Difference methods to interdiffusion models with Vegard rule

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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, $i = 1, \dots, r$ 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

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

with the initial condition and the coupled nonlinear boundary conditions

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

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

$i = 1, \dots, r$, where $\mathbf{n}$ 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].

Literatura

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