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International Journal of Heat and Mass Transfer 44 (2001) 1619-1625

www.elsevier.com/locate/ijhmt

Phase-change phenomena in porous media $-\alpha$ non-local thermal equilibrium model

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Received 1 July 1999; received in revised form 15 May 2000

Abstract

An approximate theoretical enthalpy model is developed to study the phase-change process in porous media. During the melting or the freezing process, the interface within a pore remains at the phase-change temperature until the process is completed. Since the melting process is relatively slow, the assumption of local thermal equilibrium is not universally valid. This theoretical study leads to the development of working relations. An approximate two-temperature model is studied analytically. The results provide the parametric information concerning the phase-change front. Also, the conditions that would assure the existence of local thermal equilibrium are presented. © 2001 Elsevier Science Ltd. All rights reserved.

1. Introduction

Moving boundary problems in porous media have practical relevance in nature and in the field of engineering. Applications range from freezing of biological tissues, thermal energy storage, cooling of electronic equipment to food processing. Solidification in a flow through a porous medium is commonly encountered in the formation of metal matrix composites by infiltration of molten metals into fibrous preforms [1,2]. Previous investigations conducted on flow through porous media hypothesized that the solid matrix and the primary material within the pore satisfy the local thermal equilibrium condition, thus heat transfer parameters were predicted based on the isothermal condition. Sahraoui and Kaviany [3-5] reported a one-equation model of the heat transfer process associated with the boundary between the fluid and solid phase in the porous media. The existence of a local thermal equilibrium condition in porous media becomes uncertain for applications that involve rapid heating processes, and in nuclear reactor

modeling, where the temperature gradient between the fluid and solid matrix is significant. Beckermann and Viskanta [6] investigated natural convection (solid/liquid phase change) in porous media by treating the entire domain as a single region governed by one set of conservation equations. They concluded that some de ficiencies exist between results obtained from their mathematical and experimental models.

Heat transfer analysis based on a two-equation model at the boundary between a porous medium and a homogeneous fluid has been investigated [7]. They found that flux jump conditions exist between a porous medium and a homogeneous fluid when the condition of local thermal equilibrium is invalid and, as a result, separate transport equations are required for each phase. Recently, Vafai and Sozen [8] reported a twophase equation model of flow through a porous medium. Results obtained from their study revealed a significant discrepancy between the fluid and solid phase temperature distribution.

Phase-change materials have received consideration in the defense industries for cooling of electronics and in telecommunication equipment to control internal temperature under emergency operating conditions. It is understood that electronic equipment is susceptible to failure when exposed to extreme temperatures. As an

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Nomenclature

example, telecommunication equipment located at a remote site can suffer abrupt power failure. Numerous numerical and analytical methods have been developed dealing with phase-change problems in non-porous media [9]. These methods include the perturbation method, the approximate Galerkin method, finite element method, enthalpy method, and various transformation methods. Applying a classical method to every pore is a cumbersome task. This complexity is rooted in the fact that the profiles of solid-liquid interface change from pore-topore, and the existence of non-local thermal equilibrium condition between the primary material in the pore and the solid matrix. The main thrust of this investigation is to develop an approximate method of predicting the extent of a phase-change process in a porous media assuming a non-local thermal equilibrium condition.

The phase-change materials with melting points between 40°C and 80°C usually have low thermal conductivity. For this reason, it is customary to encapsulate these materials in a sponge-like metal matrix with high thermal conductivity. The current practice is to analyze these systems assuming the existence of local thermal equilibrium, thereby the solid wall remains at the phasechange temperature while melting is in progress. This assumption is somewhat unrealistic and can be improved. A complete solution requires an extensive numerical undertaking. The objective of this work is to

introduce a linearized enthalpy model that maintains a temperature difference between the phase-change materials and the walls of a pore while it accepts a standard analytical solution technique.

2. Energy equation

A non-equilibrium phenomenon occurs during melting or freezing of phase-change materials encapsulated in a porous medium. The characteristic length to pore size and the thermophysical properties of the medium influence this non-equilibrium phenomenon. Let the subscript ``s'' identify the solid matrix and subscript ``p'' designate materials in the pores. The material in a pore can be solid, liquid, or both whose local enthalpy per unit volume is $H_p(\vec{r}, t)$. The energy equation applied to a differential element, shown in Fig. 1, is in Amiri and Vafai [10,11], and a modified form is

$$
\varepsilon \frac{\partial H_{\rm p}(\vec{\mathbf{r}},t)}{\partial t} = -\nabla \cdot q_{\rm p}(\vec{\mathbf{r}},t) + ha_c(T_{\rm s} - T_{\rm p}) + S_{\rm p}(\vec{\mathbf{r}},t),\qquad(1)
$$

$$
(1 - \varepsilon)C_{\rm s}\frac{\partial T_{\rm s}(\vec{\mathbf{r}},t)}{\partial t} = -\nabla \cdot q_{\rm s}(\vec{\mathbf{r}},t) - ha_c(T_{\rm s} - T_{\rm p}) + S_{\rm s}(\vec{\mathbf{r}},t),
$$
\n(2)

where h is the interstitial heat transfer coefficient, $a_c = \varepsilon/r_h$ and $r_h = V_p/A_p$ is the hydraulic radius. Other

Fig. 1. Schematic representation of a differential element.

parameters are defined in the nomenclature. The function $S_p(\vec{r}, t)$ and $S_s(\vec{r}, t)$ are the contribution of a source or a sink within the primary phase and the solid matrix, and $q_p(\vec{r}, t)$ and $q_s(\vec{r}, t)$ are the respective heat flux components by conduction. For this application, there is no heat generation in the solid matrix, $S_s(\vec{r}, t) = 0$.

It is clear that the temperature of the solid matrix, during a melting process, remains higher than the mean temperature of materials in the pores. During this period, the value of the volumetric heat source S_p varies with time and temperature as the liquid fraction changes in a pore. The temperature solution, using Eqs. (1) and (2), requires information as to the value of the interstitial heat transfer coefficient h . The value of h depends on the geometry of the pores and the nature of the primary phase. Because the size and shape of individual pores are different, the function T_p represents the mean temperature of solid and liquid materials occupying the pores.

2.1. A linearized theoretical model

Before the onset of the phase-change process and after its completion, there is a local thermal equilibrium condition; that is, $T_s = T_p$. During the phase-change process, the mean temperature of the phase-change materials in the pores, T_p , varies between the solid matrix temperature T_s and the phase-change temperature T_m . Assuming the lumped heat capacitance method is valid during the phase-change process, the heat flux to the materials in a pore causes a change in the enthalpy of the phase-change materials according to the relation

$$
\Delta V_{\rm p} \frac{\partial H_{\rm p}}{\partial t} = h \Delta A_{\rm p} (T_{\rm s} - T_{\rm p}). \tag{3}
$$

A mean temperature for the materials in a pore is de fined using the relation $H_p = \bar{C}_p T_p$, where \bar{C}_p is a constant. According to this definition, \overline{C}_p includes the contribution of the latent heat of the phase-change materials allowing one to consider $S_p = 0$ in Eq. (1).

Since the mean capacitance in a pore is considered to be a constant, then Eq. (3) is rewritten as

$$
T_{\rm s}(\vec{\mathbf{r}},t)=T_{\rm p}(\vec{\mathbf{r}},t)+\frac{r_{\rm h}\bar{C}_{\rm p}}{h}\frac{\partial T_{\rm p}(\vec{\mathbf{r}},t)}{\partial t}.
$$
 (4)

A mean value for the \overline{C}_p will be determined later by examining the asymptotic behavior of the solution. Eqs. (1), (2), and (4) describe the transfer of heat in a porous structure whose pores are occupied with phase-change materials. Adding Eqs. (1) and (2), replacing $q_p + q_s$ with q, and setting $S_p(\vec{r}, t) = S_s(\vec{r}, t) = 0$ yields the relation

$$
-\nabla \cdot q(\vec{\mathbf{r}},t) = \varepsilon \bar{C}_{\mathrm{p}} \frac{\partial T_{\mathrm{p}}(\vec{\mathbf{r}},t)}{\partial t} + (1-\varepsilon) C_{\mathrm{s}} \frac{\partial T_{\mathrm{s}}(\vec{\mathbf{r}},t)}{\partial t}.
$$
 (5)

In a porous medium, the equivalent thermal conductivity models often are developed for isothermal conditions. Prior to the onset of local thermal equilibrium, the Fourier thermal conduction model should be modified Tzou [12]. The Fourier conduction equation during this period is replaced by the equation

$$
q(\vec{\mathbf{r}},t) + \tau_q \frac{\partial q(\vec{\mathbf{r}},t)}{\partial t} = -k_e \bigg\{ \nabla T_p(\vec{\mathbf{r}},t) + \tau_t \frac{\partial}{\partial t} \bigg[\nabla T_p(\vec{\mathbf{r}},t) \bigg] \bigg\}.
$$
\n(6)

Comparison of Eq. (6) with Eq. (4) suggests that $\tau_t \cong r_h C_p/h$. Eliminating the heat flux vector q between Eq. (5) and Eq. (6) results in the relation [13].

$$
\nabla \cdot (k_{e} \nabla T_{p}) + \tau_{t} \frac{\partial [\nabla \cdot (k_{e} \nabla T_{p})]}{\partial t}
$$
\n
$$
= C \left[\frac{\partial T_{p}}{\partial t} + (\tau_{e} + \tau_{q}) \frac{\partial^{2} T_{p}}{\partial t^{2}} \right],
$$
\n(7)

where $\tau_e = C_s \tau_t/C$ and $C = \varepsilon \bar{C}_p + (1 - \varepsilon)C_s$.

2.2. A one-dimensional solution

Eq. (7) is linear in temperature if the thermophysical properties are considered to be independent of temperature. In the subsequent analysis, it is assumed the conduction is one-dimensional and the domain of interest is a semi-infinite body. This is mainly for convenience of demonstrating the underlying physical phenomena. During the phase change, the value of \overline{C}_p changes with T_p and the governing equation is non-linear. For a linearized solution, one needs to find an average \overline{C}_p and C. Therefore, assuming k_e and C have constant values, Eq. (7) reduces to

$$
\alpha \frac{\partial^2 T_{\mathbf{p}}}{\partial x^2} + \alpha \tau_t \frac{\partial^3 T_{\mathbf{p}}}{\partial t \partial x^2} = \frac{\partial T_{\mathbf{p}}}{\partial t} + \tau_a \frac{\partial^2 T_{\mathbf{p}}}{\partial t^2} \quad \text{for } 0 \le x < \infty,
$$
\n(8a)

where $\tau_a = \tau_e + \tau_q$ and $\alpha = k_e/C$.

Consideration is given to a semi-infinite porous medium filled with a phase-change material. The medium is initially at the melting temperature T_m and the surface temperature, at $x = 0$, increases to temperature T_0 when $t > 0$. When $r = \tau_t/\tau_a = 1$, Eq. (8a) reduces to

$$
\left(1 + \tau_t \frac{\partial}{\partial t}\right) \left(\alpha \frac{\partial^2 T_p}{\partial x^2} - \frac{\partial T_p}{\partial t}\right) = 0 \quad \text{for } 0 \leq x < \infty, \quad (8b)
$$

whose solution is

$$
\frac{T_{\rm p} - T_{\rm m}}{T_{\rm o} - T_{\rm m}} = \text{erfc}\left(\frac{x}{\sqrt{4\alpha t}}\right). \tag{9}
$$

Eq. (9) suggests a method of finding a theoretical mean value for C assuming it is independent of τ_t , τ_a and t; therefore, C should be the same for inclusion in Eqs. (8a) and (8b). In various phase-change studies, the quasisteady-state assumption is considered when time is relatively large. One can define a melt front X whose location is related to heat flux at $x = 0$ by the relation, $q(0, t) = -k_e \frac{\partial T_p}{\partial x} \approx \rho L \frac{\partial X}{\partial t}$, where L is the latent heat (J/kg). When $x/\sqrt{4\alpha t} \ll 1$, temperature is linear with error of the order of $(x/\sqrt{4at})^3$ and a quasi-steady-state assumption suggests $q(0, t) =$ $k_e(T_o - T_m)/X = \rho L\partial X/\partial t$ that, after integration, yields the relation

$$
X = \sqrt{\frac{2k_{\rm e}(T_{\rm o} - T_{\rm m})}{\rho L}} \sqrt{t}.
$$
\n(10)

Eq. (9), when t is large, one can define an equivalent front X that should approach the equilibrium solution. Following substitution of T_p from Eq. (9) in $-(k_e \partial T_p/\partial x)|_{x=0} = \rho L \partial X/\partial t$ and integration over time, one obtains

$$
X = \frac{2k_e(T_o - T_m)}{\rho L \sqrt{\pi \alpha}} \sqrt{t}.
$$
\n(11)

Equating Eqs. (10) and (11) , at the same X location, provides a mean value for the capacitance, that is,

$$
C \cong \frac{\pi \rho L}{2(T_{\text{o}} - T_{\text{m}})}.\tag{12}
$$

The parameter τ_a in Eq. (8a) has a zero value if $\tau_t = 0$ and $\tau_q = 0$; therefore, $\tau_q \neq 0$ in the presence of nonequilibrium phenomena. Accordingly, Eq. (8a), using dimensionless parameters,

$$
\xi = x/\sqrt{\alpha \tau_a}, \ \eta = t/\tau_a, \ r = \tau_t/\tau_a, \text{ and}
$$

$$
\theta = (T_p - T_m)/(T_o - T_m)
$$
(13)

reduces to

$$
\frac{\partial^2 \theta}{\partial \xi^2} + r \frac{\partial^3 \theta}{\partial \eta \partial \xi^2} = \frac{\partial \theta}{\partial \eta} + \frac{\partial^2 \theta}{\partial \eta^2} \quad \text{for } 0 \le \xi < \infty. \tag{14}
$$

The Laplace transform of θ using the conditions $\theta(\xi, 0) = 0$, $\partial \theta / \partial t |_{\eta=0} = 0$, and $\theta(0, \eta) = 1$ becomes

$$
\bar{\theta} = \mathscr{L}[\theta] = \frac{1}{s} e^{-\sqrt{s(s+1)/(rs+1)}\zeta}.
$$
 (15)

Because the sensible heat is much smaller than the latent heat, the phase-change materials are viewed as the primary consumers of the surface heat flux. In this case, a parameter X, defined as $-(k_e \partial T_p/\partial x)|_{x=0} \cong \rho L \partial X/\partial t$, can be written in dimensionless form as

$$
\frac{\partial}{\partial \eta} \left(\sqrt{\frac{\alpha}{\tau_a}} \frac{\rho L X}{k_e (T_o - T_m)} \right) = \frac{\partial X^*}{\partial \eta} = -\frac{\partial \theta}{\partial \xi} \Big|_{\xi = 0},\tag{16}
$$

where X^* in Eq. (16) is $X^* = \sqrt{\frac{\alpha}{\tau_a}} (\rho LX)/[k_e(T_o - T_m)]$. An alternative form of X^* is derived by replacing α with k_e/C and the value of C from Eq. (12) to obtain $X^* = X \sqrt{2\rho L / [\pi \tau_a k_e (T_o - T_m)]}$. The Laplace transform of X^* , using Eqs. (15) and (16) and following some algebra, the Laplace transform of X^* is

$$
\mathcal{L}[X^*] = \frac{1}{s^2} \sqrt{\frac{s(s+1)}{rs+1}}
$$

=
$$
\frac{1}{\sqrt{r}} (s^{-1/2} + s^{-3/2}) \times \frac{1}{\sqrt{s+1/r} \sqrt{s+1}}
$$
(17)

whose inverse transform, using the convolution theorem, Churchill [14] is

$$
X^* = \frac{1}{\sqrt{r}} \int_{\tau=0}^{\eta} \left(\frac{1}{\sqrt{\pi(\eta-\tau)}} + 2\sqrt{\frac{\eta-\tau}{\pi}} \right) \times \left\{ \exp\left[-\frac{1}{2} \left(1 + \frac{1}{r} \right) \tau \right] \times I_0 \left(\frac{r-1}{2r} \tau \right) \right\} d\tau. \tag{18}
$$

3. Results and discussion

Eq. (18) is well suited for a numerical study using symbolic mathematical software. A function in MATHEMATICA [15] code that provides the value of X^* , named "conv" is given in Appendix A. This MATHEMATICA [15] function was placed in a loop to provide the needed data and the output was directly transferred to a spreadsheet for a graphic presentation. Fig. 2 shows the variation of the dimensionless front X^* as a function of η for different values of the parameter r.

An examination of data in Fig. 2 shows that X^* linearly depends on $\eta^{1/2} = \sqrt{t/\tau_a}$ when η is large or when $r = 1$. Moreover, under the local thermal equilibrium condition $\tau_t = \tau_q = 0$, the r = 1 line in Fig. 2 describes the solution by setting $\tau_a = 1$ or any other non-zero constant. According to Fig. 2, when $r < 1$, the value of X^* is larger than the predicted value from a local thermal equilibrium model. Alternatively, when $r > 1$, the phase-change front progresses slower than the local thermal equilibrium model.

Three parameters C, τ_t , and τ_q emerged in this modeling. No information concerning these three

Fig. 2. Dimensionless front X^* as a function of dimensionless time η for different values of parameter r.

parameters was found in the literature. A mean value for the heat capacitance C was found earlier. The parameter τ_t is related to the interstitial heat transfer coefficient in a mean pore and the parameter τ_q is related to the thermal contact resistance across the solid matrix. In theory, it is possible to experimentally determine τ_t and τ_q . Also, it is possible to provide a theoretical determination of $\tau_t \cong r_h C_p/h$ following estimation of h. In as much as the contact resistance and subsequently τ_q depend on the structure of a specific porous matrix, the value of τ_a should be determined experimentally.

In this enthalpy model, the phase-change material has a mean temperature T_p ; and its heat capacitance, \bar{C}_p , is related to C, Eq. (12), by the relation $\overline{C}_p =$ $[C - (1 - \varepsilon)C_s]/\varepsilon$. If the material in a pore is homogeneous, the value of h is constant using only the first eigenvalue in a series solution. When the shape of a pore is a sphere, a cylindrical prism, or a square prism, Minkowycz et al. [13] reports $hr_h/k_p = 1.09$, 1.45; or 1.23. Despite the significant variance in shapes these numbers are within a narrow band; therefore, in the absence of experimental data, a mean value of 1.26 is a satisfactory approximation for hr_h/k_p .

This approximate method permits establishing a criterion for the onset of thermal equilibrium, an interesting feature of this method. Based on data in Fig. 2, as time increases, the solution approaches the lines designated by $r = 1$ and a solution that assumes local thermal equilibrium is valid. The departure from the local thermal equilibrium is viewed as

$$
X^*(\eta, r) - X^*(\eta, 1) = EX^*(\eta, 1). \tag{19}
$$

For a given pair of E and r , the root of Eq. (19) will be designated as η_0 . The parameter η_0 identifies the dimensionless time $\eta > \eta_0$ when $X^*(\eta,r)$ is within $E \times 100\%$ of $X^*(\eta, 1)$ for the same η . The parameter η_0 is computed for different values of E using MATHEM-

Fig. 3. Dimensionless time, η_0 , and phase-change front, $(X^*)_0$, when $r < 1$, for a near local thermal equilibrium condition.

Fig. 4. Dimensionless time, η_0 , and phase-change front, $(X^*)_0$, when $r > 1$, for a near local thermal equilibrium condition.

ATICA [15]. Because η_0 is large when $r > 1$ and relatively smaller when $r < 1$, two separate graphs are prepared for clarity of this presentation. When $r < 1$, the solid lines in Fig. 3 show the values of η_0 as a function of *r* for $E \times 100\% = 1\%$, 2%, 5%, and 10%. The corresponding value of $X^*(\eta_0, r)$ is also plotted as dashed lines in the same figure and it is designated as (X^*) ₀. Fig. 4 is prepared for $r > 1$ in a similar manner as that for Fig. 3.

It is notable that η_0 is nearly linear in Figs. 3 and 4 away from $r = 1$; that is,

$$
\eta_{o} = D(1 - r) \quad \text{when } r < 1,\tag{20a}
$$

and

$$
\eta_o = D(r - 1) \quad \text{when } r > 1. \tag{20b}
$$

The values of dimensionless constant D depend on E for the data in Figs. 3 and 4. The values of D , in Fig. 3, are 25.2, 12.7, 5.22, and 2.74 for 1%, 2%, 5%, and 10% deviations, respectively. For the same deviations, the corresponding values of D for the solid lines in Fig. 4 are 25.5, 13.0, 5.61, and 3.07. It is observed that the parameter D , for a given deviation E , has nearly the same value for inclusion in Eqs. (20a) and (20b). The value of D can be estimated from $D = 0.26/E$ or, for a better accuracy, from the relation $D = 3.27E^{-0.942}$. Therefore, the condition of local thermal equilibrium can be written as

$$
t > D\left|(1 - C_{\rm s}/C)\tau_t - \tau_q\right|.\tag{21}
$$

When $C_s \ll C$ and τ_a is small $(r \gg 1)$, the condition of local thermal equilibrium is achieved when

$$
t > D\tau_t = Dr_{\rm h}\bar{C}_{\rm p}/h. \tag{22}
$$

Furthermore, using X as a characteristic length, Eq. (22), in dimensionless form, reduces to $\alpha t/X^2 >$ $Dr_h\alpha\bar{C}_p/(hX^2)$. The left side of this equation is $Fo = \alpha t / X^2$, where Fo is the Fourier number whereas the right side is $D(\bar{C}_{p}/C)/Sp$, where $Sp = hX^{2}/k_{e}r_{h}$ is the Sparrow number [13]. The local thermal equilibrium may be considered when Eq. (22) is written as

 $F\!oSp > D(\bar{C}_{p}/C).$

Alternatively, assuming $hr_h/k_p \approx 1.26$, Eq. (22) yields a further simplified condition for the onset of the local thermal equilibrium condition; that is, $Fo_p =$ $k_{\rm p} t / (\bar{C}_{\rm p} r_{\rm h}^2) > 0.8D.$

4. Conclusion

A casual examination of the phase-change process in a porous medium shows that a departure from local thermal equilibrium is an existing phenomenon. The underlying heat transfer process is a complex one and requires further theoretical studies. Following a description of the physical process, this work presents an approximate method of determining the extent of a phase-change process as a function of time.

The procedure described here enables one to analyze conduction in porous media in the presence of phasechange phenomena. Upon rapid melting or solidification, there will be departure from local thermal equilibrium. This presentation quantitizes the conditions for occurrence of this local thermal equilibrium. For this analysis, three parameters are needed. First, the mean heat capacitance C that includes the effect of latent heat is predicted theoretically. Second, the parameter τ_a describes the effect of contact resistance that depends on the specific porous structure. For best melting or freezing performance, τ_q should be as small as possible, e.g. $\tau_q = 0$. The third and most important parameter, τ_t , describes the effect of the interstitial heat transfer coefficient. Presently, no experimental information is available for predicting τ_t . In the absence of experimental data, the relation $hr_h/k_p = 1.26$ enable one to predict the onset and departure from local thermal equilibrium during melting and solidification process.

Appendix A

Below is a function "conv (t_r, r_r) ", in MATHEM-ATICA [15] code, to evaluate the function X^* from Eq. (18) . The first parameter in the argument of "conv" function is η and the second parameter is r. As a numerical sample, this function is used to provide $X^*(4, 0.3) = 2.36335$ and $X^*(4, 3) = 1.90894$ at the end of the code.

```
conv[t1_{-1}, a1_{-}]: = (f1 = 1/Sqrt[Pi*x]+2*Sqrt[x/Pi];f2 = Exp[-(1+1/a1)*(t1 - x)/2]*Bess-elI[0,(a1 – 1)*(t1 – x)/2/a1];
f = f1*f2/Sqrt[a1];rt = Integrate[f, {x, 0, t1}];Return[rt])
N[conv[4,0.3]]
N[conv[4,3]]Out[1] = 2.36335Out[2] = 1.90894
```
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