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# HOMOGENIZATION FOR CHEMICAL VAPOR INFILTRATION PROCESS*

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**Abstract.** Multi-scale modeling and numerical simulations of the isothermal chemical vapor infiltration (CVI) process for the fabrication of carbon fiber reinforced silicon carbide (C/SiC) composites were presented in [Bai, Yue and Zeng, Commun. Comput. Phys., 7(3):597–612, 2010]. The homogenization theory, which played a fundamental role in the multi-scale algorithm, will be rigorously established in this paper. The governing system, which is a multi-scale reaction-diffusion equation, is different in the two stages of CVI process, so we will consider the homogenization for the two stages respectively. One of the main features is that the reaction only occurs on the surface of fiber, so it behaves as a singular surface source. The other feature is that in the second stage of the process when the micro pores inside the fiber bundles are all closed, the diffusion only occurs in the macro pores between fiber bundles and we face up with a problem in a locally periodic perforated domain.

**Keywords.** CVI process; multi-scale model; homogenization; surface reaction; locally periodic perforation.

**AMS subject classifications.** 35B27; 35J25.

## 1. Introduction

CVI process is used to produce carbon fiber reinforced silicon carbide (C/SiC) composites. Before the process, a desired preform is woven from fiber bundles. Each bundle consists of thousands of carbon fibers; see Figure 1.1 for a sample ( [26]). During the process, the preform is put into a high temperature reactor. Let the reactant gasses pass through the reactor and infiltrate into the preform. Surface reaction happens and SiC solid is generated along the fiber interface. The composite material of C/SiC is produced when almost all the pores in the preform are occluded. As 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 bundles. During the initial stage of CVI process, the deposition mainly happens in the micro pores. After the micro pores are closed as in Figure 1.2, the second stage begins and the deposition turns to happen on the surface of macro pores. Two types of diffusion equations appear in different stages. In the first stage, diffusion occurs in both macro pores and micro pores, so the diffusion region is the whole domain. In the second stage, the diffusion only occurs in the macro pores, the diffusion region is a perforated domain. During both stages, reaction always happens on the surface of fiber, so it behaves as a singular surface source, or equivalently it can be treated as an extra Robin boundary condition at the inner boundary. Modeling and simulations for CVI process have been investigated by several authors, see [15,16,24,26]. Y. Bai et al. have developed a multi-scale model to simulate CVI process. The multiscale algorithm and numerical results can be found in [2]; however, the homogenization theory is not rigorously established yet for this

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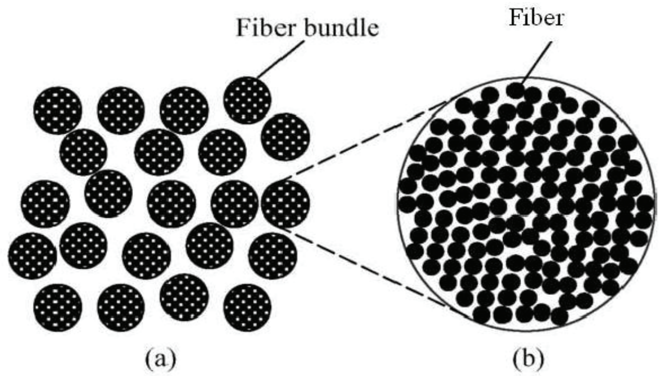


FIG. 1.1. *(a) Cross section perpendicular to randomly positioned bundles; (b) Cross section perpendicular to randomly positioned fibers inside a fiber bundle.*

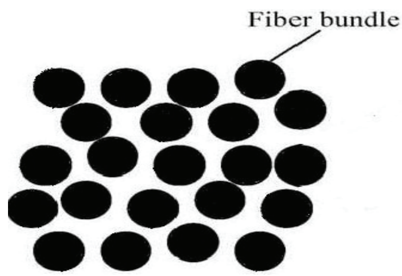


FIG. 1.2. *The pore structure of the second stage.*

model, which is the foundation of the numerical algorithm therein. In this paper we will present the homogenization theory for both stages of CVI process respectively. We assume that the media has a locally periodic structure, since even if the preform is periodically woven at the beginning, it cannot hold the periodic structure forever. The chemical reaction and deposition, which makes the micro structure change, depend on the concentration of reactant gas, which varies among the media.

General theory on homogenization can be found in books [3, 10, 14, 25]. Works on periodically perforated problems were presented in [9, 11, 19, 21]. For locally periodic perforation (the considered domain consist of periodic cells with smoothly changing perforations), the situation is more complex since the microstructure is not fixed. The asymptotic expansion technique [6, 13], two-scale convergence method [8, 22, 27] and unfolding approach [1] were applied to derive the macroscopic systems. Only in [6], the estimates were given on the convergence rate for locally periodic perforated problems with inner Robin boundary conditions. In this paper, we use a simpler and straightforward approach to handle the inner boundary condition and, furthermore, to derive the same estimate on convergence rate as in [6] under weaker assumptions on the regularity of the solutions to the homogenized systems.

The remainder of this paper is organized as follows: The multi-scale model for CVI process in [2] and the main theorems of this paper are introduced in Section 2. Section 3 is devoted to the homogenization theory for the first stage, and the results for the second stage are presented in Section 4. In both sections, we first prove the convergence results under a lower regularity assumption, then give the error estimates on the first order expansion with higher regularity. In the last section we draw conclusions and discuss certain extensions.

Throughout this paper, $A$ (with or without subscripts) denotes a generic positive constant with possibly different values in different contexts. Also we use the convention of summation on repeated indices.

## 2. Multi-scale models

In this section, we introduce the multi-scale models in [2] and present our results on the homogenization for both stages of CVI process respectively.

Even though the initial structure of the preform may be purely periodic, the structure will change as the reaction happens and solid deposits. So we assume that the media is locally periodic. In order to characterize the structure of the media, we follow some notations from Chechkin and Piatnitski [6]. Let $\Omega\subset\mathbb{R}^n$, $n\geq 2$, be the domain occupied by the media. A locally periodic function $F(x,x/\varepsilon)$ is introduced to distinguish the different regions in $\Omega$. 'Locally periodic' means, for fixed macro variable $x_0$, $F(x_0,x/\varepsilon)$ is a $\varepsilon$-period function. Here $\varepsilon\ll 1$ is the characteristic size of the macro pores. The media consist of two phases: one is all the macro pores among fiber bundles, denoted by $\Omega_\varepsilon$, where we have $F(x,x/\varepsilon)>0$; the other phase is all the fiber bundles, denoted by $\Omega\backslash\bar{\Omega}_\varepsilon$, where we have $F(x,x/\varepsilon)<0$. Denote by $S^\varepsilon=\partial\Omega^\varepsilon=\{x\in\Omega: F(x,x/\varepsilon)=0\}$ the interface between the macro pores and fiber bundles.

Let $Y=(-\frac{1}{2},\frac{1}{2})^n$ be the reference cell. Assume the interface is smooth and that, in each cell, the interface doesn't touch the cell boundary. Then we need further assumptions on $F(x,y)$. For all $x\in\Omega$ and $y\in Y$, $F(x,y)$ is sufficiently smooth and 1-periodic in $y$ such that $F(x,y)|_{y\in\partial Y}>0$, $F(x,\mathbf{0})<0$ and $\nabla_y F\neq\mathbf{0}$ as $y\in Y\backslash\{\mathbf{0}\}$.

We also need the characteristic function of macro pores. Set

$$\chi(x,y)=\begin{cases}1, & F(x,y)>0,\\ 0, & \text{otherwise.}\end{cases}$$

Then $\chi(x,\frac{x}{\varepsilon})=1$ in the macro pore region $\Omega_\varepsilon$ and $\chi(x,\frac{x}{\varepsilon})=0$ in the regions of fiber bundles. Let $\Omega_i=\varepsilon i+\varepsilon Y$, $i\in\mathbb{Z}^n$, be the small cells in $\Omega$. For each $i$, $S_i$ is the interface between the macro pore and the fiber bundle inside $\Omega_i$. $\widehat{\Omega}$ is the largest union of $\Omega_i$ cells included in $\Omega$, $\Omega_\partial^\varepsilon=\Omega\setminus\widehat{\Omega}$ is the thin boundary layer in $\Omega$ consist of cells just lying on the boundary $\partial\Omega$ and $S_\partial^\varepsilon$ is the union of surface of macro pores inside $\Omega_\partial^\varepsilon$.

Let $Y^*(x):=\{y\in Y|\chi(x,y)=1\}=\{y\in Y|F(x,y)>0\}$ be the reference macro pore area and $\Gamma^*(x):=\partial Y^*(x)\setminus\partial Y=\{y\in Y|F(x,y)=0\}$ the surface of macro pores inside a reference cell for each $x\in\Omega$.

**2.1. Multi-scale model for the first stage.** In the first stage, the diffusion happens everywhere, but with different diffusion coefficients in the bundles and in the macro pores. In micro-scale the steady reaction diffusion problem ( [2]) is

$$\begin{cases}-\nabla\cdot(D^\varepsilon\nabla C^\varepsilon)=-KC^\varepsilon\delta^\varepsilon(x)-KC^\varepsilon S_{vs}(1-\chi(x,\frac{x}{\varepsilon})) & \text{in } \Omega,\\ C^\varepsilon=C_\partial & \text{on } \partial\Omega,\end{cases}\tag{2.1}$$

where

- $C^\varepsilon$ is the concentration in $\Omega$.
- $C_\partial\in H^{1/2}(\partial\Omega)$ is the given positive concentration on $\partial\Omega$.

- $\delta^\varepsilon(x)$ is the surface Dirac delta function satisfying

$$\langle KC^\varepsilon \delta^\varepsilon(x), v(x)\rangle := \int_{S^\varepsilon} KC^\varepsilon v ds, \quad \forall\, v(x) \in H^1(\Omega).$$

- $D^\varepsilon := D(x, \frac{x}{\varepsilon})$ is the diffusion coefficient such that $D(x,\cdot)$ is periodic in $Y$, $D(\cdot, y)$ is Lipschitz continuous in $\Omega$ and there exist two positive constants $\lambda$, $\Lambda$ such that

$$\lambda|\xi|^2 \leq \xi^T D^\varepsilon(x)\xi \leq \Lambda|\xi|^2, \ \forall x \in \Omega, \ \xi \in \mathbb{R}^n. \tag{2.2}$$

  In fact, in our model $D(x,\cdot)$ is different constant in $Y^*$ and $Y \backslash Y^*$ respectively, i.e.,

$$D^\varepsilon = \chi\left(x, \frac{x}{\varepsilon}\right) D_1 + \left(1 - \chi\left(x, \frac{x}{\varepsilon}\right)\right) D_2, \tag{2.3}$$

  where $D_1$ and $D_2$ are the constant diffusion coefficients in macro pores and micro pores respectively.
- $S_{vs}$ is the effective reaction and deposition surface area of micro pores per unit volume of the fiber bundle with an order of $O(\varepsilon_1^{-1})$, where $\varepsilon_1$ is the characteristic size of the micro pores and $\varepsilon_1 = \gamma\varepsilon$ with $\gamma < 1$ is a very small positive constant.
- $K$ is the first-order surface reaction rate with a unit of m/s and with an order of $O(\varepsilon)$, see Remark 2.1 below.

LEMMA 2.1. *Problem* (2.1)-(2.2) *has a solution* $C^\varepsilon$, *which is unique and satisfies the estimate* $\|C^\varepsilon\|_{H^1(\Omega)} \leq A$, *where* $A$ *is a constant independent of* $\varepsilon$.

THEOREM 2.1. *Let* $C^\varepsilon$ *be the solution of the problem* (2.1)-(2.2). *Then as* $\varepsilon \to 0$,

$$C^\varepsilon \rightharpoonup C^0 \ \textit{weakly in } H^1(\Omega), \qquad D^\varepsilon \nabla C^\varepsilon \rightharpoonup D^0 \nabla C^0 \ \textit{weakly in } (L^2(\Omega))^n, \tag{2.4}$$

*where* $C^0$ *is the unique solution in* $H^1(\Omega)$ *of the homogenized problem*

$$\begin{cases} -\nabla \cdot (D^0(x)\nabla C^0) = -KS_{vl}C^0(x) - KS_{vs}(1-\phi_l)C^0(x) & \textit{in } \Omega, \\ C^0 = C_\partial & \textit{on } \partial\Omega. \end{cases} \tag{2.5}$$

$D^0$ *is defined as follows:*

$$D^0(x) = \frac{1}{|Y|}\int_Y D(x,y)(I + \nabla_y N(x,y))dy, \tag{2.6}$$

*with* $N(x,y)$ *a vector periodic function about* $y$, *which satisfies the following cell problem, for* $k = 1, \cdots, n$,

$$\begin{cases} -\nabla_y \cdot (D(x,y)\nabla_y(y_k + N_k)) = 0 \ \textit{in } Y, \\ N_k \ \textit{is } Y \textit{ periodic about } y \textit{ and } \int_Y N_k dy = 0. \end{cases} \tag{2.7}$$

$\phi_l = \frac{|Y^*(x)|}{|Y|}$ *is the porosity of macro pores among fiber bundles and* $S_{vl} = \frac{|\Gamma^*(x)|}{\varepsilon|Y|}$ *is the effective reaction and deposition surface area of macro pores per unit volume.*

*Further more, if we denote by* $C_1^\varepsilon$ *the first order expansion of* $C^\varepsilon$ *as*

$$C_1^\varepsilon(x) = C^0(x) + \varepsilon N_k\left(x, \frac{x}{\varepsilon}\right)\frac{\partial C^0(x)}{\partial x_k}, \quad \forall x \in \Omega,$$

*and assume that* $C^0 \in H^2(\Omega)$, *then there exists a positive constant* $A$ *independent of* $\varepsilon$ *such that*

$$\|C^\varepsilon - C_1^\varepsilon\|_{H^1(\Omega)} \le A\varepsilon^{\frac{1}{2}}. \tag{2.8}$$

REMARK 2.1. Note that $S_{vl}$ with a unit of $1/m$ is of order $O(\varepsilon^{-1})$. The unit of the quantity $KS_{vl}$ is $1/s$, which is independent of the characteristic length scale $\varepsilon$. Therefore we must have

$$K = k\varepsilon \quad \text{where } k \text{ is a constant independent of } \varepsilon. \tag{2.9}$$

Similar discussion was contained on p. 177 of [25].

REMARK 2.2. $KS_{vl}$ is of order $O(1)$ while $KS_{vs}(1-\phi_l)$ is of order $O(\varepsilon/\varepsilon_1)$, which means $KS_{vl}C^0(x)$ is much less than $KS_{vs}(1-\phi_l)C^0(x)$ since $\varepsilon_1$ is much less than $\varepsilon$, i.e., the reaction mainly occurs in the micro pores at first stage. This is consistent with the real experiment since the surface of macro pores is only a small part of the surface of all fibers.

**2.2. Multi-scale model for the second stage.** In the second stage, the micro pores inside the fiber bundles are all closed. Diffusion only occurs in the macro pores between fiber bundles, and there is no diffusion occurring inside the bundles. So we need to deal with a degenerated reaction diffusion equation in a perforated domain which is assumed to be locally periodic and with the singular surface source. In micro-scale, the steady reaction diffusion equation is

$$\begin{cases} -\nabla\cdot(D^\varepsilon \nabla C^\varepsilon) = -KC^\varepsilon \delta^\varepsilon(x) & \text{in } \Omega, \\ C^\varepsilon = C_\partial & \text{on } \partial\Omega. \end{cases} \tag{2.10}$$

The value of $D^\varepsilon$ has been changed. It no longer satisfies the previous condition (2.2), but still meets the following condition: there exist two positive constants $\lambda$, $\Lambda$ such that

$$D^\varepsilon(x) = 0,\ \forall x \in \Omega\setminus\Omega^\varepsilon; \quad \lambda|\xi|^2 \le \xi^T D^\varepsilon(x)\xi \le \Lambda|\xi|^2,\ \forall x \in \Omega^\varepsilon, \xi \in \mathbb{R}^n. \tag{2.11}$$

Actually, in our model it holds that

$$D^\varepsilon = \chi\left(x, \frac{x}{\varepsilon}\right) D_1. \tag{2.12}$$

LEMMA 2.2 ( [14]). *Let* $B_1$ *be the closure of a smooth domain, and let* $B$ *be a smooth bounded domain such that* $B_1 \subset B$ *and* $B_2 = B\setminus B_1$ *is a connected set. Then every* $u \in H^1(B_2)$ *can be extended to* $B$ *as a function* $\tilde{u} \in H^1(B)$ *such that*

$$\int_B |\nabla\tilde{u}|^2 dx \le A\int_{B_2} |\nabla u|^2 dx,$$
$$\int_B \tilde{u}^2 dx \le A\int_{B_2} u^2 dx,$$

*where the constant* $A$ *does not depend on* $u \in H^1(B_2)$.

As a corollary of Lemma 2.2 we have the following lemma.

LEMMA 2.3. *For any given* $\varphi \in H^1(\Omega^\varepsilon)$ *there is a function* $\widetilde{\varphi} \in H^1(\Omega)$ *such that* $\widetilde{\varphi} = \varphi$ *in* $\Omega^\varepsilon$, *and*

$$\|\widetilde{\varphi}\|_{H^1(\Omega)} \le A\|\varphi\|_{H^1(\Omega^\varepsilon)},$$

*where the constant $A$ does not depend on $\varphi$ and $\varepsilon$.*

LEMMA 2.4. *Problem (2.10)-(2.12) has a solution $C^\varepsilon$ such that $C^\varepsilon|_{\Omega^\varepsilon}$ is unique in $H^1(\Omega^\varepsilon)$ and $C^\varepsilon$ is uniformly bounded in $H^1(\Omega)$.*

*Proof.* (Proof sketch). The problem (2.10) is equivalent to

$$\begin{cases} -\nabla\cdot(D_1\nabla C^\varepsilon)=0 & \text{in } \Omega^\varepsilon, \\ -D_1\frac{\partial C^\varepsilon}{\partial n}=KC^\varepsilon & \text{on } S^\varepsilon, \\ C^\varepsilon=C_\partial & \text{on } \partial\Omega, \end{cases}$$

and has a weak form as: Find $C^\varepsilon\in V=\{v\in H^1(\Omega^\varepsilon):\ v=C_\partial \text{ on } \partial\Omega\}$ such that

$$\int_{\Omega^\varepsilon} D_1\nabla C^\varepsilon\nabla v dx+\int_{S^\varepsilon} KC^\varepsilon v ds=0,\quad \forall v\in V_0=\{v\in H^1(\Omega^\varepsilon):\ v=0 \text{ on } \partial\Omega\}. \tag{2.13}$$

Problem (2.13) has a solution $C^\varepsilon$, which is unique and uniformly bounded in $H^1(\Omega^\varepsilon)$. By Lemma 2.3, it can be extended from $\Omega^\varepsilon$ to $\Omega$ still denoted by $C^\varepsilon$ such that $\|C^\varepsilon\|_{H^1(\Omega)}\le A$, where $A$ is a constant independent of $\varepsilon$. □

THEOREM 2.2. *Let $C^\varepsilon\in H^1(\Omega)$ be the solution of the problem (2.10)-(2.11). Then as $\varepsilon\to 0$,*

$$C^\varepsilon\rightharpoonup C^0 \text{ weakly in } H^1(\Omega),\qquad D^\varepsilon\nabla C^\varepsilon\rightharpoonup D^0\nabla C^0 \text{ weakly in } (L^2(\Omega))^n, \tag{2.14}$$

*where $C^0$ is the unique solution in $H^1(\Omega)$ of the homogenized problem*

$$\begin{cases} -\nabla\cdot(D^0(x)\nabla C^0)=-KS_{vl}C^0(x) & \text{in } \Omega, \\ C^0=C_\partial & \text{on } \partial\Omega, \end{cases} \tag{2.15}$$

*where $D^0$ is defined as follows:*

$$D^0(x)=\frac{1}{|Y|}\int_{Y^*} D_1(I+\nabla_y M(x,y))dy, \tag{2.16}$$

*with $M(x,y)$ a vector periodic function about $y$ satisfying the following cell problem, for $k=1,\cdots,n$,*

$$\begin{cases} -\nabla_y\cdot(D_1\nabla_y(y_k+M_k(x,y)))=0 & \text{in } Y^*(x), \\ -D_1\frac{\partial(y_k+M_k(x,y))}{\partial n_y}=0 & \text{on } \Gamma^*(x), \\ M_k(x,y) \text{ is periodic in } y\in Y^*(x) \text{ and } \int_{Y^*} M_k dy=0. \end{cases} \tag{2.17}$$

*Furthermore, if we denote by $C_1^\varepsilon$ the first order expansion of $C^\varepsilon$ as*

$$C_1^\varepsilon(x)=C^0(x)+\varepsilon M_k\left(x,\frac{x}{\varepsilon}\right)\frac{\partial C^0(x)}{\partial x_k},\quad \forall x\in\Omega^\varepsilon, \tag{2.18}$$

*and assume that $C^0\in H^2(\Omega)$, then there exists a positive constant $A$ independent of $\varepsilon$ such that*

$$\|C^\varepsilon-C_1^\varepsilon\|_{H^1(\Omega^\varepsilon)}\le A\varepsilon^{\frac{1}{2}}. \tag{2.19}$$

REMARK 2.3. In this paper the derivation of the error estimates (2.8) and (2.19) relies on the assumption $C^0\in H^2(\Omega)$, while Chechkin and Piatnitski ( [6]) used a stronger assumption $C^0\in H^3(\Omega)$ to derive the same result (2.19) for locally periodic perforated media.

## 3. Homogenization for the first stage

In this section, we consider the homogenization of the first stage of CVI process and prove one of the main results, Theorem 2.1. In the beginning, we introduce the following notations:

$$\mathcal{L}^\varepsilon(C^\varepsilon) = -\nabla\cdot(D^\varepsilon\nabla C^\varepsilon) + KC^\varepsilon\delta^\varepsilon(x) + KS_{vs}C^\varepsilon\left(1-\chi\left(x,\frac{x}{\varepsilon}\right)\right),$$

$$\mathcal{L}^0(C^0) = -\nabla\cdot(D^0(x)\nabla C^0) + KS_{vl}C^0(x) + KS_{vs}C^0(1-\phi_l).$$

The following lemma is a result of the trace theorem( [5]).

LEMMA 3.1. *For any cell $\Omega_i = \varepsilon(i+Y)$, $i\in\mathbb{Z}^n$, there exists a positive constant $\tilde{A} = \tilde{A}(\Omega_i)$ such that for $v\in W^{1,p}(\Omega_i)$, $p\in[1,+\infty]$, the following inequality holds*

$$\|v\|_{L^p(S_i)} \le \tilde{A}(\Omega_i)\|v\|_{L^p(\Omega_i)}^{1-\frac{1}{p}}\|v\|_{H^{1,p}(\Omega_i)}^{\frac{1}{p}},$$

*where $S_i$ is the interface of macro pores and fibre bundles inside $\Omega_i$.*

*Furthermore, by a standard argument of scaling, we have that there exists a positive constant $A$ independent of $\varepsilon$ such that*

$$\int_{S_i}|v|^p ds \le A\varepsilon^{-1}\left(\int_{\Omega_i}|v|^p dx\right)^{1-\frac{1}{p}}\left(\int_{\Omega_i}(|v|^p+\varepsilon^p|\nabla v|^p)dx\right)^{\frac{1}{p}}. \tag{3.1}$$

LEMMA 3.2 ( [21]). *Let $\Omega$ ba a bounded domain with a smooth boundary and $\mathcal{U}_\delta = \{x\in\Omega, dist(x,\partial\Omega)<\delta\}$, $\delta>0$. Then there exists $\delta_0>0$ such that for every $\delta\in(0,\delta_0)$ and every $v\in H^1(\Omega)$ we have*

$$\|v\|_{L^2(\mathcal{U}_\delta)} \le A\delta^{\frac{1}{2}}\|v\|_{H^1(\Omega)},$$

*where $A$ is a constant independent of $\delta$ and $v$.*

LEMMA 3.3. *Let $D^\varepsilon$ satisfy the conditions (2.2)-(2.3), and let $N_k$ be the solution to the cell problem (2.7). Then $N_k(x,\cdot)\in H^1(Y)$, $N_k(\cdot,y)$ is Lipschitz continuous in $\Omega$ and $N_k(x,y)\in L^\infty(\Omega\times Y)$. Moreover, there exists a constant $A$ depending only on $n,\lambda,\Lambda$ such that*

$$\|\nabla_y N_k(x,y)\|_{L^\infty(\Omega\times Y)} \le A\|N_k(x,y)\|_{L^\infty(\Omega\times Y)}. \tag{3.2}$$

Inequality (3.2) is a direct corollary of Theorem 4.1 in [17] by Li and Vogelius. They derived an interior $W^{1,\infty}$ estimates for solutions to elliptic problems with piecewise constant coefficients. Noting that $N_k(x,y)$ is periodic with respect to $y$, the result (3.2) is actually an interior estimate, since the cell problem (2.7) is valid on the whole space $\mathbb{R}^n$. This is an extremely important result in the following estimates.

REMARK 3.1. Lemma 3.3 will be used later to bound terms like $\int_\Omega|\nabla_y N_k(x,\frac{x}{\varepsilon})v(x)|^2dx \le A\int_\Omega|v(x)|^2dx$ for all $v(x)\in L^2(\Omega)$. In fact, some efforts have been done to reduce such $W^{1,\infty}$ regularity requirements. In [28], for a *periodic* media, regarding $\nabla_y N_k(y)\in L^2(Y)$ (not $L^\infty(Y)$) as a multiplier, Zhikov proved that $\int_\Omega|\nabla_y N_k(\frac{x}{\varepsilon})v(x)|^2dx \le A\int_\Omega(|v(x)|^2+\varepsilon^2|\nabla v(x)|^2)dx$ for all $v(x)\in H^1(\Omega)$. Such idea appeared earlier in [23]. However, it can hardly extend to problems for locally periodic media here.

Du and Ming [12] considered the heterogeneous multiscale finite element method for problems with non-smooth micro-structures, where the regularity assumption $N_k(x,\cdot)\in W^{1,\infty}$ could be avoided by some subtle arguments. However, they treated a special case in which the test functions $v(x)$ in above inequalities belong to some finite element spaces, e.g., some piecewise polynomials.

The following lemma concerns on the inner boundary condition, i.e., the surface reaction term. Similar results can be found in Lemma 2 of [6].

LEMMA 3.4. *There exists a constant $A>0$ independent of $\varepsilon$ such that*

$$\left|\int_\Omega KS_{vl}u(x)v(x)dx-\int_{S^\varepsilon}Ku(x)v(x)ds\right|\le A\varepsilon\|u\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)} \tag{3.3}$$

*holds for any $u,v\in H^1(\Omega)$.*

*Proof.* In the rest of this paper, unless otherwise stated, we use $\sum_i$ to express the summation for all $i$ such that $\Omega_i\subset\widehat{\Omega}$, i.e., all inside cells.

In each cell $\Omega_i$, we first approximate $KS_{vl}(x)$ by a constant $\frac{K|S_i|}{|\Omega_i|}$, where $|S_i|$ denote the area of the surface $S_i=\{x=\varepsilon(i+y)\in\Omega_i|F(x,x/\varepsilon)=0\}$, whose counterpart in the reference cell is the surface $S_i^*=\{y\in Y|F(\varepsilon(i+y),y)=0\}$ and $|S_i|=\varepsilon^{n-1}|S_i^*|$. For each $x\in\Omega_i$, let $|\Gamma_i(x)|$ denote the area of the surface $\Gamma_i(x)=\{\varepsilon(i+y)\in\Omega_i|F(x,y)=0\}$, whose counterpart in the reference cell is the surface $\Gamma^*(x)=\{y\in Y|F(\varepsilon(i+z),y)=0\}$ for some $z\in Y$ such that $x=\varepsilon(i+z)$ and $|\Gamma_i(x)|=\varepsilon^{n-1}|\Gamma^*(x)|$. From Equation (2.9),

$$KS_{vl}=\frac{K|\Gamma_i(x)|}{|\Omega_i|}=k\frac{|\Gamma^*(x)|}{|Y|}\ \text{ and }\ \frac{K|S_i|}{|\Omega_i|}=k\frac{|S_i^*|}{|Y|}.$$

Since $F(x,y)$ is sufficiently smooth with respect to both $x$ and $y$, we have the approximation result in the reference cell that (refer to 5 for the detailed proof)

$$|(|S_i^*|-|\Gamma^*(x)|)|\le A\varepsilon. \tag{3.4}$$

Hence, we have

$$\int_{\Omega_i}\left|K\left(S_{vl}-\frac{|S_i|}{|\Omega_i|}\right)u(x)v(x)\right|dx\le A\varepsilon\|u\|_{L^2(\Omega_i)}\|v\|_{L^2(\Omega_i)}. \tag{3.5}$$

By inequality (3.5), Hölder's inequality, Equation (2.9) and Lemma 3.2,

$$\begin{aligned}
&\left|\int_\Omega KS_{vl}uvdx-\int_{S^\varepsilon}Kuvds\right|\\
=&\left|\sum_i\left(\int_{\Omega_i}KS_{vl}uvdx-\int_{S_i}Kuvds\right)+\int_{\Omega_\partial^\varepsilon}KS_{vl}uvdx-\int_{S_\partial^\varepsilon}Kuvds\right|\\
\le&\left|\sum_i\left(\int_{\Omega_i}K\frac{|S_i|}{|\Omega_i|}uvdx-\int_{S_i}Kuvds\right)\right|+\left|\int_{S_\partial^\varepsilon}Kuvds\right|+A\varepsilon\|u\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)}\\
=&\left|\sum_iK\frac{|S_i|}{|\Omega_i|}\int_{\Omega_i}(uv-\langle uv\rangle_{S_i})dx\right|+\left|\int_{S_\partial^\varepsilon}Kuvds\right|+A\varepsilon\|u\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)}\\
=&T_1+T_2+A\varepsilon\|u\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)},
\end{aligned} \tag{3.6}$$

where $\langle\cdot\rangle_{S_i}$ is the mean on $S_i$. By Lemma 3.1 with $p=1$, Equation (2.9) and Lemma 3.2, we get, for the surfaces in the boundary layer, that

$$\begin{aligned} T_2 = & \left|\sum_{S_i\in S_1^\varepsilon}\int_{S_i} Kuvds\right| \le AK\varepsilon^{-1}\int_{\Omega_\partial^\varepsilon}(|uv|+\varepsilon|\nabla(uv)|)dx \\ & \le A\|u\|_{L^2(\Omega_\partial^\varepsilon)}\|v\|_{L^2(\Omega_\partial^\varepsilon)} + A\varepsilon\|u\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)} \\ & \le A\varepsilon\|u\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)}. \end{aligned} \tag{3.7}$$

To estimate $T_1$, we first introduce a functional $G_i(\cdot)$ on $W^{1,1}(\Omega_i)$ as

$$G_i(w) = \int_{\Omega_i}(w - \langle w\rangle_{S_i})dx.$$

From Lemma 3.1, it is easy to check that $|G_i(w)|\le A\int_{\Omega_i}(|w|+|\nabla w|)dx$, where $A$ is independent of $\varepsilon$ and $G_i(w)=G_i(w+a)$, $\forall a\in\mathbb{R}^1$. Then by Bramble-Hilbert's lemma ( [4]) and the scaling argument, we have

$$|G_i(w)|\le A\inf_{a\in\mathbb{R}^1}\|w+a\|_{W^{1,1}(\Omega_i)} \le \tilde{A}(\Omega_i)\|\nabla w\|_{L^1(\Omega_i)} = A\varepsilon\|\nabla w\|_{L^1(\Omega_i)}. \tag{3.8}$$

Now we get that

$$T_1 \le \sum_i K\frac{|S_i|}{|\Omega_i|}|G_i(uv)| \le A\varepsilon\sum_i\|\nabla(uv)\|_{L^1(\Omega_i)} \le A\varepsilon\|u\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)}. \tag{3.9}$$

The lemma is now proved. ◻

REMARK 3.2. Similar results of Lemma 3.4 were given in Lemma 2 of [6]. The main ingredient in their approach is to construct the following auxiliary problem in the macro pore region

$$\begin{cases} \Delta_y\psi(x,y) = \varepsilon S_{vl} & \text{in } Y^*(x), \\ \frac{\partial\psi}{\partial n} = |Y^*(x)| & \text{on } \Gamma^*(x). \end{cases} \tag{3.10}$$

For our problem here, to follow their path, we need to construct two auxiliary problems

$$\begin{cases} \Delta_y\psi_1(x,y) = \varepsilon S_{vl} & \text{in } Y^*(x), \\ \frac{\partial\psi_1}{\partial n} = |Y^*| & \text{on } \Gamma^*(x), \end{cases} \quad \text{and} \quad \begin{cases} \Delta_y\psi_2 = \varepsilon S_{vl} & \text{in } Y\setminus Y^*(x), \\ -\frac{\partial\psi_2}{\partial n} = |Y\setminus Y^*| & \text{on } \Gamma^*(x). \end{cases}$$

In the proof of Lemma 3.4, we choose a more intuitive way.

REMARK 3.3. For purely periodic media, the approximation results (3.4) and (3.5) are not needed. We would have $|\Gamma^*(x)|\equiv \text{const.} = |S_i^*|$ and $S_{vl}(x)\equiv\text{const.} = \frac{|S_i|}{|\Omega_i|}$.

With the help of the preceding lemmas we can now prove Theorem 2.1.

*Proof.* **(Proof of Theorem 2.1).** First we prove the convergence result (2.4) by the two-scale convergence method (see [18] and references therein). The variational formulation of the problem (2.1) is

$$\begin{cases} \text{Find } C^\varepsilon\in V=\{v|v\in H^1(\Omega), v(x)=C_\partial \text{ on } \partial\Omega\} \text{ such that} \\ \int_\Omega D^\varepsilon\nabla C^\varepsilon\nabla vdx = \int_{S^\varepsilon} -KC^\varepsilon vds + \int_\Omega -KC^\varepsilon S_{vs}(1-\chi(x,\frac{x}{\varepsilon}))vdx, \quad \forall v\in H_0^1(\Omega). \end{cases} \tag{3.11}$$

It follows from Lemma 2.1 and Theorem 5.1 that there exists a subsequence, still denoted by $\varepsilon$, such that $C^\varepsilon$ two scale converges to $C^0$. Moreover, there exists $C_1=C_1(x,y)$ in $L^2(\Omega,H_{per}(Y)/\mathbb{R})$ such that, up to a subsequence, $\nabla C^\varepsilon$ two scale converges to $\nabla_x C^0+\nabla_y C_1$ by Theorem 5.2. Let $v_0(x)\in\mathcal{D}(\Omega)$ and $v_1(x,\frac{x}{\varepsilon})\in\mathcal{D}(\Omega,\mathcal{C}^\infty_{per}(Y))$, where $\mathcal{D}(\Omega)$ is the space of all indefinitely differentiable functions with compact support in $\Omega$, and $\mathcal{D}(\Omega,\mathcal{C}^\infty_{per}(Y))$ is the space of all measurable functions $v(x,y)$ on $\Omega\times Y$ such that $v(x,\cdot)\in\mathcal{C}^\infty(\overline{Y})$ is $Y$-periodic for any $x\in\Omega$, and $v(\cdot,y)\in\mathcal{D}(\Omega)$ for any $y\in Y$. Using $v_0(x)+\varepsilon v_1(x,\frac{x}{\varepsilon})$ as a test function in the problem (3.11), we obtain that

$$\begin{aligned}&\int_\Omega D^\varepsilon\nabla C^\varepsilon\left(\nabla v_0(x)+\varepsilon\nabla_x v_1\left(x,\frac{x}{\varepsilon}\right)+\nabla_y v_1\left(x,\frac{x}{\varepsilon}\right)\right)dx\\&=-\int_{S^\varepsilon}KC^\varepsilon(v_0+\varepsilon v_1)ds-\int_\Omega KC^\varepsilon S_{vs}\left(1-\chi\left(x,\frac{x}{\varepsilon}\right)\right)(v_0+\varepsilon v_1)dx.\end{aligned}$$

We can take the limit of the left-hand side and the second term of the right-hand side by using the same arguments on P183 of [10], detailed in 5. It follows from Lemmas 3.4 and 2.1 that

$$\begin{aligned}&\lim_{\varepsilon\to0}\int_{S^\varepsilon}KC^\varepsilon(x)(v_0+\varepsilon v_1)ds\\&=\lim_{\varepsilon\to0}\left[\left(\int_{S^\varepsilon}KC^\varepsilon v_0ds-\int_\Omega KS_{vl}C^\varepsilon v_0dx\right)+\int_\Omega KS_{vl}C^\varepsilon v_0dx+\int_{S^\varepsilon}KC^\varepsilon\varepsilon v_1\right]\\&=\int_\Omega KS_{vl}C^0v_0dx.\end{aligned}\tag{3.12}$$

Thus we obtain

$$\begin{aligned}&\frac{1}{|Y|}\int_\Omega\int_Y D(x,y)(\nabla C^0+\nabla_y C_1(x,y))(\nabla v_0+\nabla_y v_1(x,y))dydx\\&=-\int_\Omega KS_{vl}C^0v_0dx-\int_\Omega KS_{vs}C^0(1-\phi_l)v_0dx.\end{aligned}\tag{3.13}$$

Choosing first $v_0\equiv0$ and then $v_1\equiv0$, we obtain

$$\begin{cases}-\nabla_y\cdot(D(x,y)\nabla_yC_1(x,y))=\nabla_y(D(x,y))\nabla C^0(x)\quad\text{in }\Omega\times Y,\\-\nabla\cdot\left[\int_Y D(x,y)(\nabla C^0(x)+\nabla_yC_1(x,y))dy\right]=-KS_{vl}C^0-KS_{vs}C^0(1-\phi_l)\quad\text{in }\Omega,\\C^0=C_\partial\quad\text{on }\partial\Omega,\\C_1(x,\cdot)\quad Y-\text{periodic}.\end{cases}\tag{3.14}$$

Thus $C_1$ has the form $C_1(x,y)=N_k(x,y)\frac{\partial C^0(x)}{\partial x_k}$ with $N_k(x,y)$ satisfying cell problem (2.7). Replace $C_1(x,y)$ by $N_k(x,y)\frac{\partial C^0(x)}{\partial x_k}$ in the second line of the expression (3.14), we get $C^0$ satisfies the problem (2.5). Consequently, the whole sequence converges to $C^0$ due to the uniqueness of the solution to (2.5). So far we have proved the convergence result (2.4).

Now we will prove the error estimate (2.8) under the assumption that $C^0\in H^2(\Omega)$. First we will prove

$$\|\mathcal{L}^\varepsilon(C^\varepsilon-C_1^\varepsilon)\|_{H^{-1}(\Omega)}\le A\varepsilon,\tag{3.15}$$

where $A$ is a constant independent of $\varepsilon$. From the problems (2.1) and (2.5),

$$\|\mathcal{L}^\varepsilon(C^\varepsilon)-\mathcal{L}^\varepsilon(C_1^\varepsilon)\|_{H^{-1}(\Omega)}=\|\mathcal{L}^0(C^0)-\mathcal{L}^\varepsilon(C_1^\varepsilon)\|_{H^{-1}(\Omega)}$$

$$
\begin{aligned}
&= \|-\nabla\cdot(D^0\nabla C^0)+KS_{vl}C^0+KS_{vs}(1-\phi_l)C^0\\
&\quad +\nabla\cdot(D^\varepsilon\nabla C_1^\varepsilon)-K\delta^\varepsilon(x)C_1^\varepsilon-KS_{vs}(1-\chi)C_1^\varepsilon\|_{H^{-1}(\Omega)}\\
&\le \|\nabla\cdot(D^0\nabla C^0)-\nabla\cdot(D^\varepsilon\nabla C_1^\varepsilon)\|_{H^{-1}(\Omega)}+\|KS_{vl}C^0-K\delta^\varepsilon(x)C_1^\varepsilon\|_{H^{-1}(\Omega)}\\
&\quad +\|KS_{vs}(1-\phi_l)C^0-KS_{vs}(1-\chi)C_1^\varepsilon\|_{H^{-1}(\Omega)}\\
&= I_1+I_2+I_3.
\end{aligned}
\tag{3.16}
$$

For the first term, we have the estimate

$$
I_1 := \|\nabla\cdot(D^0\nabla C^0)-\nabla\cdot(D^\varepsilon\nabla C_1^\varepsilon)\|_{H^{-1}(\Omega)} \le A\varepsilon, \tag{3.17}
$$

which can be derived by the standard argument as employed on p. 26-27 in [14], see 5. The only difference here is that one has to treat some locally periodic functions rather than purely periodic ones, see also [7].

For all $g(x)\in H_0^1(\Omega)$,

$$
\left|\int_\Omega KS_{vl}C^0 g dx-\int_{S^\varepsilon}KC_1^\varepsilon g ds\right| \le K\left|\int_\Omega S_{vl}C^0 g dx-\int_{S^\varepsilon}C^0 g ds\right|+\left|\int_{S^\varepsilon}\varepsilon K N_k\frac{\partial C^0}{\partial x_k}g ds\right|.
$$

The first term on the right hand side can be estimated by the inequality (3.3). By Equation (2.9) and Lemmas 3.1 and 3.3, we have

$$
\left|\int_{S^\varepsilon}\varepsilon K N_k\frac{\partial C^0}{\partial x_k}g ds\right| \le A\varepsilon\|C^0\|_{H^2(\Omega)}\|g\|_{H^1(\Omega)}.
$$

Hence from Lemma 3.4, we have

$$
I_2 := \|KS_{vl}C^0-K\delta^\varepsilon(x)C_1^\varepsilon\|_{H^{-1}(\Omega)} \le A\varepsilon. \tag{3.18}
$$

Then we turn to estimate the term $I_3$. For any $g(x)\in H_0^1(\Omega)$,

$$
\begin{aligned}
&\int_\Omega \left(KS_{vs}(1-\phi_l)C^0-KS_{vs}(1-\chi)C_1^\varepsilon\right)g(x)dx\\
&= \sum_i\int_{\Omega_i}\left(KS_{vs}(1-\phi_l)C^0-KS_{vs}(1-\chi)C_1^\varepsilon\right)g(x)dx\\
&\quad +\int_{\Omega_\partial^\varepsilon}\left(KS_{vs}(1-\phi_l)C^0-KS_{vs}(1-\chi)C_1^\varepsilon\right)g(x)dx.
\end{aligned}
$$

For the inner part, we have after direct computation that

$$
\begin{aligned}
&\left|\sum_i\int_{\Omega_i}\left(KS_{vs}(1-\phi_l)C^0-KS_{vs}(1-\chi)C_1^\varepsilon\right)g(x)dx\right|\\
&\le \left|\sum_i\int_{\Omega_i}KS_{vs}\left((1-\phi_l)C^0 g-(1-\chi)C^0 g\right)dx\right|+\left|\sum_i\int_{\Omega_i}KS_{vs}(1-\chi)\varepsilon N_k\frac{\partial C^0}{\partial x_k}g dx\right|\\
&\le KS_{vs}\left(\left|\sum_i\int_{\Omega_i}(1-\phi_l)(C^0-\langle C^0\rangle_{\Omega_i})g dx\right|+\left|\sum_i\int_{\Omega_i}(1-\phi_l)\langle C^0\rangle_{\Omega_i}(g-\langle g\rangle_{\Omega_i})dx\right|\right.\\
&\quad +\left|\sum_i\int_{\Omega_i}(1-\chi)(C^0-\langle C^0\rangle_{\Omega_i})g dx\right|+\left|\sum_i\int_{\Omega_i}(1-\chi)(g-\langle g\rangle_{\Omega_i})\langle C^0\rangle_{\Omega_i}dx\right|
\end{aligned}
$$

$$+\left|\sum_i\int_{\Omega_i}(1-\chi)\varepsilon N_k\frac{\partial C^0}{\partial x_k}gdx\right|\Bigg)$$
$$\leq A\varepsilon\left(|C^0|_{H^1(\Omega)}\|g\|_{L^2(\Omega)}+\|C^0\|_{L^2(\Omega)}|g|_{H^1(\Omega)}\right).$$

For the boundary part, we have from Lemma 3.2

$$\left|\int_{\Omega_\partial^\varepsilon}\left(KS_{vs}(1-\phi_l)C^0-KS_{vs}(1-\chi)C_1^\varepsilon\right)g(x)dx\right|$$
$$\leq\left|\int_{\Omega_\partial^\varepsilon}KS_{vs}\left((1-\phi_l)C^0g-(1-\chi)C^0g\right)dx\right|+\left|\int_{\Omega_\partial^\varepsilon}KS_{vs}(1-\chi)\varepsilon N_k\frac{\partial C^0}{\partial x_k}gdx\right|$$
$$\leq A\left(\|C^0\|_{L^2(\Omega_\partial^\varepsilon)}\|g\|_{L^2(\Omega_\partial^\varepsilon)}+\varepsilon\|C^0\|_{H^1(\Omega_\partial^\varepsilon)}\|g\|_{L^2(\Omega_\partial^\varepsilon)}\right)\leq A\varepsilon\|C^0\|_{H^1(\Omega)}\|g\|_{H^1(\Omega)}.$$

So putting the above two estimates together, we get

$$I_3:=\|KS_{vs}(1-\phi_l)C^0-KS_{vs}(1-\chi)C_1^\varepsilon\|_{H^{-1}(\Omega)}\leq A\varepsilon.$$

Therefore we have proved the estimate (3.15).

If $C^\varepsilon-C_1^\varepsilon\in H_0^1(\Omega)$, then the estimate (3.15) implies the estimate (2.8) by the elliptic regularity. To treat the fact that $C^\varepsilon-C_1^\varepsilon\notin H_0^1(\Omega)$, we follow the argument on p. 28, [14]. First we introduce a cut-off function $\tau^\varepsilon(x)\in C^\infty(\overline{\Omega})$, such that

(1) $0\leq\tau^\varepsilon(x)\leq 1$, $\tau^\varepsilon(x)\equiv 1$ on $\partial\Omega$, $\tau^\varepsilon(x)\equiv 0$ in $\Omega\backslash\mathcal{U}_\varepsilon$, where $\mathcal{U}_\varepsilon=\{x\in\Omega|\text{dist}(x,\partial\Omega)<\varepsilon\}$;
(2) $\varepsilon|\nabla\tau^\varepsilon|\leq A$ in $\Omega$ , $A$ is a constant independent of $\varepsilon$.

To meet the zero Dirichlet boundary condition, let

$$\hat{C}_1^\varepsilon=C_1^\varepsilon-\varepsilon\tau^\varepsilon(x)N_k\left(x,\frac{x}{\varepsilon}\right)\frac{\partial C^0}{\partial x_k}=C^0(x)+\varepsilon(1-\tau^\varepsilon(x))N_k\left(x,\frac{x}{\varepsilon}\right)\frac{\partial C^0}{\partial x_k}.$$

Then we have $C^\varepsilon-\hat{C}_1^\varepsilon\in H_0^1(\Omega)$ and $C_1^\varepsilon-\hat{C}_1^\varepsilon=\varepsilon\tau^\varepsilon(x)N_k(x,\frac{x}{\varepsilon})\frac{\partial C^0}{\partial x_k}$. By simple calculations we have

$$\frac{\partial}{\partial x_j}(C_1^\varepsilon-\hat{C}_1^\varepsilon)=\left(\varepsilon\frac{\partial\tau^\varepsilon}{\partial x_j}N_k+\varepsilon\tau^\varepsilon\frac{\partial N_k(x,y)}{\partial x_j}\Big|_{y=\frac{x}{\varepsilon}}+\tau^\varepsilon\frac{\partial N_k(x,y)}{\partial y_j}\Big|_{y=\frac{x}{\varepsilon}}\right)\frac{\partial C^0}{\partial x_k}$$
$$+\varepsilon\tau^\varepsilon N_k\frac{\partial^2C^0}{\partial x_j\partial x_k}. \tag{3.19}$$

Noting that $\text{supp}\{\tau^\varepsilon\}\subset\mathcal{U}_\varepsilon$ and thanks to Lemmas 3.2 and 3.3, we get

$$\|C_1^\varepsilon-\hat{C}_1^\varepsilon\|_{H^1(\Omega)}\leq A\varepsilon^{\frac{1}{2}}. \tag{3.20}$$

What's left is to estimate $\|C^\varepsilon-\hat{C}_1^\varepsilon\|_{H^1(\Omega)}$. For all $g(x)\in H_0^1(\Omega)$, we have, by Lemma 3.1,

$$\int_\Omega\mathcal{L}^\varepsilon(C_1^\varepsilon-\hat{C}_1^\varepsilon)gdx$$
$$=\int_\Omega D^\varepsilon\nabla(C_1^\varepsilon-\hat{C}_1^\varepsilon)\nabla gdx+\int_{S^\varepsilon}K(C_1^\varepsilon-\hat{C}_1^\varepsilon)gds+\int_\Omega KS_{vs}(C_1^\varepsilon-\hat{C}_1^\varepsilon)(1-\chi)gds$$
$$\leq A\|C_1^\varepsilon-\hat{C}_1^\varepsilon\|_{H^1(\Omega)}\|g\|_{H^1(\Omega)}. \tag{3.21}$$

Then from the estimates (3.15) and (3.20),

$$\|\mathcal{L}^\varepsilon(C^\varepsilon-\hat{C}_1^\varepsilon)\|_{H^{-1}(\Omega)}\le\|\mathcal{L}^\varepsilon(C^\varepsilon-C_1^\varepsilon)\|_{H^{-1}(\Omega)}+\|\mathcal{L}^\varepsilon(C_1^\varepsilon-\hat{C}_1^\varepsilon)\|_{H^{-1}(\Omega)}\le A\varepsilon^{\frac{1}{2}}. \tag{3.22}$$

Thanks to $C^\varepsilon-\hat{C}_1^\varepsilon\in H_0^1(\Omega)$ and the elliptic regularity of the operator $\mathcal{L}^\varepsilon$, we have

$$\|C^\varepsilon-\hat{C}_1^\varepsilon\|_{H^1(\Omega)}\le A\varepsilon^{\frac{1}{2}}.$$

Then we finally get

$$\|C^\varepsilon-C_1^\varepsilon\|_{H^1(\Omega)}\le A\varepsilon^{\frac{1}{2}}, \tag{3.23}$$

where $A$ is a constant independent of $\varepsilon$. So we complete the proof. □

## 4. Homogenization for the second stage

This section is devoted to the homogenization theory for the second stage of the CVI process. In this stage, the micro pores inside the bundles are closed, so we face a perforated problem. Chechkin and Piatnitski ( [6]) gave the estimates on the rate of convergence for this kind of problem. We will prove the same results in a more straightforward way and under a lower regularity assumption on the homogenized concentration $C^0$.

From Equation (2.12), $D(x,y)=D_1$ is a constant in $Y^*(x)$. Since the interface $\Gamma^*$ is sufficiently smooth, we have for the cell problem (2.17), $M_k(x,\cdot)\in H^1(Y^*)$, and

$$M_k(\cdot,y)\text{ is Lipschitz continuous in }\Omega\text{ and }M_k(x,\cdot)\in W^{1,\infty}(Y^*). \tag{4.1}$$

Now we give the proof of Theorem 2.2.

*Proof.* **(Proof of Theorem 2.2).** First we prove the convergence result (2.14) by the two-scale convergence method. Recall that the problem (2.10) has a variational formulation as: Find $C^\varepsilon\in V=\{v\in H^1(\Omega^\varepsilon):\ v=C_\partial \text{ on } \partial\Omega\}$ such that

$$\int_{\Omega^\varepsilon}D_1\nabla C^\varepsilon\nabla v dx+\int_{S^\varepsilon}KC^\varepsilon v ds=0,\quad \forall v\in V_0=\{v\in H^1(\Omega^\varepsilon):\ v=0\text{ on }\partial\Omega\}. \tag{4.2}$$

It follows from Lemma 2.4, Theorem 5.1 and Theorem 5.2 that there exists a subsequence, still denoted by $\varepsilon$, such that $C^\varepsilon\in H^1(\Omega)$ two scale converges to $C^0$. Moreover, there exists $C_1=C_1(x,y)$ in $L^2(\Omega,H_{per}(Y)/\mathbb{R})$ such that, up to a subsequence, $\nabla C^\varepsilon$ two scale converges to $\nabla_x C^0+\nabla_y C_1$. Let $v_0(x)\in\mathcal{D}(\Omega)$ and $v_1(x,\frac{x}{\varepsilon})\in\mathcal{D}(\Omega,\mathcal{C}_{per}^\infty(Y))$. Using $v_0(x)+\varepsilon v_1(x,\frac{x}{\varepsilon})$ as a test function in Equation (4.2) we obtain that

$$\int_{\Omega^\varepsilon}D^\varepsilon\nabla C^\varepsilon\left(\nabla v_0(x)+\varepsilon\nabla_x v_1\left(x,\frac{x}{\varepsilon}\right)+\nabla_y v_1\left(x,\frac{x}{\varepsilon}\right)\right)dx=-\int_{S^\varepsilon}KC^\varepsilon(v_0+\varepsilon v_1)ds.$$

Hence, passing to the limit in the above equation as $\varepsilon\to 0$, we finally get

$$\frac{1}{|Y|}\int_\Omega\int_{Y^*}D(x,y)\left(\nabla C^0+\nabla_y C_1(x,y)\right)\left(\nabla v_0+\nabla_y v_1(x,y)\right)dydx=-\int_\Omega KS_{vl}C^0v_0dx.$$

Choosing first $v_0\equiv 0$ and then $v_1\equiv 0$, we obtain

$$\begin{cases}-\nabla_y\cdot(D(x,y)\nabla_y C_1(x,y))=\nabla_y(D(x,y))\nabla C^0(x), & \text{in }\Omega\times Y^*,\\ -\nabla_x\cdot\left(\int_{Y^*}D(x,y)(\nabla C^0(x)+\nabla_y C_1(x,y))dy\right)=-KS_{vl}C^0, & \text{in }\Omega,\\ C^0=C_\partial \quad \text{on }\partial\Omega,\\ C_1(x,\cdot)\quad Y-\text{periodic.}\end{cases} \tag{4.3}$$

Thus $C_1$ has the form $C_1(x,y)=M_k(x,y)\frac{\partial C^0(x)}{\partial x_k}$ in $\Omega\times Y^*$ with $M_k(x,y)$ satisfying the cell problem (2.17). Plug $M_k(x,y)\frac{\partial C^0(x)}{\partial x_k}$ in the second line of the expression (4.3), we get $C^0$ satisfies the problem (2.15). Consequently, the whole sequence converges to $C^0$ thanks to the uniqueness of the solution to the problem (2.15). So far we have proved the convergence result.

We now turn to bound the error for the first order expansion $C^\varepsilon - C_1^\varepsilon$. To meet the boundary condition, we introduce

$$\tilde{C}_1^\varepsilon = C_1^\varepsilon - \varepsilon\tau^\varepsilon(x) M_k \frac{\partial C^0}{\partial x_k} = C^0 + \varepsilon(1-\tau^\varepsilon(x)) M_k \frac{\partial C^0}{\partial x_k}, \tag{4.4}$$

where the cut-off functions $\tau^\varepsilon(x)$ have been introduced on the top of Equation (3.19). Then we have

$$C^\varepsilon - C_1^\varepsilon = C^\varepsilon - \tilde{C}_1^\varepsilon + \tilde{C}_1^\varepsilon - C_1^\varepsilon, \quad \text{and } (C^\varepsilon - \tilde{C}_1^\varepsilon)|_{\partial\Omega} = 0. \tag{4.5}$$

Similarly to Equation (3.19) and the inequality (3.20), we get from Lemma 3.2 and the condition (4.1) that

$$\|C_1^\varepsilon - \tilde{C}_1^\varepsilon\|_{H^1(\Omega^\varepsilon)} \le A\varepsilon^{\frac{1}{2}}. \tag{4.6}$$

What's left is to bound $w^\varepsilon = C^\varepsilon - \tilde{C}_1^\varepsilon$. By Lemma 2.3, we can extend $w^\varepsilon$ from $\Omega^\varepsilon$ to $\Omega$ such that

$$w^\varepsilon \in H_0^1(\Omega), \quad \|w^\varepsilon\|_{H^1(\Omega)} \le A\|w^\varepsilon\|_{H^1(\Omega^\varepsilon)}. \tag{4.7}$$

By direct computation, we have

$$\begin{aligned}
&\int_{\Omega^\varepsilon} D^\varepsilon \nabla w^\varepsilon \nabla w^\varepsilon dx \\
=&\int_{\Omega^\varepsilon} (D^\varepsilon \nabla C^\varepsilon - D^0 \nabla C^0)\nabla w^\varepsilon dx + \int_{\Omega^\varepsilon} G_{ij}\left(x,\frac{x}{\varepsilon}\right)\frac{\partial C^0}{\partial x_j}\frac{\partial w^\varepsilon}{\partial x_i} dx \\
&-\int_{\Omega^\varepsilon} \varepsilon d_{ij}\left(\frac{\partial M_k}{\partial x_j}\frac{\partial C^0}{\partial x_k} + M_k\frac{\partial^2 C^0}{\partial x_j \partial x_k}\right)\frac{\partial w^\varepsilon}{\partial x_i} dx + \int_{\Omega^\varepsilon} D^\varepsilon \nabla\left(\varepsilon\tau^\varepsilon M_k \frac{\partial C^0}{\partial x_k}\right)\nabla w^\varepsilon dx,
\end{aligned}$$

where $G_{ij} = d_{ij}^0 - d_{ij} - d_{ik}\frac{\partial M_j}{\partial y_k}$, $D^\varepsilon(x) = (d_{ij})_{n\times n} = \begin{cases} D_1 I_n, & \text{for } x\in\Omega^\varepsilon, \\ 0, & \text{for } x\in\Omega\backslash\Omega^\varepsilon \end{cases}$ and $D^0 = (d_{ij}^0)$ is given by Equation (2.16). Since $G_{ij} = d_{ij}^0$ in $\Omega\backslash\Omega^\varepsilon$, we have the following identity which plays a key role in the following estimates, with which we can avoid facing some difficulties induced by the perforated domain.

$$\begin{aligned}
&-\int_{\Omega^\varepsilon} D^0\nabla C^0 \nabla w^\varepsilon dx + \int_{\Omega^\varepsilon} G_{ij}\frac{\partial C^0}{\partial x_j}\frac{\partial w^\varepsilon}{\partial x_i} dx \\
=&-\int_{\Omega} \nabla\cdot(D^0\nabla C^0) w^\varepsilon dx + \int_{\Omega} G_{ij}\frac{\partial C^0}{\partial x_j}\frac{\partial w^\varepsilon}{\partial x_i} dx.
\end{aligned} \tag{4.8}$$

By the problems (2.10) and (2.15) and the identity (4.8), we have

$$\begin{aligned}
&\int_{\Omega^\varepsilon} D^\varepsilon \nabla w^\varepsilon \nabla w^\varepsilon dx \\
=&-\int_{S^\varepsilon} K C^\varepsilon w^\varepsilon ds + \int_{\Omega} K S_{vl} C^0 w^\varepsilon dx + \int_{\Omega} G_{ij}\frac{\partial C^0}{\partial x_j}\frac{\partial w^\varepsilon}{\partial x_i} dx \\
&-\int_{\Omega^\varepsilon} \varepsilon d_{ij}\left(\frac{\partial M_k}{\partial x_j}\frac{\partial C^0}{\partial x_k} + M_k\frac{\partial^2 C^0}{\partial x_j \partial x_k}\right)\frac{\partial w^\varepsilon}{\partial x_i} dx + \int_{\Omega^\varepsilon} D^\varepsilon \nabla\left(\varepsilon\tau^\varepsilon M_k \frac{\partial C^0}{\partial x_k}\right)\nabla w^\varepsilon dx.
\end{aligned}$$

Then there exists a constant $A_1>0$ independent of $\varepsilon$, such that

$$
\begin{aligned}
A_1\|w^\varepsilon\|^2_{H^1(\Omega^\varepsilon)} &\le \int_{\Omega^\varepsilon} D^\varepsilon \nabla w^\varepsilon \nabla w^\varepsilon dx + K\int_{S^\varepsilon} w^\varepsilon w^\varepsilon ds \\
&\le \left| -\int_{S^\varepsilon} KC_1^\varepsilon w^\varepsilon ds + \int_\Omega KS_{vl}C^0 w^\varepsilon dx \right| + \left| \int_{S^\varepsilon} K\left(\varepsilon\tau^\varepsilon M_k \frac{\partial C^0}{\partial x_k}\right) w^\varepsilon ds \right| \\
&\quad + \left| \int_\Omega G_{ij}\frac{\partial C^0}{\partial x_j}\frac{\partial w^\varepsilon}{\partial x_i} dx \right| + \left| \int_{\Omega^\varepsilon} \varepsilon d_{ij}\left(\frac{\partial M_k}{\partial x_j}\frac{\partial C^0}{\partial x_k} + M_k \frac{\partial^2 C^0}{\partial x_j \partial x_k}\right)\frac{\partial w^\varepsilon}{\partial x_i} dx \right| \\
&\quad + \left| \int_{\Omega^\varepsilon} D^\varepsilon \nabla\left(\varepsilon\tau^\varepsilon M_k \frac{\partial C^0}{\partial x_k}\right)\nabla w^\varepsilon dx \right| \\
&:= J_1 + J_2 + J_3 + J_4 + J_5.
\end{aligned}
$$

Similarly to the estimate (3.18), we get from the estimate (4.7) that

$$
|J_1| \le A\varepsilon \|w^\varepsilon\|_{H^1(\Omega)} \le A\varepsilon \|w^\varepsilon\|_{H^1(\Omega^\varepsilon)}.
$$

From Lemma 3.1, Equation (2.9) and the condition (4.1), we get

$$
|J_2| \le A\varepsilon \|w^\varepsilon\|_{H^1(\Omega)} \le A\varepsilon^{\frac{1}{2}} \|w^\varepsilon\|_{H^1(\Omega^\varepsilon)}.
$$

After carefully checking, though $M_k(x,y)$ is now a extension of the solutions of the problem (2.17), we still have

$$
\int_Y G_{ij}(x,y)dy = 0 \quad \text{and} \quad \frac{\partial G_{ij}}{\partial y_i} = 0 \quad \text{in } Y.
$$

With these properties, we can treat the third term by introducing skew-symmetric matrixes $\boldsymbol{\alpha}_j = (\alpha_{ik,j})$ such that $G_{ij} = \frac{\partial}{\partial y_k}(\alpha_{ki,j})$, $j = 1,\cdots,n$; refer to p. 6 in [14] or 5. By the same argument as in (5.10), we have

$$
|J_3| \le A\varepsilon \|w^\varepsilon\|_{H^1(\Omega)} \le A\varepsilon \|w^\varepsilon\|_{H^1(\Omega^\varepsilon)}.
$$

From the condition (4.1), we get

$$
|J_4| \le A\varepsilon \|w^\varepsilon\|_{H^1(\Omega^\varepsilon)}.
$$

For the last term, noting that $\operatorname{supp}\{\tau^\varepsilon\} \subset \mathcal{U}_\varepsilon$ and $\|\nabla(\varepsilon\tau^\varepsilon M)\|_{L^\infty(\Omega)} \le A$, we have by Lemma 3.2,

$$
|J_5| \le A\varepsilon^{\frac{1}{2}} \|C^0\|_{H^2(\Omega)} \|w^\varepsilon\|_{H^1(\Omega^\varepsilon)}.
$$

Then we obtain

$$
\|C^\varepsilon - \tilde{C}_1^\varepsilon\|_{H^1(\Omega^\varepsilon)} = \|w^\varepsilon\|_{H^1(\Omega^\varepsilon)} \le A\varepsilon^{\frac{1}{2}}. \tag{4.9}
$$

Combining the estimates (4.6) and (4.9), we obtain the estimate (2.19) and complete the proof. ∎

REMARK 4.1. The key point to derive the result (2.19) under the weaker assumption $C_0 \in H^2(\Omega)$ is that the identity (4.8) is constructed, with which we avoid some difficulties on perforated problems and we can treat the term $J_3$ with the help of skew-symmetric matrices $\boldsymbol{\alpha}$. This skew-symmetry leads to some error cancel on the fine scale; see the treatment for the first term on the right hand side of (5.10).

## 5. Conclusions and discussions

We established the homogenization theory for the two stages of CVI process, which is the foundation of the multi-scale model developed by Y. Bai et al. in [2]. In both stages, we proved the convergence results by the two-scale convergence method and then derived the estimates on the rate of convergence with the assumption $C^0 \in H^2(\Omega)$. The keys to the proofs were to handle the singular surface reaction term in both stages and to extend parts of terms in the perforated domain to the whole domain $\Omega$ in the second stage.

In this paper we have considered the homogenization for the steady state problems. The real CVI process is dynamic, i.e., the parameters are dependent on the structure of the media and the structure changes with time. So we have a nonlinear coupling system on the concentration and local porosity. The homogenization theory for the nonlinear system will be investigated in a future paper. We also expect 3-dimensional multiscale numerical simulation for the CVI process.

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**Appendix.**

**A.1.** Here we present two important theorems in [10] and prove Equation (3.13) in detail.

THEOREM 5.1. *Let $\{v^\varepsilon\}$ be a bounded sequence in $L^2(\Omega)$. Then, there exists a subsequence still denoted by $\{v^\varepsilon\}$ and a function $v_0 \in L^2(\Omega\times Y)$ such that $\{v^\varepsilon\}$ two-scale converges to $v_0$, i.e.,*

$$\lim_{\varepsilon\to 0}\int_\Omega v^\varepsilon(x)\psi\left(x,\frac{x}{\varepsilon}\right)dx = \frac{1}{|Y|}\int_\Omega\int_Y v_0(x,y)\psi(x,y)dydx, \tag{5.1}$$

*for any function $\psi = \psi(x,\frac{x}{\varepsilon}) \in \mathcal{D}(\Omega, \mathcal{C}^\infty_{per}(Y)$.*

THEOREM 5.2. *Let $\{v^\varepsilon\}$ be a sequence of functions in $H^1(\Omega)$ such that $v^\varepsilon \rightharpoonup v_0$ weakly in $H^1(\Omega)$. Then $\{v^\varepsilon\}$ two-scale converges to $v_0$ and there exists a subsequence, still denoted by $\{v^\varepsilon\}$, and $v_1 = v_1(x,y)$ in $L^2(\Omega;\mathcal{W}_{per}(Y))$ such that $\nabla v^\varepsilon$ two-scale converges to $\nabla_x v_0 + \nabla_y v_1$.*

*Proof.* **(Proof of** (3.13)**).** Since $D^\varepsilon$ is in $L^\infty(Y)$ and $\nabla v_0(x) + \nabla_y v_1(x,y)$ is in $\mathcal{D}(\Omega, \mathcal{C}^\infty_{per}(Y)$, $D^\varepsilon(\nabla v_0(x) + \nabla_y v_1(x,y))$ can be used as test function in the two-scale convergence of $\nabla C^\varepsilon$. Consequently,

$$\begin{aligned}&\lim_{\varepsilon\to 0}\int_\Omega D^\varepsilon \nabla C^\varepsilon\left[\nabla v_0(x) + \nabla_y v_1\left(x,\frac{x}{\varepsilon}\right)\right]dx\\ =&\frac{1}{|Y|}\int_\Omega\int_Y D(x,y)(\nabla C^0(x) + \nabla_y C_1(x,y))(\nabla v_0(x) + \nabla_y v_1(x,y))dydx.\end{aligned} \tag{5.2}$$

Similarly, $\nabla_x v_1(x,y)$ can be used as test function, whence

$$\lim_{\varepsilon\to 0}\int_\Omega D^\varepsilon \nabla C^\varepsilon\left[\varepsilon\nabla_x v_1\left(x,\frac{x}{\varepsilon}\right)\right]dx = 0. \tag{5.3}$$

Since $KS_{vs} \sim O(\frac{\varepsilon}{\varepsilon_1}) = O(1)$,

$$\lim_{\varepsilon\to 0}\int_\Omega K C^\varepsilon S_{vs}\left[1-\chi\left(x,\frac{x}{\varepsilon}\right)\right]\left[v_0(x) + \varepsilon v_1\left(x,\frac{x}{\varepsilon}\right)\right]dx$$

$$
\begin{aligned}
&=\lim_{\varepsilon\to 0}\frac{1}{|Y|}\int_\Omega\int_Y KS_{vs}C^0(1-\chi(x,y))(v_0(x)+\varepsilon v_1(x,y))dydx\\
&=\int_\Omega KS_{vs}C^0(1-\phi_l)v_0(x)dx.
\end{aligned}\tag{5.4}
$$

Combine the results (5.2)-(5.4) and Equation (3.12), the proof of (3.13) is complete. □

**A.2.** Now we present some definitions and results in [14], and then prove the estimate (3.17). Define the space of solenoidal periodic vector fields, setting

$$
L^2_{sol}(Y)=\{\boldsymbol{p}(y)\in L^2(Y),\quad \text{div}\ \boldsymbol{p}=0 \text{ in } \mathbb{R}^n\}.\tag{5.5}
$$

Then any solenoidal vector field $\boldsymbol{p}\in L^2_{sol}(Y)$ can be represented in the form

$$
p_j=\langle p_j\rangle+\frac{\partial}{\partial y_i}\alpha_{ij},\tag{5.6}
$$

where $\langle p_j\rangle=\frac{1}{|Y|}\int_Y p_j(y)dy$, $\boldsymbol{\alpha}$ is a skew-symmetrical matrix such that $\alpha_{ij}\in H^1(Y)$, $\langle\alpha_{ij}\rangle=0$; see p. 7, [14] for an explicit formula of $\boldsymbol{\alpha}$.

We now give the proof of the estimate (3.17). The difference from arguments on p. 27 in [14] is that some functions here are locally periodic.

$$
\begin{aligned}
&(D^\varepsilon\nabla C_1^\varepsilon)_i=d_{ij}\left(x,\frac{x}{\varepsilon}\right)\frac{\partial C_1^\varepsilon}{\partial x_j}\\
&=\left\{d_{ij}+d_{ik}\frac{\partial N_j(x,y)}{\partial y_k}\Big|_{y=\frac{x}{\varepsilon}}\right\}\frac{\partial C^0}{\partial x_j}+\varepsilon d_{ik}\frac{\partial N_j(x,y)}{\partial x_k}\Big|_{y=\frac{x}{\varepsilon}}\frac{\partial C^0}{\partial x_j}+\varepsilon d_{ij}N_k\left(x,\frac{x}{\varepsilon}\right)\frac{\partial^2 C^0}{\partial x_j\partial x_k}\\
&=d^0_{ij}\frac{\partial C^0}{\partial x_j}+g_{ij}\frac{\partial C^0}{\partial x_j}+\varepsilon d_{ik}\frac{\partial N_j(x,y)}{\partial x_k}\Big|_{y=\frac{x}{\varepsilon}}\frac{\partial C^0}{\partial x_j}+\varepsilon d_{ij}N_k\left(x,\frac{x}{\varepsilon}\right)\frac{\partial^2 C^0}{\partial x_j\partial x_k},
\end{aligned}\tag{5.7}
$$

where $g_{ij}=d_{ij}+d_{ik}\frac{\partial N_j(x,y)}{\partial y_k}\Big|_{y=\frac{x}{\varepsilon}}-d^0_{ij}$, $d_{ij}=(D^\varepsilon)_{ij}$, $d^0_{ij}=(D^0)_{ij}$. Due to Equations (2.6) and (2.7), we can get $\langle g_{ij}\rangle=0$ and $\frac{\partial g_{ij}}{\partial y_i}=0$ in $Y$. Then for each $j=1,\cdots,n$, we can introduce a skew-symmetrical matrix $B_j=(b_{ik,j}(x,y))$ such that $g_{ij}=\frac{\partial}{\partial y_k}(b_{ki,j})$. Then

$$
(D^\varepsilon\nabla C_1^\varepsilon-D^0\nabla C^0)_i=g_{ij}\frac{\partial C^0}{\partial x_j}+\varepsilon d_{ik}\frac{\partial N_j(x,y)}{\partial x_k}\Big|_{y=\frac{x}{\varepsilon}}\frac{\partial C^0}{\partial x_j}+\varepsilon d_{ij}N_k\left(x,\frac{x}{\varepsilon}\right)\frac{\partial^2 C^0}{\partial x_j\partial x_k}.\tag{5.8}
$$

For $v(x)\in H^1_0(\Omega)$,

$$
\begin{aligned}
&\int_\Omega(D^\varepsilon\nabla C_1^\varepsilon-D^0\nabla C^0)\nabla v dx\\
&=\int_\Omega g_{ij}\frac{\partial C^0}{\partial x_j}\frac{\partial v}{\partial x_i}dx+\int_\Omega\left[\varepsilon d_{ik}\frac{\partial N_j(x,y)}{\partial x_k}\Big|_{y=\frac{x}{\varepsilon}}\frac{\partial C^0}{\partial x_j}+\varepsilon d_{ij}N_k\left(x,\frac{x}{\varepsilon}\right)\frac{\partial^2 C^0}{\partial x_j\partial x_k}\right]\frac{\partial v}{\partial x_i}dx,
\end{aligned}\tag{5.9}
$$

where

$$
\begin{aligned}
\int_\Omega g_{ij}\frac{\partial C^0}{\partial x_j}\frac{\partial v}{\partial x_i}dx&=\int_\Omega\frac{\partial}{\partial y_k}(b_{ki,j})\frac{\partial C^0}{\partial x_j}\frac{\partial v}{\partial x_i}dx\\
&=\int_\Omega\varepsilon\frac{\partial}{\partial x_k}\left(b_{ki,j}\left(x,\frac{x}{\varepsilon}\right)\frac{\partial C^0}{\partial x_j}\right)\frac{\partial v}{\partial x_i}dx
\end{aligned}
$$

$$-\varepsilon \int_{\Omega} \frac{\partial b_{ki,j}(x,y)}{\partial x_k}\Big|_{y=\frac{x}{\varepsilon}} \frac{\partial C^0}{\partial x_j}\frac{\partial v}{\partial x_i}dx - \varepsilon \int_{\Omega} b_{ki,j}\left(x,\frac{x}{\varepsilon}\right)\frac{\partial^2 C^0}{\partial x_j \partial x_k}\frac{\partial v}{\partial x_i}dx. \tag{5.10}$$

Since $\frac{\partial}{\partial x_k}\left(b_{ki,j}(x,\frac{x}{\varepsilon})\frac{\partial C^0}{\partial x_j}\right)$ is a solenoidal vector field, the first term in the right-hand side of Equation (5.10) is 0. The second term and the third term on the right-hand side of Equation (5.10) are both of order $\varepsilon$. Then the first term on the right-hand side of Equation (5.9) can be bounded by $A\varepsilon$, and the other terms on the right-hand side of Equation (5.9) are all of order $\varepsilon$. So we have

$$\int_{\Omega}(D^{\varepsilon}\nabla C_1^{\varepsilon} - D^0\nabla C^0)\nabla v dx \le A\varepsilon\|\nabla v\|_{L^2(\Omega)}.$$

Thus the estimate (3.17) is proved.

**A.3.** Here we give a detailed proof of the approximation result (3.4):

$$|(|S_i^*| - |\Gamma^*(x)|)| \le A\varepsilon.$$

We denote by $n(y)$ the unit normal vector to $S_i^* = \{y\in Y | F(\varepsilon(i+y),y)=0\}$ and $\widetilde{n}(x,y) = \widetilde{n}(\varepsilon(i+z),y)$ the unit normal vector to $\Gamma^*(x) = \{y \in Y | F(\varepsilon(i+z),y)=0\}$.

$$\begin{aligned}|\Gamma^*(x)| &= \int_{\Gamma^*(x)} \widetilde{n}(x,y)\cdot\widetilde{n}(x,y)ds = \int_{Y\setminus Y^*(x)} \nabla_y\cdot\widetilde{n}(x,y)dy \\ &= \int_Y (1-\chi(x,y))\nabla_y\cdot\widetilde{n}(x,y)dy = \int_Y (1-\chi(x,y))\nabla_y \cdot \frac{\nabla_y F(x,y)}{|\nabla_y F(x,y)|}dy.\end{aligned}$$

$$\begin{aligned}|S_i^*| &= \int_{s_i^*} n(y)\cdot n(y)ds = \int_Y (1-\chi(\varepsilon(i+y),y))\nabla\cdot n(y)dy \\ &= \int_Y (1-\chi(\varepsilon(i+y),y))\nabla\cdot\frac{\nabla F(\varepsilon(i+y),y)}{|\nabla F(\varepsilon(i+y),y)|}dy \\ &= \int_Y (1-\chi(\varepsilon(i+y),y))\left(\nabla_y\cdot\frac{\nabla_y F(x,y)}{|\nabla_y F(x,y)|}\Big|_{x=\varepsilon(i+y)} + O(\varepsilon)\right)dy,\end{aligned}$$

since $F(x,y)$ is sufficiently smooth.

Let

$$Q(x,y) = \nabla_y\cdot\frac{\nabla_y F(x,y)}{|\nabla_y F(x,y)|}.$$

Then for all $x=\varepsilon(i+z)\in\Omega_i$, we have

$$\begin{aligned}|S_i^*| - |\Gamma^*(x)| &= \int_Y (1-\chi(\varepsilon(i+y),y))\cdot Q(\varepsilon(i+y),y) - (1-\chi(x,y))\cdot Q(x,y)dy + O(\varepsilon) \\ &= \int_{\{y\in Y|F(\varepsilon(i+y),y)<0 \text{ and } F(\varepsilon(i+z),y)<0\}} (Q(\varepsilon(i+y),y) - Q(\varepsilon(i+z),y))dy \\ &\quad + \int_{\{y\in Y|F(\varepsilon(i+y),y)<0 \text{ and } F(\varepsilon(i+z),y)>0\}} Q(\varepsilon(i+y),y)dy \\ &\quad + \int_{\{y\in Y|F(\varepsilon(i+y),y)>0 \text{ and } F(\varepsilon(i+z),y)<0\}} Q(\varepsilon(i+z),y)dy + O(\varepsilon).\end{aligned}$$

The first term of the right-hand side is of order $\varepsilon$ since $Q(\varepsilon(i+z),y)-Q(\varepsilon(i+y),y)=O(\varepsilon)$, and the second term and third term are of order $\varepsilon$ due to both the area of the region $\{y\in Y|F(\varepsilon(i+y),y)<0$ and $F(\varepsilon(i+z),y)>0\}$ and the area of the region $\{y\in Y|F(\varepsilon(i+y),y)>0$ and $F(\varepsilon(i+z),y)<0\}$ being $O(\varepsilon|Y|)$, since $Q$ and $F$ are smooth. Therefore we have proved $|(|S_i^*|-|\Gamma^*(x)|)|\leq A\varepsilon$.

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