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HOMOGENIZATION OF A DISCRETE NETWORK MODEL FOR CHEMICAL VAPOR INFILTRATION PROCESS*

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Abstract. Chemical vapor infiltration (CVI) is an important engineering process for manufacturing composite materials. Reaction-diffusion of the reactant gas and the structure change are two mutual influence processes. Some works have been done on the multi-scale modeling and simulation for the CVI process. The homogenization theory has not been rigorously established for the coupled nonlinear system on the concentration of the reactant gas and porosity of the media yet. In this work, we establish a discrete multi-scale node-bond network model for CVI process which contains a spatially discrete reaction-diffusion equation coupled with a spatially discrete porosity evolution equation. The tortuosity factor for the bonds in the node-bond structure is considered. The corresponding continuous homogenized system for the discrete model is given and the error estimation between the solutions of the homogenized system and the discrete one is derived.

Keywords. CVI process; Node-bond network; Homogenization; Difference operator.

AMS subject classifications. 35B27; 35K40; 35K55; 35K57.

1. Introduction

CVI process is an engineering process which is widely used in fabrication of ceramic matrix composite materials (CMCs). Take carbon fiber reinforced silicon carbide (C/SiC) as an example. A preform is woven from fiber bundles before the process, and each fiber bundle consists of thousands of carbon fibers (see Figure 1.1). During the process, reactant gas is infiltrated into the preform at elevated temperature, then surface reaction happens and SiC solid is generated along the fiber interface. The composite material of C/SiC is produced when all the pores in the preform are occluded. As shown in Figure 1.1, there are two kinds of pores in the preform: macro pores among bundles (Figure 1.1(a)) and micro pores among fibers (Figure 1.1(b)) inside the bundle. Such structure leads to two stages of CVI process. In the first stage, the deposition mainly happens in micro pores. In the second stage, the micro pores are closed and the deposition only happens on the surface of macro pores.

Some modeling and simulation works have been done to study CVI process. The multi-scale modeling of the isothermal CVI process for the fabrication of C/SiC composites was considered by Y. Bai et al. [1] where the preform was regarded as a two-phase porous media described by a dynamic pore-scale node-bond network during the fabrication process in microscopic model and a macroscopic model was formally developed without rigorous proof. Later, C.J. Zhang et al. [22] presented the homogenization theory on a simplified linear model for the CVI process, wherein they only considered the

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quasi-steady state of the gas concentration and ignored the effect of the porosity evolution. They paid more attention on the surface reaction and the effect of locally periodic perforation. W.L. Hu [7] established a multi-scale model to probe the residual pore distribution for 2-dimensional problems. The level set method was used to capture the evolution of interface on the micro scale and heterogeneous multi-scale method (HMM) was applied on the macro level. C.J. Zhang [21] proposed a seamless HMM algorithm to probe the residual pore distribution for 3-dimensional problems. Other relative works about CVI process include [9, 10, 14, 16, 18, 19].

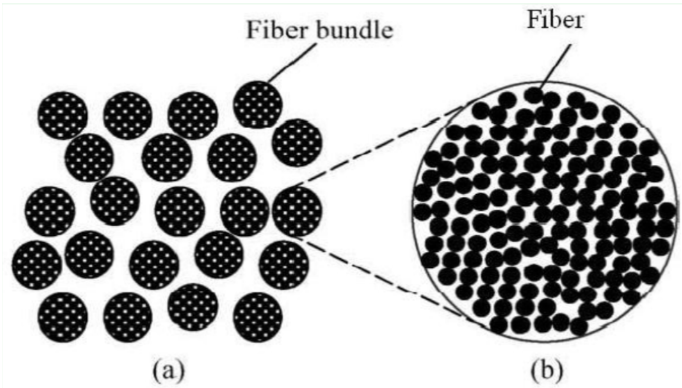

FIG. 1.1. *(a) Cross section perpendicular to randomly positioned bundles; (b) Cross section perpendicular to randomly positioned fibers inside a fiber bundle.*

This work aims to establish the homogenization theory for the second stage of CVI process, which is the foundation of the multi-scale simulation. Unlike the model in [1], where a continuous node-bond network model was applied, we develop a discrete node-bond network model, which is a coupled nonlinear evolutionary difference system on the gas concentration and the porosity and in which the tortuosity effect in the bonds is took into account. The homogenized system for the discrete model is set up and an error estimate is presented between the first order expansion and the solution of the original discrete system.

Compared with the great amount of research for continuous homogenization problems, the studies about discrete ones are relatively few. The first homogenization result for difference schemes was formulated and proved by S. Kozlov [11]. It was proved that the central limit theorem holds for symmetric random walks in random ergodic statistically homogeneous media in [12]. A. Piatnitski et al. [13] studied the asymptotic behavior, as $\varepsilon \to 0$, of the effective coefficients for a family of random difference schemes. The discrete analogue of the compensated compactness lemma was proved and the H-convergence of difference operator was established wherein. Some more results about random difference equations can be found in [4, 6, 20]. Even fewer attention was paid to the error analysis for discrete homogenization problem. An error estimate can be found in [23], where the homogenization of linear elliptic difference operators with periodic coefficients was studied.

The remainder of this paper is organized as follows: The discrete node-bond network model for CVI process and the main results on the homogenization are given in Section 2. In Section 3 the error estimate is proved.

Assume the deposition reaction in the preform is the following:

$$MTS(CH_3SiCl_{3(v)}) \xrightarrow{excess} {}^{H_2} SiC_{(s)} + 3HCl_{(v)}. \tag{1.1}$$

2. Multi-scale model

There are a lot of models to simulate the pore structure of the preform, including single pore model [5], the parallel bundle model [15], the overlap model [2] and the node-bond network model [14]. In [1], the node-bond network model was used to simulate the pore shape and distribution in the preform, and the results matched the real experiment well. Similarly, we choose node-bond network model in Figure 2.1 to simulate the fibre bundle and pore distribution. The grey part is occupied by fiber bundles and the white part is occupied by the pores. Note that Figure 2.1 is only a two dimensional schematic diagram, in three dimension the grey part (fiber bundles) is also connected. The pores can be divided into two parts, one is the "circle" which represents the node, the other is the "tube" which represents the bond. Adjacent nodes are connected by bonds. Assume the distance between the center of adjacent nodes is ε. Suppose the reactant gas (MTS) concentration $C^{\varepsilon}(x,t)$ and porosity $\phi^{\varepsilon}(x,t)$ are spatial discrete functions defined on the center point x of each node, and the pore structure is assumed to be uniquely determined by the porosity $\phi^{\varepsilon}(x,t)$, i.e., the radius of node r_n and the radius of bond r_b are only dependent on $\phi^{\varepsilon}(x,t)$. As deposition reaction goes on, the nodes and bonds gradually become smaller and smaller (see Figure 2.2).

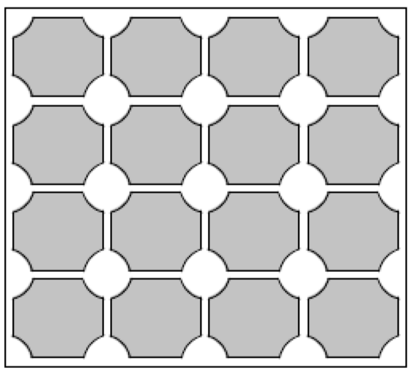

FIG. 2.1. *Node-bond network.*

(a) $t=t_0$ (b) $t=t_1>t_0$

FIG. 2.2. *Evolution of the pore. The structure of the node and bond is uniquely determined by the porosity $\phi^{\varepsilon}(x,t)$ at node x, i.e., the radius of node r_n and the radius of bond r_b are only dependent on $\phi^{\varepsilon}(x,t)$.*

First we consider the mass variation of reactant gas. Mass variation in a node is due to two factors, one is the diffusion of gas from adjacent cells, the other is the surface reaction. Denote the node by its center. For a node x_p, the set of all the adjacent linked nodes is denoted by $\Lambda(x_p)$. The conservation law of mass at node x_p has the form as

$$\frac{d(\phi^{\varepsilon}(x_p,t)C^{\varepsilon}(x_p,t))}{dt}\varepsilon^d = \sum_{x_m\in\Lambda(x_p)} F_{mp}+R_p, \tag{2.1}$$

where F_{mp} is the mass flux from node x_m to node x_p and R_p is the surface reaction term. Specifically,

$$F_{mp}=\frac{D}{\tau_{mp}}\pi(r_{b,p}\wedge r_{b,m})^2\frac{C^\varepsilon(x_m,t)-C^\varepsilon(x_p,t)}{\varepsilon}, \tag{2.2}$$

where τ_{mp} is the tortuosity factor [19] in the bond between nodes x_m and x_p, D is the constant diffusion coefficient inside the pores. $r_{b,i}$ is the radius of the bond linked to node x_i and $u\wedge w=min\{u,w\}$. The radius $r_{b,i}$ is determined by the porosity $\phi^\varepsilon(x_i,t)$, so we may write

$$F_{mp}=\frac{D}{\tau_{mp}}h(\phi^\varepsilon(x_p,t)\wedge\phi^\varepsilon(x_m,t))\varepsilon^{d-1}\frac{C^\varepsilon(x_m,t)-C^\varepsilon(x_p,t)}{\varepsilon}. \tag{2.3}$$

Function h represents the effect of the geometry change on the diffusion ability, it is positive and monotonically increasing. The deposition reaction is regarded as first order, so R_p can be given as

$$R_p=-KC^\varepsilon(x_p,t)S_{vl}(\phi^\varepsilon(x_p,t))\varepsilon^d, \tag{2.4}$$

where K is the first-order reaction rate constant and S_{vl} is the effective reaction and deposition surface area of pores per unit volume.

Then we consider the porosity evolution. Since R_p depicts the mole change of MTS per unit volume per unit time and the change rate of porosity is proportional to R_p, the evolution equation of porosity at node x_p can be written as

$$\frac{d\phi^\varepsilon(x_p,t)}{dt}=-q\frac{M}{\rho}KC^\varepsilon(x_p,t)S_{vl}(\phi^\varepsilon(x_p,t)), \tag{2.5}$$

where M is the molar mass of SiC, ρ is the density of SiC, q is the proportion between the stoichiometric coefficient of SiC and that of MTS in Equation (1.1). Actually, from (1.1) it is obvious that $q=1$, so we may omit q in some proof in the rest of the paper.

Let $\Omega\subset\mathbb{R}^d, d\geq 2$ be the domain occupied by the preform, and $\Omega_\varepsilon=\overline{\Omega}\bigcap\varepsilon\mathbb{Z}^d$ be the lattice points on $\overline{\Omega}$, $\mathring{\Omega}_\varepsilon=\{x\in\Omega_\varepsilon: x\pm\varepsilon e_i\in\Omega_\varepsilon, 1\leq i\leq d\}$ be the inner lattice points, where e_i is the unit vector along the i-th coordinate axis. $\partial\Omega_\varepsilon$ are the boundary points of Ω_ε, i.e., $\partial\Omega_\varepsilon=\Omega_\varepsilon\backslash\mathring{\Omega}_\varepsilon$. Every discrete point in Ω_ε represents a node. The difference operators are defined as

$$\begin{cases}\delta_i^{+\varepsilon}v(x)=\frac{1}{\varepsilon}(v(x+\varepsilon e_i)-v(x)), \quad \delta_i^{-\varepsilon}v(x)=\frac{1}{\varepsilon}(v(x)-v(x-\varepsilon e_i)),\\ \delta_i^{+}u(y)=u(y+e_i)-u(y), \quad \delta_i^{-}u(y)=u(y)-u(y-e_i).\end{cases}$$

Let $x(i)=x-\varepsilon e_i$ and $\widehat{\phi}^\varepsilon(x,x(i),t)=\phi^\varepsilon(x,t)\wedge\phi^\varepsilon(x(i),t)$. Then based on (2.1) and (2.5), our discrete model for CVI process is given as follows:

$$\begin{cases}\dfrac{d(\phi^\varepsilon(x,t)C^\varepsilon(x,t))}{dt}=\displaystyle\sum_{i=1}^d\delta_i^{+\varepsilon}\Big(a^\varepsilon(x,x(i))\ h(\widehat{\phi}^\varepsilon(x,x(i),t))\ \delta_i^{-\varepsilon}C^\varepsilon(x,t)\Big)\\ \qquad\qquad\qquad\qquad\qquad -KS_{vl}(\phi^\varepsilon)C^\varepsilon(x,t), \quad in\ \mathring{\Omega}_\varepsilon\times(0,T),\\ \dfrac{d\phi^\varepsilon(x,t)}{dt}=-\dfrac{M}{\rho}KS_{vl}(\phi^\varepsilon)C^\varepsilon(x,t), \quad in\ \Omega_\varepsilon\times(0,T),\\ C^\varepsilon(x,t)=C_0, \quad on\ \ \partial\Omega_\varepsilon\times(0,T),\\ C^\varepsilon(x,0)=C_0, \quad \phi^\varepsilon(x,0)=\phi_0, \quad in\ \ \Omega_\varepsilon,\end{cases} \tag{2.6}$$

where $a^\varepsilon(x,x(i)) = a(x/\varepsilon, x(i)/\varepsilon) = D/\tau_{x,x(i)}$ and $\tau_{x,x(i)}$ is the tortuosity factor between node x and node $x(i)$. ϕ_0 is the initial porosity and a positive constant. C_0 is the working concentration of the reactant gas, which is supplied by the environment in the reaction oven and is kept constant around the preform of the material.

REMARK 2.1. Note that the effective reaction surface per unit volume S_{vl} with a unit of $1/m$ is of order $O(\varepsilon^{-1})$ and the reaction speed K has a unit of m/s. So the unit of the quantity KS_{vl} is $1/s$, which has nothing to do with the spatial scale ε. Therefore we must have

$$K = k\varepsilon, \quad \text{where k is a constant independent of } \varepsilon.$$

Similar discussion was contained on page 177 of [17]. If we denote $S_{vl}(\phi^\varepsilon) = g(\phi^\varepsilon)/\varepsilon$, then

$$KS_{vl}(\phi^\varepsilon) = kg(\phi^\varepsilon) \text{ is bounded uniformly with respect to } \varepsilon. \tag{2.7}$$

REMARK 2.2. Comparing with the continuous node-bond network model in [1], the above model is a spatially discrete one with the tortuosity factor involved. The main feature of the new model is that the nonlinearity and the multi-scale oscillation are splitable. In the continuous node-bond network model, the nonlinearity comes from the changing of the diffusion area due to the surface reaction and deposition, which leads to a multi-scale free-boundary problem and is really hard to handle in the process of homogenization.

The preform is assumed to be periodic with respect to εY_1, where $Y_1 = [0,n_1]\times\cdots\times[0,n_d]$, $n_i \in \mathbb{Z}^+$, $1 \le i \le d$. Let $Y = Y_1 \bigcap \mathbb{Z}^d$ be the lattice points on Y_1, $\mathring{Y} = \{y \in Y : y \pm e_i \in Y, 1 \le i \le d\}$ be the inner lattice points, then the tortuosity factor $\tau_{x,x(i)}$ is periodic with respect to εY, i.e., $a(y, y-e_i)$ is Y-periodic. Just for simplicity, we assume that Ω consists of integer periods.

Now we present the continuous homogenized equations for (2.6) as

$$\begin{cases} \dfrac{\partial(\phi^* C^*(x,t))}{\partial t} = \nabla\cdot\big(A^* h(\phi^*(x,t))\nabla C^*(x,t)\big) - k\ g(\phi^*(x,t))C^*(x,t),\ in\ \Omega\times(0,T), \\ \dfrac{\partial\phi^*(x,t)}{\partial t} = -\dfrac{M}{\rho}k\ g(\phi^*(x,t))C^*(x,t), \quad in\ \Omega\times(0,T), \\ C^*(x,t) = C_0, \quad on\ \ \partial\Omega\times(0,T), \\ C^*(x,0) = C_0, \quad \phi^*(x,0) = \phi_0, \quad in\ \ \Omega. \end{cases} \tag{2.8}$$

The homogenized diffusion coefficient $A^* = (a^*_{ij})$, and a^*_{ij} is defined as

$$a^*_{ij} = \frac{1}{|\mathring{Y}|}\sum_{y\in\mathring{Y}}\Big(a_{ij}(y,y-e_i) + \sum_{k=1}^{d} a_{ik}(y,y-e_i)\delta_k^-\chi^j(y)\Big), \tag{2.9}$$

where

$$a_{ij}(y,y-e_i) = a(y,y-e_i)I_{ij}, \quad I_{ij} = \begin{cases} 1, & i=j, \\ 0, & i\neq 0. \end{cases}$$

and $|\mathring{Y}|$ is the number of points in $\mathring{Y}$. χ^j is the solution of the following cell problem:

$$\begin{cases} \sum\limits_{i,k=1}^{d}\delta_i^+\big(a_{ik}(y,y-e_i)\delta_k^-(\chi^j + y_j)\big) = 0, \quad y\in\mathring{Y}, \\ \chi^j(y) \text{ is Y-periodic, and } \sum\limits_{y\in\mathring{Y}}\chi^j(y) = 0. \end{cases} \tag{2.10}$$

In order to derive the error estimates between the solutions of (2.6) and (2.8), we need the following assumptions:

- (H1): $a(y,y-e_i)$ is Y-periodic and there are two positive constants a_0,a_1, such that
$$0 < a_0 \le a^\varepsilon(x,x-\varepsilon e_i) \le a_1,\ \forall\ x \in \Omega_\varepsilon.$$
- (H2): $h(s),g(s) \in \mathcal{C}^1[0,1]$ are monotonic increasing. $0 < h_0 \le h(s), s \in [0,1]$. $g(s)$ is non-negative and $g(s) \equiv 0$, $\forall s \in [0,\phi_R]$, where $\phi_R \in (0,\phi_0)$ is the residual porosity.
- (H3): $\dfrac{MC_0}{\rho} < 1$.
- (H4): The domain Ω consists of integer periods. The boundary nodes have their center lying on $\partial\Omega$.

Actually, (H3) is not too strict. Some typical values of M,C_0,ρ are 0.04 kg/mol, 0.02 mol/m^3, 3200 kg/m^3 respectively, so it holds that $\frac{MC_0}{\rho} \ll 1$. As for assumption (H2), when the porosity reaches the residual porosity ϕ_R, the whole CVI process will finish and there is no reaction any more since the effective reaction surface area becomes zero. The assumption (H4) is not essential and is just for simplified treatment.

We introduce the some discrete function spaces on Ω_ε, which will be used below.

$$L^2(\Omega_\varepsilon) = \{v^\varepsilon : \Omega_\varepsilon \to \mathbb{R}; \|v^\varepsilon\|^2_{L^2(\Omega_\varepsilon)} \triangleq \varepsilon^d \sum_{x\in\Omega_\varepsilon} |\, v^\varepsilon(x)\,|^2 < \infty\},$$
$$L^\infty(\Omega_\varepsilon) = \{v^\varepsilon : \Omega_\varepsilon \to \mathbb{R}; \|v^\varepsilon\|_{L^\infty(\Omega_\varepsilon)} \triangleq \max_{x\in\Omega_\varepsilon} |v^\varepsilon(x)| < \infty\},$$
$$W^{1,2}(\Omega_\varepsilon) = \{v^\varepsilon : \Omega_\varepsilon \to \mathbb{R}; \|v^\varepsilon\|^2_{W^{1,2}(\Omega_\varepsilon)} \triangleq \varepsilon^d \sum_{x\in\Omega_\varepsilon} |v^\varepsilon(x)|^2 + \varepsilon^d \sum_{x\in\Omega_\varepsilon}\sum_{i=1}^d |\delta_i^{-\varepsilon} v^\varepsilon(x)|^2 < \infty\},$$
$$W_0^{1,2}(\Omega_\varepsilon) = \{v^\varepsilon : \Omega_\varepsilon \to \mathbb{R}; v|_{\partial\Omega_\varepsilon} = 0,\ \|v^\varepsilon\|^2_{W_0^{1,2}(\Omega_\varepsilon)} \triangleq \varepsilon^d \sum_{x\in\Omega_\varepsilon}\sum_{i=1}^d |\,\delta_i^{-\varepsilon} v^\varepsilon(x)\,|^2 < \infty\}.$$

At the boundary point of Ω_ε, it may happen that $x(i) = x - \varepsilon e_i \notin \Omega_\varepsilon$. If so, we define $\delta_i^{-\varepsilon} v^\varepsilon(x) = 0$.

The following theorem is on the error estimates between the solutions of (2.6) and (2.8), which is the main result of this paper.

THEOREM 2.1. *Let $C^\varepsilon,\phi^\varepsilon$ be solutions of (2.6), and C^*,ϕ^* the solutions of (2.8). Suppose that $C^* \in \mathcal{C}^{3,1}(\Omega\times(0,T))$, $\phi^* \in \mathcal{C}^{1,1}(\Omega\times(0,T))$ and assumptions (H1), (H2), (H3) and (H4) hold, then we have*

$$\begin{aligned}&\|C^\varepsilon - C^*\|_{L^\infty(0,T;L^2(\Omega_\varepsilon))} + \|\phi^\varepsilon - \phi^*\|_{L^\infty(0,T;L^2(\Omega_\varepsilon))} \le Q\varepsilon,\\ &\|C^\varepsilon - C_1^\varepsilon\|_{L^2(0,T;W^{1,2}(\Omega_\varepsilon))} \le Q\sqrt{\varepsilon},\end{aligned} \tag{2.11}$$

where $C_1^\varepsilon = C^* + \varepsilon \sum_{j=1}^d \chi^j \frac{\partial C^*}{\partial x_j}$ is the first order expansion of C^ε, Q is a positive constant independent of ε.

For the rest of the paper, Q (with or without subscripts) stands for a generic positive constant independent of ε with possibly different values in different contexts.

3. Error estimate

In this section we are dedicated to proving the main result Theorem 2.1. Since the micro model (2.6) is a discrete and nonlinear system, we borrowed some ideas from the error analysis for the homogenization of elliptic difference operators [23] and the error analysis for a class of nonlinear parabolic equations [3]. Firstly, we give some a priori estimates for C^ε and ϕ^ε. The following lemma shows that the maximum principle is still valid though what we face up is a system.

LEMMA 3.1. *Suppose the assumptions (H1)-(H3) hold. If $C^\varepsilon(x,t),\phi^\varepsilon(x,t)$ are the solutions of* (2.6) *and continuous with respect to time t, then we have*

$$0\le C^\varepsilon(x,t)\le C_0,\quad 0<\phi_R\le\phi^\varepsilon\le\phi_0,\ \forall\ t\in[0,T],\ x\in\Omega_\varepsilon, \tag{3.1}$$

and

$$\frac{d\phi^\varepsilon}{dt}\in L^\infty(\Omega_\varepsilon\times(0,T)). \tag{3.2}$$

Proof. The result of (3.2) is a direct consequence of the estimates (3.1).

To prove the results (3.1), we first prove that $\phi^\varepsilon\ge\phi_R>0$, no mater whether C^ε is positive or not; then with the positiveness of ϕ^ε, we prove the discrete maximum principle for C^ε, i.e., $0\le C^\varepsilon(x,t)\le C_0$; finally the result $\phi^\varepsilon\le\phi_0$ follows naturally.

Introduce $\tilde\phi(x,t)$ such that

$$\frac{d\tilde\phi(x,t)}{dt}=-\frac{M}{\rho}k\ g(\tilde\phi)(C^\varepsilon(x,t))^+,\quad \tilde\phi(x,0)=\phi_0,$$

where $(C^\varepsilon(x,t))^+=max\{C^\varepsilon(x,t),0\}$. Noting (2.7), the above equation is just the second equation of (2.6) with the term $C^\varepsilon(x,t)$ being replaced by $(C^\varepsilon(x,t))^+$. It can be proved that $\phi^\varepsilon\ge\tilde\phi$ thanks to $C^\varepsilon(x,t)\le(C^\varepsilon(x,t))^+$. We claim that $\tilde\phi\ge\phi_R$. In fact, for fixed $x\in\Omega_\varepsilon$, $\tilde\phi(x,\cdot)$ is monotonic decreasing from its initial value ϕ_0. By the assumption (H2), $g(s)\equiv0$, for $s\in[0,\phi_R]$. So when $\tilde\phi(x,t)$ decreases to ϕ_R at some time t', $\frac{d\tilde\phi(x,t)}{dt}\equiv0$, for $t\ge t'$, i.e., $\tilde\phi(x,t)\equiv\phi_R$, for $t\ge t'$.

If C^ε is non-negative, then from the second equation of (2.6), $\phi^\varepsilon(x,t)$ is monotonic decreasing and less than its initial value ϕ_0. We have proved the results on ϕ^ε.

We now aim to prove the results on C^ε. Inserting the second equation of (2.6) into the first one, we have

$$\phi^\varepsilon\frac{dC^\varepsilon}{dt}-\sum_{i=1}^d\delta_i^{+\varepsilon}\left[a^\varepsilon\ h(\widehat{\phi^\varepsilon})\ \delta_i^{-\varepsilon}C^\varepsilon\right]+k\ g(\phi^\varepsilon)C^\varepsilon(1-\frac{MC^\varepsilon}{\rho})=0. \tag{3.3}$$

First we show that $C^\varepsilon(x,t)\ge0$ by contradiction. Suppose there exits $(x^*,t^*)\in\mathring{\Omega}_\varepsilon\times(0,T)$ such that

$$\min_{(x,t)\in\Omega_\varepsilon\times[0,T]}C^\varepsilon(x,t)=C^\varepsilon(x^*,t^*)<0, \tag{3.4}$$

then since $\phi^\varepsilon\ge\phi_R>0$, we have that

$$\phi^\varepsilon\frac{dC^\varepsilon}{dt}\bigg|_{(x^*,t^*)}\le0,\quad -\sum_{i=1}^d\delta_i^{+\varepsilon}\left[a^\varepsilon\ h(\widehat{\phi^\varepsilon})\ \delta_i^{-\varepsilon}C^\varepsilon\right]\bigg|_{(x^*,t^*)}\le0, \tag{3.5}$$

and it is obvious that

$$k\ g(\phi^\varepsilon)C^\varepsilon(1-\frac{MC^\varepsilon}{\rho})\Big|_{(x^*,t^*)}\leq 0. \tag{3.6}$$

In the last inequality, the equality may hold if $g(\phi^\varepsilon)=0$. If there exists one equality which does not hold among the three inequalities of (3.5)-(3.6), then there is a contradiction in (3.3). Otherwise, $-\sum_{i=1}^{d}\delta_i^{+\varepsilon}\left[a^\varepsilon\ h(\widehat{\phi}^\varepsilon)\ \delta_i^{-\varepsilon}C^\varepsilon\right]\Big|_{(x^*,t^*)}=0$ implies that

$$C^\varepsilon(x_p,t^*)=C^\varepsilon(x^*,t^*),\ \text{for}\ x_p\in\Lambda(x),$$

i.e., all neighbor-linked lattice points at time t^* are minimizers. Applying the above argument to the neighbor minimizers recursively, we will at least meet a contradiction in (3.3) near the boundary of Ω^ε, since all boundary points are not the minimizers. The contradiction means that

$$C^\varepsilon(x,t)\geq 0,\quad \forall\ (x,t)\in\Omega_\varepsilon\times[0,T].$$

Then we prove that $C^\varepsilon\leq C_0$ by contradiction. Suppose there exists $(x_1,t_1)\in\mathring{\Omega}_\varepsilon\times(0,T)$ such that

$$\max_{(x,t)\in\Omega_\varepsilon\times[0,t_1]}C^\varepsilon(x,t)=C^\varepsilon(x_1,t_1)>C_0. \tag{3.7}$$

Consider two cases: $C^\varepsilon(x_1,t_1)<\frac{\rho}{M}$ or $C^\varepsilon(x_1,t_1)\geq\frac{\rho}{M}$.

If $C^\varepsilon(x_1,t_1)<\frac{\rho}{M}$, we have that

$$\phi^\varepsilon\frac{dC^\varepsilon}{dt}\Big|_{(x_1,t_1)}\geq 0,\quad -\sum_{i=1}^{d}\delta_i^{+\varepsilon}\left[a^\varepsilon\ h(\widehat{\phi}^\varepsilon)\ \delta_i^{-\varepsilon}C^\varepsilon\right]\Big|_{(x_1,t_1)}\geq 0, \tag{3.8}$$

and it is clear that

$$k\ g(\phi^\varepsilon)C^\varepsilon(1-\frac{MC^\varepsilon}{\rho})\Big|_{(x_1,t_1)}\geq 0. \tag{3.9}$$

By similar argument for the minimizers, a contradiction must occur in (3.3) at some maximizer.

If $C^\varepsilon(x_1,t_1)\geq\frac{\rho}{M}$, then $\frac{MC^\varepsilon}{\rho}\geq 1$. From the assumption (H3), we know that at initial time $\frac{MC_0}{\rho}<1$, so there must exist (x_2,t_2), $0<t_2<t_1$, $x_2\in\mathring{\Omega}_\varepsilon$ such that

$$C^\varepsilon(x_2,t_2)=\max_{(x,t)\in\Omega_\varepsilon\times[0,t_2]}C^\varepsilon(x,t)<\frac{\rho}{M},\ \text{and}\ C^\varepsilon(x_2,t_2)>C_0.$$

This reduces to the first case. Then the lemma is proved. □

It can be easily shown that the following rule holds for $\delta_i^{+\varepsilon},\delta_i^{-\varepsilon}$.

$$\begin{cases}\delta_i^{+\varepsilon}(u(x)v(x))=u(x+\varepsilon e_i)\delta_i^{+\varepsilon}v(x)+v(x)\delta_i^{+\varepsilon}u(x),\\ \delta_i^{-\varepsilon}(u(x)v(x))=u(x-\varepsilon e_i)\delta_i^{-\varepsilon}v(x)+v(x)\delta_i^{-\varepsilon}u(x),\end{cases} \tag{3.10}$$

and discrete integration by parts holds: let $B=(b_{ij})$ be a $d\times d$ matrix, when $v(x)$ vanishes on $\partial\Omega_\varepsilon$, we have

$$\varepsilon^d \sum_{x\in\Omega_\varepsilon}\sum_{i,j=1}^{d}\delta_i^{+\varepsilon}\big(b_{ij}h(\widehat{\phi}^\varepsilon)\delta_j^{-\varepsilon}u\big)v=-\varepsilon^d\sum_{x\in\Omega_\varepsilon}\sum_{i,j=1}^{d}b_{ij}h(\widehat{\phi}^\varepsilon)\delta_j^{-\varepsilon}u\,\delta_j^{-\varepsilon}v. \tag{3.11}$$

Since the micro model is discrete and the homogenized model is continuous, to measure the difference between the solutions of (2.6) and (2.8), we give a discrete system for the homogenized solutions.

LEMMA 3.2. *Let C^*,ϕ^* be the solution of (2.8), and $C^*\in\mathcal{C}^{3,1}(\Omega\times(0,T))$, $\phi^*\in\mathcal{C}^{1,1}(\Omega\times(0,T))$, then there exist a bounded function $R(x,t):\Omega_\varepsilon\times(0,T)\to\mathbb{R}$ such that*

$$\begin{cases}\dfrac{d(\phi^*(x,t)C^*(x,t))}{dt}=\sum\limits_{i,j=1}^{d}\delta_i^{+\varepsilon}\big(a_{ij}^*h(\phi^*(x,t))\dfrac{\partial C^*(x,t)}{\partial x_j}\big) & \\ \qquad\qquad -kg(\phi^*(x,t))C^*(x,t)-\varepsilon R(x,t) & in\ \mathring{\Omega}_\varepsilon\times(0,T),\\ \dfrac{d\phi^*(x,t)}{dt}=-\dfrac{M}{\rho}kg(\phi^*(x,t))C^*(x,t) & in\ \Omega_\varepsilon\times(0,T),\\ C^*(x,t)=C_0 & in\ \ \partial\Omega_\varepsilon\times(0,T),\\ C^*(x,0)=C_0,\quad \phi^*(x,0)=\phi_0 & in\ \ \Omega_\varepsilon.\end{cases} \tag{3.12}$$

In the continuous case, if a vector is periodic, solenoidal, and the integration of the vector in the period is zero, then there exists an antisymmetric matrix such that the divergence of the antisymmetric matrix equals to the original solenoidal vector [8]. This property plays an important role in the proof of the error estimate because it can simplify the proof and reduce the regulation requirement on the solutions of the homogenized equations. For the discrete case, the corresponding result is also valid.

LEMMA 3.3. *Let $\mathbf{g}=(g_1,\dots,g_d)':\mathbb{Z}^d\to\mathbb{R}^d$ be a discrete solenoidal vector, i.e. $\sum\limits_{j=1}^{d}\delta_j^+g_j(y)=0$. If g_j is Y-periodic and $\frac{1}{|\mathring{Y}|}\sum\limits_{y\in\mathring{Y}}g_j(y)=0$ for $j=1,\dots,d$, then there exists an antisymmetric matrix $\mathbf{G}=(G_{jl})_{d\times d}$ such that $g_j=\sum\limits_{l=1}^{d}\delta_l^+G_{jl}$, $\forall j=1,\dots,d$, $y\in\mathring{Y}$.*

Proof. Consider the discrete Fourier transform for g_j,

$$g_j(y)=\sum_{k\in\mathring{Y}}\hat{g}_j(k)e^{2\pi iy\cdot\{\frac{k}{N}\}},\quad j=1,\dots,d,$$

where $\{\frac{k}{N}\}=(\frac{k_1}{n_1},\frac{k_2}{n_2},\dots,\frac{k_d}{n_d})'$, and $\hat{g}_j(k)=\frac{1}{|\mathring{Y}|}\sum\limits_{y\in\mathring{Y}}g_j(y)e^{-2\pi iy\cdot\{\frac{k}{N}\}}$ is the discrete Fourier coefficient.

Let $f_j^k=\delta_j^-(e^{-2\pi iy\cdot\{\frac{k}{N}\}})=h_j^ke^{-2\pi iy\cdot\{\frac{k}{N}\}}$, where $h_j^k=1-e^{-2\pi i\{\frac{k}{N}\}\cdot(-e_j)}$. Since g_j is solenoidal, we have

$$\sum_{y\in\mathring{Y}}\sum_{j=1}^{d}g_jf_j^k=\sum_{y\in\mathring{Y}}\sum_{j=1}^{d}\delta_j^-(e^{-2\pi iy\cdot\{\frac{k}{N}\}})g_j=-\sum_{y\in\mathring{Y}}\sum_{j=1}^{d}(e^{-2\pi iy\cdot\{\frac{k}{N}\}})\delta_j^+g_j=0,\ \forall k\in\mathring{Y}.$$

On the other hand, direct computation gives

$$\sum_{y\in\mathring{Y}}\sum_{j=1}^{d}g_jf_j^k=\sum_{y\in\mathring{Y}}\sum_{l\in\mathring{Y}}\sum_{j=1}^{d}\hat{g}_j(l)h_j^ke^{2\pi iy\cdot\{\frac{l-k}{N}\}}=\sum_{j=1}^{d}h_j^k\hat{g}_j(k).$$

So it follows that

$$\sum_{j=1}^{d} h_j^k \hat{g}_j(k) = 0, \qquad \forall k \in \mathring{Y}.$$

This leads to $\hat{g}_j(k) = \sum_{l=1}^{d} \alpha_{jl}^k h_l^k$, with

$$\alpha_{jl}^k = \begin{cases} \dfrac{\hat{g}_j(k) h_l^k - \hat{g}_l(k) h_j^k}{\sum\limits_{j=1}^{d} (h_j^k)^2}, & k \neq 0, \\ 0, & k = 0, \end{cases}$$

is an antisymmetric matrix. Let

$$G_{jl} = -\sum_{k \in \mathring{Y}} \alpha_{jl}^k e^{2\pi i y \cdot \{\frac{k}{N}\}},$$

then

$$\begin{aligned} \sum_{l=1}^{d} \delta_l^+ G_{jl} &= \sum_{l=1}^{d} \sum_{k \in \mathring{Y}} \alpha_{jl}^k (1 - e^{2\pi i \{\frac{k}{N}\} \cdot e_l}) e^{2\pi i y \cdot \{\frac{k}{N}\}} \\ &= \sum_{l=1}^{d} \sum_{k \in \mathring{Y}} \alpha_{jl}^k h_l^k e^{2\pi i y \cdot \{\frac{k}{N}\}} = \sum_{k \in \mathring{Y}} \hat{g}_j(k) e^{2\pi i y \cdot \{\frac{k}{N}\}} = g_j. \end{aligned}$$

So, (G_{jl}) is the required antisymmetric matrix, the lemma is proved. ∎

Introducing boundary corrector term is a common technique to treat the mismatch at the boundary in homogenization analysis. Let θ_ε be the solution of the following equation:

$$\begin{cases} \dfrac{d}{dt}(\phi^\varepsilon \theta_\varepsilon) - \sum\limits_{l=1}^{d} \delta_i^{+\varepsilon} \big(a^\varepsilon h(\widehat{\phi}^\varepsilon) \delta_i^{-\varepsilon} \theta_\varepsilon\big) = 0 & \textit{in } \mathring{\Omega}_\varepsilon \times (0,T), \\ \theta_\varepsilon = -\sum\limits_{j=1}^{d} \chi^j \dfrac{\partial C^*}{\partial x_j} & \textit{on } \partial\Omega_\varepsilon \times (0,T), \\ \theta_\varepsilon(x,0) = 0 & \textit{in } \Omega_\varepsilon. \end{cases} \tag{3.13}$$

The following lemma presents some a priori estimates for θ_ε.

Lemma 3.4. *Let θ_ε be the solution of (3.13) and $C^\star$ satisfy the regularity assumption in Theorem 2.1, then*

$$\|\varepsilon\theta_\varepsilon\|_{L^\infty(0,T;L^2(\Omega_\varepsilon))} \leq Q\varepsilon, \qquad \|\varepsilon\theta_\varepsilon\|_{L^2(0,T;W^{1,2}(\Omega_\varepsilon))} \leq Q\sqrt{\varepsilon}. \tag{3.14}$$

Proof. Let $v_\varepsilon = e^{bt}\theta_\varepsilon$, then v_ε satisfies the following equation:

$$\begin{cases} \phi^\varepsilon \dfrac{dv_\varepsilon}{dt} - \sum\limits_{l=1}^{d} \delta_i^{+\varepsilon} \big(a^\varepsilon h(\widehat{\phi}^\varepsilon) \delta_i^{-\varepsilon} v_\varepsilon\big) + v_\varepsilon \big(\dfrac{d\phi^\varepsilon}{dt} - b\phi^\varepsilon\big) = 0 & \textit{in } \mathring{\Omega}_\varepsilon \times (0,T), \\ v_\varepsilon = -e^{bt} \sum\limits_{j=1}^{d} \chi^j \dfrac{\partial C^*}{\partial x_j} & \textit{on } \partial\Omega_\varepsilon \times (0,T), \\ v_\varepsilon(x,0) = 0 & \textit{in } \Omega_\varepsilon. \end{cases} \tag{3.15}$$

From Lemma 3.1, $\frac{d\phi^\varepsilon}{dt}$ is bounded, and $\phi^\varepsilon \geq \phi_R > 0$. So we may choose $b<0$ and $|b|$ large enough to make $\frac{d\phi^\varepsilon}{dt} - b\phi^\varepsilon > 0$. The first result in (3.14) is valid by the discrete maximum principle. Next we consider the second result. Let the lattice cut-off function

$$\tau(x) = \begin{cases} 0 & x \in \mathring{\Omega}_\varepsilon, \\ 1 & x \in \partial\Omega_\varepsilon. \end{cases}$$

Obviously,

$$|\delta_j^{\pm\varepsilon}(\varepsilon\tau)| \leq 2, \quad \tau \leq 1, \quad \text{for } \forall\ x \in \mathring{\Omega}_\varepsilon.$$

Notice that $\theta_\varepsilon + \tau \sum_{j=1}^{d} \chi^j \frac{\partial C^*}{\partial x_j} \in W_0^{1,2}(\Omega_\varepsilon)$, we can choose $\theta_\varepsilon + \tau \sum_{j=1}^{d} \chi^j \frac{\partial C^*}{\partial x_j}$ as a test function in (3.13) to get

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}(\varepsilon^d \sum_{x\in\Omega_\varepsilon} \phi^\varepsilon \theta_\varepsilon^2) + \varepsilon^d \sum_{x\in\Omega_\varepsilon} \sum_{i=1}^{d} a^\varepsilon h(\widehat{\phi}^\varepsilon)(\delta_i^{-\varepsilon}\theta_\varepsilon)^2 \\
=& -\varepsilon^d \sum_{x\in\Omega_\varepsilon} \phi^\varepsilon \frac{d\theta_\varepsilon}{dt}(\tau \sum_{j=1}^{d} \chi^j \frac{\partial C^*}{\partial x_j}) - \varepsilon^d \sum_{x\in\Omega_\varepsilon} \theta_\varepsilon \frac{d\phi_\varepsilon}{dt}(\frac{1}{2}\theta_\varepsilon + \tau \sum_{j=1}^{d} \chi^j \frac{\partial C^*}{\partial x_j}) \\
&-\varepsilon^d \sum_{x\in\Omega_\varepsilon} \sum_{j=1}^{d} a^\varepsilon h(\widehat{\phi}^\varepsilon)\delta_i^{-\varepsilon}\theta_\varepsilon \delta_i^{-\varepsilon}(\tau \sum_{j=1}^{d} \chi^j \frac{\partial C^*}{\partial x_j}) \\
\equiv& R_1 + R_2 + R_3. \qquad (3.16)
\end{aligned}$$

Rewrite R_2 as

$$\begin{aligned}
R_2 =& -\frac{1}{2}\varepsilon^d \sum_{x\in\Omega_\varepsilon} \theta_\varepsilon^2 \frac{d\phi_\varepsilon}{dt} - \varepsilon^d \sum_{x\in\Omega_\varepsilon} \theta_\varepsilon \frac{d\phi_\varepsilon}{dt}(\tau \sum_{j=1}^{d} \chi^j \frac{\partial C^*}{\partial x_j}) \\
=& R_{21} + R_{22},
\end{aligned}$$

By Lemma 3.1, we have that

$$|R_{21}| \leq Q\|\theta_\varepsilon\|_{L^2(\Omega_\varepsilon)}^2 \leq \frac{Q}{\phi_R}\|\sqrt{\phi^\varepsilon}\theta_\varepsilon\|_{L^2(\Omega_\varepsilon)}^2. \qquad (3.17)$$

Denote the ε-neighbourhood of $\partial\Omega_\varepsilon$ by $\Omega_\varepsilon^\partial = \{x \in \Omega_\varepsilon : dist(x, \partial\Omega^\varepsilon) \leq \varepsilon\}$, that is just the most 2 outward layers of the lattice points in Ω_ε. Then, according to the definition of the cut-off function $\tau(x)$, the boundedness of χ^j and $\frac{\partial C^*}{\partial x_j}$, the boundedness of $\frac{d\phi_\varepsilon}{dt}$, we have

$$|R_{22}| \leq Q_1\varepsilon^d \sum_{x\in\Omega_\varepsilon} \theta_\varepsilon^2 + Q_2\varepsilon^d \sum_{x\in\Omega_\varepsilon^\partial} 1 \leq Q_3\|\sqrt{\phi^\varepsilon}\theta_\varepsilon\|_{L^2(\Omega_\varepsilon)}^2 + Q_4\varepsilon. \qquad (3.18)$$

For the term of R_3, direct calculation yields

$$\delta_i^{-\varepsilon}(\tau \sum_{j=1}^{d} \chi^j \frac{\partial C^*}{\partial x_j})$$

$$= \sum_{j=1}^{d} \big(\tau(x-\varepsilon e_i)\chi^j(y-e_i)\delta_i^{-\varepsilon}\frac{\partial C^*}{\partial x_j} + \tau(x-\varepsilon e_i)\frac{1}{\varepsilon}\delta_i^{-1}\chi^j(y)\frac{\partial C^*}{\partial x_j} + \delta_i^{-\varepsilon}\tau(x)\chi^j\frac{\partial C^*}{\partial x_j}\big).$$

From the definition of τ, the boundedness of χ^j and the regularity of C^*, we derive that

$$\begin{aligned}
&\varepsilon^d \sum_{x\in\Omega_\varepsilon} \Big(\delta_i^{-\varepsilon}\big(\tau\sum_{j=1}^{d}\chi^j\frac{\partial C^*}{\partial x_j}\big)\Big)^2 \\
&\le Q\varepsilon^d \sum_{x\in\Omega_\varepsilon^\partial} \Big(\big(\chi^j(y-e_i)\delta_i^{-\varepsilon}\frac{\partial C^*}{\partial x_j}\big)^2 + \varepsilon^{-2}\big(\delta_i^{-1}\chi^j(y)\frac{\partial C^*}{\partial x_j}\big)^2 + \varepsilon^{-2}\big(\chi^j(y)\frac{\partial C^*}{\partial x_j}\big)^2\Big) \\
&\le Q_1\varepsilon^{-1}.
\end{aligned} \tag{3.19}$$

So we have

$$|R_3| \le \frac{1}{2}\varepsilon^d \sum_{x\in\Omega_\varepsilon}\sum_{i=1}^{d} a^\varepsilon h(\widehat{\phi}^\varepsilon)(\delta_i^{-\varepsilon}\theta_\varepsilon)^2 + Q\varepsilon^{-1}. \tag{3.20}$$

Finally we consider R_1. Rewrite R_1 as

$$\begin{aligned}
R_1 = &-\frac{d}{dt}\Big(\varepsilon^d \sum_{x\in\Omega_\varepsilon} \phi^\varepsilon\theta_\varepsilon\big(\tau\sum_{j=1}^{d}\chi^j\frac{\partial C^*}{\partial x_j}\big)\Big) + \varepsilon^d \sum_{x\in\Omega_\varepsilon}\frac{d\phi^\varepsilon}{dt}\theta_\varepsilon\big(\tau\sum_{j=1}^{d}\chi^j\frac{\partial C^*}{\partial x_j}\big) \\
&+\varepsilon^d \sum_{x\in\Omega_\varepsilon}\phi^\varepsilon\theta_\varepsilon\frac{d}{dt}\big(\tau\sum_{j=1}^{d}\chi^j\frac{\partial C^*}{\partial x_j}\big) \\
&= R_{11}+R_{12}+R_{13}.
\end{aligned}$$

Notice that the initial value of $\tau\sum_{j=1}^{d}\chi^j\frac{\partial C^*}{\partial x_j}=0$, then the boundedness of $\phi^\varepsilon,\theta_\varepsilon,\tau,\chi^j$ along with the regularity of C^* leads to

$$\Big|\int_0^t R_{11}\Big| \le \varepsilon^d \sum_{x\in\Omega_\varepsilon^\partial}\Big|\phi^\varepsilon\theta_\varepsilon\big(\tau\sum_{j=1}^{d}\chi^j\frac{\partial C^*}{\partial x_j}\big)\Big| \le Q\varepsilon, \tag{3.21}$$

and

$$|R_{12}| \le Q\varepsilon, \quad |R_{13}| \le Q\varepsilon. \tag{3.22}$$

So, combining the above estimates together and multiplying (3.16) by ε^2 and integrating it with respect to time, we obtain

$$\|\sqrt{\phi^\varepsilon}\varepsilon\theta_\varepsilon\|^2_{L^2(\Omega_\varepsilon)} + \int_0^t \sum_{j=1}^{d}\|\delta_i^{-\varepsilon}\varepsilon\theta_\varepsilon\|^2_{L^2(\Omega_\varepsilon)} \le Q_1\varepsilon + Q_2\int_0^t \|\sqrt{\phi^\varepsilon}\varepsilon\theta_\varepsilon\|^2_{L^2(\Omega_\varepsilon)}.$$

Then, Gronwall inequality and the boundedness of ϕ^ε leads to the second inequality of (3.14). The lemma is proved. □

The following lemma bounds the difference between ϕ^ε and ϕ^*.

LEMMA 3.5. *Let ϕ^ε, ϕ^* be the solutions of (2.6) and (2.8) respectively, then for $\forall\, t\in(0,T)$, we have*

$$\|\phi^\varepsilon(x,t)-\phi^*(x,t)\|^2_{L^2(\Omega_\varepsilon)} \le Q\int_0^t \|C^\varepsilon - C^*\|^2_{L^2(\Omega_\varepsilon)}. \tag{3.23}$$

Proof. Let $e(\phi)=\phi^\varepsilon-\phi^*$, $e(C)=C^\varepsilon-C^*$. Subtracting the second equation of (2.8) from the second equation of (2.6) yields that

$$\begin{aligned}\frac{\partial e(\phi)}{\partial t} &= -\frac{M}{\rho}k\big(C^\varepsilon(g(\phi^\varepsilon)-g(\phi^*))+g(\phi^*)(C^\varepsilon-C^*)\big)\\ &= -\frac{M}{\rho}k\big(C^\varepsilon g'(\xi)e(\phi)+g(\phi^*)e(C)\big),\end{aligned}$$

so

$$\frac{1}{2}\frac{\partial}{\partial t}e(\phi)^2 = -\frac{M}{\rho}k\big(C^\varepsilon g'(\xi)e(\phi)^2+g(\phi^*)e(C)e(\phi)\big).$$

Since C^ε is bounded and $g(s)\in\mathcal{C}^1[0,1]$, summing the above equation for x in Ω_ε, we have

$$\frac{1}{2}\frac{d}{dt}\|e(\phi)\|^2_{L^2(\Omega_\varepsilon)} \le Q_1\|e(\phi)\|^2_{L^2(\Omega_\varepsilon)} + Q_2\|e(C)\|^2_{L^2(\Omega_\varepsilon)}.$$

By Gronwall's inequality, we have

$$\|e(\phi)(x,t)\|^2_{L^2(\Omega_\varepsilon)} \le Q\int_0^t \|e(C)\|^2_{L^2(\Omega_\varepsilon)},\ \forall\, t\in(0,T). \tag{3.24}$$

This lemma is proved. □

Proof. **(Proof of Theorem 2.1.)** Recall $C_1^\varepsilon = C^*+\varepsilon\sum_{j=1}^d \chi^j\frac{\partial C^*}{\partial x_j}$, then $C^\varepsilon - C_1^\varepsilon - \varepsilon\theta_\varepsilon$ vanishes on $\partial\Omega_\varepsilon$. Consider the following term

$$\begin{aligned}&\frac{d}{dt}(\phi^\varepsilon(C^\varepsilon - C_1^\varepsilon-\varepsilon\theta_\varepsilon)) - \sum_{i,j=1}^d \delta_i^{+\varepsilon}\big(a_{ij}^\varepsilon h(\widehat{\phi}^\varepsilon)\delta_j^{-\varepsilon}(C^\varepsilon - C_1^\varepsilon-\varepsilon\theta_\varepsilon)\big)\\
&= -kC^\varepsilon g(\phi^\varepsilon) - \frac{d}{dt}\big(\phi^\varepsilon\varepsilon\sum_{k=1}^d\chi^k\frac{\partial C^*}{\partial x_k}\big) - \frac{d}{dt}(\phi^\varepsilon C^*) + \sum_{i,j=1}^d \delta_i^{+\varepsilon}(a_{ij}^\varepsilon h(\widehat{\phi}^\varepsilon)\delta_j^{-\varepsilon}C_1^\varepsilon),\\
&= \frac{d}{dt}(\phi^* C^*) - \sum_{i=1}^d \delta_i^{+\varepsilon}\big(a_{ij}^* h(\phi^*)\frac{\partial C^*}{\partial x_j}\big) + \varepsilon R - \frac{d}{dt}(\phi^\varepsilon C^*) + \sum_{i,j=1}^d \delta_i^{+\varepsilon}(a_{ij}^\varepsilon h(\widehat{\phi}^\varepsilon)\delta_j^{-\varepsilon}C_1^\varepsilon)\\
&\quad + kC^* g(\phi^*) - kC^\varepsilon g(\phi^\varepsilon) - \frac{d}{dt}\big(\phi^\varepsilon\varepsilon\sum_{k=1}^d\chi^k\frac{\partial C^*}{\partial x_k}\big),\\
&= \sum_{i,j=1}^d \delta_i^{+\varepsilon}\big(a_{ij}^\varepsilon h(\widehat{\phi}^\varepsilon)\delta_j^{-\varepsilon}C_1^\varepsilon - a_{ij}^* h(\phi^*)\frac{\partial C^*}{\partial x_j}\big) + r^\varepsilon + \varepsilon R,\end{aligned} \tag{3.25}$$

where the first equality comes from (2.6) and (3.13), while the second equality comes from (3.12), and

$$r^\varepsilon = \big(\frac{d}{dt}(\phi^* C^*) - \frac{d}{dt}(\phi^\varepsilon C^*)\big) + \big(kC^* g(\phi^*) - kC^\varepsilon g(\phi^\varepsilon)\big) - \frac{d}{dt}\big(\phi^\varepsilon\varepsilon\sum_{k=1}^d\chi^k\frac{\partial C^*}{\partial x_k}\big)$$

$$\equiv r_1^\varepsilon + r_2^\varepsilon + r_3^\varepsilon. \tag{3.26}$$

Multiplying (3.25) by $C^\varepsilon - C_1^\varepsilon - \varepsilon\theta_\varepsilon \in W_0^{1,2}(\Omega_\varepsilon)$, taking the summation for $x \in \Omega_\varepsilon$, and we have by summation by parts that

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\varepsilon^d \sum_{x\in\Omega_\varepsilon} \big(\phi^\varepsilon (C^\varepsilon - C_1^\varepsilon - \varepsilon\theta_\varepsilon)^2\big) + \varepsilon^d \sum_{x\in\Omega_\varepsilon}\sum_{i,j=1}^d a_{ij}^\varepsilon h(\widehat{\phi}^\varepsilon)\big(\delta_j^{-\varepsilon}(C^\varepsilon - C_1^\varepsilon - \varepsilon\theta_\varepsilon)\big)^2 \\
&= -\varepsilon^d \sum_{x\in\Omega_\varepsilon}\sum_{i,j=1}^d \big(a_{ij}^\varepsilon h(\widehat{\phi}^\varepsilon)\delta_j^{-\varepsilon} C_1^\varepsilon - a_{ij}^* h(\phi^*)\frac{\partial C^*}{\partial x_j}\big)\delta_i^{-\varepsilon}(C^\varepsilon - C_1^\varepsilon - \varepsilon\theta_\varepsilon) \\
&\quad + \varepsilon^d \sum_{x\in\Omega_\varepsilon} \big(\varepsilon R + r^\varepsilon\big)(C^\varepsilon - C_1^\varepsilon - \varepsilon\theta_\varepsilon) - \frac{1}{2}\varepsilon^d \sum_{x\in\Omega_\varepsilon} \frac{d\phi^\varepsilon}{dt}(C^\varepsilon - C_1^\varepsilon - \varepsilon\theta_\varepsilon)^2 \\
&\equiv I_1 + I_2 + I_3.
\end{aligned} \tag{3.27}$$

For the first term on the right-hand side of (3.27), from the regularity assumption for C^*, there exists a bounded function $\bar{r}_j(x,t)$ such that

$$\delta_j^{-\varepsilon} C^* - \frac{\partial C^*}{\partial x_j} = \varepsilon \bar{r}_j(x,t), \text{ for } (x,t) \in \mathring{\Omega}_\varepsilon \times (0,T),$$

so

$$\delta_j^{-\varepsilon} C_1^\varepsilon = \frac{\partial C^*}{\partial x_j} + \sum_{k=1}^d \delta_j^- \chi^k \frac{\partial C^*}{\partial x_k} + \varepsilon \sum_{k=1}^d \chi^k (y - e_j)\delta_j^{-\varepsilon}\frac{\partial C^*}{\partial x_k} + \varepsilon \bar{r}_j,$$

and

$$\begin{aligned}
&\sum_{j=1}^d \big(a_{ij}^\varepsilon h(\widehat{\phi}^\varepsilon)\delta_j^{-\varepsilon} C_1^\varepsilon - a_{ij}^* h(\phi^*)\frac{\partial C^*}{\partial x_j}\big) \\
&= \sum_{j=1}^d h(\widehat{\phi}^\varepsilon)\big(a_{ij}^\varepsilon + \sum_{k=1}^d a_{ik}^\varepsilon \delta_k^- \chi^j(y) - a_{ij}^*\big)\frac{\partial C^*}{\partial x_j} + \sum_{j=1}^d a_{ij}^*(h(\widehat{\phi}^\varepsilon) - h(\phi^*))\frac{\partial C^*}{\partial x_j} \\
&\quad + \varepsilon \sum_{j=1}^d \big(\sum_{k=1}^d a_{ij}^\varepsilon \chi^k (y - e_j)\delta_j^{-\varepsilon}\frac{\partial C^*}{\partial x_k} + a_{ij}^\varepsilon \bar{r}_j\big) h(\widehat{\phi}^\varepsilon).
\end{aligned} \tag{3.28}$$

Let $g_{ij}(y) = a_{ij}(y, y - e_j) + \sum_{k=1}^d a_{ik}(y, y - e_j)\delta_k^- \chi^j(y) - a_{ij}^*$. From the cell problem (2.10) and the definition (2.9) for a_{ij}^* we know that

$$\sum_{i=1}^d \delta_i^+ g_{ij} = 0, \qquad \frac{1}{|\mathring{Y}|}\sum_{y\in\mathring{Y}} g_{ij}(y) = 0, \quad \forall j = 1,\ldots,d.$$

From Lemma 3.3, there exists an antisymmetric matrix α_{jk}^l such that

$$g_{ij}(y) = \sum_{l=1}^d \delta_l^+ \alpha_{il}^j(y).$$

So

$$\sum_{j=1}^{d}\big(a_{ij}^{\varepsilon}h(\widehat{\phi}^{\varepsilon})\delta_j^{-\varepsilon}C_1^{\varepsilon}-a_{ij}^{*}h(\phi^{*})\frac{\partial C^{*}}{\partial x_j}\big)=\varepsilon\sum_{j,l=1}^{d}\delta_l^{+\varepsilon}\big(h(\widehat{\phi}^{\varepsilon})\alpha_{il}^{j}(y)\frac{\partial C^{*}}{\partial x_j}\big)+\gamma_1+\gamma_2, \tag{3.29}$$

where

$$\gamma_1=-\varepsilon\sum_{j,l=1}^{d}\alpha_{il}^{j}(y+e_l)h(\widehat{\phi}^{\varepsilon}(x+\varepsilon e_l,x(i)+\varepsilon e_l,t))\delta_l^{+\varepsilon}\frac{\partial C^{*}}{\partial x_j}-\varepsilon\sum_{j,l=1}^{d}\alpha_{il}^{j}(y+e_l)\delta_l^{+\varepsilon}h(\widehat{\phi}^{\varepsilon})\frac{\partial C^{*}}{\partial x_j}$$
$$+\varepsilon\sum_{j=1}^{d}\big(\sum_{k=1}^{d}a_{ij}^{\varepsilon}\chi^{k}(y-e_j)\delta_j^{-\varepsilon}\frac{\partial C^{*}}{\partial x_k}+a_{ij}^{\varepsilon}\bar{r}_j\big)h(\widehat{\phi}^{\varepsilon}),$$
$$\gamma_2=\sum_{j=1}^{d}a_{ij}^{*}(h(\widehat{\phi}^{\varepsilon})-h(\phi^{*}))\frac{\partial C^{*}}{\partial x_j}.$$

From the boundedness of $\phi^{\varepsilon},\chi^{j},r_j$ and the regularity of h,C^{*}, we deduce that

$$\|\gamma_1\|^2_{L^2((0,T)\times\Omega_\varepsilon)}\le Q\varepsilon^2. \tag{3.30}$$

For γ_2, noticing that $\widehat{\phi}^{\varepsilon}(x,x(i),t)=\phi^{\varepsilon}(x,t)\wedge\phi^{\varepsilon}(x(i),t)$, we can use Lemma 3.5, Lemma 3.4, the boundedness of $\phi^{\varepsilon},\chi^{j}$ and the regularity of h,C^{*} to get

$$\begin{aligned}\|\gamma_2\|^2_{L^2(\Omega_\varepsilon)}&\le Q_1\|\phi^{\varepsilon}-\phi^{*}\|^2_{L^2(\Omega_\varepsilon)}+Q_2\varepsilon^2\\&\le Q_3\int_0^t\|C^{\varepsilon}-C^{*}\|^2_{L^2(\Omega_\varepsilon)}+Q_2\varepsilon^2\\&\le Q_4\int_0^t\|\sqrt{\phi^{\varepsilon}}(C^{\varepsilon}-C_1^{\varepsilon}-\varepsilon\theta_\varepsilon)\|^2_{L^2(\Omega_\varepsilon)}+Q_5\varepsilon^2.\end{aligned} \tag{3.31}$$

Combining (3.29)-(3.31), the first term I_1 at the right-hand side of (3.27) is bounded by

$$|I_1|=\varepsilon^d\Big|\sum_{x\in\Omega_\varepsilon}\sum_{i=1}^{d}\big(\varepsilon\sum_{j,l=1}^{d}\delta_l^{+\varepsilon}\big(h(\widehat{\phi}^{\varepsilon})\alpha_{il}^{j}(y)\frac{\partial C^{*}}{\partial x_j}\big)+\gamma_1+\gamma_2\big)\delta_i^{-\varepsilon}(C^{\varepsilon}-C_1^{\varepsilon}-\varepsilon\theta_\varepsilon)\Big| \tag{3.32}$$
$$=\varepsilon^d\Big|\sum_{x\in\Omega_\varepsilon}\sum_{i=1}^{d}(\gamma_1+\gamma_2)\delta_i^{-\varepsilon}(C^{\varepsilon}-C_1^{\varepsilon}-\varepsilon\theta_\varepsilon)\Big|$$
$$\le Q_1\int_0^t\|\sqrt{\phi^{\varepsilon}}(C^{\varepsilon}-C_1^{\varepsilon}-\varepsilon\theta_\varepsilon)\|^2_{L^2(\Omega_\varepsilon)}+Q_2\varepsilon^2+\frac{a_0h_0}{2}\|C^{\varepsilon}-C_1^{\varepsilon}-\varepsilon\theta_\varepsilon\|^2_{W_0^{1,2}(\Omega_\varepsilon)}, \tag{3.33}$$

where the constants a_0,h_0 are lower bound of a^{ε} and $h(s)$ given in the assumptions (H1) and (H2). The first term at the right-hand side of (3.32) disappears thanks to that $\sum_{j,l=1}^{d}\delta_l^{+\varepsilon}\big(h(\widehat{\phi}^{\varepsilon})\alpha_{il}^{j}(y)\frac{\partial C^{*}}{\partial x_j}\big)$ is a solenoidal vector.

Next we consider the second term I_2 in (3.27). r^{ε} is divided into 3 terms in (3.26). Rewrite r_1^{ε} as

$$r_1^{\varepsilon}=\big(\frac{d\phi^{\varepsilon}}{dt}-\frac{d\phi^{*}}{dt}\big)C^{*}+\frac{\partial C^{*}}{\partial t}(\phi^{\varepsilon}-\phi^{*})$$

$$=\frac{MkC^*}{\rho}((C^*-C^\varepsilon)g(\phi^*)+(g(\phi^*)-g(\phi^\varepsilon))C^\varepsilon)+\frac{\partial C^*}{\partial t}(\phi^\varepsilon-\phi^*).$$

We can use similar arguments for γ_2 to obtain

$$\begin{aligned}\int_0^t\|r_1^\varepsilon\|^2_{L^2(\Omega_\varepsilon)}&\le Q_1\int_0^t\|C^\varepsilon-C^*\|^2_{L^2(\Omega_\varepsilon)}+Q_2\int_0^t\|\phi^\varepsilon-\phi^*\|^2_{L^2(\Omega_\varepsilon)}\\&\le Q_3\int_0^t\|\sqrt{\phi^\varepsilon}(C^\varepsilon-C_1^\varepsilon-\varepsilon\theta_\varepsilon)\|^2_{L^2(\Omega_\varepsilon)}+Q_4\varepsilon^2,\end{aligned}\tag{3.34}$$

and for r_2^ε we also have

$$\int_0^t\|r_2^\varepsilon\|^2_{L^2(\Omega_\varepsilon)}\le Q\int_0^t\|\sqrt{\phi^\varepsilon}(C^\varepsilon-C_1^\varepsilon-\varepsilon\theta_\varepsilon)\|^2_{L^2(\Omega_\varepsilon)}+Q_1\varepsilon^2.\tag{3.35}$$

Rewrite r_3^ε as

$$r_3^\varepsilon=-\frac{d\phi^\varepsilon}{dt}\varepsilon\sum_{k=1}^d\chi^k\frac{\partial C^*}{\partial x_k}-\phi^\varepsilon\varepsilon\sum_{k=1}^d\chi^k\frac{\partial^2C^*}{\partial t\partial x_k}.$$

From the boundedness of $\phi^\varepsilon,\frac{d\phi^\varepsilon}{dt},\chi^k$ and the regularity of C^*, we derive that

$$\|r_3^\varepsilon\|^2_{L^2(\Omega_\varepsilon)}\le Q\varepsilon^2.\tag{3.36}$$

Combining (3.34)-(3.36), we have by the boundedness of $R(x,t)$ in Lemma 3.2 that

$$\int_0^t\|I_2\|^2_{L^2(\Omega_\varepsilon)}\le Q\int_0^t\|\sqrt{\phi^\varepsilon}(C^\varepsilon-C_1^\varepsilon-\varepsilon\theta_\varepsilon)\|^2_{L^2(\Omega_\varepsilon)}+Q_1\varepsilon^2.\tag{3.37}$$

The third term I_3 in (3.27) can be bounded directly by the boundedness of $\phi^\varepsilon,\frac{d\phi^\varepsilon}{dt}$ in Lemma 3.1 as

$$\|I_3\|^2_{L^2(\Omega_\varepsilon)}\le Q_1\|\sqrt{\phi^\varepsilon}(C^\varepsilon-C_1^\varepsilon-\varepsilon\theta_\varepsilon)\|^2_{L^2(\Omega_\varepsilon)}+Q_2\varepsilon^2.\tag{3.38}$$

Integrating (3.27) over time on $(0,t)$, and combining the above estimates on I_1,I_2,I_3, we deduce that

$$\begin{aligned}&\|\sqrt{\phi^\varepsilon}(C^\varepsilon-C_1^\varepsilon-\varepsilon\theta_\varepsilon)\|^2_{L^2(\Omega_\varepsilon)}+\int_0^t a_0h_0\|C^\varepsilon-C_1^\varepsilon-\varepsilon\theta_\varepsilon\|^2_{W_0^{1,2}(\Omega_\varepsilon)}\\&\le Q\varepsilon^2+Q\int_0^t\|\sqrt{\phi^\varepsilon}(C^\varepsilon-C_1^\varepsilon-\varepsilon\theta_\varepsilon)\|^2_{L^2(\Omega_\varepsilon)}.\end{aligned}$$

Then from the boundedness of ϕ^ε and Gronwall's inequality, it follows that

$$\sup_{t\in(0,T)}\|C^\varepsilon-C_1^\varepsilon-\varepsilon\theta_\varepsilon\|_{L^2(\Omega_\varepsilon)}+\|C^\varepsilon-C_1^\varepsilon-\varepsilon\theta_\varepsilon\|_{L^2(0,T;W^{1,2}(\Omega_\varepsilon))}\le Q\varepsilon.$$

So the estimates in Lemmas 3.4 and 3.5 lead to

$$\|C^\varepsilon-C^*\|_{L^\infty(0,T;L^2(\Omega_\varepsilon))}+\|\phi^\varepsilon-\phi^*\|_{L^\infty(0,T;L^2(\Omega_\varepsilon))}\le Q\varepsilon,$$

and

$$\|C^\varepsilon-C_1^\varepsilon\|_{L^2(0,T;W^{1,2}(\Omega_\varepsilon))}\le Q\sqrt{\varepsilon}.$$

Thus Theorem 2.1 is proved. □

4. Conclusion and Discussion

In this work, we establish a multi-scale node-bond network model for CVI process, which is a nonlinear system containing a spatially discrete reaction-diffusion equation coupled with a spatially discrete porosity evolution equation. The tortuosity factor for the bonds in the node-bond structure is considered. The homogenization theory is established, which is the foundation of the multi-scale simulation.

A problem, which may be discussed, is the assumption (H2) in Section 2. $h(\phi)$ represents the mobility in the bond. When the porosity reaches its residual limit ϕ_R at the ending of the whole CVI process, we have assumed that the reaction surface area $g(\phi)$ is zero. It seems to be more reasonable to also have $h(\phi)\equiv 0$, for $\phi \in [0,\phi_R]$. This will lead to degeneration for the reaction-diffusion equation. The homogenization theory for this kind of problem may be interesting and is left to future work.

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