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A multiscale domain decomposition approach for chemical vapor deposition

by

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Abstract
We consider the chemical vapor deposition process on a trenched Si-substrate. To understand the process (e.g. the layer conformality) at the trench scale (microscale), we need solutions at both the trench and reactor scales (macroscale). Due to huge difference in the sizes of these scales, straightforward numerical computations are very challenging. To overcome this difficulty, we consider a multiscale approach by introducing an intermediate scale (mesoscale). We start with time-continuous model describing the transport processes and then perform time discretization. At each time step, using the ideas of domain decomposition inspired from [4], we provide an iterative coupling conditions for these three different scales. Using weak formulation for the time-discrete equations, we prove the convergence of this iterative scheme at each time-step. The approach also provides an alternative proof for the existence of the solutions for the time-discrete formulation.

1 The motivation
This work is motivated by the chemical vapor deposition (CVD) processes involved in the manufacturing of the 3-D all-solid-state batteries. In this process, a carrier gas flows through a tube with rectangular cross-section (the reactor). A Silicon (Si) substrate is placed at the bottom of the reactor. The carrier gas transports a small amount of reactive substances, the precursors. These precursors react at the substrate, which becomes the lower part of the reactor boundary, where a solid layer is produced [6, 7, 8]. This leads to an overall transport process with reactions at the boundary. The details on the mathematical models are provided in Section 3.

To increase the energy storage capacity of the batteries, the geometries of the Si substrate is made complex. To increase the surface area, trenches are etched in the Si-substrate, which has therefore a rough surface instead of being flat. The typical size of a trench is in the order of micrometers (∼ 10 µm), whereas the substrate size is in the order ∼ 30 cm. This evidently indicates the existence of two distinct scales in the problem, the trench scale (referred as the microscale) and the reactor scale (the macroscale).

For a thorough understanding of the CVD process, in particular the conformality of the deposited layers, one needs an accurate computation of the solution at the trench scale. However, this requires computing the solution at the reactor scale as well. The scale difference (an order of ∼ 10^5) makes a direct numerical simulation computationally demanding because of the very fine mesh required for resolving the trench scale. Alternatively, we zoom-in a small region of the reactor near the region of interest, the substrate. This introduces an intermediate scale, henceforth referred to as mesoscale. Next we zoom-in a small region of the mesoscale where the trenches (the microscale) can be identified. These three domains are thus formed as a result of successive zooming-in so that the trenches are resolved only at the microscale, and the mesoscale is used only for exchanging the information from the macroscale to the microscale. To compute the solution at each scale, coupling conditions between the different scales are needed. In
doing so, we use ideas from the domain decomposition method. Our aim here is providing a numerical scheme allowing to compute the detailed solutions at each scale. The focus being on the numerics for the transport equations, we consider a simple flow model, allowing a complete decoupling from the transport equations. Further, the flow is computed only at the macroscale and projected further at the mesoscale. However, the transport equations describing the concentration of the reactants (precursor) are defined in all the three scales. The coupling between different scales is through the boundary conditions providing the continuity of the concentration and of the normal fluxes. To achieve this we first perform the time discretization of the model. Then, at each time-step, an iterative non-overlapping domain decomposition algorithm [4] is considered. The iteration involves a linear combination of the normal fluxes and the concentrations at the separating boundaries, allowing a decoupling of the models at the different scales. For the iterative scheme, rigorous convergence results are obtained by compactness arguments. This approach allows a comparison of the numerical results with the experimental results, and to identify parameters such as the diffusion coefficient and the reaction rate constants for the deposition process. This can hence be used to predict the deposition at alternative conditions and also for different geometries.

Below we briefly describe the geometry in Section 2 and provide the mathematical model in Section 3. In Section 4, we give the definitions of the weak solutions for both the time-continuous and the time-discrete equations. Next, the iterative non-overlapping domain decomposition algorithm is considered. This is followed by the proof of convergence of this iterative numerical method.

2 The mathematical model

In this section we give a simplified mathematical model for the motivating application. This model describes the reactive flow inside a reactor, with reactions taking place on the substrate being a part of the boundary. Before giving the equations we give some details regarding the geometry of the system, justifying the multi-scale approach. The scales introduced above (macro-, meso- and microscale) are involving three domains, \( \Omega_1, \Omega_2 \) and \( \Omega_3 \). Their boundaries are denoted by respectively \( \partial \Omega_j, j = 1, 2, 3 \). Each boundary \( \partial \Omega_j \) includes a part \( \Gamma_{jR} \) where reactions (depositions) take place. For the other parts of boundaries, let us first consider the microscale. We define \( \Gamma_2 = \partial \Omega_3 \setminus \Gamma_{3R} \), where the the variables in \( \Omega_2 \) and \( \Omega_3 \) are coupled. For the mesoscale, we define two parts of \( \partial \Omega_2 \), namely, \( \Gamma_1 \) and \( \Gamma_2 \). These provide the coupling with \( \Omega_3 \), respectively \( \Omega_1 \). In other words, \( \Gamma_2 = \partial \Omega_3 \cap \partial \Omega_2 \) (the interface between the micro- and the mesoscale), while \( \Gamma_1 = \partial \Omega_1 \cap \partial \Omega_2 \) (the interface between the macro- and the mesoscale). Figure 1 displays these regions and the nomenclatures.

3 The equations

The mathematical model consists of two components: the flow and the reactive transport. The reactive substance (precursor) is transported to the substrate through a combined effect of convective flow and the molecular diffusion.
The flow velocity of the carrier gas is described by the Navier-Stokes system, while the reactive transport processes are described by the linear convection-diffusion equation.

### 3.1 The flow component

The focus here is on the numerics for the reactive transport component. For the flow we consider a simplified setting, allowing a decoupling from the transport part. For instance, thermal effects are disregarded. Next, as suggested by the numerical evidences, the flow is absent in the trenches and therefore the flow is considered only at the macro- and the mesoscale, where no roughness is encountered at the boundary. Further simplifications include that the flow is laminar and incompressible, and no gravity effects are taken into account. It is also assumed that the concentration of the precursor is much smaller than the one of the carrier gas and hence, therefore the flow is not affected by the adsorption of the precursors. Finally, we only consider a steady-state, hence the flow problem needs to be solved once (in the beginning). Under the above assumptions, the flow component of the model reads

\begin{align*}
\text{Continuity:} & \quad \nabla \cdot q = 0, \\
\text{Momentum:} & \quad \nabla \cdot (\rho q q) = \nabla \cdot (\mu (\nabla q + \nabla q^T) - \frac{2}{3} \mu (\nabla \cdot q) I) - \nabla P, 
\end{align*}

in the simple domain \( \Omega_1 \cup \Omega_2 \cup \Gamma_1 \), where \( q \) is the gas velocity and \( P \) its pressure. For the boundary conditions, we provide a parabolic inlet for the velocity (at \( \Gamma_1 \)) and use no-slip boundary conditions at the side walls. We prescribe pressure at the outlet \( \Gamma_o \).

\[
q = q_d \quad \text{on} \quad \Gamma_d; \quad P = P_0 \quad \text{on} \quad \Gamma_o; \quad \text{and} \quad q = 0 \quad \text{on} \quad \Gamma_2 \cup \Gamma_{1R} \cup \Gamma_{2R} \cup \Gamma_n,
\]

for instance, in 2-D, the choice of parabolic inlet profile gives \( q_d = Q(\ell^2 - y^2) \), where \( Q \) is a positive constant.

### 3.2 The reactive transport/deposition equations

For the CVD model we restrict to the basic equations, including the convective transport and the molecular diffusion, neglect the reactions taking place in the gas phase and consider the situation when the precursor has only one species. Inside the domain \( \Omega_i \) its concentration is denoted by \( u_i \), where \( i = 1, 2, 3 \) is indexing the scale. For the boundary conditions we assume that the deposition takes place only on the bottom plate (the substrate). For simplicity, we assume a first order kinetics.

#### 3.2.1 The macroscale equations

With \( T > 0 \) standing for the maximal time, at the reactor scale the precursor is modeled by the linear convection-diffusion equation

\[
\partial_t u_1 - \Delta u_1 + q \cdot \nabla u_1 = 0 \quad \text{in} \quad \Omega_1 \times (0,T]
\]

coupled with the reactive boundary conditions

\[
-\nu \cdot \nabla u_1 = C_R u_1 \quad \text{on} \quad \Gamma_{1R} \times (0,T],
\]

where \( C_R \) is the (positive) reaction constant. The macroscale equations are coupled with the micro scale ones at \( \Gamma_1 \subset \partial \Omega_1 \). The boundary \( \partial \Omega_1 = \Gamma_d \cup \Gamma_n \cup \Gamma_o \cup \Gamma_{1R} \cup \Gamma_1 \) and the boundary part \( \Gamma_d \) has non-zero measure where Dirichlet boundary conditions are prescribed, and for \( \Gamma_n \in \Gamma_o \) homogeneous Neuman boundary conditions \( (-\nu \cdot \nabla u_3 = 0) \) are taken.

#### 3.2.2 The mesoscale equations

At the mesoscale we use the same equation for the precursor

\[
\partial_t u_2 - \Delta u_2 + q \cdot \nabla u_2 = 0 \quad \text{in} \quad \Omega_2 \times (0,T]
\]
and the reactive boundary conditions
\[-\nu \cdot \nabla u_2 = C_R u_2 \quad \text{on} \quad \Gamma_{2R} \times (0, T].\] (3.5)

Coupling conditions are imposed along \( \Gamma_2 \cup \Gamma_1 \), as explained in the next section.

### 3.2.3 The microscale equations

The geometrical dimensions of the microscale are comparable to the mean free path length of the gas particles. This means that the diffusion is no longer Fickian, but involves the Knudsen diffusion coefficient, a parameter that can be determined by comparing with experimental results. Further, we ignore the convective term for the transport in the trench as the velocity is negligible. Also, the flux at the mesoscale automatically takes into account the flux due to convection. The deposition process inside the trench is described by the following equations:
\[\partial_t u_3 = D_T \Delta u_3 \quad \text{in} \quad \Omega_3 \times (0, T] \] (3.6)

where \( D_T \) is the diffusion coefficient, outside the trench we use the Fickian diffusion while inside the trench we use different diffusion coefficient. For the boundary conditions we prescribe
\[-\nu \cdot \nabla u_3 = C_R u_3 \quad \text{on} \quad \Gamma_{3R} \times (0, T] \] (3.7)

where \( \Gamma_{3R} \) is the surface on which reactions take place. The remaining boundary part \( \partial \Omega_3 \setminus \Gamma_{3R} \) is involved in the coupling with the mesoscale, as explained below.

### 3.2.4 The coupling conditions

The different scales are coupled by the boundary conditions at non-reactive surfaces. We provide coupling conditions that are natural for this setting of the problem, namely, the flux continuity and the continuity of the concentrations. Specifically, after having fixed the normal \( \nu \) to \( \Gamma_1 \) and into \( \Omega_1 \) we have the following coupling conditions:
\[\nu \cdot (-\nabla u_2 + qu_2) = \nu \cdot (-\nabla u_1 + qu_1) \quad \text{on} \quad \Gamma_1 \] (3.8)

and
\[u_1 = u_2 \quad \text{on} \quad \Gamma_1 \] (3.9)

Similar coupling conditions are imposed at the interface \( \Gamma_2 \) between the microscale and mesoscale.
\[u_2 = u_3 \quad \text{and} \quad \nu \cdot (-\nabla u_2 + qu_2) = -D_T \nu \cdot \nabla u_3 \quad \text{on} \quad \Gamma_2. \] (3.10)

Having specified the boundary conditions, the model is closed by the initial conditions:
\[u_1(0, \cdot) = u_{10}, \quad u_2(0, \cdot) = u_{20}, \quad u_3(0, \cdot) = u_{30}. \] (3.11)

For more general coupling conditions (transmission problems), we refer to [2] and [3].

### 4 The numerical scheme

In this section we analyze the numerical scheme for solving the reactive transport model component, posed in the three sub-domains of the reactor. The scheme is based on the time Euler implicit time stepping. We start by defining the concept of weak solution for both the continuous and the time discrete cases. Then, for the resulting sequence of time discrete problems we give an iterative domain decomposition scheme, and prove its convergence based on compactness arguments.
4.1 The weak form

We start with the concept of weak solution for the coupled model in (3.2)-(3.11), involving standard notations in the functional analysis. In particular, $H^1(\Omega_t)$ is the Sobolev space of functions defined on $\Omega_t$ and having $L^2$ weak derivatives. By $H^1_{0,\Gamma_D}(\Omega_t)$ we mean the functions in $H^1(\Omega_t)$ having a vanishing trace on $\Gamma_D$, and $H^{-1}(\Omega_t)$ is its dual. Further, $L^2(0; T; X)$ is the Bochner space of functions valued in $X$, and $(\cdot, \cdot)_U$ denotes the inner product in $L^2(U)$ (with $U$ a bounded domain) or the duality pairing between $H^1_{0,\Gamma_D}$ and its dual. Finally we define the spaces

$$V_i = \{ u_i \in L^2(0; T; H^1_{0,\Gamma_D}(\Omega_t))/\partial_t u_i \in L^2(0; T; H^{-1}(\Omega_t)) \} \quad i = 1, 2, \text{ or } 3.$$ 

Also, let $\Omega^T_i := \Omega_t \times (0, T)$, $\Gamma^T_{iR} = \Gamma_{iR} \times (0, T)$ and assume that $u^0_i \in H^1_{0,\Gamma_D}(\Omega_t)$ for all $i$.

**Definition 4.1.** A weak solution of (3.2)-(3.11) is a triple $(u_1, u_2, u_3) \in V_1 \times V_2 \times V_3$ satisfying the initial conditions $u_i(0, \cdot) = u^0_i \ (i = 1, 2, \text{ or } 3)$, the boundary conditions

$$u_1 = u_2 \quad \text{at } \Gamma_1, \quad u_2 = u_3 \quad \text{at } \Gamma_2,$$

and

$$\begin{align*}
(\partial_t u_1, \phi_1)_{\Omega^T_1} + (\nabla u_1, \nabla \phi_1)_{\Omega^T_1} + (q \nabla u_1, \phi_1)_{\Omega^T_1} + (C_R u_1, \phi_1)_{\Gamma^T_{1R}} \\
(\partial_t u_2, \phi_2)_{\Omega^T_2} + (\nabla u_2, \nabla \phi_2)_{\Omega^T_2} + (q \nabla u_2, \phi_2)_{\Omega^T_2} + (C_R u_2, \phi_2)_{\Gamma^T_{2R}} \\
+ (\partial_t u_3, \phi_3)_{\Omega^T_3} + (D_T \nabla u_3, \nabla \phi_3)_{\Omega^T_3} + (C_R u_3, \phi_3)_{\Gamma^T_{3R}} = 0.
\end{align*}$$

(4.1)

for all $\phi_i \in L^2(0; T; H^1_{0,\Gamma_D}(\Omega_t))$ such that $\phi_1 = \phi_2$ at $\Gamma_1$ and $\phi_2 = \phi_3$ at $\Gamma_2$.

In this section the equalities at the non-reactive interfaces $\Gamma_1$ and $\Gamma_2$ should be interpreted in the sense of traces. Next we consider the Euler implicit time discretization of (4.1). To this aim we take $t_k = k \Delta t$ and $u^k_i$ approximating $u_i(t_k) \ (i = 1, 2, \text{ or } 3; k = 1, \ldots, N)$, the time discrete solution triple at $t = t_k$ is defined by

**Definition 4.2.** Given $u^{k-1}_i$ we seek for $u^k_i \in H^1_{0,\Gamma_D}(\Omega_t)$ satisfying

$$u^k_1 = u^k_2 \quad \text{at } \Gamma_1, \quad u^k_2 = u^k_3 \quad \text{at } \Gamma_2,$$

and

$$\begin{align*}
\frac{1}{\Delta t} (u^k_i - u^{k-1}_i, \phi_1) + (\nabla u^k_i, \nabla \phi_1) + (q \nabla u^k_i, \phi_1) + (C_R u^k_i, \phi_1)_{\Gamma^T_{1R}} \\
+ \frac{1}{\Delta t} (u^k_1 - u^{k-1}_1, \phi_2) + (\nabla u^k_2, \nabla \phi_2) + (q \nabla u^k_2, \phi_2) + (C_R u^k_2, \phi_2)_{\Gamma^T_{2R}} \\
+ \frac{1}{\Delta t} (u^k_3 - u^{k-1}_3, \phi_3) + (D_T \nabla u^k_3, \nabla \phi_3) + (C_R u^k_3, \phi_3)_{\Gamma^T_{3R}} = 0.
\end{align*}$$

(4.2)

for all $\phi_i \in H^1_{0,\Gamma_D}(\Omega_t)$, such that that $\phi_1 = \phi_2$ on $\Gamma_1$ and $\phi_2 = \phi_3$ on $\Gamma_2$.

Note that in either the continuous case or the time discrete one, the equations posed in each subdomain are coupled by imposing explicitly the continuity of the concentrations at the non-reactive surfaces $\Gamma_1 \cup \Gamma_2$. The flux continuity instead is a consequence of the fact that the test functions $\phi_i$ are also equal along these surfaces. In this way, the boundary terms along $\Gamma_1 \cup \Gamma_2$ can only vanish if the outwards normal components of the fluxes cancel each other.

The numerical iterative scheme considered here also provides proof for the existence for the time-discrete formulation. Further, one can treat more complicated reaction rates (for example, Lipschitz reaction rates) by considering Euler explicit time stepping in the reaction term. For numerical reasons, we formulate the original problem in the three (non-overlapping) domains. This allows separating the computations at the trench scale from those at the reactor scale without requiring any correlation between the meshes employed at the different scales.

Having introduced the weak solutions above, we now consider a numerical scheme to compute the solution at each time step and investigate its convergence. To simplify the presentation we fix a time step $\Delta t$ and define

$$v_i := u_i^k, \quad i = 1, 2, 3,$$

so that all the estimates are obtained in terms of $v_i$. 

5
4.2 The iterative domain decomposition scheme

Here we describe the iterative scheme used for solving the time-discrete problem (4.2). The scheme is inspired from [4, 5]. To understand its background, we consider first consider the strong form of the equation and define the quantities ($n_1$ is the normal to $\Gamma_1$ and into $\Omega_1$ $n_2$ is normal to $\Gamma_2$ and into $\Omega_2$)

\begin{align*}
g_{21} &= v_1 \cdot -\nabla v_2 + \lambda v_2 \quad \text{and} \quad g_{12} := v_1 \cdot \nabla v_1 + \lambda v_1 \quad \text{on} \quad \Gamma_1, \quad \text{(4.3)}
g_{23} &= v_2 \cdot \nabla v_2 + \lambda v_2 \quad \text{and} \quad g_{32} := -v_2 \cdot D_T \nabla v_3 + \lambda v_3 \quad \text{on} \quad \Gamma_2, \quad \text{(4.4)}
\end{align*}

where $\lambda > 0$ is a positive constant. For the convergence proof, it suffices to have $\lambda > 0$ however, its value influences the speed of convergence [1]. Note that the $g_{ij}$ terms depend on the time step $k$ and define (decoupling) boundary conditions at the non-reacting interfaces. To ensure that the solving the decoupled problems are providing a solution of the originally coupled one, additional conditions will be given later.

Based on the above we let $n \in \mathbb{N}$ denote the iteration index and construct the $n^{th}$ as the solution of

**Problem $P^n$**: Given $v_i^{n-1} \in H^1_{0, \Gamma_D}(\Omega_i)$ and $g_{ji}^{n-1} \in H^{1/2}_{1/1, \Gamma_2} (i, j = 1, 2, 3)$, find $v_i^n \in H^1_{0, \Gamma_D}(\Omega_i)$ and $g_{ij}^n (i, j = 1, 2, 3)$ such that

\begin{align*}
\frac{1}{\Delta t} (v_1^n, \phi_1) + (\nabla v_1^n, \nabla \phi_1) + (C_R u_1^n, \phi_1)_{\Gamma_1} + (g_{12}^n, \phi_1)_{\Gamma_1} &= (u_1^{k-1}, \phi_1) - (q \nabla u_1^{k-1}, \phi_1), \\
\frac{1}{\Delta t} (v_2^n, \phi_2) + (\nabla v_2^n, \nabla \phi_2) + (C_R u_2^n, \phi_2)_{\Gamma_2} + (g_{21}^n, \phi_2)_{\Gamma_2} &= (u_2^{k-1}, \phi_2) - (q \nabla u_2^{k-1}, \phi_2), \\
\frac{1}{\Delta t} (v_3^n, \phi_3) + (\nabla v_3^n, \nabla \phi_3) + (C_R u_3^n, \phi_3)_{\Gamma_3} + (g_{32}^n, \phi_3)_{\Gamma_3} &= (u_3^{k-1}, \phi_3).
\end{align*}

(4.5)

for all $\phi_i \in H^1_{0, \Gamma_D}(\Omega_i)$, such that $\phi_1 = \phi_2$ on $\Gamma_1$ and $\phi_2 = \phi_3$ on $\Gamma_2$, and

\begin{equation}
g_{ij}^n := 2\lambda v_i^{n-1} - g_{ji}^{n-1}. \tag{4.8}
\end{equation}

The iterative scheme requires a starting triple $(v_1^0, v_2^0, v_3^0)$. Since the problem under consideration is, in fact, an evolution one, a good option is $v_i^0 = u_i^{k-1}$. However, this choice is not required for the convergence proof below. Further, $g_{ij}^0 = -\nabla v_i^0 + \lambda u_i^0$ for $i \neq 3$; and $g_{ij}^2 = -\nu \cdot D_T \nabla v_3^0 + \lambda v_3$.

For the notation, we remind that $k$ is the time-step and $n$ stands for the iteration index. Thus $v_i^n$ stands for $u_i^{k,n}$, the $n$-th iterate at time step $t = t_k$. Note that at each iterative step $n$, the equations are decoupled by the boundary conditions obtained from the previous iterative step.

Before giving a rigorous convergence proof, we give a formal justification of the iterative scheme. Assuming that $v_i^n \rightarrow v_i$ and $g_{ij}^n \rightarrow g_{ij}$, passing to the limit in the updates (4.8) gives

\begin{equation}
g_{ij} = 2\lambda v_j - g_{ji}. \tag{4.9}
\end{equation}

In other words, at $\Gamma_1$ we have

\begin{equation}
g_{12} = 2\lambda v_2 - g_{21}, \quad \text{and} \quad g_{21} = 2\lambda v_1 - g_{12},
\end{equation}

implying $v_2 = v_1$. Once the continuity is established, the following simple calculation establishes the equality of normal component of diffusive fluxes at $\Gamma_1$

\begin{equation}
\nu_1 \cdot \nabla v_1 - \nu_1 \cdot \nabla v_2 + \lambda (v_1 + v_2) = g_{12} + g_{21} = 2\lambda v_1 = \lambda (v_1 + v_2).
\end{equation}

The justification of the coupling conditions at $\Gamma_2$ is completely similar.
In the formal definition of $g_{ij}$ above, we have only included the normal diffusive flux. This is because equality of normal component of diffusive flux together with the continuity of concentration also implies the equality of normal flux. Clearly,

$$\nu_1 \cdot (-\nabla u_2 + q u_2) = \nu_1 \cdot (-\nabla u_1 + q u_1) \quad \text{on } \Gamma_1$$

and similarly for $\Gamma_2$.

### 4.3 The convergence proof

We follow the ideas in [4] and the main ideas of the proof are obtaining apriori estimates for $v^n_i$ and using compactness arguments to show the $H^1$ convergence in space. Application of compact embeddings and trace inequalities lead to establishing convergence on the boundaries. It is afterwards of no particular difficulty to prove that the limits satisfy the time-discrete formulation (4.2).

We have the following theorem:

**Theorem 4.1.** As $n \to \infty$, the solutions $v^n_i$ satisfying (4.5)-(4.7) converge weakly to $v_i$ in $H^1(\Omega_i)$ norm satisfying (4.2).

#### 4.3.1 Apriori estimates

To prepare the proof of Theorem 4.1, we define the following

$$e^n_i := v^n_i - v^{n-1}_i \quad (i = 1, 2, 3), \quad (4.9)$$

$$e^n_{1,1} := g^n_{1,2} - g^{n-1}_{1,2}, \quad e^n_{2,1} = g^n_{2,1} - g^{n-1}_{2,1}, \quad (4.10)$$

$$e^n_{3,1} := g^n_{3,2} - g^{n-1}_{3,2}, \quad e^n_{4,1} = g^n_{4,2} - g^{n-1}_{4,2}, \quad (4.11)$$

$$e^{n+1}_{1,1} := [(e^n_{1,1})^2 + (e^n_{2,1})^2]^{1/2}, \quad e^{n+1}_{1,1} := [(e^n_{3,1})^2 + (e^n_{4,1})^2]^{1/2}. \quad (4.12)$$

With these definitions in mind, we have the following Lemma.

**Lemma 4.1.**

$$\sum_{n=1}^{N} \left( ||e^n_1||^2_{\Omega_1} + ||e^n_2||^2_{\Omega_1} + ||e^n_2||^2_{\Omega_2} + ||e^n_3||^2_{\Omega_2} \right) \leq C. \quad (4.13)$$

**Proof.** Subtracting (4.5) for $v^n_i - 1$ from the one for $v^n_i$ gives

$$\frac{1}{\Delta t} (v^n_i - v^{n-1}_i, \phi_i)_{\Omega_i} + (\nabla e^n_i - \nabla v^{n-1}_i, \nabla \phi_i)_{\Omega_i} + (v^n_i - v^{n-1}_i, \phi_i)_{\Gamma_i,1} + \lambda (v^n_i - v^{n-1}_i, \phi_i)_{\Gamma_i,1} - (g^n_{1,2} - g^{n-1}_{1,2}, \phi_i)_{\Gamma_i,1} = 0. \quad (4.14)$$

Taking in the above $\phi_i = e^n_i$ leads to

$$\frac{1}{\Delta t} ||e^n_i||^2_{\Omega_i} + ||\nabla e^n_i||^2_{\Omega_i} + ||e^n_i||^2_{\Gamma_i,1} + \lambda (e^n_i, e^n_i)_{\Gamma_i} = (e^n_{1,1}, e^n_{1,1})_{\Gamma_1}. \quad (4.15)$$

In a similar manner one gets

$$\frac{1}{\Delta t} ||e^n_2||^2_{\Omega_2} + ||\nabla e^n_2||^2_{\Omega_2} + ||e^n_2||^2_{\Gamma_2,1} + \lambda (e^n_2, e^n_2)_{\Gamma_2} = (e^n_{2,1}, e^n_{2,1})_{\Gamma_1} + (e^n_{3,1}, e^n_{3,1})_{\Gamma_1} \quad (4.16)$$

and

$$\frac{1}{\Delta t} ||e^n_3||^2_{\Omega_3} + ||\nabla e^n_3||^2_{\Omega_3} + ||e^n_3||^2_{\Gamma_3,1} + \lambda (e^n_3, e^n_3)_{\Gamma_3} = (e^n_{4,1}, e^n_{4,1})_{\Gamma_1} + (e^n_{5,1}, e^n_{5,1})_{\Gamma_1}. \quad (4.17)$$
Recalling the notations in (4.10)-(4.12), we have

\[
(e_{11}^{n+1})^2 = (g_{12}^{n} - g_{21}^{n})^2 + (g_{21}^{n} - g_{12}^{n})^2
\]

\[
= (2\lambda(v_2^n - v_{21}^{n-1}) - g_{21}^{n} + g_{21}^{n-1})^2 + (2\lambda(v_1^n - v_{12}^{n-1}) - g_{12}^{n} + g_{12}^{n-1})^2
\]

\[
= (2\lambda(v_2^n - v_{21}^{n-1}) - e_{21}^{n} + e_{21}^{n-1})^2 + (2\lambda(v_1^n - v_{12}^{n-1}) - e_{12}^{n} + e_{12}^{n-1})^2
\]

\[
= (e_{11}^{n} + e_{21}^{n})^2 + (e_{22}^{n})^2 + 4\lambda(\lambda(v_1^n - v_{11}^{n-1}) - e_{11}^{n})((v_1^n - v_{11}^{n-1})
\]

\[
+ 4\lambda(\lambda(v_2^n - v_{21}^{n-1}) - e_{21}^{n})((v_2^n - v_{21}^{n-1})
\]

By (4.12) this gives

\[
(e_{11}^{n+1})^2 - (e_{11}^{n})^2 = 4\lambda(\lambda(v_1^n - e_{11}^{n}) - e_{11}^{n} + (v_1^n - e_{11}^{n} - e_{11}^{n})e_{11}^{n} - 1).
\]

Similarly,

\[
(e_{22}^{n+1})^2 - (e_{22}^{n})^2 = 4\lambda(\lambda(v_2^n - e_{22}^{n}) - e_{22}^{n} + (v_2^n - e_{22}^{n} - e_{22}^{n})e_{22}^{n} - 1).
\]

With the above, adding (4.15) - (4.17) gives

\[
\frac{1}{\Delta t}||e_{11}^{n+1}||_\Omega^2 + ||\nabla e_{11}^{n+1}||^2 + ||e_{11}^{n}||^2_\Omega + ||e_{22}^{n}||^2_\Omega + ||e_{33}^{n}||^2_\Omega + \frac{1}{\Delta t}||e_{22}^{n}||^2_\Omega + ||\nabla e_{22}^{n}||^2_\Omega
\]

\[
+ \frac{1}{\Delta t}||e_{33}^{n}||^2_\Omega + ||\nabla e_{33}^{n}||^2_\Omega + \frac{1}{4\lambda} ||(e_{11}^{n+1})^2 - (e_{11}^{n})^2 - e_{11}^{n+1} - e_{11}^{n}||^2_\Omega = 0.
\]

Summing the above over \(n = 1 \cdots N\) leads to

\[
||e_{11}^{n+1}||^2 + ||e_{22}^{n+1}||^2 + 4\lambda \sum_{n=1}^{N} (||\nabla e_{11}^{n}||^2 + ||\nabla e_{22}^{n}||^2 + ||\nabla e_{33}^{n}||^2) + 4\lambda \Delta t \sum_{n=1}^{N} (||e_{11}^{n}||^2_\Omega + ||e_{22}^{n}||^2_\Omega + ||e_{33}^{n}||^2_\Omega)
\]

\[
+ ||e_{11}^{n}||^2_\Omega + ||e_{22}^{n}||^2_\Omega + ||e_{33}^{n}||^2_\Omega \leq C
\]

In particular, by the trace theorem this implies

\[
\sum_{n=1}^{N} (||e_{11}^{n}||^2_\Omega + ||e_{22}^{n}||^2_\Omega + ||e_{33}^{n}||^2_\Omega) \leq C
\]

which concludes the proof.

Lemma 4.1 implies that the series on the left of (4.13) is finite, therefore the (error) terms are converging to 0. However, this is not sufficient to prove the desired convergence result.

Lemma 4.2.

\[
\sum_{i=1}^{3} ||v_i^N||^2_{H^1(\Omega_i)} + \sum_{n=1}^{N} (||v_i^{n+1} - v_i^n||^2 + ||v_i^{n+1} - v_i^{n}||^2 + ||v_i^{n+1} - v_i^n||^2 + ||v_i^n - v_i^{n-1}||^2 + ||v_i^{n+1} - v_i^n||^2) \leq C
\]

with \(C\) independent of \(N\) and depends on the initial data.

Proof. We start by observing that

\[
g_{12}^{n+1} - g_{12}^{n-1} = 2\lambda v_2^n - 2\lambda v_{12}^{n-1}, \quad g_{21}^{n+1} - g_{21}^{n-1} = 2\lambda v_1^n - 2\lambda v_{12}^{n-1},
\]

\[
g_{23}^{n+1} - g_{23}^{n-1} = 2\lambda v_3^n - 2\lambda v_{23}^{n-1}, \quad g_{32}^{n+1} - g_{32}^{n-1} = 2\lambda v_2^n - 2\lambda v_{32}^{n-1}.
\]

Further, we have the elementary identities

\[
(v_i^{n+1} - v_i^{n-1}, v_i^{n+1}) = \frac{1}{2} ||v_i^{n+1}||^2 + \frac{1}{2} ||v_i^{n-1}||^2 - \frac{1}{2} ||v_i^{n-1}||^2,
\]

\[
(\nabla (v_i^{n+1} - v_i^{n-1}), \nabla v_i^{n+1}) = \frac{1}{2} ||\nabla v_i^{n+1}||^2 + \frac{1}{2} ||\nabla (v_i^{n+1} - v_i^{n-1})||^2 - \frac{1}{2} ||\nabla v_i^{n-1}||^2,
\]

\[
(v_i^{n+1} + v_i^{n-1} - 2v_i^n, v_i^{n+1}) = \frac{1}{2} ||v_i^{n+1}||^2 + \frac{1}{2} ||v_i^{n-1}||^2 - ||v_i^n||^2 + ||v_i^{n+1} - v_i^n||^2 - \frac{1}{2} ||v_i^{n+1} - v_i^{n-1}||^2.
\]
We now proceed as in Lemma 4.1 and subtract (4.5)-(4.7) for $v_{i}^{n-1}$ from the one for $v_{i}^{n}$, test the resulting with $\phi = v_{i}^{n+1}$, and double the resulting and summing it over $n = 1, \ldots, N$ to obtain

$$\frac{1}{\Delta t} \sum_{i=1}^{3} \left( ||v_{i}^{N+1}||_{2}^{2} + ||v_{i}^{n}||_{2}^{2} \right) + \sum_{i=1}^{3} \left( ||\nabla v_{i}^{N+1}||_{2}^{2} + ||\nabla v_{i}^{n}||_{2}^{2} \right)$$

$$+ \frac{1}{\Delta t} \sum_{n=1}^{N} \sum_{i=1}^{3} ||v_{i}^{n+1} - v_{i}^{n-1}||_{2}^{2} + \sum_{n=1}^{N} \sum_{i=1}^{3} ||\nabla v_{i}^{n+1} - \nabla v_{i}^{n-1}||_{2}^{2} + \sum_{i=1}^{3} \left( ||v_{i}^{n+1}||_{r_{1}}^{2} + ||v_{i}^{n}||_{r_{11}}^{2} \right)$$

$$+ 2 \sum_{n=1}^{N} \left( ||v_{i}^{n+1} - v_{i}^{n-1}||_{r_{11}}^{2} + ||v_{i}^{n+1} - v_{i}^{n-1}||_{r_{2}}^{2} + ||v_{i}^{n+1} - v_{i}^{n-1}||_{r_{3}}^{2} \right)$$

$$\leq C + \sum_{n=1}^{N} \left( ||v_{i}^{n+1} - v_{i}^{n-1}||_{r_{1}} + ||v_{i}^{n+1} - v_{i}^{n-1}||_{r_{2}} + ||v_{i}^{n+1} - v_{i}^{n-1}||_{r_{3}} \right).$$

Using (4.18) in the above yields

$$\sum_{i=1}^{3} \left( ||v_{i}^{N}||_{2}^{2} + ||\nabla v_{i}^{N}||_{2}^{2} \right) + \sum_{n=1}^{N} \left( ||v_{i}^{n+1} - v_{i}^{n-1}||_{2}^{2} + ||v_{i}^{n+1} - v_{i}^{n}||_{2}^{2} + ||v_{i}^{n+1} - v_{i}^{n}||_{2}^{2} + ||v_{i}^{n} - v_{i}^{n-1}||_{2}^{2} \right) \leq C$$

(4.20)

with $C$ independent of $N$ and depending only on the initial data. \hfill \Box

4.3.2 Proof of Theorem 4.1

**Proof.** Lemma 4.2 provides enough compactness to pass to the limit. Note that (4.20) implies that there exists a subsequence again denoted by $v_{i}^{n}$ such that

$$v_{i}^{n} \rightharpoonup v_{i} \quad \text{weakly in} \quad H^{1}(\Omega_{i})$$

and hence, strongly in $L^{2}(\Omega_{i})$. Further, to establish the continuity of the concentration at the boundaries, let us take for instance,

$$||v_{i} - v_{j}||_{r_{i}} \leq ||v_{i} - v_{i}^{n+1}||_{r_{i}} + ||v_{j}^{n+1} - v_{j}||_{r_{i}} + ||v_{i}^{n+1} - v_{j}^{n+1}||_{r_{i}}$$

whereby the last term on the right hand side vanishes because of estimate (4.20). The vanishing of the first two terms are consequence of weak convergence in $H^{1}$ leading to $L^{2}$ strong convergence at the boundaries. Similarly,

$$v_{2} = v_{3}$$

at the boundary $\Gamma_{2}$. From the preceding discussions, we conclude that the triple $(v_{1}, v_{2}, v_{3}) \equiv (u_{1}, u_{2}, u_{3})$ satisfies

$$\frac{1}{\Delta t} \left( u_{2}^{k} - u_{1}^{k-1}, \phi_{1} \right) + (\nabla u_{2}^{k}, \nabla \phi_{1}) - (q \nabla u_{1}^{k-1}, \phi_{1})$$

$$+ (C_{R} u_{1}^{k}, \phi_{1})_{\Gamma_{1n}} + \frac{1}{\Delta t} \left( u_{2}^{k} - u_{2}^{k-1}, \phi_{2} \right) + (\nabla u_{2}^{k}, \nabla \phi_{2}) - (q \nabla u_{2}^{k-1}, \phi_{2})$$

$$+ (C_{R} u_{2}^{k}, \phi_{2})_{\Gamma_{2n}} + \frac{1}{\Delta t} \left( u_{3}^{k} - u_{3}^{k-1}, \phi_{3} \right) + (D_{T} \nabla u_{3}^{k}, \nabla \phi_{3}) + (C_{R} u_{3}^{k}, \phi_{3})_{\Gamma_{3n}} = 0$$

for all $\phi_{i} \in H^{1}(\Omega_{i})$ such that $\phi_{1} = \phi_{2}$ at $\Gamma_{1}$ and $\phi_{2} = \phi_{3}$ at $\Gamma_{2}$. \hfill \Box

References


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