On a computational algorithm for the analysis of non-stationary diffusional phase transformation *

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Physical analysis of phase transformation of materials consisting from several (in general q substitutional and r interstitial) components, coming from the Onsager extremal thermodynamic principle, following some ideas from [2], [1] and [3], leads, as explained in [4], from the mathematical point of view, to a system of partial differential equations of evolution type, including certain integral term, with substantial differences in particular phases (α, γ) and in moving interface of finite thickness (β), in whose center the ideal liquid material behaviour can be detected. The numerical simulation of this process in MATLAB, mentioned in [5], is able to explain some phenomena (e.g. the interface velocity as a function of temperature) better than known simplified models, assuming the sharp interface and additional boundary and transfer conditions.

The evolution of $q-1+r$ molar fractions c in one dimension is characterized in a Cartesian coordinate x and in time t. The coordinate x moves from the left to the right together with the interface of constant thickness h (from $x=0$ to $x=h$); the total size of the specimen is $H >> h$, the system is assumed to be closed (with zero boundary fluxes) on the interval $\langle x_L(t), x_R(t)\rangle$. One missing molar fraction can be derived from the condition $c_1 + \dots c_q = 1$. The resulting system of equations, starting from some a priori known initial values of c, reads

$$Bc' + (K + vN)c - N\frac{C}{\tau} = vNc^\diamond - N\Omega j^\diamond - N\frac{C^\times}{\tau} \tag{1}$$

where all variables are evaluated in time t, exept $C^\times = C(t-\tau)$, τ dentotes the time interval, referring to the implicit Euler method; (the system of differential equations can be derived from such difference ones using the limit passage $\tau \to 0$), B, K and N are square matrices of order $q-1+r$, B full, K and N diagonal, B and K depending on c, N dependent on x only, Ω is the constant molar volume and

$$C(x,t) = \int_0^x c(\xi,t)\mathrm{d}\xi\,,$$

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$c^\diamond$ refers to molar fractions and $j^\diamond$ to diffusive fluxes at $x = 0$ and

$$v = \frac{\Omega}{M} \sum_{i=1}^{q+r} \int_0^h c_i \mu_i' \, \mathrm{d}x$$

for prescribed chemical potentials μ_i as complicated functions of c; a prime symbol denotes a derivative with respect to x.

The system (1) comes (after rather long computations, performed in [4]), from the mass conservation law

$$\partial c/\partial t - vc' + \Omega j' = 0\,;$$

another (more evident) its consequence is

$$(C^R - C^{R\times})/\tau - v(c^R - c^\diamond) - \Omega j^\diamond = 0\,, \qquad (C^L - C^{L\times})/\tau - v(c^L - c^\diamond) - \Omega j^\diamond = 0\,; \quad (2)$$

upper indices ^{L} and ^{R} here refer to values at x^R and x^L, respectively. As (1) generates an iterative procedure with B, K, v and x_L set by c from the preceding iteration (or time step), it is important to suggest an inexpensive solver of the system of linear algebraic equations, derived from (1), using the finite difference method. Unfortunately, such system is not triangular, thus, because of the presence of unknowns $c^\diamond$ and $j^\diamond$ it is not possible to express c in all nodes step-by-step; even $c^\diamond$ and $j^\diamond$ cannot be determined by (2) completely. However, a special decomposition of c in form $c = c^\diamond + \widetilde{c}$ where $\widetilde{c} = \widetilde{c}^O_m + \xi^I_m \widetilde{c}^I_m + \xi^{II}_m \widetilde{c}^{II}_m$, $m \in \{1, \ldots, q-1+r\}$, ξ^I and ξ^{II} contain $2(q-1+r)$ unknown parameters, suggested as multiplicative correctors of estimates of $c^\diamond$ and $j^\diamond$, and $\widetilde{c}^O$, $\widetilde{c}^I$ and $\widetilde{c}^{II}$ are solutions of (1) corresponding to special right-hand sides. All details, including a numerical example (although some theoretical existence and convergence questions are still open – cf. [5]) can be found in the extended CD-ROM version of this paper.

References

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