### Explicit and Approximated Solutions for Heat and Mass Transfer Problems with a Moving Interface

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#### 1. Introduction

The goal of this chapter is firstly to give a survey of some explicit and approximated solutions for heat and mass transfer problems in which a free or moving interface is involved. Secondly, we show simultaneously some new recent problems for heat and mass transfer, in which a free or moving interface is also involved. We will consider the following problems:

- 1. Phase-change process (Lamé-Clapeyron-Stefan problem) for a semi-infinite material:
- i. The Lamé-Clapeyron solution for the one-phase solidification problem (modeling the solidification of the Earth with a square root law of time);
- ii. The pseudo-steady-state approximation for the one-phase problem;
- iii. The heat balance integral method (Goodman method) and the approximate solution for the one-phase problem;
- iv. The Stefan solution for the planar phase-change surface moving with constant speed;
- v. The Solomon-Wilson-Alexiades model for the phase-change process with a mushy region and its similarity solution for the one-phase case;
- vi. The Cho-Sunderland solution for the one-phase problem with temperature-dependent thermal conductivity;
- vii. The Neumann solution for the two-phase problem for prescribed surface temperature at the fixed face;
- viii. The Neumann-type solution for the two-phase problem for a particular prescribed heat flux at the fixed face, and the necessary and sufficient condition to have an instantaneous phase-change process;
- ix. The Neumann-type solution for the two-phase problem for a particular prescribed convective condition (Newton law) at the fixed face, and the necessary and sufficient condition to have an instantaneous phase-change process;
- x. The similarity solution for the two-phase Lamé-Clapeyron-Stefan problem with a mushy region.
- xi. The similarity solution for the phase-change problem by considering a density jump;
- xii. The determination of one or two unknown thermal coefficients through an overspecified condition at the fixed face for one or two-phase cases.
- xiii. A similarity solution for the thawing in a saturated porous medium by considering a density jump and the influence of the pressure on the melting temperature.

- 2. Free boundary problems for the diffusion equation:
- i. The oxygen diffusion-consumption problem and its relationship with the phase-change problem;
- ii. The Rubinstein solution for the binary alloy solidification problem;
- iii. The Zel'dovich-Kompaneets-Barenblatt solution for the gas flow through a porous medium;
- iv. Luikov coupled heat and mass transfer for a phase-change process;
- A mixed saturated-unsaturated flow problem representing absorption of water by a soil with a constant pond depth at the surface and an explicit solution for a particular diffusivity;
- vi. Estimation of the diffusion coefficient in a gas-solid system;
- vii. The coupled heat and mass transfer during the freezing of the high-water content materials with two free boundaries: the freezing and sublimation fronts.

## 2. Explicit solutions for phase-change process (Lamé-Clapeyron-Stefan problem) for a semi-infinite material

Heat transfer problems with a phase-change such as melting and freezing have been studied in the last century due to their wide scientific and technological applications. A review of a long bibliography on moving and free boundary problems for phase-change materials (PCM) for the heat equation is shown in (Tarzia, 2000a). Some previous reviews on explicit or approximated solutions were presented in (Garguichevich & Sanziel, 1984; Howison, 1988; Tarzia, 1991b & 1993). Some reviews, books or booklets in the subject are (Alexiades & Solomon, 1993; Bankoff, 1964; Brillouin, 1930; Cannon, 1984; Carslaw & Jaeger, 1959; Crank, 1984; Duvaut, 1976; Elliott & Ockendon, 1982; Fasano, 1987 & 2005; Friedman, 1964; Gupta, 2003; Hill, 1987; Luikov, 1968; Lunardini, 1981 & 1991; Muehlbauer & Sunderland, 1965; Primicerio, 1981; Rubinstein, 1971; Tarzia, 1984b & 2000b; Tayler, 1986).

### 2.1 The Lamé-Clapeyron solution for the one-phase solidification problem (modeling the solidification of the Earth with a square root law of time)

We consider the solidification of semi-infinite material, represented by x > 0. We will find the interface solid-liquid x = s(t) and the temperature T = T(x, t) of the solid phase defined by

$$T(x,t) = \begin{cases} T(x,t) & \text{if } 0 < x < s(t), t > 0 \\ T_f & \text{if } s(t) \le x, t > 0 \end{cases}$$
(1)

which satisfy the following free boundary problem:

$$\rho c T_t - k T_{xx} = 0$$
,  $0 < x < s(t)$ ,  $t > 0$  (2)

$$T(0,t) = T_0 < T_f , \quad t > 0$$
(3)

$$T(s(t),t) = T_f, \quad t > 0 \tag{4}$$

$$kT_x(s(t),t) = \rho \ell \dot{s}(t), \quad t > 0$$
(5)

$$s(0) = 0 \tag{6}$$

Eq. (2) represents the heat equation for the solid phase, k is the thermal conductivity,  $\rho$  is the mass density, c is the heat capacity,  $\ell$  is the latent heat of fusion by unit of mass,  $T_0$  is the imposed temperature at the fixed face x = 0, and the material is initially at the melting temperature  $T_f$ . The problem (2)-(6) is known in literature as the one-phase Stefan problem (Lamé-Clapeyron-Stefan problem) and the condition (5) as the Stefan condition. Free boundary problems of this type were presented by the first time in (Lamé & Clapeyron, 1831) in order to study the solidification of the Earth and was continued independently by (Stefan, 1891a, b & 1990) in order to study the thickness of polar ice. We remark here that Lamé & Clapeyron found the important law for the phase-change interface with a square root of time.

<u>Theorem 1.</u> (Lamé-Clapeyron solution).

The explicit solution to the free boundary problem (2)-(6) is given by

$$T(x,t) = T_0 + \frac{T_f - T_0}{f(\xi)} erf(\frac{x}{2a\sqrt{t}}), \quad s(t) = 2a\xi\sqrt{t}$$
(7)

where  $a^2 = \alpha = \frac{k}{\rho c}$  is the diffusion coefficient and  $\xi > 0$  is the unique solution to the

equation

$$E(x) = \frac{Ste}{\sqrt{\pi}}, \quad x > 0 \tag{8}$$

with

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} \exp(-u^2) du$$
,  $E(x) = x \ erf(x) \exp(x^2)$ , (9)

$$Ste = \frac{c(T_f - T_0)}{\ell}: \text{ Stefan number ,}$$
(10)

and the total heat flux at the fixed face x = 0 is given by

$$Q(t) = \int_{0}^{t} kT_{x}(0,\tau)d\tau = \rho \ell s(t) \exp(\xi^{2}).$$
(11)

Proof. We have the following properties:

$$E(0) = 0, \quad E(+\infty) = +\infty, \quad E'(x) > 0, \quad \forall x > 0.$$
(12)

Remark 1. From (4) we have

$$T_{x}(s(t),t)\dot{s}(t) + T_{t}(s(t),t) = 0, \quad t > 0$$
(13)

and therefore the Stefan condition (5) is transformed in

$$kT_{x}^{2}(s(t),t) = -\rho\ell T_{t}(s(t),t) = -\frac{\ell k}{c}T_{xx}(s(t),t), \quad t > 0$$
(14)

which implies that the problem (2)-(6) is always a nonlinear problem (Pekeris & Slichter, 1939).

Remark 2.

A generalization of the Lamé-Clapeyron solution is given in (Menaldi & Tarzia, 2003) for a particular source in the heat equation. A study of the behaviour of the Lamé-Clapeyron solution when the latent heat goes to zero is given in (Guzman, 1982; Sherman, 1971).

#### 2.2 The pseudo-steady-state approximation for the one-phase problem

An approximated solution to problem (2)-(6) is given by the pseudo-steady-state approximation which must satisfy the following conditions: (3)-(6) and the steady-state equation

$$T_{xx} = 0$$
,  $0 < x < s(t)$ ,  $t > 0$ . (15)

Theorem 2 (Stefan, 1989a)

The solution to the problem (15), (3)-(6) is given by

$$T(x,t) = T_0 + \frac{T_f - T_0}{s(t)}x, \qquad 0 < x < s(t), \quad t > 0$$
(16)

$$s(t) = 2a\xi_{ap}\sqrt{t}, \qquad \xi_{ap} = \sqrt{\frac{Ste}{2}}$$
(17)

Proof.

The solution to (15), (3) and (4) is given by (16). Therefore the condition (5) is transformed in the ordinary differential equation

$$k(T_f - T_0) / s(t) = \rho \lambda \dot{s}(t) \tag{18}$$

with the initial condition (6), whose solution is given by

$$s^{2}(t) = 2k(T_{f} - T_{0})t / (\rho \ell) = 4a^{2} \frac{Ste}{2}t$$
(19)

that is

$$s(t) = \sqrt{\frac{2k(T_f - T_0)}{\rho\ell}t}$$
(20)

<u>Remark 3.</u>

If the Stefan number is very small, i.e.

$$Ste = \frac{c(T_f - T_0)}{\ell} \ll 1 \tag{21}$$

then the solution  $\xi$  to the equation (8) for the Lamé-Clapeyron solution can be taken as  $\xi_{ap}$ , given in (17). This can be obtained by using the following first approximation:

$$\exp(x^2) \approx 1, \qquad f(x) \approx \frac{2}{\sqrt{\pi}}x, \quad 0 < x << 1$$
. (22)

Remark 4.

A study of sufficient conditions on data to estimate the occurrence of a phase-change process is given in (Solomon et al., 1983; Tarzia & Turner, 1992 & 1999).

## 2.3 The heat balance integral method (Goodman method) and the approximate solution for the one-phase problem

An approximated solution for the following fusion problem (similar to the solidification problem (2)-(6))

$$\rho c T_t - k T_{xx} = 0$$
,  $0 < x < s(t)$ ,  $t > 0$  (23)

$$T(0,t) = T_0 > 0, \quad t > 0$$
 (24)

$$T(s(t),t) = 0, \quad t > 0$$
 (25)

$$kT_{x}(s(t),t) = -\rho\ell\dot{s}(t), \quad t > 0$$
<sup>(26)</sup>

$$s(0) = 0$$
 (27)

is given by the heat balance integral method, known by the Goodman method (Goodman,1958). This method consists of replacing the Stefan condition (26) by

$$T_x^2(s(t),t) = \frac{\ell}{c} T_{xx}(s(t),t), \quad t > 0$$
(28)

and the heat equation (23) by its integral on the domain (0, s(t)) given by

$$\frac{d}{dt} \int_{0}^{s(t)} T(x,t) dx = \int_{0}^{s(t)} T_{t}(x,t) dx + T(s(t),t) \dot{s}(t) = \int_{0}^{s(t)} T_{t}(x,t) dx = \frac{k}{\rho c} \int_{0}^{s(t)} T_{xx}(x,t) dx$$

$$= \frac{k}{\rho c} [T_{x}(s(t),t) - T_{x}(0,t)] = -\frac{k}{\rho c} [\frac{\rho \lambda}{k} \dot{s}(t) + T_{x}(0,t)]$$
(29)

that is

$$\frac{d}{dt} \int_{0}^{s(t)} T(x,t) dx = -\frac{k}{\rho c} \left[ \frac{\rho \ell}{k} \dot{s}(t) + T_{x}(0,t) \right].$$
(30)

In order to solve (30), (28), (24), (25) and (27), we propose an approximated temperature profile

$$T(x,t) = \alpha(t)(s(t) - x) + \beta(t)(s(t) - x)^2, \quad 0 < x < s(t), \ t > 0$$
(31)

where  $\alpha = \alpha(t)$ ,  $\beta = \beta(t)$ , and s = s(t) are real functions to be determined. Firstly, we can obtain  $\alpha$  and  $\beta$  as a function of s and, therefore, we solve the corresponding ordinary differential equation for s = s(t).

#### Theorem 3.

The Goodman approximated solution is given by:

$$\alpha(t) = \frac{\ell}{c} \frac{\sqrt{1 + 2Ste} - 1}{s(t)} , \ \beta(t) = \frac{\alpha(t)s(t) + T_0}{s^2(t)}$$
(32)

$$s(t) = 2a\xi_g \sqrt{t}, \quad \xi_g = \sqrt{3} \frac{1 + 2Ste - \sqrt{1 + 2Ste}}{5 + Ste + \sqrt{1 + 2Ste}}, \quad Ste = \frac{cT_0}{\ell}$$
(33)

Remark 5.

Other refinements of the Goodman method are given in (Bell, 1978; Lunardini, 1981; Lunardini 1991). In (Reginato & Tarzia, 1993; Reginato et al, 1993; Reginato et al., 2000) the heat balance method was applied to root growth of crops and the modelling nutrient uptake. In (Tarzia, 1990a) the heat balance method was applied to obtain the exponentially fast asymptotic behaviour of the solutions in heat conduction problems with absorption.

## 2.4 The Stefan solution for the planar phase-change surface moving with constant speed

When the phase-change interface is moving with constant speed we can consider the following inverse Stefan problem: find the temperature T = T(x,t) and f(t) = T(0,t) such that:

$$\alpha T_{xx} = T_t, \qquad 0 < x < s(t), \quad t > 0 \quad (\alpha = \frac{k}{\rho c})$$
(34)

$$T(s(t), t) = 0, t > 0$$
 (35)

$$kT_x(s(t),t) = \rho\ell\dot{s}(t), \qquad t > 0 \tag{36}$$

$$\dot{s}(t) = m > 0, \quad s(0) = 0 \quad (s(t) = mt)$$
(37)

<u>Theorem 4.</u> (Stefan, 1989b & 1991) The solution to (34)-(37) is given by

$$T(x,t) = \frac{\ell}{c} [1 - \exp(\frac{m}{\alpha}(mt - x))]$$
(38)

and the temperature at the fixed face is variable in time given by the expression:

$$f(t) = T(0,t) = -\frac{\ell}{c} \left[ \exp(\frac{m^2 t}{\alpha}) - 1 \right] < 0 = T_f, \quad t > 0.$$
(39)

Remark 6.

More details with respect to the inverse Stefan problem can be found in (Quilghini, 1967).

## 2.5 The Solomon-Wilson-Alexiades model for the phase-change process with a mushy region and its similarity solution for the one-phase case

We consider a semi-infinite material in the liquid phase at the melting temperature  $T_f$ . We impose a temperature  $T_0 < T_f$  at the fixed face x = 0, and the solidification process begins, and three regions can be distinguished, as follows (Solomon et al., 1982):

- i. the liquid phase, at temperature  $T = T_t$ , occupying the region x > r(t), t > 0;
- ii. the solid phase, at temperature  $T(x,t) < T_t$ , occupying the region 0 < x < s(t), t > 0;
- iii. the mushy zone, at temperature  $T_f$ , occupying the region s(t) < x < r(t), t > 0. We make the following two assumptions on its structure:
- a. the material in the mushy zone contains a fixed fraction  $\epsilon \ell$  (with constant  $0 < \epsilon < 1$ ) of the total latent heat  $\ell$ .
- b. the width of the mushy zone is inversely proportional (with constant  $\gamma > 0$ ) to the temperature gradient at s(t).

Therefore the problem consists of finding the free boundaries x = s(t) and x = r(t), and the temperature T = T(x, t) such that the following conditions are satisfied:

$$\rho c T_t - k T_{xx} = 0$$
,  $0 < x < s(t)$ ,  $t > 0$  (40)

$$T(0,t) = T_0 < T_f , \quad t > 0 ; \ s(0) = r(0) = 0$$
(41)

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

$$\tag{42}$$

$$kT_x(s(t),t) = \rho\ell[\varepsilon\dot{s}(t) + (1-\varepsilon)\dot{r}(t)], \quad t > 0$$
(43)

$$T_{x}(s(t),t)(r(t)-s(t)) = \gamma, \quad t > 0.$$
(44)

Theorem 5. (Solomon et al., 1982):

The explicit solution to problem (40)-(44) is given by:

$$T(x,t) = T_0 + \frac{(T_f - T_0)}{erf(\xi)} erf(\frac{x}{2a\sqrt{t}}), \quad s(t) = 2\xi a\sqrt{t}, \quad r(t) = 2\mu a\sqrt{t}$$
(45)

where

$$\mu = \xi + \frac{\gamma \sqrt{\pi}}{2(T_f - T_0)} erf(\xi) exp(\xi^2), \quad a = \sqrt{\frac{k}{\rho c}}$$
(46)

and  $\xi > 0$  is the unique solution to the equation

$$D(x) = \frac{Ste}{\sqrt{\pi}}, \quad x > 0 \quad \left(Ste = \frac{c(T_f - T_0)}{\ell}\right)$$
(47)

with

$$D(x) = xerf(x)\exp(x^{2}) + \frac{\gamma(1-\varepsilon)\sqrt{\pi}}{2(T_{f} - T_{0})}[\exp(x^{2})erf(x)]^{2}.$$
(48)

Remark 7.

The classical Lamé-Clapeyron solution can be obtained for the particular case  $\varepsilon = 1$ ,  $\gamma = 0$ . If the Stefan number is small, then an approximated solution for  $\xi$  and  $\mu$  is given by:

$$\xi = \left[\frac{Ste}{2[1 + \gamma(1 - \varepsilon) / (T_f - T_0)]}\right]^{\frac{1}{2}}, \quad \mu = \xi[1 + \gamma / (T_f - T_0)] \quad .$$
(49)

#### 2.6 The Cho-Sunderland solution for the one-phase problem with temperaturedependent thermal conductivity

We consider the following solidification problem for a semi-infinite material

$$\rho c T_t(x,t) = (k(T)T_{\chi}(x,t))_{\chi}, \quad 0 < x < s(t), t > 0$$
(50)

$$T(0,t) = T_0 < T_f , \quad t > 0$$
(51)

$$T(s(t),t) = T_f, \quad t > 0$$
 (52)

$$k(T_{f}) T_{\chi}(s(t), t) = \rho \ell \dot{s}(t) , \quad t > 0$$
(53)

where T(x,t) is the temperature of the solid phase,  $\rho > 0$  is the density of mass,  $\ell > 0$  is the latent heat of fusion by unity of mass, c > 0 is the specific heat, x=s(t) is the phase-change interface,  $T_f$  is the phase-change temperature,  $T_o$  is the temperature at the fixed face x=0. We suppose that the thermal conductivity has the following expression:

$$k = k(T) = k_0 [1 + \beta (T - T_0) / (T_f - T_0)] \quad , \ \beta \in \mathbb{R}.$$
 (54)

Let  $a_o = k_o / \rho c$  be the diffusion coefficient at the temperature  $T_o$ . We observe that if  $\beta = 0$ , the problem (50)-(53) becomes the classical one-phase Lamé-Clapeyron-Stefan problem.

Theorem 6. (Cho & Sunderland, 1974)

The solution to problem (50)-(54) is given by:

$$T(x,t) = T_0 + \frac{(T_f - T_0)}{\Phi(\lambda)} \Phi(\eta) \quad , \quad \eta = \frac{x}{2\sqrt{\alpha_0 t}} \quad , \quad 0 < \eta < \lambda$$
(55)

$$s(t) = 2\lambda \sqrt{\alpha_o t} \tag{56}$$

where  $\Phi = \Phi(x) = \Phi_{\delta}(x)$  is the modified error function, for  $\delta > -1$ , the unique solution to the following boundary value problem in variable *x*, i.e:

$$\begin{cases} i) \ [(1+\delta \Phi'(x))\Phi'(x)]' + 2x\Phi'(x) = 0, & x > 0, \\ ii) \ \Phi(0^+) = 0 & , \ \Phi(+\infty) = 1 \end{cases}$$
(57)

and the unknown thermal coefficients  $\lambda$  and  $\delta$  must satisfy the following system of equations:

$$\beta - \delta \Phi(\lambda) = 0 \tag{58}$$

$$[1 + \delta \Phi(\lambda)] \frac{\Phi'(\lambda)}{\lambda \Phi(\lambda)} - \frac{2\ell}{c(T_f - T_o)} = 0 \quad .$$
(59)

Remark 8.

Explicit solutions are given in (Briozzo et al., 2007 & 2010; Briozzo & Tarzia, 2002; Natale & Tarzia, 2006; Rogers & Broadbridge, 1988; Tirskii, 1959; Tritscher & Broadbridge, 1994) where nonlinear thermal coefficients are considered and in (Natale & Tarzia, 2000; Rogers, 1986) for Storm's materials.

## 2.7 The Neumann solution for the two-phase problem for prescribed surface temperature at the fixed face

We consider a semi-infinite material with null melting temperature  $T_f = 0$ , with an initial temperature -C < 0 and having a temperature boundary condition B > 0 at the fixed face x = 0. The model for the two-phase Lamé-Clapeyron-Stefan problem is given by: find the free boundary x = s(t), defined for t > 0, and the temperature T = T(x, t) defined by

$$T(x,t) = \begin{cases} T_2(x,t) > T_f & \text{if } 0 < x < s(t), t > 0\\ T_f & \text{if } x = s(t), t > 0\\ T_1(x,t) < T_f & \text{if } s(t) < x, t > 0 \end{cases}$$
(60)

for x > 0 and t > 0, such that (i=1: solid phase; i=2: liquid phase):

$$\rho c_2 T_{2_t} - k_2 T_{2_{xx}} = 0, \qquad 0 < x < s(t), \quad t > 0,$$
(61)

$$\rho c_1 T_{1_t} - k_1 T_{1_{xx}} = 0, \qquad x > s(t), \quad t > 0 , \qquad (62)$$

$$T_1(x,0) = -C < 0, \qquad x > 0, \tag{63}$$

$$T_2(0,t) = B > 0, \qquad t > 0,$$
 (64)

$$T_1(s(t),t) = T_f = 0, \qquad t > 0,$$
 (65)

$$T_2(s(t),t) = T_f = 0, \qquad t > 0,$$
 (66)

$$k_1 T_{1_v}(s(t), t) - k_2 T_{2_v}(s(t), t) = \rho \ell \dot{s}(t), \quad t > 0 ,$$
(67)

$$s(0) = 0$$
. (68)

<u>Theorem 7.</u> (Neumann solution (Webber, 1901)) The explicit solution to problem (61)-(68) is given by:

$$T_{2}(x,t) = B - \frac{B}{erf(\sigma / a_{2})} erf(\frac{x}{2a_{2}\sqrt{t}}), \quad 0 \le x \le s(t), t > 0$$
(69)

$$T_1(x,t) = -C + \frac{B}{erfc(\sigma / a_1)} erfc(\frac{x}{2a_1\sqrt{t}}), \quad s(t) \le x, \quad t > 0$$
(70)

$$s(t) = 2\sigma\sqrt{t}$$
  $(a_2^2 = \frac{k_2}{\rho c_2}, a_1^2 = \frac{k_1}{\rho c_1})$  (71)

where  $\sigma > 0$  is the unique solution to the following equation:

$$F(x) = x, \quad x > 0 \tag{72}$$

where

$$F(x) = \frac{Bk_2}{\rho \ell a_2 \sqrt{\pi}} F_2(\frac{x}{a_2}) - \frac{Ck_1}{\rho \ell a_1 \sqrt{\pi}} F_1(\frac{x}{a_1})$$
(73)

$$F_1(x) = \frac{exp(-x^2)}{erfc(x)}, \quad F_2(x) = \frac{exp(-x^2)}{erf(x)}, \quad erfc(x) = 1 - erf(x).$$
(74)

#### Remark 9.

It is very interesting to answer the following question: When is the Neumann solution for a semi-infinite material applicable to a finite material  $(0, x_0)$ ? (Solomon, 1979).

Taking into account that  $erf(x) \cong 1$  for  $2 \le x$ , we have an affirmative answer for a short period of time because  $T_1(x_0, t) \cong -C$  is equivalent to

$$erf(\frac{x_0}{2a_1\sqrt{t}}) \approx 1 \tag{75}$$

that is

$$t \le \frac{x_0^2}{16a_1^2} \,. \tag{76}$$

Remark 10.

A generalization of Neumann solution is given in (Briozzo et al, 2004 & 2007b) for particular sources in the heat equations for both phases. A study of the behaviour of the Neumann solution when the latent heat goes to zero is given in (Tarzia & Villa, 1991). A generalization of Neumann solution in multi-phase media is given in (Sanziel & Tarzia, 1989; Weiner, 1955; Wilson, 1978 & 1982), and when we have shrinkage or expansion (Fi & Han, 2007; Natale et al., 2010; Wilson & Solomon, 1986).

## 2.8 The Neumann-type solution for the two-phase problem for a particular prescribed heat flux at the fixed face, and the necessary and sufficient condition to have an instantaneous phase-change process

If we consider the problem (61)-(68) by changing the boundary condition (64) at x = 0 by a heat flux condition of the type

$$k_2 T_{2_x}(0,t) = -\frac{q_0}{\sqrt{t}} \tag{77}$$

then we can obtain the following result: <u>Theorem 8.</u> (Tarzia, 1981)

i. If  $q_0$  verifies the inequality

$$q_0 > \frac{Ck_1}{a_1 \sqrt{\pi}} \tag{78}$$

then we have an instantaneous change of phase and the corresponding explicit solution is given by:

$$T_2(x,t) = A_2 + B_2 erf(\frac{x}{2a_2\sqrt{t}}), \quad 0 \le x \le s(t), \ t > 0$$
(79)

$$T_1(x,t) = A_1 + B_1 erf(\frac{x}{2a_1\sqrt{t}}), \quad s(t) \le x, \ t > 0$$
(80)

$$s(t) = 2w\sqrt{t} \qquad \left(a_2^2 = \frac{k_2}{\rho c_2}, a_1^2 = \frac{k_1}{\rho c_1}\right)$$
(81)

where

$$A_{1}(w) = C \frac{erf(w / a_{1})}{erfc(w / a_{1})}, \quad B_{1}(w) = \frac{-C}{erfc(w / a_{1})}$$
(82)

$$A_{2}(w) = \frac{a_{2}q_{0}\sqrt{\pi}}{k_{2}} erf(w / a_{2}), \quad B_{2}(w) = -\frac{a_{2}q_{0}\sqrt{\pi}}{k_{2}}$$
(83)

and w > 0 is the unique solution to the equation

$$F_0(x) = x, \quad x > 0,$$
 (84)

where

$$F_0(x) = \frac{q_0}{\rho \lambda} \exp(-x^2 / a_2^2) - \frac{Ck_1}{\rho \lambda a_1 \sqrt{\pi}} F_1(x / a_1) .$$
(85)

ii. If  $q_0 \le Ck_1 / a_1 \sqrt{\pi}$  the corresponding problem represents only a heat conduction problem for the initial solid phase, and the temperature is given by

$$T(x,t) = T_1(x,t) = -C + \frac{q_0 a_1 \sqrt{\alpha \pi}}{k_1} \operatorname{erfc}(\frac{x}{2a_1 \sqrt{\alpha t}}), \quad x > 0, t > 0.$$
(86)

Corollary 9 (Tarzia, 1981)

The coefficient  $\sigma$  that characterizes the free boundary  $s(t) = 2\sigma\sqrt{t}$  of Neumann solution (69)-(74) must satisfy the following inequality:

$$erf\left(\frac{\sigma}{a_2}\right) < \frac{B}{C} \sqrt{\frac{k_2 c_2}{k_1 c_1}} .$$
(87)

## 2.9 The Neumann-type solution for the two-phase problem for a particular prescribed convective condition (Newton law) at the fixed face, and the necessary and sufficient condition to have an instantaneous phase-change process

We consider the following free boundary problem: find the solid-liquid interface x = s(t) and the temperature T(x,t) defined by

$$T(x,t) = \begin{cases} T_s(x,t) & \text{if } 0 < x < s(t), \quad t > 0, \\ T_f & \text{if } x = s(t), \quad t > 0, \\ T_l(x,t) & \text{if } x > s(t), \quad t > 0, \end{cases}$$
(88)

which satisfy the following equations and boundary conditions

$$T_{s_t} = \alpha_s T_{s_{v_t}}, \quad 0 < x < s(t), \ t > 0$$
(89)

$$T_{l_{t}} = \alpha_{l} T_{l_{yy}}, \quad x > s(t), \ t > 0$$
(90)

$$T_{s}(s(t),t) = T_{l}(s(t),t) = T_{f}, \quad x = s(t), \quad t > 0$$
(91)

$$T_{l}(x,0) = T_{l}(+\infty,t) = T_{i}, \quad x > 0, \quad t > 0$$
(92)

$$k_{s}T_{s_{x}}(0,t) = \frac{h_{0}}{\sqrt{t}}(T_{s}(0,t) - T_{\infty}), \quad t > 0$$
(93)

$$k_{s}T_{s_{x}}(s(t),t) - k_{l}T_{l_{x}}(s(t),t) = \rho\ell\dot{s}(t), \quad t > 0$$
(94)

$$s(0) = 0$$
 (95)

where the subscripts *s* and *l* represent the solid and liquid phases respectively,  $\rho$  is the common density of mass and  $\ell$  is the latent heat of fusion, and  $T_{\infty} < T_f < T_i$ . We have the following results:

Theorem 10. (Tarzia, 2004)

If the coefficient  $h_0$  verifies the inequality

$$h_0 > \frac{k_l}{\sqrt{\pi\alpha_l}} \frac{T_i - T_f}{T_i - T_{\infty}}$$
(96)

there exists an instantaneous solidification process and then the free boundary problem (89)-(95) has the explicit solution to a similarity type given by

$$s(t) = 2\lambda \sqrt{\alpha_l t} \tag{97}$$

$$T_{s}(x,t) = T_{\infty} + \frac{(T_{f} - T_{\infty})\left[1 + \frac{h_{0}\sqrt{\pi\alpha_{s}}}{k_{s}}erf(\frac{x}{2\sqrt{\alpha_{s}t}})\right]}{1 + \frac{h_{0}\sqrt{\pi\alpha_{s}}}{k_{s}}erf(\lambda\sqrt{\frac{\alpha_{l}}{\alpha_{s}}})}$$
(98)

$$T_{l}(x,t) = T_{i} - (T_{i} - T_{f}) \frac{\operatorname{erfc}(\frac{x}{2\sqrt{\alpha_{i}t}})}{\operatorname{erfc}(\lambda)}$$
(99)

and the dimensionless parameter  $\lambda > 0$  satisfies the following equation

$$F(x) = x, \quad x > 0 \tag{100}$$

where function F and the b's coefficients are given by

$$F(x) = b_1 \frac{\exp(-bx^2)}{1 + b_2 erf(x\sqrt{b})} - b_3 \frac{\exp(-x^2)}{erfc(x)}$$
(101)

$$b = \frac{\alpha_l}{\alpha_s} > 0; \quad b_1 = \frac{h_0(T_f - T_\infty)}{\rho \ell \sqrt{\alpha_l}} > 0$$
(102)

$$b_{2} = \frac{h_{0}}{h_{s}} \sqrt{\pi \alpha_{s}} > 0; \quad b_{3} = \frac{c_{l}(T_{i} - T_{f})}{\ell \sqrt{\pi}} > 0$$
(103)

Proof.

Function *F* has the following properties:

$$F(0^{+}) = b_1 - b_3 = \frac{h_0(T_f - T_{\infty})}{\rho \ell \sqrt{\alpha_l}} - \frac{c_l(T_i - T_f)}{\ell \sqrt{\pi}}$$
(104)

$$F(+\infty) = -\infty, \quad F'(x) < 0, \quad \forall x > 0 \tag{105}$$

Therefore, there exists a unique solution  $\lambda > 0$  of the Eq. (100) if and only if  $F(0^+) > 0$ , that is inequality (96) holds.

## 2.10 The similarity solution for the two-phase Lamé-Clapeyron-Stefan problem with a mushy region

We consider a semi-infinite material initially in the solid phase at the temperature  $-C < T_f = 0$ . We impose a temperature  $B > T_f = 0$  at the fixed face x = 0, and the fusion process begins, and three regions can be distinguished, as follows: (Tarzia, 1990b):

- i. the liquid phase, at temperature  $T_2 = T_2(x,t) > 0$ , occupying the region  $0 < x \le s(t), t > 0$ ;
- ii. the solid phase, at temperature  $T_1 = T_1(x, t) < 0$ , occupying the region x > r(t), t > 0;
- iii. the mushy zone, at temperature  $T_f = 0$ , occupying the region s(t) < x < r(t), t > 0. We make the following two assumptions on its structure:
- a. the material in the mushy zone contains a fixed fraction  $\epsilon \ell$  (with constant  $0 < \epsilon < 1$ ) of the total latent heat  $\ell$ ;
- b. the width of the mushy zone is inversely proportional (with constant  $\gamma > 0$ ) to the temperature gradient at s(t).

Therefore, the problem consists of finding the free boundaries x = s(t), x = r(t), and the temperature:

$$T(x,t) = \begin{cases} T_2(x,t) > 0 & \text{if } 0 < x < s(t), t > 0 \\ 0 & \text{if } s(t) \le x \le r(t), t > 0 \\ T_1(x,t) < 0 & \text{if } r(t) < x, t > 0 \end{cases}$$
(106)

defined for x > 0 and t > 0, such that the following conditions are satisfied:

$$\alpha_2 T_{2_{xx}} = T_{2_t}, \qquad 0 < x < s(t), t > 0 \tag{107}$$

$$s(0) = r(0) = 0, \tag{109}$$

$$T_2(s(t),t) = T_1(r(t),t) = 0, \quad t > 0$$
(110)

$$k_1 T_{1_x}(r(t), t) - k_2 T_{2_x}(s(t), t) = \rho \ell [(1 - \varepsilon)\dot{s}(t) + \varepsilon \dot{r}(t)],$$
(111)

$$-T_{2_{\gamma}}(s(t),t)(r(t)-s(t)) = \gamma, \quad t > 0$$
(112)

$$T_1(x,0) = T_1(+\infty,t) = -C, \quad x > 0, t > 0$$
(113)

$$T_2(0,t) = B > 0, \quad t > 0$$
 (114)

Theorem 11. (Tarzia, 1990b)

i. The explicit solution to the problem (107)-(114) is given by

$$T_1(x,t) = A_1 + B_1 erf(\frac{x}{2a_1\sqrt{t}}), \quad T_2(x,t) = A_2 + B_2 erf(\frac{x}{2a_2\sqrt{t}})$$
(115)

$$s(t) = 2\sigma\sqrt{t}, \quad r(t) = 2\omega\sqrt{t} \quad (a_2^2 = \frac{k_2}{\rho c_2}, \quad a_1^2 = \frac{k_1}{\rho c_1})$$
 (116)

where

$$A_{2} = B, \quad B_{2} = -\frac{B}{erf(\frac{\sigma}{a_{2}})}, \quad A_{1} = \frac{Cerf(\frac{\omega}{a_{1}})}{erfc(\frac{\omega}{a_{1}})}, \quad B_{1} = -\frac{C}{erfc(\frac{\omega}{a_{1}})}$$
(117)

$$\omega = \omega(\sigma) = \sigma + \frac{\gamma a_2 \sqrt{\pi}}{2B} \exp(\frac{\sigma^2}{a_2^2}) erf(\frac{\sigma}{a_2})$$
(118)

where  $\sigma > 0$  is the unique solution to the equation

$$K_1(x) = K_2(x), \quad x > 0 \tag{119}$$

with

$$K_{1}(x) = \frac{k_{2}B}{a_{2}\sqrt{\pi}}F_{2}(\frac{x}{a_{2}}) - \frac{k_{1}B}{a_{1}\sqrt{\pi}}F_{1}(\frac{\omega(x)}{a_{1}}), \quad F_{1}(x) = \frac{\exp(-x^{2})}{erfc(x)}$$

$$K_{2}(x) = \rho\ell[x + \frac{\varepsilon\gamma a_{2}\sqrt{\pi}}{2B}\exp(\frac{x^{2}}{a_{2}^{2}})erf(\frac{x}{a_{2}})], \quad F_{2}(x) = \frac{\exp(-x^{2})}{erf(x)}$$
(120)

Proof.

We have the following properties

$$K_1(0^+) = +\infty, \quad K_1(+\infty) = -\infty, \quad K'_1 < 0, \forall x > 0,$$
 (121)

$$K_2(0^+) = 0, \quad K_2(+\infty) = +\infty, \quad K'_2 < 0, \forall x > 0,$$
 (122)

and the thesis holds.

<u>Remark 11</u>

If the boundary condition (114) is replaced by a heat flux condition of the type (77) then we will have an instantaneous change of phase if and only if the coefficient  $q_0$  that characterizes the heat flux (77) verifies an inequality (Tarzia, 1990b).

## 2.11 The similarity solution for the phase-change problem by considering a density jump

We will consider the two-phase Lamé-Clapeyron-Stefan problem for a semi-infinite material taking into account the density jump under the change of phase. We will find the interface s = s(t) > 0 (free boundary), defined for t > 0, and the temperature

$$\theta(x,t) = \begin{cases} \theta_1(x,t) < 0 & \text{if } 0 < x < s(t), \quad t > 0, \\ 0 & \text{if } x = s(t), \quad t > 0, \\ \theta_2(x,t) > 0 & \text{if } x > s(t), \quad t > 0, \end{cases}$$
(123)

defined for x > 0 and t > 0, such that they satisfy the following conditions:

$$\alpha_1 \theta_{1_{xx}} = \theta_{1_t}, \qquad 0 < x < s(t), t > 0 \tag{124}$$

$$\alpha_2 \theta_{2_{xx}} + \frac{\rho_1 - \rho_2}{\rho_2} \dot{s}(t) \theta_{2_x} = \theta_{2_t}, \quad x > s(t), \quad t > 0$$
(125)

$$\theta_1(s(t), t) = 0, \quad t > 0$$
  
 $\theta_2(s(t), t) = 0, \quad t > 0$ 
(126)

$$k_1 \theta_{1_y}(s(t), t) - k_2 \theta_{2_y}(s(t), t) = \rho_1 \ell \dot{s}(t), \quad t > 0$$
(127)

$$\theta_2(x,0) = \theta_0 > 0, \quad x > 0 \tag{128}$$

$$s(0) = 0$$
 (129)

$$\theta_1(0,t) = -d < 0, \quad t > 0.$$
(130)

<u>Theorem 12</u> (Carslaw & Jaeger, 1959; Rubinstein, 1971) The explicit solution to the free boundary problem (124)-(130) is given by

$$\begin{cases} \theta_1(x,t) = A_1 + B_1 erf(\frac{x}{2a_1\sqrt{t}})\\ \theta_2(x,t) = A_2 + B_2 erf(\delta_1 + \frac{x}{2a_2\sqrt{t}})\\ s(t) = 2\gamma\sqrt{t}, \qquad \gamma > 0 \end{cases}$$
(131)

where

$$A_1(\gamma) = -d, \qquad B_1(\gamma) = \frac{d}{erf(\gamma/a_1)},$$
 (132)

$$A_2(\gamma) = \frac{-\theta_0 \operatorname{erf}(\gamma/a_0)}{\operatorname{erfc}(\gamma/a_0)}, \qquad B_2(\gamma) = \frac{\theta_0}{\operatorname{erfc}(\gamma/a_0)}, \tag{133}$$

$$\varepsilon = \frac{\rho_1 - \rho_2}{\rho_2}, \quad \delta_1 = \frac{\gamma}{a_2} |\varepsilon|, \quad a_0 = \frac{a_2}{1 + |\varepsilon|}, \quad (134)$$

and  $\gamma$  is the unique solution to the following equation:

$$F(x) = x, \qquad x > 0$$
, (135)

with

$$F(x) = \frac{k_1}{\ell \rho_1 a_1 \sqrt{\pi}} B_1(x) \exp\left(\frac{-x^2}{a_1^2}\right) - \frac{k_2}{\ell \rho_1 a_2 \sqrt{\pi}} B_2(x) \exp\left(\frac{-x^2}{a_0^2}\right).$$
 (136)

Proof.

We have the following properties:

$$F(0^{+}) = +\infty, \qquad F(+\infty) = -\infty, \qquad F'(x) < 0, \, \forall x > 0.$$
(137)

Theorem 13 (Bancora & Tarzia, 1985)

i. If we replace the boundary condition (130) by the following one given by:

$$k_1 \theta_{1_x}(0,t) = \frac{q_0}{\sqrt{t}}, \quad t > 0,$$
(138)

then there exists an explicit solution corresponding to the free boundary problem (124)-(130) and (138) if and only if the coefficient  $q_0$  satisfies the inequality

$$q_0 > \theta_0 \sqrt{\frac{k_2 \rho_2 c_2}{\pi}} . \tag{139}$$

In this case the explicit solution is given by:

$$\begin{cases} \theta_{1}(x,t) = C_{1} + D_{1}erf(\frac{x}{2a_{1}\sqrt{t}}) \\ \theta_{2}(x,t) = C_{2} + D_{2}erf(\delta_{2} + \frac{x}{2a_{2}\sqrt{t}}) \\ s(t) = 2w\sqrt{t}, \qquad w > 0 \end{cases}$$
(140)

where

$$C_1(w) = -\frac{a_1 q_0 \sqrt{\pi}}{k_1} \operatorname{erf}(\frac{w}{a_1}), \qquad D_1(w) = \frac{a_1 q_0 \sqrt{\pi}}{k_1}, \tag{141}$$

$$C_2(w) = \frac{-\theta_0 \operatorname{erf}(w/a_0)}{\operatorname{erfc}(w/a_0)}, \qquad D_2(\gamma) = \frac{\theta_0}{\operatorname{erfc}(w/a_0)}, \tag{142}$$

$$\varepsilon = \frac{\rho_1 - \rho_2}{\rho_2}, \quad \delta_2 = \frac{\gamma}{a_2} |\varepsilon|, \quad a_0 = \frac{a_2}{1 + |\varepsilon|}, \quad (143)$$

and w is the unique solution to the following equation:

$$F_0(x) = x, \qquad x > 0,$$
 (144)

with

$$F_0(x) = \frac{q_0}{\ell \rho_1} \exp\left(\frac{-x^2}{a_1^2}\right) - \frac{k_2}{\ell \rho_1 a_2 \sqrt{\pi}} B_2(x) \exp\left(\frac{-x^2}{a_0^2}\right).$$
(145)

Proof.

We have the following properties:

$$F_0(0^+) = \frac{1}{\ell \rho_1} \left( q_0 - \frac{k_2 \theta_0}{a_2 \sqrt{\pi}} \right), \qquad F(+\infty) = -\infty, \qquad F_0'(x) < 0, \, \forall x > 0.$$
(146)

#### Remark 12 .

When the boundary condition at the fixed face x = 0 is given by (93) the explicit solution was given in (Tarzia, 2007).

#### 2.12 The determination of one or two unknown thermal coefficient through an overspecified condition at the fixed face for one or two-phase cases

We consider the one-phase Lamé-Clapeyron-Stefan problem with unknown thermal coefficients. If we give an overspecified boundary condition at the fixed face x = 0 we can determine one or two unknown coefficients following (Arderius et al., 1996; Cannon, 1963 & 1964; Garguichevich et al., 1985; Jones, 1962 & 1963; Tarzia, 1982,1983 & 1984)).

#### 2.12.1 Determination of one unknown thermal coefficient through a one-phase case

The problem consists of finding the free boundary x = s(t), the temperature T = T(x,t), and one unknown thermal coefficient chosen among  $\{k, \rho, c, \ell\}$  such that they must satisfy the following conditions (we have a free boundary problem):

$$T_t = \alpha T_{xx}, \qquad 0 < x < s(t), \quad t > 0 \quad (a^2 = \alpha = k/\rho c)$$
 (147)

$$T(s(t),t) = 0, t > 0$$
 (148)

$$kT_x(s(t),t) = \rho \ell \dot{s}(t), \qquad t > 0,$$
 (149)

$$T(0,t) = T_0 > 0 \tag{150}$$

$$kT_x(0,t) = -\frac{q_0}{\sqrt{t}}, \quad t > 0 ,$$
 (151)

$$s(0) = 0$$
 , (152)

where  $q_0$  is the coefficient that characterizes the heat flux at the fixed face x = 0 and it must be obtained experimentally.

Theorem 14 (Tarzia, 1982)

Let  $T_0$  and  $q_0$  be determinated experimentally. The solution for the determination of one thermal coefficient is given by:

$$T(x,t) = T_0 - \frac{T_0}{erf(\frac{\sigma}{a})} erf(\frac{x}{2a\sqrt{t}}), \quad 0 < x < s(t), \ t > 0 \quad ,$$
(153)

$$s(t) = 2\sigma\sqrt{t}, \quad t > 0 \quad , \tag{154}$$

where  $\sigma$  and the unknown thermal coefficient are computed in the summarized way in the following Table 1:

Case #	Formulae for unknown coefficients	Parameter $\xi$ is the unique solution to the equation	Restrictions on data
1	$\sigma = \xi \sqrt{\frac{k}{\rho c}}$ $\ell = \frac{q_0}{\rho} \sqrt{\frac{\rho c}{k}} \frac{\exp(-\xi^2)}{\xi}$	$erf(x) = \frac{T_0}{q_0} \sqrt{\frac{k\rho c}{\pi}}$ $x > 0$	$\frac{T_0}{q_0} \sqrt{\frac{k\rho c}{\pi}} < 1$
2	$\sigma = \frac{kT_0}{q_0\sqrt{\pi}} \frac{\xi}{erf(\xi)}$ $\rho = \frac{\pi q_0^2}{kcT_0^2} erf^2(\xi)$	$E(x) = \frac{cT_0}{\ell\sqrt{\pi}}$ $x > 0$	
3	$\sigma = \frac{q_0}{\rho \ell} \exp(-\xi^2)$ $k = \frac{\pi q_0^2}{\rho c T_0^2} erf^2(\xi)$	As in Case 2	
4	$\sigma = \frac{q_0}{\rho \ell} \exp(-\xi^2)$ $c = \frac{\pi q_0^2}{\rho k T_0^2} erf^2(\xi)$	$\frac{erf(x)}{x} = \frac{k\rho\ell T_0}{q_0^2\sqrt{\pi}}\exp(x^2)$ x > 0	$\frac{k ho\ell T_0}{2q_0^2} < 1$

Table 1. Summary of the determination of one thermal coefficient through a one-phase Lamé-Clapeyron-Stefan problem (4 cases)

Remark 13.

The determination of one unknown thermal coefficient for phase-change problems with temperature-dependent thermal conductivity of the type (54) was given in (Tarzia, 1998).

#### 2.12.2 Determination of two unknown thermal coefficients for the one-phase case

If the interface solid-liquid is given by the law:

$$s(t) = 2\sigma\sqrt{t}, \quad t > 0 \tag{155}$$

where the coefficient  $\sigma > 0$  was determined experimentally then the problem consists of finding the temperature T = T(x,t) and two unknown thermal coefficients chosen among  $\{k, \rho, c, \ell\}$  such that they satisfy the conditions (147)-(152) (we have a moving boundary problem).

Theorem 15 (Tarzia, 1983)

Let  $T_0$ ,  $\sigma$  and  $q_0$  be determined experimentally. The solution for the determination of two thermal coefficients is given by

$$T(x,t) = T_0 - \frac{T_0}{erf(\frac{\sigma}{a})} erf(\frac{x}{2a\sqrt{t}}), \quad 0 < x < s(t), \ t > 0,$$
(156)

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Case #	Formulae for unknown coefficients	Parameter $\xi$ is the unique solution to the equation	Restrictions on data
1	$c = \frac{q_0 \sqrt{\pi}}{\rho \sigma T_0} \xi \operatorname{erf}(\xi)$ $k = \frac{\sigma q_0 \sqrt{\pi}}{T_0} \frac{\operatorname{erf}(\xi)}{\xi}$	$\xi = \sqrt{\log(\frac{q_0}{\rho\ell\sigma})}$	$\frac{q_0}{\rho\ell\sigma} > 1$
2	$\ell = \frac{q_0}{\rho\sigma} \exp(-\xi^2)$ $k = \frac{\rho c \sigma^2}{\xi^2}$	$xerf(x) = \frac{\rho c \sigma T_0}{q_0 \sqrt{\pi}}$ $x > 0$	
3	$\rho = \frac{q_0}{\ell\sigma} \exp(-\xi^2)$ $k = \frac{q_0 c\sigma}{\ell} \frac{\exp(-\xi^2)}{\xi^2}$	$E(x) = \frac{cT_0}{\ell\sqrt{\pi}}$ $x > 0$	
4	$c = \frac{k}{\rho \sigma^2} \xi^2$ $\ell = \frac{q_0}{\rho \sigma} \exp(-\xi^2)$	$\frac{erf(x)}{x} = \frac{kT_0}{\sigma q_0 \sqrt{\pi}}$ $x > 0$	$\frac{kT_0}{2\sigma q_0} < 1$
5	$\rho = \frac{k}{c\sigma^2} \xi^2$ $\ell = \frac{c\sigma q_0}{k} \frac{\exp(-\xi^2)}{\xi^2}$	As in case 4	As in case 4
6	$\rho = \frac{q_0}{\ell \sigma} \exp(-\xi^2)$ $c = \frac{k\ell}{\sigma q_0} \xi^2 \exp(\xi^2)$	As in case 4	As in case 4

and the two coefficients are computed in the summarized way in the following Table 2.

Table 2. Summary of the simultaneous determination of two thermal coefficients through a one-phase Lamé-Clapeyron-Stefan problem (6 cases)

#### Remark 14.

The determination of thermal coefficients for the Solomon-Wilson-Alexiades mushy region was obtained in (Tarzia, 1987). The simultaneous determination of two unknown thermal coefficients for phase-change problems with temperature-dependent thermal conductivity of the type (54) was given in (Salva & Tarzia, 2010) with a sensitivity analysis.

## 2.12.3 Determination of one or two unknown thermal coefficients through a two-phase Lamé-Clapeyron-Stefan problem

The determination of one or two unknown thermal coefficients for a two-phase solidification or fusion problem was obtained in (Stampella & Tarzia, 1989). The

determination of one or two unknown thermal coefficients for a mushy region was obtained in (González & Tarzia, 1996). Another variant for the simultaneous determination of the thermal coefficients is given in (Tarzia, 1991a).

#### Remark 15.

Explicit solutions for the determination of unknown coefficients are given in (Briozzo et al., 1999) for Storm's type materials.

## 2.13 A similarity solution for the thawing in a saturated porous medium by considering a density jump and the influence of the pressure on the melting temperature

We consider the problem of thawing of a partially frozen porous medium, saturated with an incompressible liquid. For a detailed exposition of the physical background we refer to (Charach & Rubinstein, 1992; Fasano et al. 1993; Fasano & Primicerio, 1984; Nakano, 1990; O'Neill & Miller, 1985; Talamucci, 1997 & 1998). More specifically, we deal with the following situations:

- i. a sharp interface between the frozen part and the unfrozen part of the domain exists (sharp, in the macroscopic sense);
- ii. the frozen phase is at rest with respect to the porous skeleton, which will be considered to be undeformable;
- iii. due to the density jump between the liquid and solid phases, thawing can induce either desaturation or water movement in the melting region. We will consider the latter situation, assuming that liquid is continuously supplied to keep the medium saturated.

The unknowns of the problem are the function x=s(t), representing the free boundary, and the two functions u(x, t) and v(x, t) representing the temperature of the unfrozen and of the frozen zone respectively which must satisfy the following conditions:

$$u_t = a_1 u_{xx} - b\rho \dot{s}(t) u_x, \qquad 0 < x < s(t), \quad t > 0$$
(157)

$$v_t = a_2 v_{xx}, \quad x > s(t), \quad t > 0$$
 (158)

$$u(s(t),t) = v(s(t),t) = d\rho s(t)\dot{s}(t), \quad t > 0$$
(159)

$$k_F v_x(s(t), t) - k_U u_x(s(t), t) = \alpha \dot{s}(t) + \beta \rho s(t) (\dot{s}(t))^2, \quad t > 0$$
(160)

$$u(0,t) = B > 0, \quad t > 0.$$
(161)

$$v(x,0) = v(+\infty,t) = -A < 0, \quad x > 0, t > 0$$
(162)

$$s(0) = 0$$
 (163)

with

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$$a_{1} = \alpha_{1}^{2} = \frac{k_{U}}{\rho_{U}c_{U}}, \quad a_{2} = \alpha_{2}^{2} = \frac{k_{F}}{\rho_{F}c_{F}}, \quad b = \frac{\varepsilon\rho_{W}c_{W}}{\rho_{U}c_{U}}, \quad d = \frac{\varepsilon\gamma\mu}{K}$$

$$\rho = \frac{\rho_{W} - \rho_{I}}{\rho_{W}}, \quad \alpha = \varepsilon\rho_{I}\ell, \quad \beta = \frac{\varepsilon^{2}\rho_{I}\gamma\mu(c_{W} - c_{I})}{K} = \varepsilon d\rho_{I}(c_{W} - c_{I})$$
(164)

where

 $\varepsilon$ : porosity,

 $\rho_W$  and  $\rho_I$ : density of water and ice,

*c*: specific heat at constant density,

 $k_{u}$  and  $k_{F}$ : conductivity of the unfrozen and frozen zones,

u=v=0: the melting point at atmospheric pressure,

 $\ell$  : latent heat at  $u{=}0$  ,

 $\gamma$  : coefficient in the Clausius-Clapeyron law,

 $\mu > 0$ : viscosity of liquid,

*K*>0: hydraulic permeability,

B>0: boundary temperature at the fixed face x=0,

-*A*<0: initial temperature.

Theorem 16 (Fasano et al., 1999)

The free boundary problem (157) - (163) has the similarity solution

$$s(t) = 2\xi \alpha_1 \sqrt{t}, \qquad (165)$$

$$u(x,t) = B + \frac{m\xi^2 - B}{g(p,\xi)} \int_{0}^{\frac{x}{2}/2\alpha_1 \sqrt{t}} \exp(-r^2 + pr\xi) dr$$
(166)

$$v(x,t) = \frac{m\xi^2 erfc\left(\frac{x}{2\alpha_2\sqrt{t}}\right) + A\left(erf(\gamma_0\xi) - erf\left(\frac{x}{2\alpha_2\sqrt{t}}\right)\right)}{erfc(\gamma_0\xi)}$$
(167)

if and only if the coefficient  $\xi > 0$  satisfies the following equation:

$$K_1(B - my^2)H(p, y) - K_2F(m, y) = \delta y + \upsilon y^3, \quad y > 0,$$
(168)

where

$$g(p,y) = \int_{0}^{y} \exp(-r^{2} + pyr) dr, \qquad H(p,y) = \frac{\exp((p-1)y^{2})}{2\sqrt{\pi}g(p,y)}$$
(169)

$$F(m,y) = (A + my^{2}) \frac{\exp(-\gamma_{0}^{2}y^{2})}{erfc(\gamma_{0}y)}$$
(170)

and the constants  $K_1, K_2, \gamma_0, \delta, p, m$  and v are defined as follows:

$$K_1 = \frac{k_U}{\alpha_1 \sqrt{\pi}} > 0, \quad K_2 = \frac{k_F}{\alpha_2 \sqrt{\pi}} > 0, \quad \gamma_0 = \frac{\alpha_1}{\alpha_2} > 0, \quad \delta = \alpha \alpha_1 > 0$$
 (171)

$$p = 2b\rho, \quad m = 2d\rho\alpha_1^2 > 0, \quad \upsilon = 2\beta\rho\alpha_1^3$$
 (172)

Moreover, the existence and uniqueness of the unknown coefficient  $\xi > 0$  depends on the sign of the three parameters p,m and v of the problem.

If we replace the boundary condition (161) by the following one:

$$k_{U}u_{x}(0,t) = -\frac{q_{0}}{\sqrt{t}}, \quad t > 0 , \qquad (173)$$

then we can consider the free boundary problem (157) - (160), (173), (162)-(163) and we can obtain the following result.

Theorem 17 (Lombardi & Tarzia, 2001)

The free boundary problem (157) – (160), (173), (162)-(163) has the following similarity solution:

$$s(t) = 2\xi^* \alpha_1 \sqrt{t}, \qquad (174)$$

$$u(x,t) = m(\xi^*)^2 + \frac{2q_0\alpha_1}{K_U}g(p,\xi^*) - \frac{2q_0\alpha_1}{K_U}\int_0^{\frac{N}{2}(2\alpha_1\sqrt{t})} \exp(-r^2 + pr\xi^*) dr$$
(175)

$$v(x,t) = \frac{m(\xi^*)^2 + Aerf(\gamma_0\xi^*)}{erfc(\gamma_0\xi^*)} - \frac{m(\xi^*)^2}{erfc(\gamma_0\xi^*)}erf\left(\frac{x}{2\alpha_1\sqrt{t}}\right)$$
(176)

if and only if the coefficient  $\xi^* > 0$  satisfies the following equation:

$$q_0 \exp((p-1)y^2) - K_2 F(m, y) = \delta y + \upsilon y^3, \quad y > 0,$$
(177)

or its equivalent

$$Q_0(y) = q_0, \quad y > 0 , \tag{178}$$

where

$$Q_0(y) = \frac{K_2 F(m, y) + \delta y + \upsilon y^3}{\exp((p-1)y^2)}, \quad y > 0.$$
(179)

Moreover, the existence and uniqueness of the unknown coefficient  $\xi^* > 0$  depends on the sign of the three parameters p, m and v of the problem.

#### 3. Explicit solutions for free boundary problems for the diffusion equation

Heat and mass transfer with phase change problems, taking place in a porous medium, such as evaporation, condensation, freezing, melting, sublimation and desublimation, have wide application in separation processes, food technology, heat and mixture migration in soils and grounds, etc. Due to the non-linearity of the problem, solutions usually involve mathematical difficulties and only a few exact solutions have been found. Mathematical formulation of the heat and mass transfer in capillary porous bodies has been established by (Luikov, 1964, 1966, 1975 & 1978). Some books or booklets on the subject for the diffusion equation are (Crank, 1975; Duvaut, 1976; Fasano, 2005; Fasano & Primicerio, 1986; Froment & Bischoff, 1979; Levenspiel, 1962; Primicerio & Gianni, 1989; Szekely et al., 1976).

#### 3.1 The oxygen diffusion-consumption problem and its relationship with the phasechange problem

The diffusion-consumption of oxygen in absorbing tissue consists in finding the free boundary x=s(t) and the concentration C(x,t) such that they satisfy the following conditions (Crank & Gupta, 1972; Crank, 1984; Liapis et al., 1982):

$$C_t - C_{xx} = -1, \quad 0 < x < s(t), \quad 0 < t < T_0$$
 (180)

$$C(x,0) = H(x), \quad 0 \le x \le 1,$$
 (181)

$$C_x(0,t) = -G(t) \qquad (C(0,t) = F(t)), \quad 0 < t < T_0,$$
(182)

$$C(s(t),t) = 0, \qquad 0 < t < T_0,$$
(183)

$$C_x(s(t),t) = 0, \qquad 0 < t < T_0,$$
(184)

$$s(0) = 1, \qquad 0 < t < T_0.$$
 (185)

<u>Remark 16.</u>

We remark that  $\dot{s}(t)$  does not appear in both conditions (183) and (184) on the free boundary x=s(t) and for this reason the free boundary problem is of an implicit type; the Lamé-Clapeyron-Stefan problem is one of an explicit type.

<u>Theorem 18.</u> (Fasano, 1974; Schatz, 1966)

The free boundary problem of the diffusion-consumption of oxygen in absorbing tissue is equivalent to the following Lamé-Clapeyron-Stefan problem:

$$z_t - z_{xx} = 0, \quad 0 < x < s(t), \quad 0 < t < T_0$$
(186)

$$z(x,0) = h(x), \quad 0 \le x \le 1$$
 (187)

$$z_x(0,t) = -g(t) \quad (z(0,t) = f(t)), \quad 0 < t < T_0$$
(188)

$$z(s(t),t) = 0, \qquad 0 < t < T_0 \tag{189}$$

$$z_x(s(t), t) = -\dot{s}(t), \quad 0 < t < T_0$$
(190)

$$s(0) = 1, \qquad 0 < t < T_0.$$
 (191)

i. If  $(s, z, T_0)$  is a solution to the problem (186) – (191) then  $(s, C, T_0)$  is solution to the problem (180) – (185) where we define:

$$C(x,t) = \int_{x}^{s(t)} d\xi \int_{\xi}^{s(t)} [1 + z(y,t)] dy, \qquad (192)$$

$$H(x) = \int_{x}^{1} d\xi \int_{\xi}^{1} [1 + h(y)] dy, \quad F(t) = H(0) + \int_{0}^{t} f(\tau) d\tau$$
(193)

$$G(t) = 1 + \int_{0}^{1} h(x)dx + \int_{0}^{t} g(\tau)d\tau,$$
(194)

ii. If  $(s,C,T_0)$  is a solution to the problem (180) – (185) then  $(s,z,T_0)$  is solution to the problem (186) – (191) where we define:

$$z(x,t) = C_t(x,t) \tag{195}$$

$$h(x) = H''(x) - 1, \quad g(t) = G'(t), \quad f(t) = F'(t)$$
 (196)

Remark 17.

The oxygen diffusion-consumption free boundary problem was applied to the anaerobiosis in saturated soil aggregates in (González et al., 2008).

#### 3.2 The Rubinstein solution for the binary alloy solidification problem

We consider a semi-infinite slab of a binary alloy consisting of two components *A*, *B*. Let *C* be the concentration of "*A*". We suppose that solidification of the alloy is governed by an equilibrium phase diagram consisting of liquidus curve  $T = f_L(C)$ , and a solidus curve  $T = f_S(C)$ , 0 < C < 1 and we assume  $f_L, f_S$  to be monotonically increasing,  $f_L(C) > f_S(C)$  and  $f_L(0) = f_S(0) = T_{cr}^A$ ,  $f_L(1) = f_S(1) = T_{cr}^B$ . Material is in its solid state if  $T \le f_S(C)$  and liquid if  $f_L(C) \le T$ . If  $f_S(C) < T < f_L(C)$  then the material state is not well defined (it is known as mushy region).

We consider that the semi-infinite alloy is initially liquid at constant temperature  $T_{in}$  and concentration  $C_{in}$ , for which  $f_L(C_{in}) \le T_{in}$ . Beginning at time t = 0, a cold temperature  $T_B < T_{cr}^A$  is imposed at x = 0. Freezing occurs with, in principle, a sharp phase change front s = s(t) separating solid alloy (x < s(t)) from liquid alloy (x > s(t)). The mathematical formulation of the solidification process is given in (Rubinstein, 1971) as follows:

Find temperature T(x,t), concentration C(x,t) and phase-change front x = s(t), such that the following conditions must be satisfied:

$$C_{S_t} = D_S C_{S_{yy}}, \quad 0 < x < s(t), \quad t > 0$$
(197)

$$C_{\ell_{\ell}} = D_{\ell}C_{\ell_{yy}}, \quad x > s(t), \quad t > 0$$
 (198)

$$T_{s_t} = \alpha_s T_{s_{vv}}, \quad 0 < x < s(t), \quad t > 0$$
(199)

$$T_{\ell_t} = \alpha_{\ell} T_{\ell_{xx}}, \quad x > s(t), \quad t > 0$$
(200)

$$T_{cr} = T_{s}(s(t), t) = f_{s}[C_{s}(s(t), t)], \quad t > 0$$
(201)

$$T_{cr} = T_{\ell}(s(t), t) = f_{L}[C_{\ell}(s(t), t)], \quad t > 0$$
(202)

$$D_{\ell}C_{\ell_{x}}(s(t),t) - D_{s}C_{s_{x}}(s(t),t) = [C_{s}(s(t),t) - C_{\ell}(s(t),t)]\dot{s}(t), \quad t > 0$$
(203)

$$k_{s}T_{s_{x}}(s(t),t) - k_{\ell}T_{\ell_{x}}(s(t),t) = \rho\ell\dot{s}(t), \quad t > 0$$
(204)

$$T_{s}(0,t) = T_{B} < T_{cr}^{A}, \quad t > 0$$
(205)

$$T_{\ell}(x,0) = T_{in} > f_{L}(C_{in}), \quad t > 0$$
(206)

$$C_{\ell}(x,0) = C_{in}, \quad x > 0$$
 (207)

$$C_{S_{v}}(0,t) = 0, \quad t > 0$$
 (208)

$$s(0) = 0$$
 (209)

where  $\rho$ , k,  $\alpha$ , D,  $\ell$  represent the mass density, the thermal conductivity, the thermal diffusivity, the mass diffusion and the latent heat of fusion, being *S* and  $\ell$  the subscripts that denote the solid and liquid phase respectively.

Theorem 19 (Rubinstein, 1971; Solomon et al., 1983)

There exists a unique solution to the coupled free boundary problem (197)-(209), moreover, the solidus  $C_1(s(t),t)$  and liquidus  $C_2(s(t),t)$  concentrations as well as the phase-change temperature  $T_{C_r} = T_1(s(t),t) = T_2(s(t),t)$  are constants in time. The explicit solution is given by the following expressions:

$$s(t) = 2\lambda \sqrt{\alpha_1 t} \tag{210}$$

$$C_{S}(x,t) = C_{S}, \quad T_{cr} = f_{S}(C_{S}) = f_{L}(C_{L}),$$
 (211)

$$C_{\ell}(x,t) = C_{in} + (C_L - C_{in}) \frac{erfc(x/2\sqrt{D_{\ell}t})}{erfc(\lambda\sqrt{\alpha_s/D_{\ell}})}$$
(212)

$$T_{S}(x,t) = T_{B} + (T_{cr} - T_{B}) \frac{erf(x/2\sqrt{\alpha_{S}t})}{erf(\lambda)}$$
(213)

$$T_{\ell}(x,t) = T_{in} + (T_{cr} - T_{in}) \frac{erf(x/2\sqrt{\alpha_{\ell}t})}{erf(\lambda\sqrt{\alpha_{s}/\alpha_{\ell}})}$$
(214)

where  $\lambda$  and  $T_{cr}$  (or equivalently  $C_s$  and  $C_\ell$ ) must satisfy the following conditions:

$$\frac{C_{in} - C_L}{C_s - C_L} = Q(\lambda \sqrt{\alpha_s / D_\ell}), \quad T_{cr} = W_1(\lambda)$$
(215)

where

$$Q(x) = \sqrt{\pi} x \exp(x^2) \operatorname{erfc}(x), \quad A = \rho \ell \alpha_\ell / k_\ell$$
(216)

$$W_{1}(x) = T_{B} + [(T_{in} - T_{B}) + AQ(x\sqrt{\alpha_{S} / \alpha_{\ell}})] \frac{\Psi(x)}{1 + \Psi(x)}$$
(217)

$$\Psi(x) = \frac{k_{\ell}\alpha_{s}\sqrt{\pi}}{k_{s}\alpha_{\ell}} \frac{E(x)}{Q(x\sqrt{\alpha_{s}/\alpha_{\ell}})}$$
(218)

Proof.

The system of equations (215) has a unique solution because of the following properties

$$Q(0^+) = 0, \quad Q(+\infty) = 1, \quad Q' > 0$$
 (219)

$$W_1(0^+) = T_B, \quad W_1(+\infty) = T_{in} + \frac{\ell}{c_\ell}, \quad W_1' > 0.$$
 (220)

Remark 18.

Some other references on the binary alloy solidification problems are (Alexandrov & Malygin, 2006; Gupta et al., 1997; Tien & Geigen, 1967; Tien & Koump, 1970; Tsubaki & Boley, 1977; Voller, 2006, 2008 a&b; White, 1985; Wilson et al., 1982). In (Cirelli & Tarzia, 2010) the binary alloy solidification problem (197)-(209) is solved by changing the boundary condition (205) at the fixed face by a heat flux boundary condition of the type (77) or a convective boundary condition of the type (93).

## 3.3 The Zel'dovich-Kompaneets-Barenblatt solution for the gas flow through a porous medium

The porous medium equation for a unidimensional material is given by

$$u_t = (u^m)_{xx}, \quad m > 1$$
 (221)

which appears in a natural way, mainly to describe processes involving fluid flow, heat transfer or diffusion, the flow of a gas through a porous medium and groundwater infiltration (Vázquez, 2007). The diffusion coefficient of the equation (221) is

$$D(u) = mu^{m-1} \tag{222}$$

assuming  $0 \le u$ . Equation (221) is parabolic only at those points where  $u \ne 0$  and it is in general a degenerate parabolic equation because degenerates wherever u = 0.

Its main qualitative property with respect to the classical heat or diffusion equation is the finite propagation which implies the appearance of a free boundary that separates the regions where the solution u > 0 (where there is gas, according to the standard interpretation of u as a gas density), from the empty region where u = 0.

There exists an explicit solution to the Eq. (221) with a free boundary given by:

Theorem 20 (Zel'dovich & Kompaneets, 1950; Barenblatt, 1952; Pattle, 1959)

The function

$$u(x,t) = \begin{cases} \frac{1}{s(t)} \left[ 1 - \left(\frac{x}{s(t)}\right)^2 \right]^{\frac{1}{m-1}} & \text{for } |x| \le s(t), \ 0 \le t \\ 0 & \text{for } |x| > s(t), \ 0 \le t \end{cases}$$
(223)

with

$$s(t) = \left[\frac{2m(m+1)}{m-1}(t+1)\right]^{\frac{1}{m+1}}$$
(224)

is a solution to the Cauchy problem for the equation (221) with initial data  $u(x,0) = u_0(x), x \in \mathbb{R}$  given by

$$u_{0}(x) = \begin{cases} \frac{1}{s(0)} \left[ 1 - \left( \frac{x}{s(0)} \right)^{2} \right]^{\frac{1}{m-1}} & for \quad |x| \le s(0) \\ 0 & for \quad |x| > s(0) \end{cases}$$
(225)

## 3.4 The Luikov solution for the coupled heat and mass transfer for a phase-change process

#### 3.4.1 Drying with coupled phase-change in a porous medium

A semi-infinite porous medium is dried by maintaining a heat flux condition at x = 0 of the type  $-\frac{q_0}{\sqrt{t}}$ , with  $q_0 > 0$ . Initially, the whole body is at uniform temperature  $t_0$  and uniform moisture potential  $u_0$ . The moisture is assumed to evaporate completely at a constant temperature, evaporation point  $t_v$ . It is also assumed that the moisture potential in the first region  $0 < x < s(\tau)$ , is constant at  $u_v$ , where  $x = s(\tau)$  locates the evaporation front at time  $\tau > 0$ . It is further assumed that the moisture in vapour form does not take away any appreciable amount of heat from the system. Neglecting mass diffusion due to temperature variation, the problem can be expressed as (Cho, 1975; Gupta, 1974; Luikov, 1978; Santillan Marcus & Tarzia, 2003):

$$\frac{\partial t_1}{\partial \tau}(x,\tau) = \alpha_1 \frac{\partial^2 t_1}{\partial x^2}(x,\tau), \qquad 0 < x < s(\tau), \ \tau > 0 \tag{226}$$

$$u_1 = u_v, \quad 0 < x < s(\tau), \ \tau > 0$$
 (227)

$$\frac{\partial t_2}{\partial \tau}(x,\tau) = \alpha_2 \frac{\partial^2 t_2}{\partial x^2} + \frac{\varepsilon L c_m}{c_2} \frac{\partial u_2}{\partial \tau}, \qquad x > s(\tau), \tau > 0$$
(228)

$$\frac{\partial u_2}{\partial \tau}(x,\tau) = \alpha_m \frac{\partial^2 u_2}{\partial x^2}(x,\tau), \qquad x > s(\tau), \ \tau > 0$$
(229)

$$k_1 \frac{\partial t_1}{\partial x} = -\frac{q_0}{\sqrt{\tau}}, \quad \text{at} \quad x = 0, \, \tau > 0$$
 (230)

$$t_2 = t_0$$
 in  $x > 0, \tau = 0$  (231)

$$u_2 = u_0$$
 in  $x > 0, \tau = 0$  (232)

$$t_1(s(\tau), \tau) = t_2(s(\tau), \tau) = t_v > t_0$$
 on  $x = s(\tau)$  (233)

$$u_1(s(\tau), \tau) = u_2(s(\tau), \tau) = u_v < u_0 \quad \text{on } x = s(\tau)$$
 (234)

$$-k_1 \frac{\partial t_1}{\partial x}(s(\tau),\tau) + k_2 \frac{\partial t_2}{\partial x}(s(\tau),\tau) = (1-\varepsilon)\rho_m L \frac{ds}{dt} \quad \text{on} \quad x = s(\tau)$$
(235)

where  $t_1$ : temperature of the dried porous medium;  $t_2$ : temperature of the humid porous medium;  $u_2$ :mass-transfer potential of the humid porous medium;  $\alpha_i$  (i = 1, 2): thermal diffusivity of the phase i;  $\alpha_{12}$ : ratio of thermal diffusivities from phase 1 to phase 2;  $\alpha_m$ : moisture diffusivity;  $c_m$ : specific mass capacity;  $c_2$ : specific heat capacity;  $k_i$  (i = 1, 2): thermal conductivity of the phase i;  $k_{21} = \frac{k_2}{k_1}$ ;  $K_0 = Lc_m \frac{(u_0 - u_v)}{c_2(t_v - t_0)}$ : Kossovitch number; L: latent heat evaporation of liquid per unit mass-transfer potential;  $\varepsilon$ : coefficient of internal evaporation;  $\rho_m$ : density of moisture;  $L_u = \alpha_m / \alpha_1$ : Luikov number, and  $v = (1 - \varepsilon) L \rho_m \alpha_1 / k_1 (t_v - t_0) > 0$ .

Theorem 21 (Santillan Marcus & Tarzia, 2003)

i. If the Luikov number is equal to one, and the coefficient  $q_0$  verifies the condition

$$q_{0} > \frac{k_{2}(t_{v} - t_{0})}{2\sqrt{\pi\alpha_{1}}} (\varepsilon K_{0} + 2) \quad ,$$
(236)

then there exists one and only one solution  $\lambda > 0$  to the following equation:

$$\frac{k_{21}}{\sqrt{\pi}}F_1(x)\left[-\frac{2\varepsilon K_0}{\sqrt{\pi}}xF_1(x)+2\varepsilon K_0x^2-\varepsilon K_0-2\right]+\frac{2\sqrt{\alpha_1}q_0}{k_1(t_v-t_0)}\exp(-x^2)=2\nu x, \quad x>0$$
(237)

Furthermore, the solution to the problem (226)-(235) is given by:

$$u_1(x,\tau) = u_v, \quad 0 < x < s(\tau), \ \tau > 0, \quad \eta = \frac{x}{2\sqrt{\alpha_1 \tau}}$$
 (238)

$$t_1(x,\tau) = 1 + \frac{q_0 \sqrt{\pi \alpha_1}}{k_1(t_v - t_0)} (erf(\lambda) - erf(\eta)), \quad 0 < x < s(\tau), \quad \tau > 0$$
(239)

$$u_{2}(x,\tau) = \frac{erfc\left(\frac{\eta}{\sqrt{L_{u}}}\right)}{erfc(\lambda)}, \qquad x > s(\tau), \quad \tau > 0$$
(240)

$$t_{2}(\eta) = \frac{\varepsilon K_{0}}{\sqrt{\pi} \operatorname{erfc}(\lambda)} [\lambda \exp(-\lambda^{2}) \frac{\operatorname{erfc}(\eta)}{\operatorname{erfc}(\lambda)} - \eta \exp(-\eta^{2})] + \frac{\operatorname{erfc}(\eta)}{\operatorname{erfc}(\lambda)}, \quad x > s(\tau), \tau > 0$$
(241)

$$s(\tau) = 2\lambda \sqrt{\alpha_1 \tau} . \tag{242}$$

ii. If the Luikov number is different than one, (that is  $\alpha_m \neq \alpha_1$ ) and the coefficient  $q_0$  verifies the condition

$$q_0 > k_2 \left( 1 + \frac{\sqrt{L_u \varepsilon K_0}}{1 + \sqrt{L_u}} \right) \frac{t_v - t_0}{\sqrt{\pi \alpha_1}}$$
(243)

then there exist one and only one solution  $\lambda > 0$  to the equation:

$$\phi(x) = \varphi(x), \quad x > 0,$$
 (244)

where

$$\phi(x) = \frac{\sqrt{\pi\alpha_1}q_0}{(t_v - t_0)} \exp(-x^2) + P(x)$$
(245)

$$\varphi(x) = k_2 F_1(x) + \sqrt{\pi} k_1 \nu x \tag{246}$$

$$P(x) = \frac{L_u \varepsilon K_0}{L_u - 1} k_2 \left( \frac{1}{\sqrt{L_u}} F_1(\frac{x}{\sqrt{L_u}}) - F_1(x) \right).$$
(247)

Furthermore, the solution to the problem (226)-(235) is given by (238)-(240) , (242) and  $\left(\eta=\frac{x}{2\sqrt{\alpha_1\tau}}\right)$ 

$$t_{2}(\eta) = \frac{\varepsilon K_{0}L_{u}}{L_{u}-1} \left[ -\frac{erfc\left(\frac{x}{\sqrt{L_{u}}}\right)}{erfc\left(\frac{\lambda}{\sqrt{L_{u}}}\right)} + \frac{erfc(\eta)}{erfc(\lambda)} \right] + \frac{erfc(\eta)}{erfc(\lambda)}, \quad x > s(\tau), \quad \tau > 0.$$
(248)

iii. If the Luikov number  $L_u$  verifies the condition

$$L_u > \frac{1}{\varepsilon K_0 + 1} \tag{249}$$

then the temperature distribution  $t_2$  reaches to a minimum value which is smaller than the initial temperature or its limit value at  $+\infty$ . The minimum value is attained when the dimensionless variable  $\eta = \frac{x}{2\sqrt{\alpha_1 \tau}}$  takes the value

$$\eta = \sqrt{\left(\frac{L_u}{L_u - 1}\right) \log \left(\frac{\left(\left(\varepsilon K_0 + 1\right)L_u - 1\right)}{\varepsilon K_0 \sqrt{L_u}} \frac{\operatorname{erfc}\left(\frac{\lambda}{\sqrt{L_u}}\right)}{\operatorname{erfc}(\lambda)}\right)}.$$
(250)

#### 3.4.2 Other free boundary problem in a porous medium

There are some explicit solutions for the following free boundary problems for the diffusion equation corresponding to evaporation, freezing, sublimation or desublimation processes in (Lin, 1981, 1982a & 1982b; Mikhailov, 1975 & 1976; Santillan Marcus & Tarzia, 2000a & b). The simultaneous determination of one or two unknown thermal coefficients of a semiinfinite material through a desublimation process with coupled heat and moisture flows is given in (Santillan Marcus & Tarzia, 2007; Santillan Marcus, et al., 2008).

## 3.5 A mixed saturated-unsaturated flow problem representing absorption of water by a soil with a constant pond depth at the surface and an explicit solution for a particular diffusivity

In wet soils, zones of saturation develop naturally in the vicinity of impermeable strata, surface ponds and subterranean cavities. Hydrology must be concerned with transient flow through coexisting unsaturated and saturated zones. Models of advancing saturated zones necessarily involve a nonlinear free boundary problem (Broadbridge & White, 1990; Knigh & Philip, 1974; Philip, 1957 & 1958; Warrick & Broadbridge, 1992).

We consider a homogeneous soil which initially has some uniform volumetric water content  $\theta_n$ . At times t > 0, water is supplied at the surface x = 0 under pressure head  $\psi_0$ . Then, a mixed saturated-unsaturated flow problem representing absorption of water by a soil with constant pond depth at the surface is presented. At any time t the zone of saturation extends from x = 0 to x = s(t). Assuming Darcy's law and neglecting gravity, the water flux is given by

$$v = -K(\psi)\frac{\partial\psi}{\partial x} \tag{251}$$

where  $\psi$  is the soil water matric potential and *K* is the hydraulic conductivity. In the saturated zone we have

$$\psi(x,t) = \psi_0 - \frac{\psi_0 - \psi_s}{s(t)}, \quad 0 < x < s(t)$$
(252)

and we obtain a free boundary problem for the unsaturated zone:

$$\theta(s(t)^+, t) = \theta_s, \quad t > 0 \tag{253}$$

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left[ D(\theta) \frac{\partial \theta}{\partial x} \right], \quad x > s(t), \quad t > 0$$
(254)

$$-D(\theta)\frac{\partial\theta}{\partial x}(s(t)^{+},t) = K_{s}\frac{\psi_{0} - \psi_{s}}{s(t)}, \quad t > 0$$
(255)

$$\theta(x,0) = \theta(+\infty,t) = \theta_n, \quad x > s(t), \quad t > 0$$
(256)

$$s(0) = 0$$
 (257)

where

- x: spatial coordinate,
- t: time,

 $\theta$ : volumetric water content,

- $\theta_n$ : initial volumetric water content,
- $\theta_s$ : volumetric water content at saturation,
- $\psi$ : soil water matric potential,

 $\psi_0$ : pond depth,

 $\psi_s$ : soil water potential at x = s(t),  $\psi_s < \psi < \psi_0$ 

K : hydraulic conductivity,

 $K_s$ : hydraulic conductivity at saturation,

*D* : soil water diffusivity  $(D = K \frac{d\psi}{d\theta})$ .

We consider the free boundary (253)-(257) where the position s(t) of the free boundary and the water content field  $\theta(x,t)$  must be determined; and we restrict our attention to the special functional form of the soil water diffusivity

$$D(\theta) = \frac{a}{\left(b - \theta\right)^2} \tag{258}$$

where a, and b are positive constants. With this form of diffusivity the nonlinear diffusion equation (254) may be transformed to a linear diffusion equation. We consider the following parameter:

$$C = \frac{b - \theta_n}{\theta_s - \theta_n} > 1 .$$
<sup>(259)</sup>

<u>Remark 19.</u>

In (Briozzo & Tarzia, 1998) a closed-form analytic solution can be obtained for a nonlinear diffusion model under conditions of ponding surface. The explicit solution depends on a parameter *C* (determined by the data of the problem ), according to two cases:  $1 < C < C_1$  or  $C_1 \leq C$ , where  $C_1$  is a constant which is obtained as the unique solution to an equation. This results complements the study given in (Broadbridge, 1990) in order to established when the explicit solution is available. The behaviour of the bifurcaton parameter  $C_1$  as a function of the driving potential is studied with the corresponding limits for small and large

values. We also prove that the sorptivity is continuously differentiable as a function of variable C.

#### 3.6 Estimation of the diffusion coefficient in a gas-solid system

Looking for a competitive separation process like as the permeation, the development and optimal choice of membrane materials become necessary. On this subject, equations modelling the permeation process are required. The parameters contained in such a model must be obtained from simple experiments. The knowledge of solubility and diffusivity are very important to solve the separation problem.

We consider a polymeric membrane swelling for a hydrocarbon solution. The following assumptions are considered: Once the gaseous component reaches a threshold concentration on the gas-polymer interface, it diffuses through the membrane in the *x* direction being immobilized by a quickly and irreversible transformation. Then a swelling front is generated whose position is given by the free boundary x = s(t), t > 0 with the initial condition s(0)=0.

Moreover, the hydrocarbon diffusion coefficient D in the saturated o swollen region of the polymer is considered a constant for each experimental condition. A free boundary model (Castro et al., 1987; Crank, 1975; Villa, 1987) with an overspecified condition for the one-dimensional diffusion equation under the preceding assumptions is given:

$$c_t = Dc_{xx}, \qquad 0 < x < s(t), \quad t > 0$$
(260)

$$c(s(t),t) = 0, t > 0$$
 (261)

$$Dc_x(s(t),t) = -\beta \dot{s}(t), \quad t > 0,$$
 (262)

$$c(0,t) = C_0 > 0, \quad t > 0 \tag{263}$$

$$A\int_{0}^{t} Dc_{x}(0,\tau)d\tau = -\alpha\sqrt{t}, \quad t > 0, \qquad (264)$$

$$s(0) = 0$$
 , (265)

where c=c(x,t) denotes the concentration profile of the hydrocarbon in the swollen area, s(t) gives the position at time t of the free interface and separates the two regions in the membrane, the saturated and unsaturated, D is the unknown diffusion coefficient in the system, and  $C_0$ ,  $\alpha$  and  $\beta$  are positive parameters and A is a positive constant which must be obtained experimentally.

Theorem 22. (Destefanis et al., 1993)

The concentration profile and the free boundary position are given by:

$$c(x,t) = C_0 - \frac{C_0}{erf(\frac{\sigma}{\sqrt{D}})} erf(\frac{x}{2\sqrt{Dt}}), \quad 0 < x < s(t), \ t > 0,$$
(266)

$$s(t) = 2\sigma\sqrt{t}, \quad t > 0 , \qquad (267)$$

and the unknown coefficients D and  $\sigma$  are obtained by the following expressions:

$$D = \frac{\pi \alpha^2}{4A^2 C_0} \operatorname{erf}(\xi) = \frac{\alpha^2}{4A^2 \beta^2} \frac{\exp(-2\xi^2)}{\xi^2}$$

$$\sigma = \frac{\alpha \sqrt{\pi}}{2AC_0} \xi \operatorname{erf}(\xi) = \frac{\alpha}{2A\beta} \exp(-\xi^2)$$
(268)

where  $\xi$  is the unique solution to the equation:

$$E(x) = \frac{C_0}{\beta \sqrt{\pi}}, \quad x > 0.$$
 (269)

Remark 20.

The methodology used in this determination of the unknown diffusion coefficient is a variant of those developed in (Tarzia, 1982 & 1983) for the determination of thermal coefficients for a semi-infinite material through a phase-change process.

## 3.7 The coupled heat and mass transfer during the freezing of high-water content materials with two free boundaries: the freezing and sublimation fronts

Ice sublimation takes place from the surface of high water-content systems like moist soils, aqueous solutions, vegetable or animal tissues and foods that freeze uncovered or without an impervious and tight packaging material. The rate of both phenomena (solidification and sublimation) is determined both by material characteristics (mainly composition, structure, shape and size) and cooling conditions (temperature, humidity and rate of the media that surrounds the phase change material). The sublimation process, in spite of its magnitude being much less than that of freezing process, determines fundamental features of the final quality for foods and influences on the structure and utility of frozen tissues. Modelling of these simultaneous processes is very difficult owed to the coupling of the heat and mass transfer balances, the existence of two moving phase change fronts that advance with very different rates and to the involved physical properties which are, in most cases, variable with temperature and water content.

When high water-content materials like foods, tissues, gels, soils or water solutions of inorganic or organic substances, held in open, permeable or untightly-sealed containers are refrigerated to below their initial solidification temperature, two simultaneous physical phenomena take place:

- Liquid water solidifies (freeze), and
- Surface ice sublimates.

For the description of the freezing process, the material can be divided into three zones: unfrozen, frozen and dehydrated. Freezing begins from the refrigerated surface/s, at a temperature  $(T_{if})$  lower than that of pure water, due to the presence of dissolved materials, and continues along an equilibrium line. Simultaneously, ice sublimation begins at the frozen surface and a dehydration front penetrates the material, whose rate of advance is again determined by all the abovementioned characteristics of the material and environmental conditions. Normally this rate is much lower than that of the freezing front. A complete mathematical model has to solve both, the heat transfer (freezing) and the mass transfer (weight loss) simultaneously (Campañone et al., 2005a & b).

Phase change is accounted for in the following way:

- Solidification (freezing) as a freezing front ( $x = s_f(t)$ ) located in the point where material temperature reaches the initial freezing temperature ( $T_{if}$ ), determined by material composition. For temperatures lower than  $T_{if}$  (the zone nearer to the refrigerated surface) the amount of ice formed is determined by an equilibrium line (ice content vs temperature and water content) specific to the material.
- On the dehydration front  $(x = s_d(t))$  we impose Stefan-like conditions for temperature distribution and vapor concentration.

We consider a semi-infinite material with characteristics similar to a very dilute gel (whose properties can be supposed equal to those of pure water). The system has initial uniform temperature equal to  $T_{if}$  and uncovered flat surface which at time t=0 is exposed to the surrounding medium (with constant temperature  $T_s$  (lower than  $T_{if}$ ) and heat and mass transfer coefficients h and  $K_m$ ). We assume that  $T_s < T_0(t) < T_{if}$ , t > 0 where  $T_0(t)$  is the unknown sublimation temperature.

To calculate the evolution of temperature and water content in time, we will consider the following free boundary problem: Find the temperatures  $T_d = T_d(x,t)$  and  $T_f = T_f(x,t)$ , the concentrations  $C_{va} = C_{va}(x,t)$ , the free boundaries  $s_d = s_d(t)$  and  $s_f = s_f(t)$  and the temperature  $T_0 = T_0(t)$  at the sublimation front  $x = s_d(t)$  which must satisfy the following:

• Differential equations at the dehydrated region:

$$\rho_d C_{p_d} \frac{\partial T_d}{\partial t} = k_d \frac{\partial^2 T_d}{\partial x^2}, \quad 0 < x < s_d(t), \quad t > 0$$
(270)

$$\varepsilon \frac{\partial C_{va}}{\partial t} = D_{ef} \frac{\partial^2 C_{va}}{\partial x^2}, \quad 0 < x < s_d(t), \quad t > 0$$
(271)

• Differential equations at the frozen region:

$$\rho_f C_{p_f} \frac{\partial T_f}{\partial t} = k_f \frac{\partial^2 T_f}{\partial x^2}, \quad s_d(t) < x < s_f(t), \quad t > 0$$
(272)

Free boundary conditions at the sublimation front  $x = s_d(t)$ :

$$T_{d}(s_{d}(t),t) = T_{f}(s_{d}(t),t) = T_{0}(t), \quad t > 0$$
(273)

$$k_{f} \frac{\partial T_{f}\left(s_{d}\left(t\right),t\right)}{\partial x} - k_{d} \frac{\partial T_{d}\left(s_{d}\left(t\right),t\right)}{\partial x} = L_{s}m_{s}\dot{s}_{d}\left(t\right), \quad t > 0$$

$$(274)$$

$$D_{ef} \frac{\partial C_{va}(s_d(t), t)}{\partial x} = m_s \dot{s}_d(t)$$
(275)

$$C_{va}(s_{d}(t),t) = \frac{MP_{sat}(T)}{R_{g}T_{0}(t)} = M a \frac{\exp\left(b - \frac{c}{T_{0}(t)}\right)}{R_{g}T_{0}(t)}$$
(276)

where  $C_{va}(s_d(t),t)$  is the equilibrium vapor concentration at  $T_0(t)$  and the saturation pressure  $P_{sat}(T)$  is evaluated according to (Fennema & Berny, 1974). Free boundary conditions at the freezing front  $x = s_f(t)$ :

$$T_f(s_f(t), t) = T_{if}, \quad t > 0$$
 (277)

$$k_f \frac{\partial T_f(s_f(t), t)}{\partial x} = m_f L_f \dot{s}_f(t), \quad t > 0$$
(278)

• The convective boundary conditions at the fixed interphase x = 0:

$$k_{d} \frac{\partial T_{d}(0,t)}{\partial x} = h \left( T_{d}(0,t) - T_{s} \right), \quad t > 0$$
(279)

$$D_{ef} \frac{\partial C_{va}(0,t)}{\partial x} = K_m \left( C_{va}(0,t) - C_a \right), \quad t > 0$$
(280)

• The initial conditions at t = 0:

$$s_f(0) = s_d(0) = 0 \tag{281}$$

$$T = T_{if} \quad \text{for } x \ge 0 \,. \tag{282}$$

We will solve the system (270) - (282) by using the quasi-steady method. In general, it is a good approximation when the Stefan number tends to zero, i.e. when the latent heat of the material is high with respect to the heat capacity of the solid material. This approximation has often been used when modelling the freezing of high-water content materials.

<u>Theorem 23</u>. (Olguin et al., 2008)

The temperatures  $T_f$ ,  $T_d$  and the concentration  $C_{va}$  are given by the following expressions:

$$T_d(x,t) = A(t) + B(t)x, \quad 0 < x < s_d(t), \quad t > 0$$
(283)

$$C_{v_a}(x,t) = D(t) + E(t)x, \quad 0 < x < s_d(t), \quad t > 0$$
(284)

$$T_f(x,t) = F(t) + G(t)x, \quad s_d(t) < x < s_f(t), \quad t > 0$$
(285)

where A(t), B(t), D(t) and E(t) as a function of  $T_0(t)$  and  $s_d(t)$ , as well as F(t) and G(t) as a function of  $T_0(t)$ ,  $s_d(t)$  and  $s_f(t)$ , given by the following expressions:

$$A(t) = \frac{T_0(t) + T_s \frac{h}{k_d} s_d(t)}{1 + \frac{h}{k_d} s_d(t)}, \quad B(t) = \frac{h}{k_d} \frac{T_0(t) - T_s}{1 + \frac{h}{k_d} s_d(t)}$$
(286)

$$D(t) = \frac{\frac{K_m}{D_{ef}}C_a s_d(t) + M a \frac{\exp\left(b - \frac{c}{T_0(t)}\right)}{R_g T_0(t)}}{1 + \frac{K_m}{D_{ef}}s_d(t)}, \quad E(t) = \frac{K_m}{D_{ef}} \frac{M a \frac{\exp\left(b - \frac{c}{T_0(t)}\right)}{R_g T_0(t)} - C_a}{1 + \frac{K_m}{D_{ef}}s_d(t)}$$
(287)

$$F(t) = \frac{T_0(t)s_f(t) - T_{if}s_d(t)}{s_f(t) - s_d(t)}, \quad G(t) = \frac{T_{if} - T_0(t)}{s_f(t) - s_d(t)}$$
(288)

and we obtain the following system of two ordinary differential equations and one algebraic equation for  $s_d(t)$ ,  $s_f(t)$  and  $T_0(t)$  given by:

$$1 + \frac{h}{k_{f}} \frac{T_{s}}{T_{if}} s_{f}(t) + h s_{d}(t) \left( \frac{1}{k_{d}} - \frac{T_{s}}{T_{if} k_{f}} \right) - \frac{T_{0}(t)}{T_{if}} \left[ 1 + \frac{h}{k_{f}} s_{f}(t) + h s_{d}(t) \left( \frac{1}{k_{d}} - \frac{1}{k_{f}} \right) \right] =$$

$$= \frac{L_{s} K_{m}}{T_{if} k_{f}} \frac{\left( 1 + \frac{h}{k_{f}} s_{f}(t) \right) \left( s_{f}(t) - s_{d}(t) \right)}{1 + \frac{K_{m}}{D_{ef}} s_{d}(t)} \left[ M a \frac{\exp \left( b - \frac{c}{T_{0}(t)} \right)}{R_{g} T_{0}(t)} - C_{a} \right]$$
(289)

$$\dot{s}_{d}(t) = \frac{k_{f}T_{if}}{m_{s}L_{s}} \frac{1 + \frac{h}{k_{f}}\frac{T_{s}}{T_{if}}s_{f}(t) + hs_{d}(t)\left(\frac{1}{k_{d}} - \frac{T_{s}}{k_{f}T_{if}}\right) - \frac{T_{0}(t)}{T_{if}}\left[1 + \frac{h}{k_{f}}s_{f}(t) + hs_{d}(t)\left(\frac{1}{k_{d}} - \frac{1}{k_{f}}\right)\right]}{\left(1 + \frac{h}{k_{d}}s_{f}(t)\right)\left(s_{f}(t) - s_{d}(t)\right)}$$
(290)

$$\dot{s}_{f}(t) = \frac{k_{f}T_{if}}{m_{f}L_{f}} \frac{1 - \frac{T_{o}(t)}{T_{if}}}{s_{f}(t) - s_{d}(t)}$$
(291)

$$s_f(0) = s_d(0) = 0$$
. (292)

Remark 21.

There exist some approximate or explicit solutions for some other free boundary problems for the heat-diffusion equation, e.g.: model for a single nutrient uptake by a growing root system by using a moving boundary approach; explicit estimate for the asymptotic behavior of the solution of the porous media equation with absorption (reaction-diffusion processes of a gas inside a chemical reactor); penetration of solvents in polymers; filtration of water through oil in a porous medium; the Wen model for an isothermal monocatalytic diffusion-reaction process of a gas with a solid. The solid is chemically attacked from its surface with a quick and irreversible reaction and, at the same time, a free boundary begins, etc.

#### 4. Conclusion

We have given a review on explicit and approximated solutions for heat and mass transfer problems in which a free or moving interface is involved. We have also showed some new recent problems for heat and mass transfer in which a free or moving interface is also involved.

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### Advanced Topics in Mass Transfer

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This book introduces a number of selected advanced topics in mass transfer phenomenon and covers its theoretical, numerical, modeling and experimental aspects. The 26 chapters of this book are divided into five parts. The first is devoted to the study of some problems of mass transfer in microchannels, turbulence, waves and plasma, while chapters regarding mass transfer with hydro-, magnetohydro- and electro- dynamics are collected in the second part. The third part deals with mass transfer in food, such as rice, cheese, fruits and vegetables, and the fourth focuses on mass transfer in some large-scale applications such as geomorphologic studies. The last part introduces several issues of combined heat and mass transfer phenomena. The book can be considered as a rich reference for researchers and engineers working in the field of mass transfer and its related topics.

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