On a special integro-differential problem occurring in diffusional phase transformation *

Jiří Vala

Brno University of Technology, Faculty of Civil Engineering
Department of Mathematics and Descriptive Geometry
602 00 Brno, Žižkova 17, Czech Republic
e-mail: Vala.J@fce.vutbr.cz

Most problems from continuum mechanics, from the mathematical point of view, are formulated as boundary and/or initial problems for certain special classes of (ordinary or partial) differential equations. However, come considerations, typically those incorporating the thermal behaviour of material at high temperature, insert non-local (integral) terms into such equations, which brings complication both to the existence theory and to the design of effective algorithms for numerical simulations. Such one-dimensional stationary model problem, taken from [5], includes the physical analysis of diffusive and massive phase transformation in substitutional alloys for an arbitrary finite number $r+1$ of components where $r \in \{1, 2, \ldots\}$ under the assumption of the finite positive thickness h of the interface between two different material phases. It is needed to find a vector of molar fractions c of all components, in practice of all except the last one which are allowed to be completed a posteriori. Consequently $c(x)$ have values in the r-dimensional Euclidean space R^r where $0 \leq x \leq H$; $H > h$ is some positive length. We have to know all initial values c_0 as the values of c for $x = 0$ (where the phase transformation starts) and consider the interface for $x \leq h$ and the final phase for $x > h$.

The proper mathematical theory of diffusional phase transformation has been published only for very special cases, as in [4]. The general case with a non-negligible interface thickness and with $r > 1$ seems to be uncovered by any available mathematical literature. The aim of this paper is to demonstrate, at least for sufficiently small nonlinear terms, how the effective algorithm for numerical simulations can be suggested and how its mathematical correctness can be verified. An original MATLAB- (and partially also MAPLE-) supported software solver has been created; some numerical results have been presented in [5], a more extensive study (covering non-stationary analysis, interstitial components, etc.) is being prepared.

The basic simplified differential equation for stationary phase transformation, in various forms repeated several times in [5], defined for $0 \leq x \leq H$, is

$$B(c)c' + K(c)c + vN(x)c = vN(x)c_0\,; \tag{1}$$

c' is the brief notation for $\mathrm{d}c/\mathrm{d}x$ and

*This research is supported by the Grant Agency of the Czech Republic, Reg. No. 103/05/0292.

$$v = \int_0^h \mu(c)\,\mathrm{d}x\,. \tag{2}$$

In this equation c has to be found from a subspace V of Sobolev space $W^{1,2}((0,H),R^r)$ satisfying $c(0) = c_0$; consequently c' belongs to the Lebesque space $L^2((0,H),R^r)$ and, by the Sobolev imbedding theorem, discussed in [1], p. 134, c is even absolutely continuous on $(0,H)$. The values of $\mu(c)$ are real numbers, supposed to be bounded and non-negative. Some additional assumptions must be accepted also for $B(c)$, $K(c)$ and $N(x)$, whose values are real matrices of order r: B and K map V to the Lebesgue space $L^\infty((0,H),R^{r\times r})$, N can be taken from $L^\infty((0,H),R^{r\times r})$ directly.

The full text of this paper (see the attached CD-ROM) shows that the above sketched problem can be solved using the following iterative procedure, based on the discrete versions of (1) and (2), coming from the finite difference method and from the standard numerical quadrature. The initial estimate of c is the extension of c_0 to the whole interval $(0,H)$. Then v can be calculated from (2). Consequently, c in (1) can be evaluated, step by step, in particular nodes; the result is the better estimate of c. The mathematical analysis is based on the weak and strong convergence in special Sobolev spaces, namely on the Eberlein-Shmulyan theorem, studied in [1], and on the classical and discrete versions of the Gronwall lemma by [3] and [2].

The results of [5] show that even relatively simple equations can give new both qualitative and quantitative results. The overview of facultative generalizations is contained in [6]. However, the characteristics B, K and μ (as very complicated functions of c, prepared automatically by symbolic software manipulations) are derived from chemical potentials, whose identification is rather difficult; the same is true for the interface mobility hidden in μ and diffusive characteristics contained in N. The still open questions are now intensively studied in the collaboration of the Montan University of Leoben (Austria), of the Institute of Physics of Materials (Czech Academy of Sciences, Brno), and of the Brno University of Technology.

References

[1] S. Fučík and A. Kufner. *Nonlinear Differential Equations.* Elsevier Amsterdam, 1985.

[2] W.-S. Cheung and J. Ren. Discrete non-linear inequalities and applications to boundary value problems. *Journal of Mathematical Analysis and Applications*, **319**: 708-724, 2006.

[3] M. Greguš, M. Švec and M. Šeda. *Obyčajné diferenciálne rovnice.* Alfa Bratislava, 1980.

[4] U. F. Mayer and G. Simonett. Classical solutions for diffusion-induced grain boundary motion. *Journal of Mathematical Analysis and Applications*, **234**: 660–674, 1999.

[5] J. Svoboda, J. Vala, E. Gamsjäger and F.-D. Fischer. A thick-interface model for diffusive and massive phase transformation in substitutional alloys. *Acta Materialia*, **54**: 3953-3960, 2006.

[6] J. Vala. Thermodynamic modelling of phase transformation in a multi-component system. *Proceedings of ICNAAM 2007 in Corfu*, in print.