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On a numerical approach to Stefan problem

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Abstract. — A one-dimensional Stefan problem for a spherical particle moving in a plasma jet is solved by approximating the enthalpy formulation of the problem by $C^0$ piecewise linear finite elements in space combined with a semi-implicit scheme in time.

Introduction.

In [1] a new numerical approach to bidimensional Stefan-like problems was proposed. Our aim is to show efficiency of this approach by modifying the resultant numerical scheme to a solution of a one-dimensional (radial) heat transfer equation (HTE) in a spherical particle with temperature dependent material parameters. As an example, we consider the particle of alumina ($\text{Al}_2\text{O}_3$) moving in a water plasma jet.

When speaking about Stefan problem we mean that the particle melts and resolidifies and thus a sharp moving solid-liquid boundary occurs. Two additional conditions have to be satisfied on this boundary: the temperature $T$ equals a melting temperature $T_m$ and the heat flow exhibits a jump corresponding to the absorption or liberation of a latent heat of fusion $L_m$ (Stefan condition) [2, 3].

The finite difference schemes of the temperature formulated problem usually involve both these conditions as new equations in addition to the HTE and use deforming grids in order to follow the interphase boundary [4, 5]. Nevertheless, it is well-known that the numerical modelling of the temperature formulated problem can be simplified by avoiding these difficulties; it only suffices to redefine suitably the specific heat in a neighbourhood of the melting point [6]. An alternative approach is to use the enthalpy formulation of the problem in which case no explicit conditions on the temperature and the heat flow at the solid-liquid interface need to be accounted for and the fixed grid can be used as well. However, there are first-order discontinuities of the thermal parameters of particle at melting point and one is led to a weak formulation of both the temperature and enthalpy formulated problem [1, 2].

The enthalpy formulation in [1] is based on a physically nice fact that the temperature is an
Increasing function of enthalpy, \( T = \beta(u) \), whose graph has a flat part at melting point \( T_m \), and for our purposes similarly at boiling point \( T_b \), as shown in figure 1. The differences \( u_2 - u_1 \), \( u_4 - u_3 \) correspond with the latent heat of fusion and evaporation \( L_m \) and \( L_v \), respectively. The weak formulation is approximated by continuous piecewise linear finite elements in space combined with a semi-implicit scheme in time.

Before presenting the numerical study we point out that the behaviour of solid particles in high pressure (thermal) plasmas has been extensively studied. We refer the reader to overviews [7, 8] for details and to the Appendix where the necessary transport coefficients are summarized.

From now on, we let \( p \) to denote the density, \( \lambda \) the thermal conductivity, \( c_p \) the specific heat at constant pressure, \( \nu \) the viscosity, \( \nu \) the kinematic viscosity, \( r \) the radial coordinate and \( r_p(t) \) the (time dependent) particle radius. The subscripts \( g, v \) are let to denote “gas” and “vapour”, respectively.

Weak formulation of the problem.

The HTE is written in terms of the enthalpy \( u = \int_{T_m}^{T} c_p(T')dT' \) (which is defined up to an additive constant; see also Fig. 1) as follows:

\[
\frac{\partial u}{\partial t} = \nabla \cdot (\lambda \nabla T) = \nabla \cdot (\lambda \frac{d\beta}{du} \nabla u) .
\]

We suppose that the initial temperature of particle is equal to a constant \( T_0 \) which is different from melting or boiling temperature and we set the initial condition

\[
u(\cdot, 0) = u_0 = \beta^{-1}(T_0) \quad \text{on } \Omega_0 = [0, r_p(0)].
\]

We assume the following boundary and symmetry conditions:

\[
\lambda \nabla_n T = h_T (T_g - T) - \varepsilon \sigma (T^4 - T^4) - j \cdot n [L_v + c_p v (T_g - T)] \Theta(u_2) \quad \text{RHS}
\]

\[
\nabla T = 0 \quad \text{at } r = r_p(t),
\]

\[
\nabla T = 0 \quad \text{at } \quad r = 0.
\]

Here \( n \) denotes the outer normal to the surface of the particle, \( \varepsilon \) the surface emissivity, \( \sigma \) the Stefan-Boltzmann constant, \( T_g \) the temperature of an environment surrounding the jet and \( \Theta \) the Heaviside function. The heat transfer coefficient \( h_T \) and the vapour mass flow density \( j \)
are defined in the Appendix. The three terms in RHS describe the heat flow due to forced convection, the radiative and the evaporative heat losses, respectively. The particle vapours are assumed to be heated to the temperature \( T_h \) of the carrier gas.

Moreover, we suppose that the temperature dependent parameters \( \rho, \ c_p, \ \lambda \) are strictly positive and that the function \( \beta \) is piecewise \( C^1 \) function satisfying the conditions \( \beta(\xi) = T_m \) (resp. \( T_b \)) for all \( \xi \in [u_1, u_2] \) (resp. \( \xi \in [u_3, u_4] \)) and \( 0 < \beta'(\xi) \leq B \), where \( B \) is some finite number, for all \( \xi \notin [u_1, u_2] \cup [u_3, u_4] \) - see figure 1.

Denoting \( \phi = \int_0^\infty \phi \psi r^2 dr, \ (\phi, \psi) = \int_S \phi \psi dS = \phi \psi r_p^2 \) (one-dimensionality of the problem!) we get in a standard way the weak formulation of (1-4) (see [1] and [2] for mathematical details):

Find \( u \) such that

\[
\left( \frac{\partial u}{\partial t}, \phi \right) + (\lambda \beta' \nabla u, \nabla \phi) = \langle \text{RHS}, \phi \rangle, \quad u(\cdot, 0) = u_0 \quad \text{on} \ \Omega_0
\]

(5)

for all suitable test functions \( \phi \) and almost every \( t \in (0, t_F) \), where \( t_F \) is a fixed positive time.

**Numerical scheme.**

We solve (5) in a class of \( C^0 \) piecewise linear functions on \( \Omega_t = [0, r_p(t)] \). We let \( I_h \) to denote the decomposition of \( \Omega_t \) into \( M + 1 \) intervals \( I_i = [(i - 1)h, ih], \ i = 1, \ldots, M, M \geq 0, \) and \( R_i = ir_p(t)/(M + 1) =ih, \ i = 0, \ldots, M + 1, \) its equidistant nodal points.

We consider the finite element space

\[
V_h = \{ \psi \in C^0(\Omega_t); \ \psi|_I \text{ is a polynomial function of degree} \\
\leq 1 \text{ on all } I \in I_h \text{ and } \nabla \psi = 0 \text{ at } r = 0 \}
\]

with the basis generated by the set \( \{ \psi_i \}_{i=0}^{M+1} \) of "pyramidal" functions \( \psi_i(r) = (R_{i+1} - r)/h \) on \( I_{i+1}, \ \psi_i(r) = (r - R_{i-1})/h \) on \( I_i, \ \psi_i = 0 \) otherwise, which are orthogonal with respect to the discrete inner product

\[
(\phi, \chi)_h = \sum_{I \in I_h} \int_I r_h(\phi \chi) r^2 dr = \sum_{I \in I_h} \int_I \sum_{R_k^I} (\phi \chi)(R_k^I) \psi_k r^2 dr.
\]

\( R_k^I \) denote the nodal points belonging to the interval \( I \) and \( r_h \) is the interpolation operator related to \( V_h \).

**Remark 1.** — Notice the possible time dependence of \( h \) which takes into account the decrease of particle due to vaporization or even due to intense evaporation at boiling point.

Setting the time step \( \tau = t_F/N \), where the integer \( N > 0, t^n = n\tau, \) and following [1] we obtain the space-time discretization of (5):

Find \( (U^n)_{n=0}^{N-1}, U^n \in V_h \) such that

\[
\left( \frac{\rho(U^n)U^{n+1} - U^n}{\tau}, \phi \right)_h + (a(U^n) \nabla U^{n+1}, \nabla \phi)_h = \langle \text{RHS}(U^n), \phi \rangle \quad \text{for all} \ \phi \in V_h,
\]

(6)

where

\[
a(U^n)|I = \begin{cases} \\
(\lambda \beta')(U^n) & \text{if } \nabla U^n = 0 \text{ on } I \in I_h, \\
\lambda(U^n) \frac{\nabla (U^n) \cdot \nabla U^n}{\nabla U^n \cdot \nabla U^n} & \text{if } \nabla U^n \neq 0 \text{ on } I \in I_h.
\end{cases}
\]
and where the notation \( h = h^{n+1} \) is used for brevity.

If \( U^n \) is constant, equal to \( u_1, u_2 \) or \( u_3 \) on \( I \in I_h \), we can arbitrarily set \( \beta'(U^n) = \beta'(u_1 - 0) \) if \( U^n = u_1 \), \( \beta'(U^n) = \beta'(u_2 + 0) \) if \( U^n = u_2 \) and \( \beta'(U^n) = \beta'(u_3 - 0) \) if \( U^n = u_3 \).

The matrix form of (6) is obtained by putting \( \phi = \psi \), \( U^n = \sum_{i=0}^{N+1} U^n_i \psi_i \), where \( U^n_i \equiv U^n(R_i) \), and by remembering that \( U^n_0 = U^n_1 \) (symmetry at \( r = 0 \)). The result is as follows:

\[
\frac{D^n U^{n+1} - U^n}{\tau} + R^n U^{n+1} = F^n
\]

or equivalently

\[
(1 + \tau \cdot (D^n)^{-1} R^n) U^{n+1} = U^n + \tau \cdot (D^n)^{-1} F^n, \quad n = 0, \ldots, N - 1. \tag{7}
\]

The \((M+1)\)-dimensional column vectors \( U^n \) and \( F^n \) have their components \( U^n_i \) and \( F^n_i \) respectively.

The \((M+1)\times(M+1)\) matrix \( D^n \) is diagonal with strictly positive elements

\[
d_{11}^n = (\rho^n(\psi_0 + \psi_1), \psi_0 + \psi_1)_h = \rho^n_i (B_0 + A_1 + B_1) h^3,
\]

\[
d_{ii}^n = (\rho^n \psi_i, \psi_i)_h = \rho^n_i (A_i + B_i) h^3, \quad i = 2, \ldots, M,
\]

\[
d_{(M+1)(M+1)}^n = (\rho^n \psi_{M+1}, \psi_{M+1})_h = \rho^n_{M+1} A_{M+1} h^3.
\]

The square matrix \( R^n \) is symmetric tridiagonal with the elements

\[
r_{11}^n = (a^n \nabla (\psi_0 + \psi_1), \nabla (\psi_0 + \psi_1))_h = (a^n_{1,R} B_1 + a^n_{2,L} A_2) h,
\]

\[
r_{ii}^n = (a^n \nabla \psi_i, \nabla \psi_i)_h = (a^n_{i-1,R} B_{i-1} + a^n_{i-1,L} A_i + a^n_{i,R} B_i + a^n_{i+1,L} A_{i+1}) h, \quad i = 2, \ldots, M,
\]

\[
r_{M+1,M+1}^n = (a^n \nabla \psi_{M+1}, \nabla \psi_{M+1})_h = (a^n_{M,R} B_M + a^n_{M+1,L} A_{M+1}) h,
\]

\[
r_{i(i+1)}^n = (a^n \nabla \psi_i, \nabla \psi_{i+1}) = -(a^n_{i,R} B_i + a^n_{i+1,L} A_{i+1}) h, \quad i = 1, \ldots, M.
\]

In the above formulae, the strictly positive coefficients \( A_i \) and \( B_i \) are given by the equations

\[
A_i = \frac{1}{h^3} \int_{I_i} \psi_i r^2 dr = \frac{i^4 - (i - 1)^4}{4} - \frac{(i - 1)^3 - (i - 1)^3}{3}, \quad i = 1, \ldots, M + 1,
\]

\[
B_i = \frac{1}{h^3} \int_{I_{i+1}} \psi_i r^2 dr = (i + 1)^3 - \frac{(i + 1)^3 - i^3}{3} - \frac{(i + 1)^4 - i^4}{4}, \quad i = 0, \ldots, M.
\]

The \( a^n_{i,R} \) and \( a^n_{i,L} \) denote the (positive) \( a^n_i \)'s with the derivatives \( \beta' \) taken at the point \( R_i \) from the right and from the left, respectively.

The matrix \( R^n \) is easily shown to be diagonally dominant (one has \( r_{ii}^n \geq 0, r_{i(i+1)}^n \leq 0 \). Thus the semi-implicit scheme (6) is positive and it is shown to be stable whenever (in nondimensional units) \( \tau B / h^2 \leq c \), where \( c \) is an arbitrary positive constant. Moreover, the solution of (6) converges strongly (in a corresponding space) to the solution of problem (5) whenever \( \tau \) and \( h \) tend to zero in such a way that \( \tau / h^2 \) tends to zero [1].
Numerical results.

To set the correct space and time steps in (7), it is convenient to proceed to the dimensionless variables \( r^* = r/r_p(0), \quad t^* = Fo \cdot Ste, \quad u^* = u/L_m, \quad T^* = (T - T_0)/(T_m - T_0). \)

\( Fo = \lambda_s t/(\rho_s c_p s r^2_p(0)) \) and \( Ste = c_p s (T_m - T_0)/L_m \) are the Fourier and Stefan number, respectively. We also define the dimensionless density \( \rho^* = \rho/\rho_s \), the specific heat capacity \( c_p^* = c_p/c_p s \) and the heat conductivity \( \lambda^* = \lambda/\lambda_s \) (the subscript \( s \) refers to solidus). The only change in equation (7) is that all the parameters in matrices \( D^n \) and \( R^n \) are replaced by their nondimensional equivalents, \( U^n \) is replaced by \( U^{*n} \), \( R^n \) is divided by \( Ste \) and \( F^n \) is divided by \( r_0 \lambda_s (T_m - T_0). \)

Remark 2. — As the information about whether the particle is melted or not does not depend on the units used, we plot the results by means of nondimensional variables.

We set \( T_m = 2326 \) K, \( T_b = 3800 \) K, \( T_0 = T_a = 300 \) K, \( L_m = 1.065 \) MJ/kg, \( L_v = 24.7 \) MJ/kg, \( \rho_s = 3900 \) kg/m\(^3\), \( \rho_l = 2750 \) kg/m\(^3\), \( c_p s = 1.419 \) kJ/(kgK), \( c_p v = 0.967 \) kJ/(kgK), \( \lambda_s = 9.66 \) J/(msK), \( u^*_1 = 0, \quad u^*_2 = 1, \quad u^*_3 = 2.96, \quad u^*_4 = 26.16. \) The Stefan number \( Ste = 2.7. \)

To mimic experimental conditions, we suppose that the jet temperature and velocity decrease rapidly from 12000 K and 600 m/s at the jet origin \( x = 0.0 \) m to 1000 K and 240 m/s at \( x = 0.3 \) m.

We present results for particles of the initial diameter 30 and 120 \( \mu \)m and of the initial velocity 10 m/s. In both cases, we set the space step \( h = 1/25 \) and the time step \( \tau = h/20. \)

The results were obtained by solving the set of linear algebraic equations (7) for \( U^{n+1}. \) Our program was written in Fortran and its flow diagram is similar to that in [5]. The particle motion is supposed to be one-dimensional, parallel to that of the gas in which case the equation of motion is integrated analytically; provided that the gas velocity and temperature are constant over the short time step \( \tau. \) The moving grid is only used if the particle decreases by vaporization or evaporation. The intense evaporation is taken into account by “switching-off” the

Fig.2. — Particle velocity, radius, surface (thick line) and central (thin line) temperature vs. the distance from the jet origin. Label 30 (120) - particle diameter 30 (120) \( \mu \)m. Unlabelled lines - gas.
Fig. 3. — Enthalpy (above) and temperature (below) history of an Al$_2$O$_3$ particle - diameter 30 μm. Time $1 \approx 4.8 \times 10^{-5}$ s.
mass flow density \( j \) whenever the particle surface reaches the boiling point and by "cutting-off" the thin surface layer whose temperature exceeds \( T_b \). The vaporization is negligible unless the surface temperature is above 3700 K.

Both the enthalpy and temperature histories of the particles were calculated. The dependence of some remarkable parameters of the particles on a distance from the jet origin is shown in figure 2. To this purpose, the dimensionless velocity \( v^* = v/100 \; m/s \) and the \( x \)-axis coordinate \( x^* = x/1m \) were defined. We conclude that while the smaller particle is partially evaporated and resolidified at \( x^* = 0.3 \), the greater one is melted and unevaporated.

Comparison of the enthalpy and temperature history of the particle is shown in figure 3. The melting or solidification front is defined at time \( t^n \) as the set of points \( \{ r \in \Omega_t^n; u_1 \leq U^n \leq u_2 \} \). The enthalpy history is seen to be advantageous for determining where this front lies - see figure 3.

As pointed out in [1], the choice of \( a(U^n) \) is made in order to avoid small oscillations of the solution to problem (6). It is argued that the oscillations observed near the melting point are caused by the discontinuity of the solution to problem (5) at this point, while in (6) the continuity and piecewise linearity are required. Our numerical tests show that the oscillations of the solution of (6) are actually smaller if the recommended \( a(U^n) \) is used. Moreover, the two solutions of (6) with and without the corrected form of \( a(U^n) \) are shown to be identical away from the melting point.

Conclusion.

The straightforward modification to different one or two-dimensional problems (including those with nonlinear source term, nonhomogeneous Dirichlet or Neumann boundary conditions, solidification of alloys etc.), the economy in numerical modelling requirements (no moving grids, continuity, piecewise linearity) and the behaviour of our results make the numerical approach in [1] useful to all those who are concerned with Stefan-like problems.

Appendix.

The heat transfer coefficient \( h_T \) is given by the semi-empirical formula

\[
h_T = \frac{\bar{\lambda}_g}{2r_p} (2 + 0.6Re_p^{1/2}Pr^{1/3}) \left( \frac{\bar{\nu}_g}{\nu_g} \right)^{0.15},
\]

where

\[
Pr = \frac{\bar{\mu}_g \bar{c}_{pg}}{\bar{\lambda}_g}
\]

and

\[
Re_p = \frac{2r_p \bar{\rho}_g |\bar{v}_g - v|}{\bar{\mu}_g}
\]

are the Prandtl and Reynolds number, respectively. The bar over the gas parameters means that they are calculated at the mean gas-surface temperature \( (T_s + T_g)/2 \).

To determine the particle velocity and position in a gas, we assume the equation of motion

\[
m \frac{dv}{dt} = \frac{1}{2} \pi r_p^2 \bar{\rho}_g |\bar{v}_g - v| (\bar{v}_g - v) C_D.
\]
The drag coefficient $C_D$ is given for $\text{Re}_p \in [1, 1000]$ by the formula

$$C_D = \frac{24}{\text{Re}_p} \left(1 + 0.15 \text{Re}_p^{0.687}\right) \left(\frac{\nu_g}{\nu_s}\right)^{0.15}$$

The mass flow density $j$ is defined by the equation

$$j = h_M(\rho_s - \rho_\infty)n,$$

where $\rho_s$ and $\rho_\infty$ are the vapour density at the surface and away from the surface, respectively. The mass transfer coefficient $h_M$ is given by the formula for $h_T$ with $\bar{\lambda}$ replaced by the vapour-gas diffusivity $\bar{D}$ and with $\text{Pr}$ replaced by the Schmidt number

$$\text{Sc} = \frac{\nu_g}{\rho_g \bar{D}}.$$

When combined with the equation of state of an ideal gas and with the Clausius-Clapeyron's equation of first-order phase transitions the equation for $j$ can be rewritten in terms of the partial pressures of vapours.

References