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ESTIMATION OF THE OCCURANCE OF THE PHASE-CHANGE PROCESS IN SPHERICAL COORDINATES

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ABSTRACT

We study heat conduction problems in spherical coordinates with mixed boundary conditions. We obtain sufficient and/or necessary conditions among the data in order to get a phase-change process. For the spherical coordinates case we consider a problem in a hollow sphere $r_1 < r < r_2$, where the boundary conditions are the heat flux ($q > 0$) on the surface $r = r_1$ and the temperature the surface ($b > 0$) on the surface $r = r_2$, and an initial condition in the hollow sphere is also considered. We analyse both, the case with or without source. We explicit the relation between the heat flux q, the fixed temperature b and the thermal conductivity k of the initial phase, in order to have a change of phase in the material. © 1999 Elsevier Science Ltd

Introduction

Heat transfer problems with phase-change such as melting and freezing have been studied in the last century due to their wide scientific and technological applications. The modeling of solidification systems is a problem of a great mathematical and industrial significance. Phase-change problems appear frequently in industrial process and other problems of technological interest [1,3,5,9,10]. For example, a review of a long bibliography on moving and free boundary problems for the heat equation, particulary concerning the Stefan problem, is presented in [17] with a large bibliography.

We study heat conduction problems in spherical coordinates with mixed boundary conditions. We obtain sufficient and/or necessary conditions among the data in order to estimate the occurance of a phase-change process. We consider a heat conduction problem in a hollow sphere $r_1 < r < r_2$, where the boundary conditions are the heat flux ($q > 0$) on the surface $r = r_1$ and the temperature ($b > 0$) on the surface $r = r_2$, and an initial condition in the hollow sphere is also considered. We analyse both, the case with or without source. We explicit the relation among the heat flux q, the fixed temperature b and the thermal conductivity k of the initial phase, in order to have a change of phase in the material. We suppose, without loss of generality, that the phase-change temperature is $0°C$. By the data monotonicity the corresponding phase-change interface begins at $r = r_1$.

We study the following heat conduction problem: we consider a hollow sphere with radii r_1, r_2 with $r_1 \leq r_2$ the initial temperature $\theta_0 = \theta_0(r) \geq 0$, having a heat flux $q = q(t) > 0$ on the internal surface ($r = r_1$) and a temperature condition $b = b(t) > 0$ on the external surface ($r = r_2$). Then the heat conduction problem for the initial (liquid) phase is given by the following mathematical conditions:

Problem Ps:

$$k(\theta_{rr} + \tfrac{2}{r}\theta_r) = \rho c \theta_t, \qquad r_1 < r < r_2, \qquad t > 0; \tag{1.1}$$

$$\theta(r, 0) = \theta_0(r), \qquad r_1 \leq r \leq r_2; \tag{1.2}$$

$$k\theta_r(r_1, t) = q(t), \qquad t > 0; \tag{1.3}$$

$$\theta(r_2, t) = b(t), \qquad t > 0. \tag{1.4}$$

We assume that the data satisfy the hypotheses that ensure the existence and uniqueness of the solution of the Problem Ps.

Moreover, the following two possibilities can occur:

a) the heat conduction problem is defined for all $t > 0$;

b) there exists a time $T_w < \infty$ (called, a waiting-time) such that another phase (i.e., the solid phase) appears for $t > T_w$ and then we will have a solidification process, i.e. a two-phase Stefan problem. In this case, there exists a front (free-boundary) $r = s(t)$ which separates the liquid and the solid phases whose initial position is given by $s(T_w) = r_1$. Moreover, for $t < T_w$ we have a heat conduction problem for the initial liquid phase.

These two only possibilities depend on the data θ_0, q, k, b. We try to clarify this dependence by finding necessary or sufficient conditions on data in order to estimate the different possibilities.

In [6,12,13] the unidimensional one-phase Stefan problem with prescribed flux or convective boundary conditions at $x = 0$ is studied. This paper was motivated by [2,14,16], where some explicit results were obtained for the one-dimensional case. First we analyse the heat conduction problem in spherical coordinates (Ps), and then we study the corresponding problem with a source term.

Heat Conduction Problems in Spherical Coordinates

Without a Source Term

In order to study the possibilities a) and b) for the problem Ps we consider the steady-state heat conduction problem (called Problem P_∞), corresponding to (1.1)-(1.4), which is given by :

$$\theta''_\infty + \frac{2}{r}\theta'_\infty = 0, \quad r_1 \leq r \leq r_2;$$

$$\theta_\infty(r_2) = b > 0; \qquad k\theta'_\infty(r_1) = q > 0,$$

where b and q are positive constants.

The solution of Problem P_∞ is given by:

$$\theta_\infty(r) = b + \tfrac{q}{k}r_2^2(\tfrac{1}{r_2} - \tfrac{1}{r}), \quad r_1 \leq r \leq r_2. \tag{2.1}$$

The temperature at the interior surface $r = r_1$ is given by $\theta_\infty(r_1) = b + \frac{q}{k}r_2^2(\frac{1}{r_2} - \frac{1}{r_1})$ and we can conclude that if the heat flux q satisfies the following inequality,

$$q > Q_\infty = kb\tfrac{r_2}{r_1}\tfrac{1}{(r_2 - r_1)}, \tag{2.2}$$

then the temperature $\theta_\infty(r_1) < 0$, that means that we have a steady state phase-change process [14]. This condition is also a necessary condition to have a change of phase [15]. From this, it is natural to think that we can expect to have a change of phase for the evolution case (Problem Ps), *if* $q > Q(t)$ (with $Q(t) > Q_\infty$) for $t > t_Q$, for a suitable positive time t_Q.

The answer to this question is given below.

First we will obtain sufficient condition on data of problem (Ps) in order to get a waiting time, i.e. the possibility b).

Property 1:

If the data $q = q(t), \theta_0 = \theta(r)$, and $b = b(t)$ verify the following conditions:

(i) $0 < q(t) \leq q_0$, $0 < t \leq t_0$;
(ii) $0 < \beta_0 \leq \theta_0(r) \leq \beta_1$, $\theta_0'(r) \geq 0$, $\qquad r_1 \leq r \leq r_2$;
(iii) $b(t) \geq \beta_1$, $\dot{b}(t) \geq 0, t > 0$;

there exists a "waiting time" $T_\omega > 0$ for Problem (Ps) and its expression is given by $T_W = min(t_0, T_W^*)$ where

$$T_w^* = \left\{ \begin{array}{lc} +\infty \quad if & 1 - \dfrac{\beta_0 k}{r_1 q_0} \leq 0 \\ \frac{r_1^2}{\alpha}\left(H_1^{-1}(1 - \frac{\beta_0 k}{r_1 q_0})\right)^2 \text{ if } & -\dfrac{\beta_0 k}{r_1 q_0} + 1 > 0. \end{array} \right\} \tag{2.3}$$

where H_1^{-1} is the inverse function of H_1 where $H_1(x) = exp(x^2)erfc(x)$.

Proof.

In orden to prove the result it is sufficient to show that $\theta(r,t) \geq 0$ for $r_1 \leq r \leq r_2$ and $0 \leq t \leq T_\omega$.

Remark 1.

i) The waiting time T_w increases with the parameter β_0 (the lower bound for the initial temperature).

ii) The Property 1 implies that the model of heat conduction, given by problem Ps, under the assumption (i-iii) is only valid for $t < T_w$.

The temperature θ, the solution of Problem Ps, is a non decreasing function of variable r, by the maximun principle, ie. $\theta_r(r,t) \geq 0$ for all $r_1 \leq r \leq r_2, t > 0,$, when the following conditions

(i) $\theta_0'(r) \geq 0$, $\qquad r_1 \leq r \leq r_2$;
(ii) $\dot{b}(t) \geq 0$, $\qquad t > 0$;
(iii) $q = q(t) > 0$, $\quad t > 0$.
are satisfied.

The temperature θ can be written as $\theta = \theta_\infty + U_0 + \frac{q}{k}U_1$, where U_0 and U_1 satisfy the following problems:

Problem Pu_0	Problem Pu_1
$\alpha(U_{o_{rr}} + \frac{2}{r}U_{o_r}) = U_{o_t}$	$\alpha(U_{1_{rr}} + \frac{2}{r}U_{1r}) = U_{1_t}$
$U_0(r,0) = \theta_0(r) - b \le 0$	$U_1(r,0) = -r_1^2\left(\frac{1}{r_2} - \frac{1}{r}\right) > 0$
$U_{0_r}(r_1,t) = 0$	$U_{1_r}(r_1,t) = 0$
$U_0(r_2,t) = 0$	$U_1(r_2,t) = 0.$

By the maximun principle $U_0 \le 0$ and $U_1 \ge 0$. Using [11] the solution U_1 can be written down as:

$$U_1(r,t) = \frac{1}{r}\sum_{m=1}^{\infty}\frac{R(\beta_m r)}{N(\beta_m)}\, e^{-\alpha\beta_m^2 t}\int_{r_1}^{r_2}\rho(r_1^2\Big(\frac{1}{\rho} - \frac{1}{r_2}\Big)R(\beta_m\rho)d\rho, \qquad r_1 < r < r_2,\, t > 0 \tag{2.4}$$

where
$$R(\beta_m r) = \beta_m\, cos(\beta_m(r - r_1)) + \frac{1}{r_1}sin(\beta_m(r - r_1)), \tag{2.5}$$

$$\frac{1}{N(\beta_m)} = \frac{2}{(\beta_m^2 + \frac{1}{r_1^2})(r_2 - r_1) + \frac{1}{r_1}}\ ; \tag{2.6}$$

with $\beta_m > 0$ (for $m \in N$) are the solutions of the equation:

$$tg(\beta_m(r_2 - r_1)) = -\beta_m\, r_1, \text{ and } \beta_m > 0. \tag{2.7}$$

By some computation and taking into account (2.7) the function R can be written only in sine terms as:

$$R(\beta_m r) = -\sqrt{\beta_m^2 + \frac{1}{r_1^2}}\ \ \sin\,(\beta_m(r_2 - r)), \tag{2.8}$$

and then we can compute the integral

$$\int_{r_1}^{r_2}\rho r_1^2\Big(\frac{1}{\rho} - \frac{1}{r_2}\Big)R(\beta_m\rho)d\rho = \frac{r_1^2}{\beta_m}\sqrt{\beta_m^2 + \frac{1}{r_1^2}}\ cos(\beta_m(r_1 - r_2)). \tag{2.9}$$

Therefore U_1 can be written as

$$U_1(r,t) = -\frac{r_1^2}{r}\sum_{m=1}^{\infty}\Big(\frac{\beta_m^2 + \frac{1}{r_1^2}}{N(\beta_m}\Big)e^{-\alpha\beta_m^2 t}\ \frac{sin(\beta_m(r_2 - r))cos(\beta_m(r_2 - r_1)}{\beta_m} \tag{2.10}$$

for $r_1 < r < r_2, t > 0$ and then we have

$$U_1(r_1,t) = -\sum_{m=1}^{\infty}\frac{e^{-\alpha\beta_m^2 t}}{N(\beta_m)}, t > 0. \tag{2.11}$$

Theorem 2.

Let θ be the solution of Problem Ps, with the initial and boundary data satisfying the following hypotheses:

(i) $\theta_0(r) \leq b(0), \quad r_1 \leq r \leq r_2;$

(ii) $\theta_0'(r) \geq 0, \quad r_1 < r < r_2;$

(iii) $b(t) > 0, \quad \dot{b}(t) > 0, \ t > 0;$

(iv) $q(t) > 0, \quad t > 0.$

Then there exists a curve $q = Q(t)$ in the first quadrant of the plane (q,t) such that if $q > Q(t)$, and $t > t^*$, we have a phase change process for the material where t^* is defined by

$$t^* = \frac{1}{\alpha\beta_1^2} log\Big(\frac{\sum_{m=1}^{\infty}\frac{1}{N(\beta_m)}}{r_1^2(\frac{1}{r_1}-\frac{1}{r_2})}\Big), \tag{2.12}$$

for any $\gamma = \frac{r_2}{r_1} \in (1, \gamma_0]$ with a suitable $\gamma_0 > 1$.

Proof.

Since $\theta_r \geq 0$ we will only check the temperature θ at $r = r_1$, that is

$$\theta(r_1,t) \leq b + \frac{q}{k}\Big(\sum_{m=1}^{\infty}\frac{e^{-\alpha\beta_1^2 t}}{N(\beta_m)} + r_1^2(\frac{1}{r_2}-\frac{1}{r_1})\Big),$$

because $U_0(r_1,t) \leq 0$, and β_m is increasing with m.

Therefore we have $\theta(r_1,t) \leq 0$ when

$$q \geq Q(t) = \frac{bk}{r_1^2\Big(\frac{1}{r_1}-\frac{1}{r_2}\Big) - e^{-\alpha\beta_1^2 t}\sum_{m=1}^{\infty}\frac{1}{N(\beta_m)}}$$

for $t > t^*$, where t^* is the value that makes

$$r_1^2\Big(\frac{1}{r_2}-\frac{1}{r_1}\Big) + e^{-\alpha\beta_1^2 t^*}\sum_{1}^{\infty}\frac{1}{N(\beta_m)} = 0,$$

that is (2.12).

The value t^* is great than zero if and only if $H_2(\gamma) > 1$, where $H_2(x)$ is defined by the following expression

$$H_2(x) = 2\frac{\sum_{m=1}^{\infty}\frac{1}{1+\frac{\lambda_m^2}{x(x-1)}}}{x-1};$$

$$\lambda_m = \beta_m(r_2 - r_1); \ \gamma = \frac{r_2}{r_1}.$$

After some mathematical manipulation we can conclude that $H_2(\gamma) > 1$ for some $\gamma \in (1, \gamma_0]$ with an adequate constant $\gamma_0 > 1$.

Remark 2.

i) If we consider the (t,q) plane and we define the following set $S = \{(t,q)/q > Q(t), t \geq t^*\}$, in the first quadrant then we have a two-phase problem for all $(t,q) \in S$, and $\frac{r_2}{r_1} \in (1, \gamma_0]$.

ii) We can obtain an upper estimation of the time t^* defined by (2.12). Since $\beta_m \geq \left(\frac{2m-1}{2(r_2-r_1)}\right)\pi$ we can deduce

$$\sum_{m=1}^{\infty} \frac{1}{\left(\beta_m^2 + \frac{1}{r_1^2}\right)(r_2 - r_1) + \frac{1}{r_1}} \leq \sum_{m=1}^{\infty} \frac{4(r_2 - r_1)}{\left(2m-1\right)^2 \pi^2} = \frac{r_2 - r_1}{2}.$$

Then the upper bound for t_Q is given by the following inequality

$$t_Q \leq \frac{1}{\alpha\beta_1} log\left(\frac{r_2}{r_1}\right). \tag{2.13}$$

Heat Conduction Problems in Spherical Coordinates With a Source Term

Let θ be the solution of the following heat conduction problem with a constant source term g in spherical coordinates:

Problem P_g:

$\theta_t - \alpha(\theta_{rr} + \frac{2}{r}\theta_r) = \frac{g}{\rho c}$, $r_1 < r < r_2, t > 0$;

$\theta(r,0) = \theta_0(r)$, $r_1 < r < r_2$;

$k\theta_r(r_1,t) = q > 0$, $t > 0$; $\theta(r_2,t) = b > 0$, $t > 0$.

The steady-state solution for the problem Pg is given by [8]

$$\begin{aligned} \theta_\infty(r) &= -\frac{g}{6k}r^2 - \left(\frac{g}{3k}r_1^3 + \frac{q}{k}r_1^2\right)\frac{1}{r} + b + \frac{g}{6k}r_2^2 + \frac{q}{k}\frac{r_1^2}{r_2} + \frac{g}{3k}\frac{r_1^3}{r_2} \\ &= b + \frac{g}{k}\left[\frac{-r^2}{6} + \frac{r_2^2}{6} - \frac{r_1^3}{3r} + \frac{r_1^3}{3r_2}\right] + \frac{q}{k}\left[\frac{-r_1^2}{r} + \frac{r_1^2}{r_2}\right], \quad r_1 < r < r_2. \end{aligned} \tag{2.14}$$

Property 3:

We obtain the following properties in order to determine the sign of the steady-state temperature θ_∞ (i.e. the phase of the material).

(i) If $q > 0$, then the function θ_∞ is of non-constant sign (there are two-phases within the material) if and only if $\theta_\infty(r_1) < 0$, that is $q > Q_\infty^g = \frac{kr_2}{r_1(r_2-r_1)}\left[b + \frac{g}{k}\left(\frac{r_1^3}{3r_2} + \frac{r_2^2}{6} - \frac{r_1^2}{2}\right)\right]$ and $g > g_0$ with $g_0 = \frac{b\,k}{-\frac{r_1^2}{2} + \frac{r_2^2}{6} + \frac{r_1^3}{3r_2}} > 0$.

(ii) If $q < 0$, then θ_∞ if of non-constant sign if and only if $g < 0$ and $\theta_\infty(r_m) < 0$, where r_m is the unique solution of the equation $\theta'_\infty(r_m) = 0$ in (r_1, r_2), where $r_m = \sqrt[3]{r_1^3 + 3\frac{q}{gr_1}}$ and $\theta_\infty(r_m) < 0$ with $(\frac{r_2}{r_1})^3 > 1 + \frac{3q}{gr_1}$.

Remark 3

For all $r_2 > r_1$ we have that $\frac{{r_1}^2}{2} + \frac{{r_2}^2}{6} + \frac{{r_1}^3}{3r_2} > 0$.

Now we shall consider the possibility of the occurence of the phase-change process in the evolution problem Pg. From the above results it is natural to think that we can expect to have a change of phase in the evolution case if $q \geq Q^g(t) \geq Q^g_\infty > 0$ for $t > t_{Q,g}$, with $t_{Q,g} > 0$.

Theorem 4.

Let $\theta(x,t)$ be the solution of the problem Pg with the hypotheses of the Theorem 2 then there exists a curve $q = Q^g(t)$ in the (q,t) plane (for each positive g) such that if $q > Q^g(t)$ and $t \geq t^*$, we have a change of phase for a suitable $t^* > 0$

Proof.

The temperature θ is given by $\theta = \theta_\infty + u_0 + \frac{g}{k}u_1 + \frac{q}{k}u_2$, where u_0 satisfies problem Pu with the initial data $u_0(r,0) = \theta_0(r) - b \leq 0, r_1 < r < r_2$; u_1 satisfies problem Pu with the initial data $u_1(r,0) = \frac{r^2}{6} + \frac{r_1^3}{3r} - \left(\frac{r_1^3}{3r_2} + \frac{r_2^2}{6}\right)$; and u_2 satisfies the problem Pu with the initial data $u_2(r,0) = r_1^2\left[\frac{1}{r} - \frac{1}{r_2}\right]$.

We can compute the temperature at r_1 and we get

$$\theta(r_1,t) = u_0(r_1,t) + \frac{g}{k}u_1(r_1 t) + \frac{q}{k}u_2(r_1 t) +$$

$$-\frac{g}{6k}r_1^2 - \left(\frac{g}{3k}r_1^3 + \frac{q}{k}r_1^2\right)\frac{1}{r_1} + b + \frac{g}{6k}r_2^2 + \frac{gr_1^3}{3kr_2} + \frac{qr_1^2}{kr_2} \leq$$

$$\leq \frac{q}{k}\left[\sum_{m=1}^{\infty}\frac{e^{-\alpha\beta m^2 t}}{N(\beta m)} - r_1 + \frac{r_1^2}{r_2}\right] + b + \frac{g}{k}\left[-\frac{r_1^2}{2} + \frac{r_2^2}{6} + \frac{r_1^3}{3r_2}\right]$$

$$\leq \frac{q}{k}\left[e^{-\alpha\beta_1^2 t}\sum_{m=1}^{\infty}\frac{1}{N(\beta_m)} - r_1\frac{(r_2 - r_1)}{r_2}\right] + b + \frac{g}{k}\left[-\frac{r_1^2}{2} + \frac{r_2^2}{6} + \frac{r_1^3}{3r_2}\right] \leq 0,$$

taking $t > t^* = t_Q$ such that

$$q \geq k \frac{b + \frac{g}{k}\left[\frac{r_2^2}{6} - \frac{r_1^2}{2} + \frac{r_1^3}{3r_2}\right]}{(-e^{-\alpha\beta_1^2 t})\sum_{m=1}^{\infty}\frac{1}{N(\beta_m)} + \frac{r_1}{r_2}(r_2 - r_1)}.$$

and t^* given by the solution of the equation $e^{-\alpha\beta_1^2 t^*}\sum_{m=1}^{\infty}\frac{1}{N(\beta m)} - \frac{r_1}{r_2}(r_2 - r_1) = 0$, that is

$$t^* = \frac{1}{\alpha\beta_1^2} log\Big(\frac{\sum_{m=1}^{\infty}\frac{1}{N(\beta_m)}}{r_1^2(\frac{1}{r_1} - \frac{1}{r_2})}\Big),$$

which is great than zero by the same argument used in the proof of the Theorem 2.

Conclusion

We have obtained sufficient condition on data for a heat conduction problem with mixed boundary conditions in order to estimate a phase-change process for a hollow sphere with radii $r_2 > r_1$ with or without a constant heat source within the domain.

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Nomenclature

c specific heat, $[J/Kg^oK]$

k thermal conductivity , $[W/m^oK]$

t time, $[s]$

r radial space variable, $[m]$

q heat flux on the face $r = r_1$,$[Kg/s^3]$

b temperature on the face $r = r_2$, $[^oK]$

Greek symbols

ρ mass density,$[Kg/m^3]$

θ temperature, $[^oK]$

θ_0 initial temperature ,$[^oK]$

$\gamma = \frac{r_2}{r_1} > 1$ adimensional constant.

$\alpha = \frac{k}{\rho k}$ thermal diffusivity,$[m^2/s]$

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