The properties of the difference method to the interdiffusion model

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Abstract

We study some new model of interdiffusion. Let a region $\Omega \subset \mathbb{R}^n$, $n \in \mathbb{N}$ with the smooth boundary $\partial \Omega$, T > 0 and $r \in \mathbb{N} \setminus \{1\}$ be fixed. Moreover, let diffusion coefficients D_i , partial molar volumes Ω_i , initial concentrations c_{0i} and flows on the boundaries j_i of the ith components of a mixture, $i = 1, \ldots, r$ be given. The unknowns are concentrations c_i and the potential F of a drift velocity v^d .

The local mass conservation law for fluxes with the Darken drift term and the Vegard rule lead to the parabolic-elliptic system of strongly coupled nonlinear differential equations

$$\begin{cases} \partial_t c_i + \operatorname{div}\left(-D_i(c_1, \dots, c_r)\nabla c_i + c_i\nabla F\right) = 0 & \text{on} \quad [0, T] \times \Omega, \\ \Delta F = \operatorname{div}\left(\sum_{k=1}^r \Omega_k D_k(c_1, \dots, c_r)\nabla c_k\right) & \text{on} \quad [0, T] \times \Omega, \\ \int_\Omega F dx = 0 & \text{on} \quad [0, T], \end{cases}$$
(1)

with the initial condition and the coupled nonlinear boundary conditions

$$c_i(0,x) = c_{0i}(x) \quad \text{on} \quad \Omega, \tag{2}$$

$$\begin{cases} -D_i(c_1, ..., c_r)\frac{\partial c_i}{\partial \mathbf{n}} + c_i\frac{\partial F}{\partial \mathbf{n}} = j_i(t, x) \quad \text{on} \quad [0, T] \times \partial\Omega, \\ \frac{\partial F}{\partial \mathbf{n}} = \sum_{k=1}^r \Omega_k (D_k(c_1, ..., c_r)\frac{\partial c_k}{\partial \mathbf{n}} + j_k(t, x)) \quad \text{on} \quad [0, T] \times \partial\Omega, \end{cases}$$
(3)

i = 1, ..., r, where **n** is the outside normal to the boundary $\partial \Omega$. This model was introduced in [1]. In one dimensional case it can be transformed to the well-known model studied in [3], [2].

We will present the finite implicit difference method (FDM) for the differential problem (1)-(3) studied in [4]. The theorems on existence and uniqueness of solutions of the implicit difference schemes, and the theorems concerned convergence and stability will be proved.

Literatura

- L. Sapa, B. Bożek, M. Danielewski, Weak solutions to interdiffusion models with Vegard rule, AIP Conference Proceedings 1926 (2018), 020039-1–020039-9.
- [2] L. Sapa, B. Bożek, M. Danielewski, Existence, uniqueness and properties of global weak solutions to interdiffusion with Vegard rule, Topol. Methods Nonlinear Anal. 52, No 2 (2018), 423–448.
- [3] K. Holly K., M. Danielewski, Interdiffusion and free-boundary problem for r-component ($r \ge 2$) onedimensional mixtures showing constant concentration, Phys. Rev. B 50 (1994), 13336–13346.
- B. Bożek, L. Sapa, M. Danielewski, Difference methods to one and multidimensional interdiffusion models with Vegard rule, Mathematical Modelling and Analysis 24, No 2 (2019), 276–296.