneous shape of the liquid-solid interface, which becomes one of the key unknowns in each problem [26]. Equation (14) is derived by considering the Neumann-problem with conduction only. Thus, we will try to derive, in this work, the entransy dissipation of phase-change with convection being the dominant heat transfer mode. For this, a 2D enclosure is considered as shown in Fig. 3, with $T_s(t)$ applied on the left side and having the fluid initially in solid state and at T_m. The other sides are considered adiabatic. At the beginning the conduction mode will be dominant, nevertheless, it is worth noting that an infinitesimally small convection heart transfer effect is present even when time tends to zero [26]. From here, we assume that considering the effect of convection for minimizing the entransy dissipation is crucial.

4.2. Entransy dissipation in convection dominated phase-change

The main difference in between conduction and convection melting is the shape and mode of propagation of the melting front. Under the effect of convection the upper part of the front recedes faster due to clockwise rotating velocity of the fluid. From [26], the vertical velocity scale of this very slender counter flow, v, is determined by the balance between the vertical buoyancy effect $g\beta(T_s - T_f)$, where T_f is the temperature at the melting front, and the vertical friction effect of thickness equal to that of the formed fluid, δ. Thus, the resulting velocity scale is at a time t,

$$v(t) \approx \frac{g\beta\left[T_s(t) - T_f\right]}{\nu} d^2 = \frac{k Ra(t)}{\rho c_p d}. \qquad (21)$$

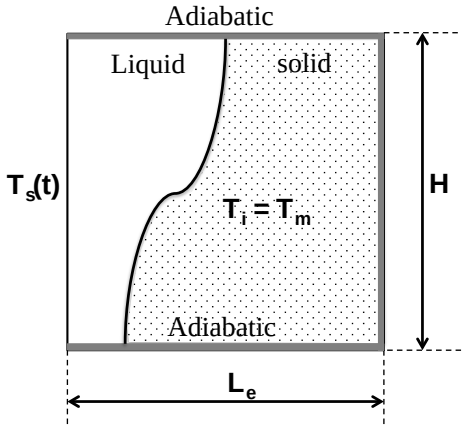

Fig. 3. 2D convection dominated solid-liquid phase-change schema.

The convective heat transfer rate carried upward by this counter flow is [26],

$$Q_c(t) \approx (\rho v \delta) c_p \left[T_s(t) - T_f\right], \qquad (22)$$

in which $(\rho v \delta)$ represents the vertical mass flow rate of one branch. The convective heat current Q_c originates from the bottom end of the hot wall, flows vertically through the fluid gap and is then absorbed by the top end of the liquid-solid interface. The total heat transfer rate in the horizontal direction is the sum of the conduction and convection contributions [26],

$$Q(t) \gg kH \frac{T_s(t) - T_f}{\delta} + Q_c(t). \qquad (23)$$

Dividing the enclosure in Fig. 3 to finite number of thin slabs, the position of the velocity of the melting front of slab *i* is now determined by [26],

$$\rho L \delta_i'(t) \gg k \frac{T_s(t) - T_f}{\delta} + \delta \rho v c_p \frac{T_s(t) - T_f}{\delta}. \quad (24)$$

Then we can substitute (21) to get,

$$\rho L \delta_i'(t) \gg k \frac{T_s(t) - T_f}{\delta}\bigg|_{cond} + kRa(t) \frac{T_s(t) - T_f}{\delta}\bigg|_{conv}. \qquad (25)$$

We will divide the rate of phase propagation as that caused by conduction effect and that caused by convection as, $\delta' = \delta'_{cond} + \delta'_{conv}$.

$$k \frac{T_s(t) - T_f}{\delta \rho L}\bigg|_{cond} = \delta' - \delta'_{conv}. \qquad (26)$$

Since we intend to minimize the entransy for a fixed period of time, the entransy caused by conduction should be minimized. This is because that caused by convection is always increasing as time passes, since it depends on *Ra(t)*. Hence, the scaling of (14) insures the following equation for the entransy dissipation of phase change in the presence of convection:

$$\Delta E = r^2 L^2 k^{-1} \int_0^{t_0} d(\delta' - \delta'_{conv})^2. \qquad (27)$$

The applied temperature of a slab *i* at any time *t*, is given as functions f_1 and f_2 ,

$$T_s(t) = f_1(cond \cdot d\delta') + f_2(conv \cdot Ra^{2/3} \cdot \delta^2). \qquad (28)$$

So, if δ is of exponent *n* then $T_s(t)$ is of exponent *2n*.

4.3. Optimization procedure

Similarly to the previous case, the optimization problem is done by minimizing (27) using Euler-Lagrange equation. This results in,

$$\delta'^3 + 2d\delta'\delta'' - 2a\left(\delta^3\delta'\delta'' + 3\delta^2\delta'^2\right) + 5b\delta^4\delta' = 0. \qquad (29)$$

Let $\delta = A(t/t_0)^n$ and substitute for δ, δ', and δ'' in (29). The parameters *a* and *b* are constants to be derived from the initial conditions and are function of material properties and temperature gradient. Their calculation in this stage is not necessary. It should be noted here that in (27) δ'_{conv} is replaced by a function of δ and b, according to (25) and (26). The resultant optimum solution is for $n = 1/4$. This means that the external temperature reads as,

$$T_s(t) \approx T_m + B\left(\frac{t}{t_1}\right)^{1/2}, \qquad (28)$$

with *B* being function of material properties, $B = f(k,L,Pr,c_p,t_1)$, and t_1 here denotes the end of convection plus conduction regime. It is important to mention that here the heat transfer regime is considered with conduction and convection modes. When we have fully convection regime, the above optimisation is no more valid and the entransy dissipation always increases with time until reaching the steady state. Unlike, our heating strategy optimisation during transient states, which is independent of the parameters (since we consider only conduction), the optimisation at steady state can be done with respect to shape or material parameters and is unique for every material. Moreover, the external temperature is the same for all slabs *i*. Its optimisation is based on the minimization of the total entransy dissipation, which leads to a profile with exponent *n* independent of slab's position *i*. However, the value of parameter B may differ from one slab to another depending on the local Ra.

4.4. Numerical results for convective melting

To test if the numerical results match the theoretical hypothesis, the problem of Fig. 3 is simulated via the thermal Lattice Boltzmann for the case of Octadecane with $Pr = 50$, Stefan number $Ste(t) = 0.0084(T_s(t) - T_m)$, $Ra(t_1) = 10^4$, and $H = L_e$. The results are presented in Fig. 4. It is important to

assure that we do not pass to the fully convective regime the condition brought by [26] is respected, which is, $Ra(t)^{1/4} < H/L_e = 1$. Hence, we simulate for $n = 0$ till 1, however we estimate numerically the interval of n where we insure that starting from, at least $0.2t_1$ to have a significant minimum, the convection is dominant and thus we insure conduction plus convective mode. This interval is $0 < n < 0.7$, hereafter the optimal numerical solution should be in this interval. To explain more, for n > 0.7, the convection mode dominates in a fast period of time and this will affect the previously proposed assumptions, i.e. conduction plus convection regime. To recall, when the dominant mode is convection the entransy dissipation increases with time and no minimum will exist. As illustrated in Fig. 4, the numerical results match the theoretical scaling with the optimum heating strategy being of exponent $n = 0.5 = 1/2$.

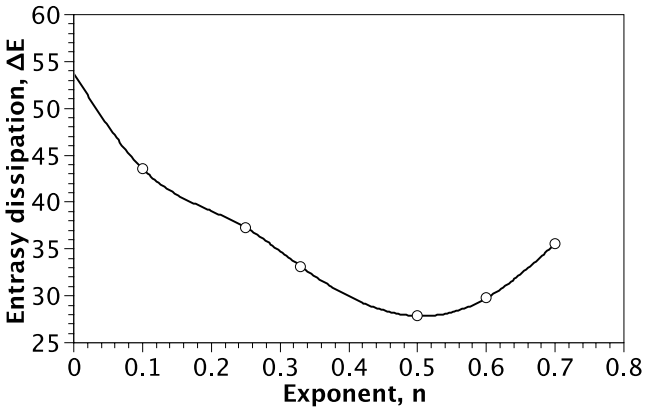

Fig. 2. Conduction & convection: Entransy dissipation of phase-change versus the exponent n.

5. Practical employment of the optimum heating/cooling strategy in (PCMs) applications

The first type of integration is in a latent heat storage system, where there exists a reservoir containing a fluid surrounding the PCM. Here the external reservoir temperature is controllable and the benefit of the optimum heating/cooling strategies is straightforward. However, in the passive (PCMs) application, the thermal loading is due to solar energy. The time and external temperature are directly related to the climatic data. In this case, we can test how far the climatic thermal load is from the optimal strategy. However, for this there can be another optimisation procedure by fixing the exponent n and assessing t_0, which is the time necessary for fusion, by selecting adequate material properties. We recall that if the (PCM) mass is overestimated, the time needed for the heat to penetrate it could become larger than the sunshine period, and the melting process cannot be completed. Thereby, insufficient thermal storage is faced when (PCM) does not totally solidify or totally melt within the heating/cooling period.

Conclusion

In this work, we calculated analytically and numerically the optimal heating/cooling paths for (PCM) for the pure conduction and conduction plus convection cases. The numerical simulations were done via a thermal lattice Boltzmann model and using single relaxation time (SRT) collision operator. The derived theoretical and numerical optimal strategies are confounded, which proves the adequacy of the optimisation procedure. For the case of pure conduction, the optimal heating is via a hyperbolic function of exponent $(n = 0.33)$. On the other hand, for the mixed conduction plus convection regime, the optimal path is via a hyperbolic function of $(n = 0.5)$. In the light of the obtained results, we can propose an optimisation for the external fluid temperature surrounding (PCM) within a latent heat storage system.

Nomenclature

Most of the symbols are defined directly when used, however, here is a list of most used symbols.

c_p specific heat, J/(kg K)

k conductivity, W/(m K)

H height, m

L_e length, m

L latent heat of fusion, J/kg

t time, s

T temperature, K

T_m melting temperature, K

T_s external temperature, K

Greek symbols

ρ density, kg/m^3

δ position of fusion front

δ' rate of propagation of fusion front

Subscripts and superscripts

cond conduction

conv convection

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