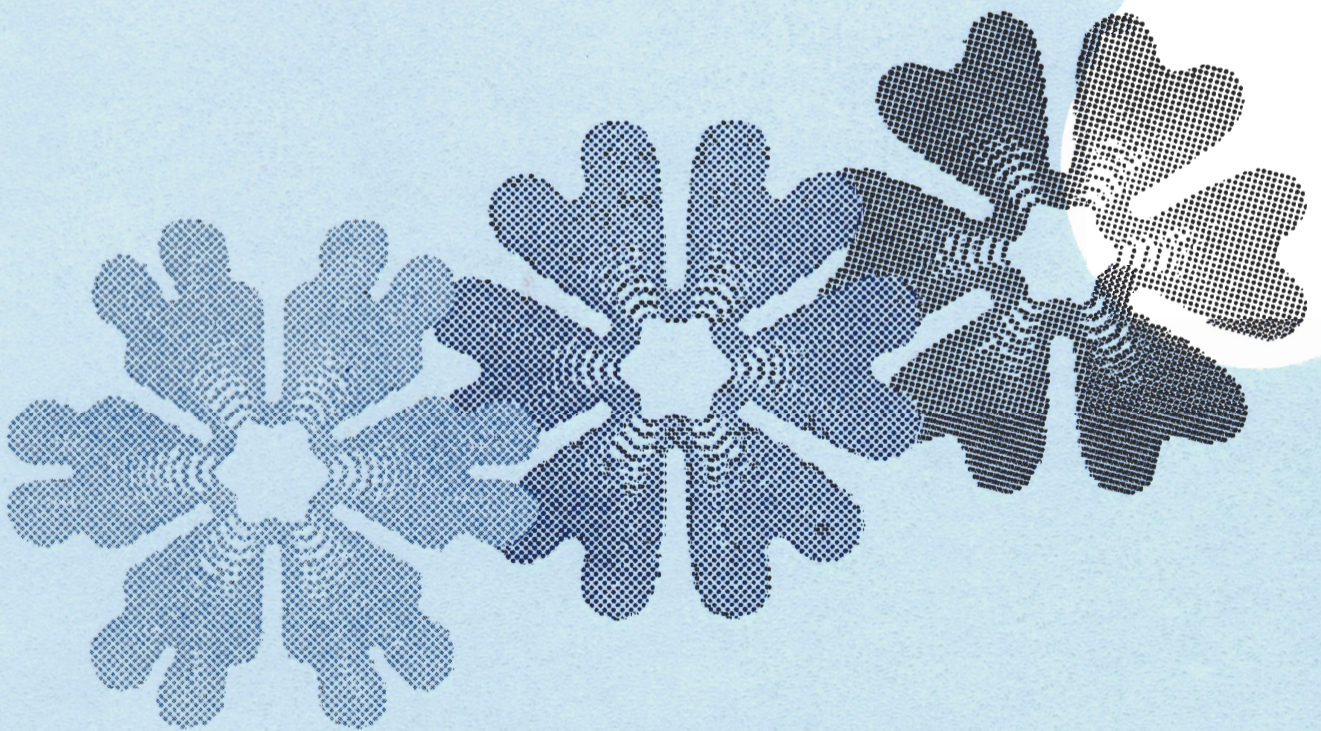


Computational Modelling of Free and Moving Boundary Problems III

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On the determination of the unknown coefficients through phase-change processes

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Abstract

We present two different approaches on the determination of thermal coefficients of a semi-infinite material through a phase-change process with an overspecified heat flux condition on the fixed face.

1) We use a simple mushy zone model in a two-phase solidification problem (Stefan problem) for the simultaneous determination of some unknown coefficients. We also find the necessary and sufficient conditions for the existence of a solution and the corresponding formulae for the unknown coefficients.

2) We use approximate methods (heat balance integral and variational methods) for a one-phase Stefan problem for the simultaneous determination of some unknown coefficients. We propose a convex linear expansion (with a parameter to be also determined) of the first and second order approximation solutions for the temperature. We also find the necessary and sufficient conditions for the existence of a solution and the corresponding formulae for the unknown coefficients .

1 Introduction

Heat transfer problems with phase-change such as melting and freezing have been studied in the last century because of their wide scientific and technological

applications (e.g. Alexiades & Solomon [1], Lunardini [10], Rubinstein [11]). For example, a review of a long bibliography on moving and free boundary problems for the heat equation, particularly concerning the Stefan problem, is presented in Tarzia [16] with a large bibliography (we are now preparing an updated one with approximately 4500 references).

First, we shall consider a semi-infinite material with mass densities $\rho > 0$ equal in both solid and liquid phases and we assume, without loss of generality, that the phase-change temperature is 0°C .

If the material is initially assumed to be liquid at the constant temperature $E > 0$ and a constant temperature $-D < 0$ is imposed on the fixed face $x=0$, then three distinct regions can be distinguished (for a mathematical and properties description of this simple model see Tarzia [20]; for the one-phase model see Solomon, Wilson & Alexiades [12]) :

(H₁) The liquid phase, at temperature $\theta_2 = \theta_2(x, t) > 0$, occupying the region $x > r(t)$, $t > 0$.

(H₂) The solid phase, at temperature $\theta_1 = \theta_1(x, t) < 0$, occupying the region $0 < x < s(t)$, $t > 0$.

(H₃) The mushy zone, at temperature 0, occupying the region $s(t) \leq x \leq r(t)$, $t > 0$.

We make two assumptions on its structure :

(a) The material in the mushy zone contains a fixed fraction ϵh (with $0 < \epsilon < 1$) of the total latent heat $h > 0$, i.e.,

$$k_1 \theta_{1x}(s(t), t) - k_2 \theta_{2x}(r(t), t) = \rho h \left(\epsilon \dot{s}(t) + (1 - \epsilon) \dot{r}(t) \right), \quad t > 0. \quad (1)$$

(b) The width of the mushy zone is inversely proportional (with constant $\gamma > 0$) to the temperature gradient at the point $(s(t), t)$, i.e.,

$$\theta_{1x}(s(t), t) (r(t) - s(t)) = \gamma, \quad t > 0. \quad (2)$$

We suppose that the temperature $\theta = \theta(x, t)$ of the material is defined by

$$\theta(x, t) = \begin{cases} \theta_1(x, t) < 0 & \text{if } 0 < x < s(t), t > 0 \\ 0 & \text{if } s(t) \leq x \leq r(t), t > 0 \\ \theta_2(x, t) > 0 & \text{if } x > r(t), t > 0. \end{cases} \quad (3)$$

The governing differential equations take the following forms for the solid and liquid phases :

$$\alpha_1 \theta_{1xx}(x, t) = \theta_{1t}(x, t), \quad 0 < x < s(t), t > 0, \quad (4)$$

$$\alpha_2 \theta_{2_{xx}}(x,t) = \theta_{2_t}(x,t) \quad , \quad x > r(t), t > 0 \quad , \quad (5)$$

where $c_i > 0$, $k_i > 0$ and $\alpha_i = a_i^2 = k_i / \rho c_i > 0$ are the specific heat, the thermal conductivity and the diffusion coefficient for the phase i ($i = 1$: solid phase; $i = 2$: liquid phase) respectively.

The conditions at the solid-mushy interface $x=s(t)$ and the mushy-liquid interface $x = r(t)$ are given by (1), (2) and the requirement of the continuity of the temperature, i.e.,

$$\theta_1(s(t),t) = \theta_2(r(t),t) = 0 \quad , \quad t > 0. \quad (6)$$

The initial and boundary conditions are given by

$$\theta_1(0,t) = -D < 0 \quad , \quad t > 0 \quad , \quad (7)$$

$$\theta_2(x,0) = \theta_2(+\infty,t) = E > 0 \quad , \quad x > 0 \quad , \quad t > 0 \quad , \quad (8)$$

$$s(0) = r(0) = 0. \quad (9)$$

We consider an overspecified heat flux condition (e.g. Cannon [4], Tarzia [15]) on the fixed face $x=0$ which is given by (e.g. Stampella & Tarzia [14], Tarzia [17–19], Solomon, Wilson & Alexiades [13])

$$k_1 \theta_{1_x}(0,t) = \frac{q_0}{\sqrt{t}} \quad , \quad t > 0 \quad , \quad \text{with } q_0 > 0. \quad (10)$$

Moreover, the coefficients $q_0 > 0$ (which characterizes the heat flux at the fixed face $x=0$) and $T_0 > 0$ (which is the temperature at the fixed face $x = 0$) must be found through an experimental phase-change process (e.g. Arderius, Lara & Tarzia [1]). If by means of a phase-change experiment we are able to measure these quantities, then we shall find formulae for the determination of the unknown coefficients (ϵ , γ : parameters of the mushy zone; h , ρ , c_1 , c_2 , k_1 , k_2 : thermal coefficients of the material). Moreover, it does exist iff some complementary conditions for the corresponding data are verified. We generalize some of the results obtained in Stampella & Tarzia [14] for the particular case $\epsilon=1$ and $\gamma=0$ (i.e., for a sharp interphase, without mushy region) and those obtained in Tarzia [19] for the one-phase case. In Tarzia [18] several references on the determination of physical coefficients were given. We shall only consider here the respective properties for the determination of the thermal conductivity k_2 of the liquid phase (initial phase) or the parameter $\epsilon \in (0,1)$ which characterizes the free boundary condition (1). Other cases will be

considered in Gonzalez & Tarzia [8].

Secondly, we shall consider the determination of the unknown coefficients through approximate methods (heat balance integral and variational methods) corresponding to the one-phase Stefan problem. We consider the following melting problem for a semi-infinite material with an overspecified condition on the fixed face :

$$\rho c T_t = k T_{xx} , \quad 0 < x < s(t) , t > 0, \quad (11)$$

$$s(0) = 0 , \quad (12)$$

$$T(0, t) = T_0 > 0 , t > 0 , \quad (13)$$

$$T(s(t), t) = 0 , t > 0 , \quad (14)$$

$$k T_x(s(t), t) = - \rho h \dot{s}(t) , t > 0 , \quad (15)$$

$$k T_x(0, t) = - \frac{q_0}{\sqrt{t}} , t > 0 , \quad (16)$$

where $T = T(x, t)$ is the temperature of the liquid phase.

In Tarzia [17,18] one or two thermal coefficients were determined, and formulae for the unknown coefficients were given by using the exact Lamé-Clapeyron solution. In Garguichevich, Sanziel & Tarzia[7] the approximate solution is given by using the quasi-stationary, heat balance integral and variational methods. Now, we shall consider the heat balance integral and variational methods (e.g. Goodman [9], Biot [3]) for the determination of one thermal coefficient. We propose a different approach to the one proposed before by considering a convex linear expansion (with a parameter to be also determined) of the first and second order approximation solutions for the temperature. We also find the necessary and sufficient conditions for the existence of a solution and the corresponding formulae for the unknown coefficients. In Castellini & Tarzia [6] comparison results are obtained for the quasi-stationary, heat balance integral and variational methods.

II Determination of one unknown thermal coefficient through a mushy zone model for the two-phase Stefan problem

Taking into account the hypothese $(H_1) - (H_3)$ we can formulate the following

Problem (P_1) : Find the free boundaries $x=s(t)$ and $x=r(t)$, defined for $t > 0$ with $0 < s(t) < r(t)$ and $s(0) = r(0) = 0$, the temperature $\theta = \theta(x, t)$, defined by (3) for $x > 0$ and $t > 0$, and k_2 or c such that they satisfy the conditions (1), (2), (4) – (10) where $D > 0$, $E > 0$ and $q_0 > 0$ are data and they must be known or determined by an

experience of phase-change.

The solution of this problem is given by (e.g. Carslaw & Jaeger [5], Rubinstein [11], Solomon, Wilson & Alexiades [12], Tarzia [15, 20])

$$\theta_1(x,t) = -D + \frac{D}{f\left(\frac{\sigma}{a_1}\right)} f\left(\frac{x}{2 a_1 \sqrt{t}}\right), \quad (17)$$

$$\theta_2(x,t) = \frac{-E f\left(\frac{\omega}{a_2}\right)}{1 - f\left(\frac{\omega}{a_2}\right)} + \frac{E}{1 - f\left(\frac{\omega}{a_2}\right)} f\left(\frac{x}{2 a_2 \sqrt{t}}\right), \quad (18)$$

$$s(t) = 2 \sigma \sqrt{t}, \quad \sigma > 0, \quad (19)$$

$$r(t) = 2 \omega \sqrt{t}, \quad \omega > \sigma, \quad (20)$$

the coefficient ω is given by

$$\omega = \omega(\sigma) = a_1 W\left(\frac{\sigma}{a_1}\right), \quad (21)$$

and, the coefficient σ and the unknown thermal coefficient k_2 or ϵ are obtained by solving the following system of equations

$$\frac{q_0}{h \rho a_1} \exp\left(-\frac{\sigma^2}{a_1^2}\right) - \frac{E k_2}{h \rho a_1 a_2 \sqrt{\pi}} F_1\left(\frac{\omega(\sigma)}{a_2}\right) = G\left(\frac{\sigma}{a_1}\right), \quad (22)$$

$$\frac{a_1}{k_1} f\left(\frac{\sigma}{a_1}\right) = \frac{D}{q_0 \sqrt{\pi}} \quad (23)$$

where

$$f(x) = \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt, \quad F_1(x) = \frac{\exp(-x^2)}{1 - f(x)}, \quad (24)$$

$$W(x) = x + \frac{\gamma \sqrt{\pi}}{2 D} f(x) \exp(x^2), \quad G(x) = x + \frac{(1 - \epsilon) \gamma \sqrt{\pi}}{2 D} f(x) \exp(x^2). \quad (25)$$

Theorem 1. – (i) (Determination of k_2) The necessary and sufficient condition for Problem (P₁), with σ and k_2 unknown, to have a unique solution is that data $D > 0$, $E > 0$, $q_0 > 0$, mushy zone coefficients $0 < \epsilon < 1$ and $\gamma > 0$, and thermal coefficients of the phase-change material $h, \rho, c_1, c_2, k_1 > 0$ do verify the condition

$$\frac{D k_1}{q_0 a_1 \sqrt{\pi}} < f(p), \quad (26)$$

where p is the unique positive zero of function P . In such case, the solution is given by (17) – (20) with

$$k_2 = \frac{k_1 c_2}{c_1} \frac{W^2(\xi_1)}{B^2}, \quad \sigma = a_1 \xi_1, \quad \omega = a_1 W(\xi_1), \quad (27)$$

where ξ_1 is the unique solution of the equation

$$f(x) = \frac{D k_1}{q_0 a_1 \sqrt{\pi}}, \quad x > 0. \quad (28)$$

and B is the only solution of the equation

$$\frac{1}{Q(x)} = \frac{h}{E c_2} \frac{H(\xi_1)}{W(\xi_1)}, \quad x > 0. \quad (29)$$

where

$$H(x) = \frac{q_0}{h \rho a_1} \exp(-x^2) - G(x), \quad Q(x) = \sqrt{\pi} x \exp(x^2) (1 - f(x)), \quad (30)$$

$$P(x) = \frac{q_0}{E \rho a_1 c_2} \exp(-x^2) - \left(1 + \frac{(1 - \epsilon) h}{E c_2}\right) \frac{\gamma \sqrt{\pi}}{2 D} f(x) \exp(x^2) - \left(1 + \frac{h}{E c_2}\right) x. \quad (31)$$

(ii) (Determination of ϵ) The necessary and sufficient condition for Problem (P_1) , with σ and ϵ unknown, to have a unique solution is that data $D > 0$, $E > 0$, $q_0 > 0$, mushy zone coefficient $\gamma > 0$ and thermal coefficients of the phase-change material h , ρ , c_1 , c_2 , k_1 , $k_2 > 0$ do verify the conditions

$$q_0 > \frac{E k_2}{a_2 \sqrt{\pi}}, \quad f(v) < \frac{D k_1}{q_0 a_1 \sqrt{\pi}} < f(u), \quad (32)$$

where u and v are the unique positive zeros of functions U and V respectively, which are defined by

$$U(x) = \frac{q_0}{h \rho a_1} \exp(-x^2) - x - \frac{E k_2}{h \rho a_1 a_2 \sqrt{\pi}} F_1\left(\frac{a_1}{a_2} W(x)\right), \quad (33)$$

$$V(x) = \frac{\gamma \sqrt{\pi}}{2 D} f(x) \exp(x^2) - U(x), \quad F_2(x) = \frac{\exp(-x_2)}{f(x)}. \quad (34)$$

In such case, the solution is given by (17) – (20) with

$$\epsilon = \frac{2 D}{\gamma \sqrt{\pi}} F_2(\xi_1) V(\xi_1), \quad \sigma = a_1 \xi_1, \quad \omega = a_1 W(\xi_1), \quad (35)$$

where ξ_1 is the unique solution of the eqn (28).

III Determination of one unknown thermal coefficient through the heat balance integral method in a one-phase Stefan problem

By using the heat balance integral method (e.g. Goodman [9]) we replace eqn (11) by

$$\frac{d}{dt} \left(\int_0^{s(t)} \theta(x,t) dx \right) = - \frac{k}{\rho c} \left(\frac{\rho h}{k} \dot{s}(t) + \theta_x(0,t) \right), \quad 0 < x < s(t), \quad t > 0, \quad (36)$$

and condition (15) by

$$\theta_{xx}(s(t),t) = \frac{c}{h} \theta_x^2(s(t),t), \quad t > 0. \quad (37)$$

We can formulate the following

Problem (P₂) : Find the free boundary $x=s(t)$, defined for $t > 0$, the temperature $\theta=\theta(x,t)$, defined for $0 < x < s(t)$, $t > 0$, and one of the four thermal coefficient k , ρ , h and c such that they satisfy the conditions (12) – (14), (16), (36) and (37).

If we choose a convex linear expansion for the temperature profile given by

$$\theta(x,t) = \theta_0 \left[\lambda \left(1 - \frac{x}{s(t)} \right)^2 + \left(1 - \lambda \right) \left(1 - \frac{x}{s(t)} \right) \right], \quad 0 < \lambda < 1, \quad (38)$$

the free boundary of problem (P₂) is given by

$$s(t) = 2 \sigma \sqrt{t} = 2 \mu \sqrt{\alpha t}, \quad \alpha = \frac{k}{\rho c}, \quad (39)$$

where $\sigma > 0$ is the coefficient which characterizes the free boundary and the unknown coefficients λ , σ (or μ) and one of the four elements $\{k, \rho, h, c\}$ must satisfy the following system of equation

$$\mu^2 = \frac{\frac{Ste}{2} (1 + \lambda)}{1 + \frac{Ste}{2} (1 - \frac{\lambda}{3})}, \quad Ste = \frac{c T_0}{h}, \quad (40)$$

$$\lambda = \beta - \sqrt{\beta^2 - 1}, \quad \beta = 1 + \frac{1}{Ste}, \quad (41)$$

$$T_0^2 k \rho c = \frac{4 \mu^2}{(1 + \lambda)^2} q_0^2, \quad (42)$$

Theorem 2. – The solution of the four cases is summarized in Table 1.

Unknown Coefficients	Restriction	Solution
k, σ	—	$k = \frac{4 q_0^2}{\rho c \theta_0^2} \frac{\mu^2}{(1 + \lambda)^2}, \quad \sigma = \frac{2 q_0}{\rho c \theta_0} \frac{\mu^2}{(1 + \lambda)^2}$ <p>where μ, λ are given by (40) and (41) respectively.</p>
ρ, σ	—	$\rho = \frac{4 q_0^2}{k c \theta_0^2} \frac{\mu^2}{(1 + \lambda)^2}, \quad \sigma = \frac{k \theta_0 (1 + \lambda)}{2 q_0}$ <p>where μ, λ are given by (40) and (41) respectively.</p>
c, σ	$\frac{k \rho h T_0}{2 q_0^2} < 1$	$\sigma = \sqrt{\frac{3 k \theta_0}{2 \rho h}} \sqrt{\frac{\lambda + 1}{2 \lambda^2 - 3 \lambda + 3}} (1 - \lambda),$ $c = \frac{h}{\theta_0} \frac{2 \lambda}{(1 - \lambda)^2},$ <p>where λ is the unique solution of the equation</p> $M(\lambda) = \frac{k \rho h \theta_0}{6 q_0^2}, \quad 0 < \lambda < 1.$
h, σ	$\frac{k \rho c T_0^2}{2 q_0^2} < 1$	$h = c \theta_0 \frac{(1 - \lambda)^2}{2 \lambda}, \quad \sigma = \sqrt{\frac{k}{\rho c}} \sqrt{\frac{3 \lambda (\lambda + 1)}{2 \lambda^2 - 3 \lambda + 3}}$ <p>where λ is the unique solution of the equation</p> $N(\lambda) = \frac{1}{12} \frac{\rho c k \theta_0^2}{q_0^2}, \quad 0 < \lambda < 1.$

Table 1. Restrictions and formulae for the unknown thermal coefficients through the heat balance integral method, where M and N are defined by

$$M(\lambda) = \frac{(1 - \lambda)^2}{(1 + \lambda)(2 \lambda^2 - 3 \lambda + 3)}, \quad N(\lambda) = \frac{\lambda}{(1 + \lambda)(2 \lambda^2 - 3 \lambda + 3)}$$

and verify the conditions

$$M(0) = \frac{1}{3}, \quad M(1) = 0, \quad M'(\lambda) < 0 \text{ in } (0, 1) \quad ; \quad N(0) = 0, \quad N(1) = \frac{1}{4}, \quad N'(\lambda) > 0 \text{ in } (0, 1).$$

IV Determination of one unknown thermal coefficient through the Biot's variational method in a one-phase Stefan problem

By using the variational method (e.g. Biot [3]) we replace condition (15) by (37) and eqn (11) by

$$\frac{\partial V_o}{\partial s} + \frac{\partial D_o}{\partial \dot{s}} = Q, \quad 0 < x < s(t), \quad t > 0, \quad (43)$$

where

$$V_o = \frac{1}{2} \int_0^{s(t)} \rho c \theta^2(x, t) \, dx : \text{thermal potential}, \quad (44)$$

$$D_o = \frac{1}{2} \int_0^{s(t)} \frac{1}{k} (\dot{H}_o(x, t))^2 \, dx : \text{dissipation function}, \quad (45)$$

$$Q_o = \theta_o \frac{\partial H_o}{\partial s}(0, t) : \text{thermal forces}, \quad (46)$$

where H_o is the heat displacement defined as the solution of the problem

$$\frac{\partial H_o}{\partial x} = -\rho c \theta, \quad H_o(s(t), t) = \rho L s(t). \quad (47)$$

We can then formulate the following

Problem (P₃) : Find the free boundary $x=s(t)$, defined for $t > 0$, the temperature $\theta=\theta(x, t)$, defined for $0 < x < s(t)$, $t > 0$, and one of the four thermal coefficient k , ρ , h and c such that they satisfy the conditions (12) – (14), (16), (37) and (43).

If we choose a convex linear expansion for the temperature profile given by (38), then the free boundary of problem (P₃) is given by (39) and the unknown coefficients λ , σ (or μ) and one of the four elements $\{k, \rho, h, c\}$ must satisfy the following system of equation

$$\mu^2 = \frac{21}{2} \lambda R(\lambda), \quad T_o^2 k \rho c = \frac{4 \mu^2}{(1+\lambda)^2} q_o^2, \quad \frac{c T_o}{h} = \frac{2 \lambda}{(1-\lambda)^2} \quad (48)$$

where

$$R(\lambda) = \frac{30 - 40 \lambda + 25 \lambda^2 - \lambda^3}{315 - 840 \lambda + 10008 \lambda^2 - 574 \lambda^3 + 143 \lambda^4} \quad (49)$$

$$R(0) = \frac{2}{21}, \quad R(1) = \frac{7}{26}, \quad R'(1) = 0, \quad R' > 0 \text{ in } (0, 1). \quad (50)$$

Theorem 3. – The solution of the four cases is summarized in Table 2.

Unknown Coefficients	Restriction	Solution
k, σ	—	$k = \frac{42 q_0^2}{\rho c \theta_0^2} \frac{\lambda R(\lambda)}{(1 + \lambda)^2}, \quad \sigma = \frac{21 q_0}{\rho c \theta_0} \frac{\lambda R(\lambda)}{1 + \lambda}$ where λ is given by (41).
ρ, σ	—	$\rho = \frac{42 q_0^2}{k c \theta_0^2} \frac{\lambda R(\lambda)}{(1 + \lambda)^2}, \quad \sigma = \frac{k \theta_0 (1 + \lambda)}{2 q_0}$ where λ is given by (41).
c, σ	$\frac{k \rho h T_0}{2 q_0^2} < 1$	$c = \frac{2 h}{\theta_0} \frac{\lambda}{(1 - \lambda)^2}, \quad \sigma = \frac{k \theta_0}{2 q_0} (1 + \lambda)$ where λ is the unique solution of the equation $\frac{(1 - \lambda)^2 R(\lambda)}{(1 + \lambda)^2} = \frac{k \rho h \theta_0}{21 q_0^2}, \quad 0 < \lambda < 1.$
h, σ	$\frac{52 k \rho c T_0^2}{147 q_0^2} < 1$	$h = \frac{c \theta_0}{2} \frac{(1 - \lambda)^2}{\lambda}, \quad \sigma = \frac{k \theta_0}{2 q_0} (1 + \lambda)$ where λ is the unique solution of the equation $\frac{\lambda R(\lambda)}{(1 + \lambda)^2} = \frac{k \rho c \theta_0^2}{42 q_0^2}, \quad 0 < \lambda < 1.$

Table 2. Restrictions and formulae for the unknown thermal coefficients through the variational method.

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