

HOMOGENIZATION AND DIMENSION REDUCTION OF FILTRATION COMBUSTION IN HETEROGENEOUS THIN LAYERS

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ABSTRACT. We study the homogenization of a reaction-diffusion-convection system posed in an ε -periodic δ -thin layer made of a two-component (solid-air) composite material. The microscopic system includes heat flow, diffusion and convection coupled with a nonlinear surface chemical reaction. We treat two distinct asymptotic scenarios: (1) For a fixed width $\delta > 0$ of the thin layer, we homogenize the presence of the microstructures (the classical periodic homogenization limit $\varepsilon \rightarrow 0$); (2) In the homogenized problem, we pass to $\delta \rightarrow 0$ (the vanishing limit of the layer's width). In this way, we are preparing the stage for the simultaneous homogenization ($\varepsilon \rightarrow 0$) and dimension reduction limit ($\delta \rightarrow 0$) with $\delta = \delta(\varepsilon)$. We recover the reduced macroscopic equations from [25] with precise formulas for the effective transport and reaction coefficients. We complement the analytical results with a few simulations of a case study in smoldering combustion. The chosen multiscale scenario is relevant for a large variety of practical applications ranging from the forecast of the response to fire of refractory concrete, the microstructure design of resistance-to-heat ceramic-based materials for engines, to the smoldering combustion of thin porous samples under microgravity conditions.

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1. Introduction.

1.1. Aim of the paper. We wish to investigate the sub-sequential homogenization and dimension reduction limits for a reaction-diffusion-convection system coupled with a non-linear differential equation posed in a periodically-distributed array of microstructures; see [25, 24] for details on the smoldering combustion context inspiring this paper. To prove the homogenization limit we employ the two-scale convergence (cf. e.g. [8, 33, 19]). Relying on the estimates obtained here, we hope to be able to deal at a later stage with the boundary layers occurring during the simultaneous homogenization-dimension reduction procedure. We expect that the concept of two-scale convergence for thin heterogeneous layers (see [36]) and appropriate scaling arguments, somewhat similar to the spirit of [5, 10], are applicable. A similar strategy would be to use a periodic unfolding operator depending on two parameters [14]. It is worth noting that the simultaneous homogenization and dimension reduction limit is a relevant research topic related to the rigorous derivation of plate theories, but also away from the elasticity framework; see e.g. [20, 1, 34] and references cited therein.

This paper prepares a framework where such a simultaneous limit can be done for a filtration combustion scenario.

1.2. Mathematical background. Homogenization of problems depending on two or more small parameters is a useful averaging tool when dealing for instance with reticulated structures (see e.g. [15]) or with porous media with thin fractures (see e.g. [5]). Often in such cases, the small parameters correspond to scale-separated processes and can therefore be treated as being independent of each other. The most challenging mathematical situation is when the two small parameters are interrelated, i.e. $\delta = \delta(\varepsilon)$ where $\varepsilon > 0$ takes into account the periodicity scale (or the length scale of a reference elementary volume) and $\delta > 0$ a typical length scale of the microstructure. This kind of scaling dependence $\delta = \delta(\varepsilon)$ with $\delta > \varepsilon > 0$ makes such setting resemble a boundary layer case. Essentially, due to the lack of scale separation, one can easily imagine that when passing to $\delta \rightarrow 0$ one loses the information at the ε -scale; like for instance, in the balance of measures setting discussed in [41].

1.3. Estimating the heat response of materials with microstructure. Homogenization of heat transfer scenarios has attracted the attention of many researchers in the last years; see for instance the references indicated in [49, 33, 4] as well as in the doctoral thesis by Habibi [21] (where the focus is on the radiative transfer of heat). For a closely related multiscale setting where convection interplays with diffusion and chemistry, we refer the reader to the elementary presentation of the main issues given in [47]. For a computational approach to heat conduction in multiscale solids, see [40].

The practical application we have in mind needs the multiscale modeling of reverse smoldering combustion, aiming at understanding the behavior of fingering patterns that arise from a controlled experimental study of smoldering combustion of thin porous samples under microgravity conditions. The details of such an experimental scenario have been reported previously in [51, 39], and treated mathematically in different contexts [26, 18, 32, 50]. In all these papers, the models are introduced directly at the macroscopic scale and less attention is paid on the choice of microstructures as well as to the influence of physical processes at the pore scale. Our paper wishes to fill some gaps in this direction. There are also other

related studies [43, 38] dealing with averaging of combustion processes. Closely related application areas include the design of microstructures for refractory concrete – a composite heterogeneous material with special chemical composition (meant to postpone de-hydration [44]), also referred to as blast furnace. The refractory concrete materials are expected to sustain high temperatures and moderate convection, typical of situations arising in the furnace of steel factories; for more details see [7] and references cited therein.

1.4. Organization of the material. We proceed as follows: We first ensure the solvability of the microscopic combustion model. Then we check how the model responds to the application of the two-scale convergence as $\varepsilon \rightarrow 0$ for the case $\delta = \mathcal{O}(1)$ recovering in this way the structure of the averaged model equations obtained in [25] by means of formal asymptotics homogenization. Then as next step, the limit $\delta \rightarrow 0$ turns to be a regular perturbation scenario that we approach with techniques inspired by the averaging of reticulated geometries; see [15]. Using the macroscopic equations obtained in the case $\varepsilon \rightarrow 0$ for $\delta \rightarrow 0$, we illustrate numerically the instability of combustion fingers as observed experimentally in [51]. Finally, we conclude the paper with a brief enumeration of a couple of open problems arising from this filtration combustion scenario.

The paper is organized in the following fashion:

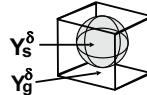
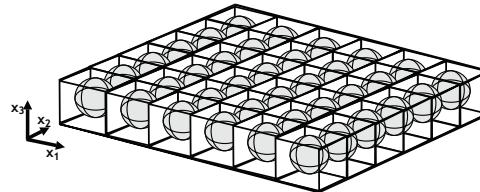
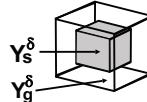
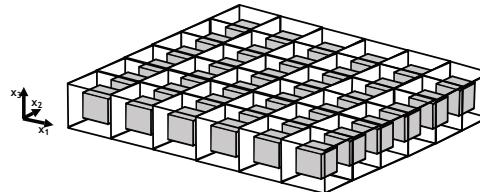
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2. Notations. Choice of microstructures. Unknowns. The geometry of the porous material we have in mind is depicted in Figure 2 and in Figure 4. It is basically obtained by replicating and then glueing periodically the unit cell/pore structures shown in Figure 1 and Figure 3.

To describe the porous structure of the medium, the following notations will be used (very much in the spirit of [23]): The time interval of interest is $[0, T]$, $0 < T < \infty$. Assume the scale factors $\varepsilon > 0$ and $\delta > 0$ to be given³. A straightforward

³Actually, ε and δ are sequences of strictly positive numbers going to zero such that $(\frac{1}{\varepsilon}, \frac{1}{\delta}) \in \mathbb{N}^2$.

FIGURE 1. δ -cell (ball microscopic fabric).FIGURE 2. Periodically-distributed array of cells contained in a ε -thin layer.FIGURE 3. δ -cell (parallelepiped microscopic fabric).FIGURE 4. Periodically-distributed array of cells contained in a ε -thin layer.

dimensional analysis connects them with the characteristic length and time scales in the system; see the scaling discussion on the meaning of ε from Section 3.2 in [24].

Our representative pore, Y^δ , contains two phases: a connected solid phase Y_s^δ and a connected gas phase such that $Y^\delta = Y_g^\delta \cup \overline{Y_s^\delta}$; see Figure 1 and Figure 3 for sketches of admissible microstructures Y^δ . To fix ideas, take now Y^δ to be the δ -cell

$$Y^\delta := \left\{ \sum_{i=1}^3 \lambda_i e_i : 0 < \lambda_i < 1 (i = 1, 2), -\frac{\delta}{2} < \lambda_3 < \frac{\delta}{2} \right\},$$

where e_i is the i th unit vector in \mathbb{R}^3 . Correspondingly, $Y^\delta := Y_g^\delta \cup \overline{Y_s^\delta}$, where Y_g^δ and Y_s^δ are δ -dilated versions of Y_g and Y_s . Two options of microstructures model here the internal structure of the solid fabrics: (1) Figure 1 indicates that Y^δ contains a ball that does not touch ∂Y^δ , and (2) Figure 3 indicates that Y^δ contains a solid parallelepiped (cuboid) that does not touch ∂Y^δ . Note, for instance, that plant

cells have pores looking like rectangular cuboids. Also, many epithelial tissues have structures that can be well approximated by arrays of cubes; see e.g. [2].

For subsets X of Y^δ and integer vectors $k = (k_1, k_2, k_3) \in \mathbb{Z}^3$ we denote the e_1, e_2 -directional shifted subset by

$$X^k := X + \sum_{i=1}^3 k_i e_i.$$

The geometry within our layer Ω^δ includes the pore skeleton $\Omega_s^{\delta\varepsilon}$ and the pore space $\Omega_g^{\delta\varepsilon}$. Obviously, we have

$$\Omega^\delta := \Omega_g^{\delta\varepsilon} \cup \overline{\Omega}_s^{\delta\varepsilon}$$

with

$$\Gamma^{\delta\varepsilon} := \partial\Omega_s^{\delta\varepsilon}$$

as the (total) gas-solid boundary. As indicated in the above Figures, the microstructures are not allowed to touch neither themselves nor the outer boundary of the layer Ω^δ .

Finally, note that

$$\partial\Omega^\delta = \Gamma_D^\delta \cup \Gamma_N^\delta \cup \Gamma^{\delta\varepsilon},$$

that is the boundary of the layer Ω^δ can be split into the exterior Dirichlet and Neumann boundaries (Γ_D^δ and Γ_N^δ) and the inner gas-solid boundary $\Gamma^{\delta\varepsilon}$.

On the other hand, w.l.o.g. assume that we can take Ω a bounded domain in \mathbb{R}^2 as side for the layer Ω^δ such that $\Omega^\delta := \Omega \times [-\frac{\delta}{2}, \frac{\delta}{2}]$. Later on in section 6, when taking $\delta \rightarrow 0$ we will understand that $\Omega^\delta \rightarrow \Omega \times \{0\}$ (the dimension reduction step) with $Y^\delta \rightarrow Y \times \{0\}$, where $\Omega, Y \subset \mathbb{R}^2$. We will write for the reduced homogenized problem Ω , Y , etc. instead of $\Omega \times \{0\}$ and $Y \times \{0\}$ and so on. Also, denote $\hat{\Omega} := \Omega \times [-\frac{1}{2}, \frac{1}{2}]$.

By χ_Θ we denote the characteristic function of the set Θ . Typical choices for the set Θ will be Y_g^δ, Y_s^δ , etc.

Given $\mathbf{u}^{\delta\varepsilon} : \Omega_g^{\delta\varepsilon} \rightarrow \mathbb{R}^3$ velocity of the flow, the unknowns of the microscopic model are: $C^{\delta\varepsilon} : \Omega_g^{\delta\varepsilon} \rightarrow \mathbb{R}$ – the concentration of the active species (typically oxygen), $T_g^{\delta\varepsilon} : \Omega_g^{\delta\varepsilon} \rightarrow \mathbb{R}$ and $T_s^{\delta\varepsilon} : \Omega_s^{\delta\varepsilon} \rightarrow \mathbb{R}$ – the temperatures corresponding to the solid and gas phases of the material, and $R^{\delta\varepsilon} : \Gamma^{\delta\varepsilon} \rightarrow \mathbb{R}$ – the solid reaction product.

For the sake of a simpler notation, for the case $\delta = \mathcal{O}(1)$, we omit to write the dependence of the solution vector $(C^{\delta\varepsilon}, T^{\delta\varepsilon}, R^{\delta\varepsilon})$ [with $T^{\delta\varepsilon} := (T_g^{\delta\varepsilon}, T_s^{\delta\varepsilon})$] on the scale factor δ ; we just write $(C^\varepsilon, T^\varepsilon, R^\varepsilon)$ but still keep the presence of δ in the definition of the space domain.

3. Setting of the microscopic equations - the model $(\mathcal{P}^{\delta\varepsilon})$. We investigate the model equations proposed in [25] to describe the smoldering combustion of a porous medium and pose it now in the thin layer Ω^δ (see Figure 2 or Figure 4) as follows: Find the triplet $(C^{\delta\varepsilon}, T^{\delta\varepsilon}, R^{\delta\varepsilon})$ satisfying

$$\begin{cases} \partial_t C^{\delta\varepsilon} + \nabla \cdot (\mathbf{u}^{\delta\varepsilon} C^{\delta\varepsilon} - D^{\delta\varepsilon} \nabla C^{\delta\varepsilon}) = 0 & \text{in } \Omega_g^{\delta\varepsilon}, \\ C_g^{\delta\varepsilon} \partial_t T_g^{\delta\varepsilon} + \nabla \cdot (C_g^{\delta\varepsilon} \mathbf{u}^{\delta\varepsilon} T_g^{\delta\varepsilon} - \lambda_g^{\delta\varepsilon} \nabla T_g^{\delta\varepsilon}) = 0 & \text{in } \Omega_g^{\delta\varepsilon}, \\ C_s^{\delta\varepsilon} \partial_t T_s^{\delta\varepsilon} - \nabla \cdot (\lambda_s^{\delta\varepsilon} \nabla T_s^{\delta\varepsilon}) = 0 & \text{in } \Omega_s^{\delta\varepsilon}, \\ \partial_t R^{\delta\varepsilon} = W(T^{\delta\varepsilon}, C^{\delta\varepsilon}) & \text{on } \Gamma^{\delta\varepsilon}, \end{cases} \quad (1)$$

together with initial and boundary conditions

$$\begin{cases} C^{\delta\varepsilon}(0, x) = C^0 & \text{in } \{t = 0\} \times \Omega_g^{\delta\varepsilon} \\ T_i^{\delta\varepsilon}(0, x) = T_i^0 & \text{in } \{t = 0\} \times \Omega_i^{\delta\varepsilon}, i \in \{g, s\} \\ R^{\delta\varepsilon}(0, x) = R^0 & \text{on } \{t = 0\} \times \Gamma^{\delta\varepsilon} \\ (\lambda_g^{\delta\varepsilon} \nabla T_g^{\delta\varepsilon} - \lambda_s^{\delta\varepsilon} \nabla T_s^{\delta\varepsilon}) \cdot \nu = \varepsilon QW(T^{\delta\varepsilon}, C^{\delta\varepsilon}) & \text{on } \Gamma^{\delta\varepsilon}, \\ T_g^{\delta\varepsilon} = T_s^{\delta\varepsilon} & \text{on } \Gamma^{\delta\varepsilon}, \\ D^{\delta\varepsilon} \nabla C^{\delta\varepsilon} \cdot \nu = -\varepsilon W(T^{\delta\varepsilon}, C^{\delta\varepsilon}) & \text{on } \Gamma^{\delta\varepsilon}, \end{cases} \quad (2)$$

and

$$\begin{cases} T_i^{\delta\varepsilon} = T_u, \quad C^{\delta\varepsilon} = C_u & \text{on } \Gamma_D^{\delta\varepsilon} \\ \nabla T_i^{\delta\varepsilon} \cdot \nu = 0, \quad \nabla C^{\delta\varepsilon} \cdot \nu = 0 & \text{on } \Gamma_N^{\delta\varepsilon}. \end{cases} \quad (3)$$

The heat production term, i.e. in terms $T^{\delta\varepsilon}$, or the mass consumption rate of the gaseous oxidizer $C^{\delta\varepsilon}$ due to the chemical reaction at the surface is denoted by

$$W(T^{\delta\varepsilon}, C^{\delta\varepsilon}) := AC^{\delta\varepsilon} f(T^{\delta\varepsilon}). \quad (4)$$

The physical assumption for the reaction rate (4) is that the solid porous sample is available in abundance and the gaseous oxidizer concentration is limited in amount. Since, we also look to an the exothermic chemical oxidation of the porous sample, the chemical kinetics (4) is thus governed by a one-step first order Arrhenius law. For further information of the reaction term (4), we refer to [27] and for a detailed treatment of chemical kinetics, we refer to [46]. We refer to this microscopic model as the $(\mathcal{P}^{\delta\varepsilon})$ -model.

4. Solvability of the $(\mathcal{P}^{\delta\varepsilon})$ -model.

4.1. Working hypotheses. Before performing any asymptotics, we wish to ensure that the microscopic model $(\mathcal{P}^{\delta\varepsilon})$ is well-posed. To do so, we introduce a set of restrictions on data and parameters, which we collect as *Assumptions (A)*.

We assume the following set of assumptions, to which we refer to as **Assumptions (A)**:

(A1) $D^\delta, \lambda_g^\delta, \lambda_s^\delta \in L^\infty(Y^\delta)^{3 \times 3}$, $(D^\delta(x)\xi, \xi) \geq D^0|\xi|^2$ for $D^0 > 0$, $(\lambda_g^\delta(x)\xi, \xi) \geq \lambda_g^0|\xi|^2$ for $\lambda_g^0 > 0$, $(\lambda_s^\delta(x)\xi, \xi) \geq \lambda_s^0|\xi|^2$ for $\lambda_s^0 > 0$ and every $\xi \in \mathbb{R}^3$, $y \in Y^\delta$.

(A2) f is a bounded Lipschitz function. Furthermore

$$f(\alpha) = \begin{cases} \text{positive, if } \alpha > 0, \\ 0, \text{ otherwise.} \end{cases}$$

(A3) $C_g^{\delta\varepsilon}, C_s^{\delta\varepsilon}$ are bounded from below by C_g^0, C_s^0 , respectively.

(A4) $C^0, C_g^0, C_s^0 \in H^1(\Omega^\delta) \cap L_\infty^1(\Omega^\delta)$, $R \in L_\infty^1(\Gamma^\delta)$. $C^0, T_g^0, T_s^0 \in H^1(\Omega^\delta) \cap L_\infty^1(\Omega^\delta)$ and $R \in L_\infty^1(\Gamma^\delta)$.

(A5) $\operatorname{div}(\mathbf{u}^{\delta\varepsilon}) = 0$, $\|\mathbf{u}^{\delta\varepsilon}\|_{L^2([0, T] \times \Omega^\delta)} \leq M_u < \infty$ and $\mathbf{u}^{\delta\varepsilon} \rightarrow \mathbf{u}^\delta$ strongly as $\varepsilon \rightarrow 0$.

(A6) $C_u, T_u \in H^1(0, T; H^1(\Omega_g^{\delta\varepsilon})) \cap L_\infty^1((0, T) \times \Omega_g^{\delta\varepsilon})$.

Remark 1. Assumption (A1) and (A3) are physical by nature, while (A2), (A4), and (A6) are technical, needed to ensure a proper functional setting. By involving (A5), we basically circumvent the use of Stefan-Maxwell equations (see [45], e.g.) to describe how the multicomponent reactive mixture responds to changes in temperature. Involving the Stefan-Maxwell equations would probably lead to a better phenomenological model, at least if the transport coefficients were known.

However, as far as we are aware, there is not yet a general theory able to provide global-in-time weak solutions to general classes of Stefan-Maxwell equations. The situation seems to be better what strong solutions are concerned, but they are not useful in the context of averaging processes in contrast media.

We define the following uniform in δ constants

$$\begin{aligned} M_C &:= \|C^0\|_{L^\infty(\Omega^\delta)}, \\ M_T &:= \max\{\|T_g^0\|_{L^\infty(\Omega^\delta)}, \|T_s^0\|_{L^\infty(\Omega^\delta)}\}, \\ M_R &:= \max\{\|R^0\|_{L^\infty(\Gamma^\delta)}, M_T\}. \end{aligned} \quad (5)$$

Definition 4.1. We call $(C^{\delta\varepsilon}, T_g^{\delta\varepsilon}, T_s^{\delta\varepsilon}, R^{\delta\varepsilon})$ a weak solution to (1)–(2) if $C^{\delta\varepsilon} \in C_u + L^2(0, T; H_\Gamma^1(\Omega_g^{\delta\varepsilon}))$, $\partial_t C^{\delta\varepsilon} \in \partial_t C_u + L^2(0, T; L^2(\Omega_g^{\delta\varepsilon}))$, $T_g^{\delta\varepsilon} \in T_u + L^2(0, T; H_\Gamma^1(\Omega_g^{\delta\varepsilon}))$, $\partial_t T_g^{\delta\varepsilon} \in \partial_t T_g + L^2(0, T; L^2(\Omega_g^{\delta\varepsilon}))$, $T_s^{\delta\varepsilon} \in L^2(0, T; H^1(\Omega_s^{\delta\varepsilon})) \cap H^1(0, T; L^2(\Omega_s^{\delta\varepsilon}))$, and $R^{\delta\varepsilon} \in H^1(0, T; L^2(\Gamma^{\delta\varepsilon}))$ satisfies a.e. in $(0, T)$ the following formulation

$$\begin{aligned} &\int_{\Omega_g^{\delta\varepsilon}} \partial_t C^{\delta\varepsilon} \phi dx + \int_{\Omega_g^{\delta\varepsilon}} D^{\delta\varepsilon} \nabla C^{\delta\varepsilon} \nabla \phi dx + \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \nabla C^{\delta\varepsilon} \phi dx = -\varepsilon \int_{\Gamma^{\delta\varepsilon}} W(T^{\delta\varepsilon}, C^{\delta\varepsilon}) \phi d\gamma, \\ &\int_{\Omega_g^{\delta\varepsilon}} C_g^{\delta\varepsilon} \partial_t T_g^{\delta\varepsilon} \varphi dx + \int_{\Omega_g^{\delta\varepsilon}} \lambda_g^{\delta\varepsilon} \nabla T_g^{\delta\varepsilon} \nabla \varphi dx + \int_{\Omega_g^{\delta\varepsilon}} C_g^{\delta\varepsilon} \mathbf{u}^{\delta\varepsilon} \nabla T_g^{\delta\varepsilon} \varphi dx + \int_{\Omega_g^{\delta\varepsilon}} C_s^{\delta\varepsilon} \partial_t T_s^{\delta\varepsilon} \varphi dx \\ &\int_{\Omega_s^{\delta\varepsilon}} \lambda_s^{\delta\varepsilon} \nabla T_s^{\delta\varepsilon} \nabla \varphi dx = \varepsilon \int_{\Gamma^{\delta\varepsilon}} QW(T^{\delta\varepsilon}, C^{\delta\varepsilon}) \varphi d\gamma, \\ &\int_{\Gamma^{\delta\varepsilon}} \partial_t R^{\delta\varepsilon} \psi d\gamma = \int_{\Gamma^{\delta\varepsilon}} W(T^{\delta\varepsilon}, C^{\delta\varepsilon}) \psi d\gamma, \end{aligned}$$

for all $\phi \in L^2(0, T; H_\Gamma^1(\Omega_g^{\delta\varepsilon}))$, $\varphi \in L^2(0, T; H_\Gamma^1(\Omega_g^{\delta\varepsilon})) \times L^2(0, T; H^1(\Omega_s^{\delta\varepsilon}))$, $\psi \in L^2((0, T) \times \Gamma^{\delta\varepsilon})$ and $C^{\delta\varepsilon}(t) \rightarrow C^0$, $T_g^{\delta\varepsilon}(t) \rightarrow T_g^0$ in $L^2(\Omega_g^{\delta\varepsilon})$, $T_s^{\delta\varepsilon}(t) \rightarrow T_s^0$ in $L^2(\Omega_s^{\delta\varepsilon})$, $R^{\delta\varepsilon}(t) \rightarrow R^0$ in $L^2(\Gamma^{\delta\varepsilon})$ as $t \rightarrow 0$.

4.2. Basic estimates and results.

Lemma 4.2. (Energy estimates) Assume (A1)–(A4), then the weak solution to the microscopic problem $(\mathcal{P}^{\delta\varepsilon})$ in the sense of Definition 4.1 satisfies the following a priori estimates

$$\|C_g^{\delta\varepsilon}\|_{L^2(0, T; L^2(\Omega_g^{\delta\varepsilon}))} + \|\nabla C_g^{\delta\varepsilon}\|_{L^2(0, T; L^2(\Omega_g^{\delta\varepsilon}))} \leq C, \quad (6)$$

$$\|T_i^{\delta\varepsilon}\|_{L^2(0, T; L^2(\Omega_i^{\delta\varepsilon}))} + \|\nabla C_i^{\delta\varepsilon}\|_{L^2(0, T; L^2(\Omega_i^{\delta\varepsilon}))} \leq C, \text{ for } i \in \{g, s\} \quad (7)$$

$$\sqrt{\varepsilon} \|R^{\delta\varepsilon}\|_{L^\infty((0, T) \times \Gamma^{\delta\varepsilon})} + \sqrt{\varepsilon} \|\partial_t R^{\delta\varepsilon}\|_{L^2((0, T) \times \Gamma^{\delta\varepsilon})} \leq C \quad (8)$$

Proof. We test with $\phi = C^{\delta\varepsilon}$ to get

$$\begin{aligned} &\int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |C^{\delta\varepsilon}|^2 dx d\tau + 2D^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\nabla C^{\delta\varepsilon}|^2 dx d\tau + \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \cdot \nabla C^{\delta\varepsilon} C^{\delta\varepsilon} dx d\tau \\ &\leq 2\varepsilon A \int_{\Gamma^{\delta\varepsilon}} |C^{\delta\varepsilon}|^2 f(T^{\delta\varepsilon}) d\gamma d\tau. \end{aligned}$$

Convection term in (9) vanishes. This follows from

$$\begin{aligned} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \nabla C^{\delta\varepsilon} C^{\delta\varepsilon} dx d\tau &= \frac{1}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \nabla |C^{\delta\varepsilon}|^2 dx d\tau \\ &= \frac{1}{2} \int_0^t \int_{\Gamma^{\delta\varepsilon}} n \cdot \mathbf{u}^{\delta\varepsilon} |C^{\delta\varepsilon}|^2 dx d\tau - \frac{1}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \nabla \cdot \mathbf{u}^{\delta\varepsilon} |C^{\delta\varepsilon}|^2 dx d\tau. \end{aligned}$$

Using the boundedness of f , the fact that $\mathbf{u}^{\delta\varepsilon}$ is divergence-free and zero on the boundary and the trace inequality, we obtain

$$\int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |C^{\delta\varepsilon}(t)|^2 dx d\tau + (2D^0 - \varepsilon^2 C) \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\nabla C^{\delta\varepsilon}|^2 dx d\tau \leq C \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |C^{\delta\varepsilon}(t)|^2 dx d\tau.$$

Choosing ε small enough and applying Gronwall's inequality, we obtain the desired result. Let us take $\phi = (T_g^{\delta\varepsilon}, T_s^{\delta\varepsilon}) \in L^2(0, T; H_\Gamma^1(\Omega_g^{\delta\varepsilon})) \times L^2(0, T; H^1(\Omega_s^{\delta\varepsilon}))$ to get

$$\begin{aligned} &C_g^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |T_g^{\delta\varepsilon}|^2 dx d\tau + 2\lambda_g^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\nabla T_g^{\delta\varepsilon}|^2 dx d\tau + C_g^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \nabla |T_g^{\delta\varepsilon}|^2 dx d\tau \\ &+ C_s^0 \int_0^t \int_{\Omega_s^{\delta\varepsilon}} \partial_t |T_s^{\delta\varepsilon}|^2 dx d\tau + 2\lambda_s^0 \int_0^t \int_{\Omega_s^{\delta\varepsilon}} |\nabla T_s^{\delta\varepsilon}|^2 dx d\tau \\ &\leq 2\varepsilon A Q \int_0^t \int_{\Gamma^{\delta\varepsilon}} f(T^{\delta\varepsilon}) C^{\delta\varepsilon} T^{\delta\varepsilon} d\gamma d\tau \leq \varepsilon C \int_0^t \int_{\Gamma^{\delta\varepsilon}} C^{\delta\varepsilon} T^{\delta\varepsilon} d\gamma d\tau. \end{aligned} \tag{9}$$

The convection term disappears by the argument given above. Furthermore, we estimate the integral on right hand side as follows:

$$\begin{aligned} &\varepsilon C \int_0^t \int_{\Gamma^{\delta\varepsilon}} C^{\delta\varepsilon} T^{\delta\varepsilon} d\gamma d\tau \leq \varepsilon C \int_0^t \int_{\Gamma^{\delta\varepsilon}} (|C^{\delta\varepsilon}|^2 + |T^{\delta\varepsilon}|^2) d\gamma d\tau \\ &\leq C \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|C^{\delta\varepsilon}|^2 + \varepsilon^2 |\nabla C^{\delta\varepsilon}|^2 + |T_g^{\delta\varepsilon}|^2 + \varepsilon^2 |\nabla T_g^{\delta\varepsilon}|^2) dx d\tau \\ &\quad + C \int_0^t \int_{\Omega_s^{\delta\varepsilon}} (|T_s^{\delta\varepsilon}|^2 + \varepsilon^2 |\nabla T_s^{\delta\varepsilon}|^2) dx d\tau. \end{aligned}$$

(9) becomes

$$C_g^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |T_g^{\delta\varepsilon}|^2 dx d\tau + (2\lambda_g^0 - \varepsilon^2 C) \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\nabla T_g^{\delta\varepsilon}|^2 dx d\tau$$

$$\begin{aligned}
& + C_s^0 \int_0^t \int_{\Omega_s^{\delta\varepsilon}} \partial_t |T_s^{\delta\varepsilon}|^2 dx d\tau + (2\lambda_s^0 - \varepsilon^2 C) \int_0^t \int_{\Omega_s^{\delta\varepsilon}} |\nabla T_s^{\delta\varepsilon}|^2 dx d\tau \\
& \leq C \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|C^{\delta\varepsilon}|^2 + \varepsilon^2 |\nabla C^{\delta\varepsilon}|^2 + |T_g^{\delta\varepsilon}|^2) dx d\tau + C \int_0^t \int_{\Omega_s^{\delta\varepsilon}} |T_s^{\delta\varepsilon}|^2 dx d\tau.
\end{aligned}$$

Choose ε conveniently. Using then the estimates (6) and applying Gronwall's inequality, we get

$$\int_{\Omega_i^{\delta\varepsilon}} |T_i^{\delta\varepsilon}(t)|^2 dx + \int_0^t \int_{\Omega_i^{\delta\varepsilon}} |\nabla T_i^{\delta\varepsilon}|^2 dx d\tau \leq C \quad i \in \{g, s\}.$$

We set as a test function $\psi = R^{\delta\varepsilon}$ and get

$$\begin{aligned}
\varepsilon \int_0^t \int_{\Gamma^{\delta\varepsilon}} \partial_t |R^{\delta\varepsilon}|^2 d\gamma d\tau &= 2\varepsilon A \int_0^t \int_{\Gamma^{\delta\varepsilon}} f(T^{\delta\varepsilon}) C^{\delta\varepsilon} R^{\delta\varepsilon} d\gamma d\tau \\
&\leq \varepsilon C \int_0^t \int_{\Gamma^{\delta\varepsilon}} (|C^{\delta\varepsilon}|^2 + |R^{\delta\varepsilon}|^2) d\gamma d\tau.
\end{aligned}$$

Applying Gronwall's inequality together with trace inequality, we have

$$\varepsilon \int_{\Gamma^{\delta\varepsilon}} |R^{\delta\varepsilon}(t)|^2 d\gamma \leq C \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|C^{\delta\varepsilon}|^2 + \varepsilon^2 |\nabla C^{\delta\varepsilon}|^2) dx$$

Using (6), we have the result. Now, we take as a test function $\psi = \partial_t R^{\delta\varepsilon}$ and obtain

$$\begin{aligned}
\varepsilon \int_0^t \int_{\Gamma^{\delta\varepsilon}} |\partial_t R^{\delta\varepsilon}|^2 d\gamma d\tau &= \varepsilon A \int_0^t \int_{\Gamma^{\delta\varepsilon}} f(T^{\delta\varepsilon}) C^{\delta\varepsilon} \partial_t R^{\delta\varepsilon} d\gamma d\tau \\
&\leq \varepsilon A \int_0^t \int_{\Gamma^{\delta\varepsilon}} \left(\frac{1}{2\xi} |C^{\delta\varepsilon}|^2 + \frac{\xi}{2} |\partial_t R^{\delta\varepsilon}|^2 \right) d\gamma d\tau \\
\varepsilon(1 - \frac{A\xi}{2}) \int_0^t \int_{\Gamma^{\delta\varepsilon}} |\partial_t R^{\delta\varepsilon}|^2 d\gamma d\tau &\leq \frac{A}{2\xi} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|C^{\delta\varepsilon}|^2 + \varepsilon^2 |\nabla C^{\delta\varepsilon}|^2) dx.
\end{aligned}$$

Choosing ξ conveniently and using (6) to obtain

$$\sqrt{\varepsilon} \|\partial_t R^{\delta\varepsilon}\|_{L^2((0,T) \times \Gamma^{\delta\varepsilon})} \leq C.$$

□

Lemma 4.3. (Positivity) Assume (A1)-(A4), and let $t \in [0, T]$ be arbitrarily chosen. Then the following estimates hold:

(i) $C^{\delta\varepsilon}(t), T_g^{\delta\varepsilon}(t) \geq 0$ a.e. in $\Omega_g^{\delta\varepsilon}$, $T_s^{\delta\varepsilon}(t) \geq 0$ a.e. in $\Omega_s^{\delta\varepsilon}$ and $R^{\delta\varepsilon}(t) \geq 0$ a.e. on $\Gamma^{\delta\varepsilon}$.

(ii) $C^{\delta\varepsilon}(t) \leq M_C$, $T_g^{\delta\varepsilon}(t) \leq M_T$ a.e. in $\Omega_g^{\delta\varepsilon}$, $T_s^{\delta\varepsilon}(t) \leq M_T$ a.e. in $\Omega_s^{\delta\varepsilon}$ and $R^{\delta\varepsilon}(t) \leq M_R$ a.e. on $\Gamma^{\delta\varepsilon}$, where M_C , M_T and M_R are defined in 5.

Proof. (i) We test with $\phi = -[C^{\delta\varepsilon}]^-$ and obtain the following inequality

$$\begin{aligned} & \frac{1}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |[C^{\delta\varepsilon}]^-|^2 dx d\tau + D^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\nabla [C^{\delta\varepsilon}]^-|^2 dx d\tau + \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \nabla C^{\delta\varepsilon} [C^{\delta\varepsilon}]^- dx d\tau \\ & \leq \varepsilon A \int_0^t \int_{\Gamma^{\delta\varepsilon}} |[C^{\delta\varepsilon}]^-|^2 d\gamma d\tau. \end{aligned} \quad (10)$$

The convection term in (10) vanishes. Apply the trace inequality to the expression on the right hand side gives

$$\begin{aligned} & \frac{1}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |[C^{\delta\varepsilon}]^-|^2 dx d\tau + D^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\nabla [C^{\delta\varepsilon}]^-|^2 dx d\tau \\ & \leq C \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|[C^{\delta\varepsilon}]^-|^2 + \varepsilon^2 |\nabla [C^{\delta\varepsilon}]^-|^2) dx d\tau. \end{aligned}$$

Choosing ε conveniently and applying Gronwall's inequality together with the positivity of the initial data, we conclude that $C^{\delta\varepsilon} \geq 0$ a.e. in $(0, T) \times \Omega_g^{\delta\varepsilon}$. Testing with $\varphi = (-[T_g^{\delta\varepsilon}]^-, [T_s^{\delta\varepsilon}]^-)$ leads to

$$\begin{aligned} & \frac{C_g^0}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |[T_g^{\delta\varepsilon}]^-|^2 dx d\tau + \lambda_g^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\nabla [T_g^{\delta\varepsilon}]^-|^2 dx d\tau \\ & + \frac{C_g^0}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \nabla |[T_g^{\delta\varepsilon}]^-|^2 dx d\tau \\ & + \frac{1}{2} C_s^0 \int_0^t \int_{\Omega_s^{\delta\varepsilon}} \partial_t |[T_s^{\delta\varepsilon}]^-|^2 dx d\tau + \lambda_s^0 \int_0^t \int_{\Omega_s^{\delta\varepsilon}} |\nabla [T_s^{\delta\varepsilon}]^-|^2 dx d\tau \\ & \leq -\varepsilon Q A \int_0^t \int_{\Gamma^{\delta\varepsilon}} f(T^{\delta\varepsilon}) C^{\delta\varepsilon} [T_g^{\delta\varepsilon}]^- d\gamma d\tau \leq 0. \end{aligned} \quad (11)$$

The expression on right hand side of (11) is zero by assumption (A). Note that the convection term on left hand side vanishes as well. Gronwall's inequality together with the positivity of the initial data provides that $T_g^{\delta\varepsilon} \geq 0$ a.e. in $(0, T) \times \Omega_g^{\delta\varepsilon}$ and $T_s^{\delta\varepsilon} \geq 0$ a.e. in $(0, T) \times \Omega_s^{\delta\varepsilon}$. Let us test with $\psi = -[R^{\delta\varepsilon}]^-$

$$\frac{1}{2} \partial_t \int_{\Gamma^{\delta\varepsilon}} |[R^{\delta\varepsilon}]^-|^2 d\gamma = - \int_{\Gamma^{\delta\varepsilon}} W(T^{\delta\varepsilon}, C^{\delta\varepsilon}) [R^{\delta\varepsilon}]^- d\gamma \leq 0. \quad (12)$$

We conclude that $R^{\delta\varepsilon} \geq 0$ a.e. on $(0, T) \times \Gamma^{\delta\varepsilon}$.

(ii) Taking $[C^{\delta\varepsilon} - M_C]^+$, we get

$$\begin{aligned}
& \frac{1}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |[C^{\delta\varepsilon} - M_C]^+|^2 dx d\tau + D^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\nabla [C^{\delta\varepsilon} - M_C]^+|^2 dx d\tau \\
& \quad + C_g^0 \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \nabla C^{\delta\varepsilon} \cdot [C^{\delta\varepsilon} - M_C]^+ dx d\tau \\
& \leq -\varepsilon A \int_0^t \int_{\Gamma^{\delta\varepsilon}} C^{\delta\varepsilon} f(T^{\delta\varepsilon}) [C^{\delta\varepsilon} - M_C]^+ d\gamma d\tau \leq 0. \tag{13}
\end{aligned}$$

Arguing as before, we observe that the convection term vanishes. Applying Gronwall's inequality together with $C^0 \leq M_C$ a.e. in $\Omega_g^{\delta\varepsilon}$, we end up with the boundedness of the $C^{\delta\varepsilon} \leq M_C$ a.e. in $\Omega_g^{\delta\varepsilon}$ for all $t \in (0, T)$. Note that since $C^{\delta\varepsilon} \in L^2(0, T; H_\Gamma^1(\Omega_g^{\delta\varepsilon})) \cap L^\infty((0, T) \times \Omega_g^{\delta\varepsilon})$, by Claim 5 in [19] we have $C^{\delta\varepsilon} \in L^\infty((0, T) \times \Gamma^{\delta\varepsilon})$. Testing with $([T_g^{\delta\varepsilon} - M_T]^+, [T_s^{\delta\varepsilon} - M_T]^+)$ and the resulting inequalities

$$\begin{aligned}
& \frac{C_g^0}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |[T_g^{\delta\varepsilon} - M_T]^+|^2 dx d\tau + \frac{C_s^0}{2} \int_0^t \partial_t \int_{\Omega_s^{\delta\varepsilon}} |[T_s^{\delta\varepsilon} - M_T]^+|^2 dx d\tau \\
& + \lambda_g^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\nabla [T_g^{\delta\varepsilon} - M_T]^+|^2 dx d\tau + \lambda_s^0 \int_0^t \int_{\Omega_s^{\delta\varepsilon}} |\nabla [T_s^{\delta\varepsilon} - M_T]^+|^2 dx d\tau \\
& + \frac{1}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \nabla |[T_g^{\delta\varepsilon} - M_T]^+|^2 dx d\tau \leq \varepsilon Q A \int_0^t \int_{\Gamma^{\delta\varepsilon}} f(T^{\delta\varepsilon}) C^{\delta\varepsilon} [T^{\delta\varepsilon} - M_T]^+ d\gamma d\tau \\
& \leq \varepsilon Q A M_c \int_0^t \int_{\Gamma^{\delta\varepsilon}} |[T^{\delta\varepsilon} - M_T]^+|^2 d\gamma d\tau. \tag{14}
\end{aligned}$$

Recall the boundedness of $C^{\delta\varepsilon}$ on $\Gamma^{\delta\varepsilon}$ and the sublinearity of f . Applying the trace inequality, leads to

$$\begin{aligned}
& \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |[T_g^{\delta\varepsilon} - M_T]^+|^2 dx d\tau + \int_0^t \int_{\Omega_s^{\delta\varepsilon}} \partial_t |[T_s^{\delta\varepsilon} - M_T]^+|^2 dx d\tau \\
& + \left(\frac{2\lambda_g^0}{C_g^0} - C\varepsilon^2 \right) \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\nabla [T_g^{\delta\varepsilon} - M_T]^+|^2 dx d\tau \\
& + \left(\frac{2\lambda_s^0}{C_s^2} - C\varepsilon^2 \right) \int_0^t \int_{\Omega_s^{\delta\varepsilon}} |\nabla [T_s^{\delta\varepsilon} - M_T]^+|^2 dx d\tau \\
& \leq C \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |[T_g^{\delta\varepsilon} - M_T]^+|^2 dx d\tau + C \int_0^t \int_{\Omega_s^{\delta\varepsilon}} |[T_s^{\delta\varepsilon} - M_T]^+|^2 dx d\tau.
\end{aligned}$$

Let us choose ε small enough. Applying again Gronwall's inequality, we obtain $T_g^{\delta\varepsilon} \leq M_T$ a.e. in $\Omega_g^{\delta\varepsilon}$ and $T_s^{\delta\varepsilon} \leq M_T$ a.e. in $\Omega_s^{\delta\varepsilon}$. Now we test with $[R^{\delta\varepsilon} - (t + 1)M_R]^+$ and obtain

$$\begin{aligned} & \int_{\Gamma^{\delta\varepsilon}} (\partial_t [R^{\delta\varepsilon} - (t + 1)M_R]^+)^2 + M_R [R^{\delta\varepsilon} - (t + 1)M_R]^+ d\gamma \\ & \leq C \int_{\Gamma^{\delta\varepsilon}} M_c [R^{\delta\varepsilon} - (t + 1)M_R]^+ d\gamma \\ & \int_{\Gamma^{\delta\varepsilon}} \partial_t [R^{\delta\varepsilon} - (t + 1)M_R]^+ d\gamma \leq (CM_c - M_R) \int_{\Gamma^{\delta\varepsilon}} [R^{\delta\varepsilon} - (t + 1)M_R]^+ d\gamma \end{aligned}$$

Using (A5) and Gronwall's inequality to get $R^{\delta\varepsilon} \leq M_R$ a.e. in $(0, T) \times \Gamma^{\delta\varepsilon}$. \square

Remark 2. Based on $C^{\delta\varepsilon} \in L^\infty((0, T) \times \Omega_g^{\delta\varepsilon}) \cap L^2(0, T; H^1(\Omega_g^{\delta\varepsilon}))$, we use Claim 5 in [19] to obtain $C^{\delta\varepsilon} \in L^\infty((0, T) \times \Gamma^{\delta\varepsilon})$.

Lemma 4.4. *Consider Assumption (A). There exists a unique weak solution in the sense of Definition 4.1.*

Proof. With minor modifications, the proof follows the lines of the corresponding result in [19]. For the complete calculations, see Theorem 4.3.5 in [24]. \square

Theorem 4.5. (Global Existence) *Assume the hypothesis of Lemma 4.4. Then there exists at least a global-in-time weak solution in the sense of Definition 4.1.*

Proof. The proof is based on the Galerkin argument. Since $W(T^{\delta\varepsilon}, C^{\delta\varepsilon})$ is globally Lipschitz function in both variables, this makes the proof rather standard. \square

Lemma 4.6. (Additional a priori estimates) *Assume the hypothesis of Lemma 4.4. The following ε -independent bounds hold:*

$$\| \partial_t C^{\delta\varepsilon} \|_{L^2(0, T; L^2(\Omega_g^{\delta\varepsilon}))} + \| \partial_t T_i^{\delta\varepsilon} \|_{L^2(0, T; L^2(\Omega_i^{\delta\varepsilon}))} \leq C, \quad i \in \{g, s\}, \quad (15)$$

where C a generic constant independent of ε .

Proof. To obtain the estimates (15), we consider a sufficiently regular extension of the Dirichlet data C_u, T_u to the whole $\overline{\Omega}^\delta$. We test with $\phi = \partial_t(C^{\delta\varepsilon} - C_u)$ to get

$$\begin{aligned} & \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\partial_t C^{\delta\varepsilon}|^2 dx d\tau + \frac{D^0}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |\nabla C^{\delta\varepsilon}|^2 dx d\tau + \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \cdot \nabla C^{\delta\varepsilon} \partial_t C^{\delta\varepsilon} dx d\tau \\ & \leq \frac{1}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (\xi |\partial_t C^{\delta\varepsilon}|^2 + \frac{1}{\xi} |\partial_t C_u|^2) dx d\tau + \frac{D^0}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|\nabla C^{\delta\varepsilon}|^2 + |\nabla \partial_t C_u|^2) dx d\tau \\ & + \frac{M_u}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|\nabla C^{\delta\varepsilon}|^2 + |\partial_t C_u|^2) dx d\tau - \varepsilon A \int_0^t \int_{\Gamma^{\delta\varepsilon}} C^{\delta\varepsilon} f(T^{\delta\varepsilon}) \partial_t (C^{\delta\varepsilon} - C_u) dx d\tau. \end{aligned}$$

$$\begin{aligned}
& (1 - \frac{C\xi}{2}) \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\partial_t C^{\delta\varepsilon}|^2 dx d\tau + \frac{D^0}{2} \int_{\Omega_g^{\delta\varepsilon}} |\nabla C^{\delta\varepsilon}(t)|^2 dx \\
& \leq \frac{D^0}{2} \int_{\Omega_g^{\delta\varepsilon}} |\nabla C^{\delta\varepsilon}(0)|^2 dx + \frac{1}{2\xi} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\partial_t C_u|^2 dx d\tau \\
& + \frac{D^0}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|\nabla C^{\delta\varepsilon}|^2 + |\nabla \partial_t C_u|^2) dx d\tau + \frac{M_u}{2\delta} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\nabla C^{\delta\varepsilon}|^2 dx d\tau \\
& + \frac{M_u}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|\nabla C^{\delta\varepsilon}|^2 + |\partial_t C_u|^2) dx d\tau \\
& + \varepsilon C \int_0^t \int_{\Gamma^{\delta\varepsilon}} (\partial_t |C^{\delta\varepsilon}|^2 + |C^{\delta\varepsilon}|^2 + |\partial_t C_u|^2) dx d\tau. \\
& (1 - \frac{C\xi}{2}) \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\partial_t C^{\delta\varepsilon}|^2 dx d\tau + \frac{D^0}{2} \int_{\Omega_g^{\delta\varepsilon}} |\nabla C^{\delta\varepsilon}(t)|^2 dx \\
& \leq \frac{D^0}{2} \int_{\Omega_g^{\delta\varepsilon}} |\nabla C^{\delta\varepsilon}(0)|^2 dx + C \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|\nabla C^{\delta\varepsilon}|^2 + |\nabla \partial_t C_u|^2 + |\partial_t C_u|^2) dx d\tau \\
& + C \int_{\Omega_g^{\delta\varepsilon}} (|C^{\delta\varepsilon}(t)|^2 + \varepsilon^2 |\nabla C^{\delta\varepsilon}(t)|^2 + |C^{\delta\varepsilon}(0)|^2 + \varepsilon^2 |\nabla C^{\delta\varepsilon}(0)|^2) dx \\
& + C \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|C^{\delta\varepsilon}|^2 + \varepsilon^2 |\nabla C^{\delta\varepsilon}|^2 + |\partial_t C_u|^2 + \varepsilon |\nabla \partial_t C_u|^2) dx d\tau.
\end{aligned}$$

Choosing ξ conveniently and using the inequalities in Lemma 4.2 together with (A4) and (A6), we get

$$\| \partial_t C^{\delta\varepsilon} \|_{L^2(0,T;L^2(\Omega_g^{\delta\varepsilon}))} \leq C.$$

Now we take as a test function

$$(\partial_t(T_g^{\delta\varepsilon} - T_u), \partial_t T_s^{\delta\varepsilon}) \in L^2(0,T;L^2(\Omega_g^{\delta\varepsilon})) \times L^2(0,T;L^2(\Omega_s^{\delta\varepsilon}))$$

and have

$$\begin{aligned}
& C_g^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\partial_t T_g^{\delta\varepsilon}|^2 dx d\tau + \frac{\lambda_g^0}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \partial_t |\nabla T_g^{\delta\varepsilon}|^2 dx d\tau \\
& + C_g^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \cdot \nabla T_g^{\delta\varepsilon} \partial_t T_g^{\delta\varepsilon} dx d\tau + C_s^0 \int_0^t \int_{\Omega_s^{\delta\varepsilon}} |\partial_t T_s^{\delta\varepsilon}|^2 dx d\tau
\end{aligned}$$

$$\begin{aligned}
& + \frac{\lambda_s^0}{2} \int_0^t \int_{\Omega_s^{\delta\varepsilon}} \partial_t |\nabla T_s^{\delta\varepsilon}|^2 dx d\tau \\
& \leq \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \lambda_g^{\delta\varepsilon} \nabla T_g^{\delta\varepsilon} \nabla \partial_t T_u dx d\tau + \int_0^t \int_{\Omega_g^{\delta\varepsilon}} C_g^{\delta\varepsilon} \partial_t T_g^{\delta\varepsilon} \partial_t T_u dx d\tau \\
& + C_g^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \mathbf{u}^{\delta\varepsilon} \cdot \nabla T_g^{\delta\varepsilon} \partial_t T_u dx d\tau + \varepsilon Q A \int_0^t \int_{\Gamma^{\delta\varepsilon}} C^{\delta\varepsilon} f(T^{\delta\varepsilon}) \partial_t T^{\delta\varepsilon} dx d\tau \\
& C_g^0 \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\partial_t T_g^{\delta\varepsilon}|^2 dx d\tau + \frac{\lambda_g^0}{2} \int_{\Omega_g^{\delta\varepsilon}} |\nabla T_g^{\delta\varepsilon}(t)|^2 dx \\
& + C_s^0 \int_0^t \int_{\Omega_s^{\delta\varepsilon}} |\partial_t T_s^{\delta\varepsilon}|^2 dx d\tau + \frac{\lambda_s^0}{2} \int_{\Omega_s^{\delta\varepsilon}} |\nabla T_s^{\delta\varepsilon}(t)|^2 dx \\
& \leq \frac{\lambda_g^0}{2} \int_{\Omega_g^{\delta\varepsilon}} |\nabla T_g^{\delta\varepsilon}(0)|^2 dx + \frac{\lambda_s^0}{2} \int_{\Omega_s^{\delta\varepsilon}} |\nabla T_s^{\delta\varepsilon}(0)|^2 dx \\
& + \frac{M_u}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \left(\frac{1}{\xi} |\nabla T_g^{\delta\varepsilon}|^2 + \xi |\partial_t T_g^{\delta\varepsilon}|^2 \right) dx d\tau \\
& + \frac{C_g^0}{2} \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \left(\delta |\partial_t T_g^{\delta\varepsilon}|^2 + \frac{1}{\xi} |\partial_t T_u|^2 \right) dx d\tau \\
& + C \int_0^t \int_{\Omega_g^{\delta\varepsilon}} \left(|\nabla T_g^{\delta\varepsilon}|^2 + |\partial_t T_u|^2 + |\nabla \partial_t T_u|^2 \right) dx d\tau \\
& + \varepsilon C \int_0^t \int_{\Gamma^{\delta\varepsilon}} \partial_t |T^{\delta\varepsilon}|^2 d\gamma d\tau
\end{aligned}$$

Making use of the boundedness of $C^{\delta\varepsilon}$ on $(0, T) \times \Gamma^{\delta\varepsilon}$ and of the sub-linearity of f

$$\begin{aligned}
& (C_g^0 - \frac{M_u \xi}{2}) \int_0^t \int_{\Omega_g^{\delta\varepsilon}} |\partial_t T_g^{\delta\varepsilon}|^2 dx d\tau + \frac{\lambda_g^0}{2} \int_{\Omega_g^{\delta\varepsilon}} |\nabla T_g^{\delta\varepsilon}(t)|^2 dx \\
& + C_s^0 \int_0^t \int_{\Omega_s^{\delta\varepsilon}} |\partial_t T_s^{\delta\varepsilon}|^2 dx d\tau + \frac{\lambda_s^0}{2} \int_{\Omega_s^{\delta\varepsilon}} |\nabla T_s^{\delta\varepsilon}(t)|^2 dx \\
& \leq \frac{\lambda_g^0}{2} \int_{\Omega_g^{\delta\varepsilon}} |\nabla T_g^{\delta\varepsilon}(0)|^2 dx + \frac{\lambda_s^0}{2} \int_{\Omega_s^{\delta\varepsilon}} |\nabla T_s^{\delta\varepsilon}(0)|^2 dx
\end{aligned}$$

$$\begin{aligned}
& + C \int_0^t \int_{\Omega_g^{\delta\varepsilon}} (|\nabla T_g^{\delta\varepsilon}|^2 + |\partial_t T_g^{\delta\varepsilon}|^2 + |\nabla \partial_t T_g^{\delta\varepsilon}|^2) dx d\tau \\
& + C \int_{\Omega_s^{\delta\varepsilon}} (|T_s^{\delta\varepsilon}(t)|^2 + \varepsilon^2 |\nabla T_s^{\delta\varepsilon}(t)|^2 + |T_s^{\delta\varepsilon}(0)|^2 + \varepsilon^2 |\nabla T_s^{\delta\varepsilon}(0)|^2) dx.
\end{aligned}$$

Choosing ξ conveniently and using the inequalities in Lemma 4.2 together with (A4), we get

$$\|\partial_t T_g^{\delta\varepsilon}\|_{L^2(0,T;L^2(\Omega_g^{\delta\varepsilon}))} + \|\partial_t T_s^{\delta\varepsilon}\|_{L^2(0,T;L^2(\Omega_s^{\delta\varepsilon}))} \leq C. \quad (16)$$

□

Remark 3. We can use the Cauchy-Schwarz inequality together with (16) to show the boundedness from above of the *microscopic instantaneous bulk burning rate*

$$V^{\delta\varepsilon}(t) := \int_{\Omega^\delta} |\partial_t T^{\delta\varepsilon}(t, x)| \frac{1}{\delta} dx \quad (17)$$

as well as its time average

$$\langle V^{\delta\varepsilon}(t) \rangle_t := \frac{1}{t} \int_0^t V^{\delta\varepsilon}(s) ds \quad (18)$$

with

$$T^{\delta\varepsilon}(x, t) := \begin{cases} T_g^{\delta\varepsilon}(x, t), & \text{if } x \in \Omega_g^{\delta\varepsilon} \\ T_s^{\delta\varepsilon}(x, t), & \text{if } x \in \Omega_s^{\delta\varepsilon}, \end{cases}$$

for any $t \in (0, T)$. We refer the reader to [16] for the terminology and use of such bulk burning rates.

5. The homogenization limit $\varepsilon \rightarrow 0$. The case $\delta > \varepsilon > 0$, $\delta = \mathcal{O}(1)$.

5.1. Extensions to Ω^δ . Our main interest in this section lies in the passing to the homogenization limit $\varepsilon \rightarrow 0$. Before passing to this limit, we extend all the unknowns of the problem to the whole space Ω^ε . Using a standard extension result due to D. Ciorănescu and J. Saint Jean Paulin [13], we extend the concentration defined in Ω_g^ε inside the solid grains; see also Lemma 2.4 in [33] for a related result. The temperature extends naturally in the whole domain by taking the extended temperature field

$$T^\varepsilon(x, t) := \begin{cases} T_g^\varepsilon(x, t), & \text{if } x \in \Omega_g^\varepsilon \\ T_s^\varepsilon(x, t), & \text{if } x \in \Omega_s^\varepsilon. \end{cases}$$

Since the nonlinearity imposed at the microstructure boundary turns to be globally Lipschitz, there are no problems in stating the existence of the extended temperature field. We refer the reader to [28] for a situation where, due to the presence of (boundary) multivalued functions, a more detailed investigation of the existence of the extension is needed. If more effects are introduced at the microscopic solid-gas interfaces like temperature jumps, or heating delays (etc), effects that could require the introduction of a second temperature (see e.g. [18, 33]), then the extension step requires a special care.

5.2. Two-scale convergence step.

Definition 5.1. (Two-scale convergence; cf. [3, 37]) Let $\{u^\varepsilon\}$ be a sequence of functions in $L^2((0, T) \times \Omega)$ (Ω being an open set of \mathbb{R}^N) where ε being a sequence of strictly positive numbers tends to zero. $\{u^\varepsilon\}$ is said to two-scale converge to a unique function $u_0(t, x, y) \in L^2((0, T) \times \Omega \times Y)$ if and only if for any $\psi \in C_0^\infty((0, T) \times \Omega, C_\#^\infty(Y))$, we have

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_\Omega u^\varepsilon(t, x) \psi(t, x, \frac{x}{\varepsilon}) dx dt = \frac{1}{|Y|} \int_\Omega \int_Y u_0(t, x, y) \psi(t, x, y) dy dx dt. \quad (19)$$

We denote (19) by $u^\varepsilon \xrightarrow{2} u_0$.

Theorem 5.2. (Two-scale compactness on volumes; cf. [3, 37])

- (i) From each bounded sequence $\{u^\varepsilon\}$ in $L^2((0, T) \times \Omega)$, one can extract a subsequence which two-scale converges to $u_0(t, x, y) \in L^2((0, T) \times \Omega \times Y)$.
- (ii) Let $\{u^\varepsilon\}$ be a bounded sequence in $H^1((0, T) \times \Omega)$, then there exists $\tilde{u} \in L^2((0, T) \times \Omega; H_\#^1(Y)/\mathbb{R})$ such that up to a subsequence $\{u^\varepsilon\}$ two-scale converges to $u_0(t, x) \in L^2((0, T) \times \Omega)$ and $\nabla u^\varepsilon \xrightarrow{2} \nabla_x u_0 + \nabla_y \tilde{u}$.

Definition 5.3. (Two-scale convergence for ε -periodic hypersurfaces; cf. [35]) A sequence of functions $\{u^\varepsilon\}$ in $L^2((0, T) \times \Gamma_\varepsilon)$ is said to two-scale converge to a limit $u_0 \in L^2((0, T) \times \Omega \times \Gamma)$ if and only if for any $\psi \in C_0^\infty((0, T) \times \Omega, C_\#^\infty(\Gamma))$ we have

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\Gamma_\varepsilon} u^\varepsilon(t, x) \psi(t, x, \frac{x}{\varepsilon}) d\sigma_x dt = \frac{1}{|Y|} \int_\Omega \int_Y u_0(t, x, y) \psi(t, x, y) d\sigma_y dx dt.$$

Theorem 5.4. (Two-scale compactness on hypersurfaces; cf. [35])

- (i) From each bounded sequence $\{u^\varepsilon\} \in L^2((0, T) \times \Gamma_\varepsilon)$, one can extract a subsequence u^ε which two-scale converges to a function $u_0 \in L^2((0, T) \times \Omega \times \Gamma)$.
- (ii) If a sequence of functions $\{u^\varepsilon\}$ is bounded in $L^\infty((0, T) \times \Gamma_\varepsilon)$, then u^ε two-scale converges to a function $u_0 \in L^\infty((0, T) \times \Omega \times \Gamma)$.

The estimates stated in Lemma 4.2 and Lemma 4.6 ensure the following convergence results:

Lemma 5.5. Assume (A1)–(A6). Then, for any fixed $\delta > 0$, we have as $\varepsilon \rightarrow 0$ the following convergences (up to subsequences):

- (a) $C^{\delta\varepsilon}, T^{\delta\varepsilon} \rightharpoonup C^\delta, T^\delta$ weakly in $L^2(0, T; H^1(\Omega^\delta))$,
- (b) $C^{\delta\varepsilon}, T^{\delta\varepsilon} \xrightarrow{2} C^\delta, T^\delta$ weakly in $L^\infty((0, T) \times \Omega^\delta)$,
- (c) $\partial_t C^{\delta\varepsilon}, \partial_t T^{\delta\varepsilon} \rightharpoonup \partial_t C^\delta, \partial_t T^\delta$ weakly in $L^2((0, T) \times \Omega^\delta)$,
- (d) $C^{\delta\varepsilon}, T^{\delta\varepsilon}$ strongly in $L^2(0, T; H^\beta(\Omega^\delta))$ for $\frac{1}{2} < \beta < 1$,
also $\sqrt{\varepsilon} \|C^{\delta\varepsilon} - C^\delta\|_{L^2((0, T) \times \Gamma^{\delta\varepsilon})} \rightarrow 0$ and $\sqrt{\varepsilon} \|T^{\delta\varepsilon} - T^\delta\|_{L^2((0, T) \times \Gamma^{\delta\varepsilon})} \rightarrow 0$ as $\varepsilon \rightarrow 0$.
- (e) $C^{\delta\varepsilon}, T^{\delta\varepsilon} \xrightarrow{2} C^\delta, T^\delta, \nabla C^{\delta\varepsilon} \xrightarrow{2} \nabla_x C^\delta + \nabla_y \tilde{C}^\delta, \tilde{C}^\delta \in L^2((0, T) \times \Omega^\delta; H_\#^1(Y_g)/\mathbb{R})$,
 $\nabla T^{\delta\varepsilon} \xrightarrow{2} \nabla_x T^\delta + \nabla_y \tilde{T}^\delta, \tilde{T}^\delta \in L^2((0, T) \times \Omega^\delta; H_\#^1(Y^\delta)/\mathbb{R})$,
- (f) $R^{\delta\varepsilon} \xrightarrow{2} R^\delta$, and $R^\delta \in L^\infty((0, T) \times \Omega^\delta \times \Gamma^\delta)$,
- (g) $\partial_t C^{\delta\varepsilon}, \partial_t T^{\delta\varepsilon} \xrightarrow{2} \partial_t C^\delta, \partial_t T^\delta$, and $\partial_t R^{\delta\varepsilon} \xrightarrow{2} \partial_t R^\delta \in L^2((0, T) \times \Omega^\delta \times \Gamma^\delta)$.

Proof. (a) and (b) are obtained as a direct consequence of the fact that $C^{\delta\varepsilon}, T^{\delta\varepsilon}$ are bounded in $L^2(0, T; H^1(\Omega^\delta)) \cap L^\infty((0, T) \times \Omega^\delta)$. Up to a subsequence (still denoted by $C^{\delta\varepsilon}, T^{\delta\varepsilon}$), $C^{\delta\varepsilon}, T^{\delta\varepsilon}$ converge weakly to C^δ, T^δ in $L^2(0, T; H^1(\Omega^\delta)) \cap L^\infty((0, T) \times \Omega^\delta)$.

Ω^δ . A similar argument gives (c). To get (d), we use the compact embedding $H^{\beta'}(\Omega^\delta) \hookrightarrow H^\beta(\Omega^\delta)$, for $\beta \in (\frac{1}{2}, 1)$ and $0 < \beta < \beta' \leq 1$ (since Ω^δ has Lipschitz boundary). We have $W := \{C^{\delta\varepsilon}, T^{\delta\varepsilon} \in L^2(0, T; H^1(\Omega^\delta)) \text{ and } \partial_t C^{\delta\varepsilon}, \partial_t T^{\delta\varepsilon} \in L^2((0, T) \times \Omega^\delta)\}$. For a fixed ε , W is compactly embedded in $L^2(0, T; H^\beta(\Omega^\delta))$ by the Lions-Aubin Lemma; cf. e.g. [31]. Using the trace inequality for oscillating surfaces

$$\begin{aligned} \sqrt{\varepsilon} \| C^{\delta\varepsilon} - C^\delta \|_{L^2((0, T) \times \Gamma_{\delta\varepsilon})} &\leq C \| C^{\delta\varepsilon} - C^\delta \|_{L^2(0, T; H^\beta(\Omega_g^{\delta\varepsilon}))} \\ &\leq C \| C^{\delta\varepsilon} - C^\delta \|_{L^2(0, T; H^\beta(\Omega^\delta))} \end{aligned}$$

where $\| C^{\delta\varepsilon} - C^\delta \|_{L^2(0, T; H^\beta(\Omega^\delta))} \rightarrow 0$ as $\varepsilon \rightarrow 0$. Similar argument holds for the rest of (d). To investigate (e), (f) and (g), we use the notion of two-scale convergence as indicated in Definition 5.1 and 5.3. Since $C^{\delta\varepsilon}$ are bounded in $L^2(0, T; H^1(\Omega^\delta))$, up to a subsequence $C^{\delta\varepsilon} \rightharpoonup C^\delta$ in $L^2((0, T) \times \Omega^\delta)$, and $\nabla C^{\delta\varepsilon} \rightharpoonup \nabla_x C^\delta + \nabla_y \tilde{C}^\delta$, $\tilde{C}^\delta \in L^2((0, T) \times \Omega^\delta; H_\#^1(Y_g^\delta)/\mathbb{R})$. By Theorem 5.4, $R^{\delta\varepsilon}$ in $L^\infty((0, T) \times \Gamma^{\delta\varepsilon})$ converges two-scale to $R^\delta \in L^\infty((0, T) \times \Omega^\delta \times \Gamma^\delta)$ and $\partial_t R^{\delta\varepsilon}$ converges two-scale to $\partial_t R^\delta$ in $L^2((0, T) \times \Omega^\delta \times \Gamma^\delta)$. \square

5.3. Derivation of upscaled limit equations. To be able to formulate the limit (upscaled) equations in a compact manner, we define two classes of *cell problems* (local auxiliary problems) very much in the spirit of [22].

Definition 5.6. The *cell problems for the gaseous part* are given by

$$\begin{cases} -\nabla_y \cdot (D(y) \nabla_y \omega^k) &= \sum_{i=1}^3 \partial_{y_k} D_{ki}(y) \text{ in } Y_g^\delta, \\ -D(y) \frac{\partial \omega^k}{\partial n} &= \sum_{i=1}^3 D_{ki}(y) n_i \text{ on } \Gamma^\delta, \end{cases} \quad (20)$$

for all $k \in \{1, 2, 3\}$ and ω^k are Y^δ -periodic in y .

$$\begin{cases} -\nabla_y \cdot (\lambda_g(y) \nabla_y \omega_g^k) &= \sum_{i=1}^3 \partial_{y_k} \lambda_{gki}(y) \text{ in } Y_g^\delta, \\ -\lambda_g(y) \frac{\partial \omega_g^k}{\partial n} &= \sum_{i=1}^3 \lambda_{gki}(y) n_i \text{ on } \Gamma^\delta, \end{cases} \quad (21)$$

for all $k \in \{1, 2, 3\}$ and ω_g^k are Y^δ -periodic in y . The *cell problems for the solid part* are given by

$$\begin{cases} -\nabla_y \cdot (\lambda_s(y) \nabla_y \omega_s^k) &= \sum_{i=1}^3 \partial_{y_k} \lambda_{ski}(y) \text{ in } Y_s^\delta, \\ -d\lambda_s(y) \frac{\partial \omega_s^k}{\partial n} &= \sum_{i=1}^3 \lambda_{ski}(y) n_i \text{ on } \Gamma^\delta \end{cases} \quad (22)$$

for all $k \in \{1, 2, 3\}$, ω_s^k are Y^δ -periodic in y .

Standard theory of linear elliptic problems with periodic boundary conditions ensures the weak solvability of the families of cell problems (20) – (22); see e.g. Ref. [12].

The main result of this section is the following:

Theorem 5.7. The sequence of weak solutions of the microscopic problem (in the sense of Definition (4.1)) converges as $\varepsilon \rightarrow 0$ to the triplet $(C^\delta, T^\delta, R^\delta)$, where $C^\delta \in C_u + L^2(0, T; H_\Gamma^1(\Omega^\delta))$, $\partial_t C^\delta \in \partial_t C_u + L^2(0, T; L^2(\Omega^\delta))$, $T^\delta \in T_u + L^2(0, T; H_\Gamma^1(\Omega^\delta))$, $\partial_t T^\delta \in \partial_t T_u + L^2(0, T; L^2(\Omega^\delta))$, and $R^\delta \in H^1(0, T; L^2(\Omega^\delta \times \Gamma^\delta))$ satisfying weakly the following macroscopic equations a.e. in Ω^δ for all $t \in (0, T)$

$$\partial_t C^\delta + \nabla \cdot (-\mathfrak{D} \nabla C^\delta + \mathbf{u}^\delta C^\delta) = -\frac{|\Gamma^\delta|}{|Y_g^\delta|} W(T^\delta, C^\delta), \quad (23)$$

$$\mathfrak{C} \partial_t T^\delta + \nabla \cdot (-\mathfrak{L} \nabla T^\delta + \langle C_g \rangle_{Y_g^\delta} \mathbf{u}^\delta T^\delta) = \frac{|\Gamma^\delta|}{|Y_g^\delta|} QW(T^\delta, C^\delta), \quad (24)$$

$$\partial_t \langle R^\delta \rangle_{\Gamma^\delta} = W(T^\delta, C^\delta), \quad (25)$$

where

$$\langle R^\delta \rangle_{\Gamma^\delta}(t, x) := \frac{1}{|\Gamma^\delta|} \int_{\Gamma^\delta} R^\delta(t, x, y) d\gamma$$

and

$$\langle C_g \rangle_{Y_g^\delta} := \frac{1}{|Y_g^\delta|} \int_{Y_g^\delta} C_g(y) dy$$

for all $x \in \Omega^\delta$ and all $t \in (0, T)$. Furthermore, the effective heat capacity \mathfrak{C} , the effective diffusion tensor \mathfrak{D} , and the effective heat conduction tensor \mathfrak{L} are given by

$$\mathfrak{C} := \int_{Y^\delta} [C_g(y) \chi_{Y_g^\delta}(y) + C_s(y) \chi_{Y_g^\delta}(y)] dy \quad (26)$$

$$(\mathfrak{D})_{jk} := \frac{1}{|Y_g^\delta|} \sum_{\ell=1}^3 \int_{Y_g^\delta} (D)_{jk} + (D)_{\ell k} \partial_{y_\ell} \omega_g^j dy \quad (27)$$

$$(\mathfrak{L})_{jk} := (\Lambda_g)_{jk} + (\Lambda_g)_{jk} \quad (28)$$

$$(\Lambda_g)_{jk} := \sum_{\ell=1}^3 \int_{Y^\delta} ((\lambda_g)_{jk} + (\lambda_g)_{\ell k} \partial_{y_\ell} \omega_g^j) \chi_{Y_g^\delta}(y) dy$$

$$(\Lambda_s)_{jk} := \sum_{\ell=1}^3 \int_{Y^\delta} ((\lambda_s)_{jk} + (\lambda_s)_{\ell k} \partial_{y_\ell} \omega_s^j) \chi_{Y_s^\delta}(y) dy$$

with ω^j, ω_i^j being solutions of the cell problems defined in Definition 5.6. Here $i \in \{g, s\}$ and $j, k \in \{1, 2, 3\}$. The initial values

$$\begin{aligned} C^\delta(0, x) &= C^0(x), & T_g^\delta(0, x) &= T^0(x) \text{ for } x \in \Omega^\delta \\ R^\delta(0, x, y) &= R^0(x, y) \text{ for } (x, y) \in \Omega^\delta \times \Gamma^\delta, \end{aligned}$$

together with the boundary conditions

$$C^\delta = C_u \quad \text{on } \Gamma_D^\delta, \quad (29)$$

$$-\mathfrak{D} \nabla C^\delta \cdot \nu = 0 \quad \text{on } \Gamma_N^\delta, \quad (30)$$

$$T^\delta = T_u \quad \text{on } \Gamma_D^\delta, \quad (31)$$

$$-\mathfrak{L} \nabla T^\delta \cdot \nu = 0 \quad \text{on } \Gamma_N^\delta. \quad (32)$$

complete the formulation of the macroscopic problem.

Furthermore, it exists at most one triplet $(C^\delta, T^\delta, R^\delta)$ satisfying the above properties.

Proof. Relying on Lemma 5.5, we apply the two-scale convergence results stated in Definition 5.1 and Definition 5.3 to derive the weak and strong formulations of the wanted upscaled model equations. We take as test functions incorporating the following oscillating behavior $\bar{\phi}(t, x) = \phi(t, x) + \varepsilon \tilde{\phi}(t, x, \frac{x}{\varepsilon})$, with $\phi \in C_0^\infty([0, T] \times \overline{\Omega^\delta})$

and $\tilde{\phi} \in C_0^\infty([0, T] \times \overline{\Omega^\delta}; C_\#^\infty(Y_g^\delta))$. Applying the concept of two-scale convergence yields

$$\begin{aligned} & |Y_g^\delta| \int_0^T \int_{\Omega^\delta} \partial_t C \phi(t, x) + \int_0^T \int_{\Omega^\delta} \int_{Y_g^\delta} D(\nabla_x C^\delta(t, x) + \nabla_y \tilde{C}^\delta(t, x, y))(\nabla_x \phi(t, x) + \nabla_y \tilde{\phi}(t, x, y)) \\ & - |Y_g^\delta| \int_0^T \int_{\Omega^\delta} \mathbf{u}^\delta \cdot \nabla_x C^\delta \phi(t, x) dx dt = - \lim_{\varepsilon \rightarrow 0} \varepsilon \int_0^T \int_{\Gamma^{\delta\varepsilon}} W(T^{\delta\varepsilon}, C^{\delta\varepsilon}) \phi d\gamma dt, \\ & = - |\Gamma^\delta| \int_0^T \int_{\Omega^\delta} W(T^\delta, C^\delta) \phi dx dt. \end{aligned} \quad (33)$$

Now, we take $\bar{\varphi}(t, x) = \varphi(t, x) + \varepsilon \tilde{\varphi}(t, x, \frac{x}{\varepsilon})$ with $\varphi \in C_0^\infty([0, T] \times \overline{\Omega^\delta})$, $\tilde{\varphi} \in C_0^\infty([0, T] \times \overline{\Omega^\delta}; C_\#^\infty(Y^\delta))$. We thus get

$$\begin{aligned} & \int_0^T \int_{\Omega^\delta} \int_{Y^\delta} [C_g(y) \chi_{Y_g^\delta}(y) + C_s(y) \chi_{Y_s^\delta}(y)] \partial_t T^\delta(t, x) \varphi(t, x) + \\ & \int_0^T \int_{\Omega^\delta} \int_{Y^\delta} [\lambda_g \chi_{Y_g^\delta}(y) + \lambda_s \chi_{Y_s^\delta}(y)] (\nabla_x T^\delta(t, x) + \nabla_y \tilde{T}^\delta(t, x, y)) (\nabla_x \varphi(t, x) + \nabla_y \tilde{\varphi}(t, x, y)) \\ & + \int_0^T \int_{\Omega^\delta} \int_{Y_g^\delta} C_g(y) \mathbf{u}^\delta(t, x) \cdot \nabla_x T^\delta(t, x) \varphi(t, x) dx dy dt = \int_0^T \int_{\Omega^\delta} \int_{\Gamma^\delta} QW(T^\delta, C^\delta) \varphi dx d\gamma dt. \end{aligned}$$

Take now $\psi(t, x, \frac{x}{\varepsilon}) \in C^\infty([0, T] \times \overline{\Omega^\delta}, C_\#^\infty(\Gamma^\delta))$ and pass to the limit in the ordinary differential equations for R^ε and choose in the respective weak form $\psi = 1$. Then averaging over the variable y leads to (25). To proceed further, we set $\phi = 0$ in (33) to calculate the expression of the unknown (corrector) function \tilde{C}^δ and obtain

$$\int_0^T \int_{\Omega^\delta} \int_{Y_g^\delta} D(y) (\nabla_x C^\delta(t, x) + \nabla_y \tilde{C}^\delta(t, x, y)) \nabla_y \tilde{\phi}(t, x, y) dx dy dt = 0.$$

Since \tilde{C}^δ depends linearly on $\nabla_x C^\delta$, it can be defined as

$$\tilde{C}^\delta := \sum_{j=1}^3 \partial_{x_j} C^\delta \omega^j,$$

where the cell function ω^j is the unique solution of the corresponding cell problem defined in Definition 5.6. Similarly, we have $\tilde{T}^\delta := \sum_{j=1}^3 \partial_{x_j} T^\delta(\omega_s^j + \omega_g^j)$, where ω_g^j and ω_s^j are the cell solutions. Setting $\tilde{\phi} = 0$ in (33), we get

$$\begin{aligned} & \int_0^T \int_{\Omega^\delta} \int_{Y_g^\delta} \sum_{j,k=1}^3 D_{jk}(y) (\partial_{x_k} C^\delta(t, x) + \sum_{m=1}^3 \partial_{y_k} \omega^m \partial_{x_m} C^\delta(t, x)) \partial_{x_j} \phi(t, x) dy dx dt \\ & = |Y_g^\delta| \int_0^T \int_{\Omega^\delta} \sum_{j,k=1}^3 (\mathfrak{D})_{jk} \partial_{x_k} C^\delta(t, x) \partial_{x_j} \phi(t, x) dx dt. \end{aligned}$$

Hence, the coefficients entering the effective diffusion tensor \mathfrak{D} (for the active gaseous species) is given by

$$(\mathfrak{D})_{jk} := \frac{1}{|Y_g^\delta|} \sum_{\ell=1}^3 \int_{Y_g^\delta} (D)_{jk} + (D)_{\ell k} \partial_{y_\ell} \omega_g^j) dy.$$

Similarly, we obtain the following coefficients

$$(\Lambda_g)_{jk} := \sum_{\ell=1}^3 \int_{Y_g^\delta} ((\lambda_g)_{jk} + (\lambda_g)_{\ell k} \partial_{y_\ell} \omega_g^j) dy.$$

and

$$(\Lambda_s)_{jk} := \sum_{\ell=1}^3 \int_{Y_s^\delta} ((\lambda_s)_{jk} + (\lambda_s)_{\ell k} \partial_{y_\ell} \omega_s^j) dy.$$

defining the heat conduction tensor \mathfrak{L} cf. (28). The uniqueness of weak solutions follows in a straightforward way; see related comments in Remark 5. \square

Remark 4. The tensors \mathfrak{D} and \mathfrak{L} are symmetric and positive definite, see [12]. Note that a similar estimate as the one reported in Remark 3 holds also for the *macroscopic instantaneous burn bulk rates* and for their time averages.

Remark 5. From now on, let us refer to the homogenized equations (23)–(32) as problem $(\mathcal{P}^{\delta 0})$. Note that the compactness results associated with the two-scale convergence guarantee the existence of positive weak solutions to $(\mathcal{P}^{\delta 0})$. On top of this, Tietze's extension result ensures that the obtained weak solutions also satisfy a weak maximum principle (so, we have L^∞ bounds on the temperature, reaction product and on the concentration). Having this in view, proving the uniqueness of weak solutions to our semilinear parabolic system $(\mathcal{P}^{\delta 0})$ becomes a simple exercise, and therefore we omit the proof of the uniqueness statement.

6. The dimension reduction limit $\delta \rightarrow 0$. In this section, we wish to pass to the dimension reduction limit $\delta \rightarrow 0$. To do this, we follow the main line of the ideas from [11], i.e. we use a scaling argument and employ weak convergence methods (δ -independent estimates) to derive the structure of the limit equations for the reduced problem – (\mathcal{P}^{00}) . Closely related ideas are included in section 4 of [48]. We refer here also to [6] for remotely related regular and singular perturbation settings treated in a rigorous manner for linear evolution equations.

Consider the following set of restrictions, collected as *Assumptions (B)*:

- (B1) The microstructures are chosen such that the ratios $\frac{|\Gamma_g^\delta|}{|Y_g^\delta|}$ and $\frac{|\Gamma_s^\delta|}{|Y_s^\delta|}$ are of order of $\mathcal{O}(1)$; Choose the microstructure shown in Figure 3.
- (B2) u^δ is δ -independent. We refer to it as u^0 .
- (B3) Assume all model parameters ($\mathfrak{D}, \mathfrak{L}, \mathfrak{C}$, etc.) to be constant in the Oz -coordinate. The same holds for the initial data R^0, C^0, T^0 and for the Dirichlet boundary values T_u and C_u .
- (B4) $\lim_{\delta \rightarrow 0} \langle C_g \rangle_{Y_g^\delta} = \langle C_g \rangle_{Y_g}$.

Remark 6. The assumption (B1) is basically imposed by the way we passed to the homogenization limit, i.e. if one wants to pass to either of the limits $\delta \rightarrow 0$ or $\varepsilon \rightarrow 0$, the microstructures cannot be too small. This is a simplification avoiding the occurrence of boundary layers. The conditions (B2)–(B4) are technical assumptions

that can potentially be replaced by less restrictive ones. We choose them for the simplicity of the presentation.

We introduce now the bijective mapping

$$\Omega^\delta \ni (x, y, z) \rightarrow (X, \frac{w}{\delta}) \in \hat{\Omega} := \Omega \times [0, 1] \quad (34)$$

for any $\delta > 0$, where $X := (x, y)$. $\hat{\Gamma}$ will denote the transformation of Γ^δ under this mapping. The main role of this transformation is to fix the width of the layer independently on δ with the price of having some δ -dependent coefficients multiplying derivatives in the Oz direction, i.e. (34) transforms $\nabla \varphi$ into $\nabla_X \varphi + \delta \nabla_w \varphi$ for any sufficiently smooth choice of φ . This way the dimension reduction problem is reformulated as an anisotropic singular perturbation problem.

After applying (34) to the averaged equations, we can rewrite Theorem 5.7 in a slightly modified form as:

Theorem 6.1. *Let Assumptions (A) and Assumptions (B) to hold. There exists a unique triplet $(C^\delta, T^\delta, R^\delta)$, where $C^\delta \in C_u + L^2(0, T; H_\Gamma^1(\hat{\Omega}))$, $\partial_t C^\delta \in \partial_t C_u + L^2(0, T; L^2(\hat{\Omega}))$, $T^\delta \in T_u + L^2(0, T; H_\Gamma^1(\hat{\Omega}))$, $\partial_t T^\delta \in \partial_t T_u + L^2(0, T; L^2(\hat{\Omega}))$, and $R^\delta \in H^1(0, T; L^2(\hat{\Omega} \times \hat{\Gamma}))$ satisfying weakly the following macroscopic equations a.e. in $\hat{\Omega}$ for all $t \in (0, T)$*

$$\partial_t C^\delta + \nabla_X \cdot (-\mathfrak{D} \nabla_X C^\delta + \mathbf{u}^\delta C^\delta) + \frac{1}{\delta^2} \nabla_w \cdot (-\mathfrak{D} \nabla_w C^\delta) = -\frac{|\Gamma^\delta|}{|Y_g^\delta|} W(T^\delta, C^\delta), \quad (35)$$

$$\begin{aligned} \mathfrak{C} \partial_t T^\delta &+ \nabla_X \cdot (-\mathfrak{L} \nabla_X T^\delta + \langle C_g \rangle_{Y_g^\delta} \mathbf{u}^\delta T^\delta) \\ &+ \frac{1}{\delta^2} \nabla_w \cdot (-\mathfrak{L} \nabla_w T^\delta + \langle C_g \rangle_{Y_g^\delta} \mathbf{u}^\delta T^\delta) = \frac{|\Gamma^\delta|}{|Y_g^\delta|} QW(T^\delta, C^\delta), \end{aligned} \quad (36)$$

$$\partial_t \langle R^\delta \rangle_{\Gamma^\delta} = W(T^\delta, C^\delta). \quad (37)$$

The main result of this section is the following:

Theorem 6.2. *Consider the hypothesis of Theorem 6.1. There exists a subsequence $(C^\delta, T^\delta, R^\delta)$, where $C^\delta \in C_u + L^2(0, T; H_\Gamma^1(\hat{\Omega}))$, $\partial_t C^\delta \in \partial_t C_u + L^2(0, T; L^2(\hat{\Omega}))$, $T^\delta \in T_u + L^2(0, T; H_\Gamma^1(\hat{\Omega}))$, $\partial_t T^\delta \in \partial_t T_u + L^2(0, T; L^2(\hat{\Omega}))$, and $R^\delta \in H^1(0, T; L^2(\hat{\Omega}))$ converging weakly to the weak solution of the following reduced equations a.e. in Ω for all $t \in (0, T)$*

$$\partial_t C^0 + \nabla_X \cdot (-\mathfrak{D} \nabla_X C^0 + \mathbf{u}^0 C^0) = -\frac{|\Gamma|}{|Y_g|} W(T^0, C^0), \quad (38)$$

$$\mathfrak{C} \partial_t T^0 + \nabla_X \cdot (-\mathfrak{L} \nabla_X T^0 + \langle C_g \rangle_{Y_g} \mathbf{u}^0 T^0) = \frac{|\Gamma|}{|Y|} QW(T^0, C^0), \quad (39)$$

$$\partial_t \mathcal{R}^0 = W(T^0, C^0). \quad (40)$$

Proof. The proof of this Theorem is rather lengthy and uses anisotropic singular perturbations. We only sketch here the main steps:

Step 1. Derivation of δ -independent estimates. This step consists in a few technical Lemmas that we state in what follows.

Lemma 6.3. *For all $t \geq 0$, it exists a constant $c > 0$ such that the following energy estimates holds*

$$\|C^\delta(t)\|_{L^2(\hat{\Omega})}^2 + \|\nabla_X C^\delta(t)\|_{L^2(\hat{\Omega})}^2 + \frac{1}{\delta^2} \|\nabla_w C^\delta(t)\|_{L^2(\hat{\Omega})}^2 \leq c \quad (41)$$

$$\|T^\delta(t)\|_{L^2(\hat{\Omega})}^2 + \|\nabla_X T^\delta(t)\|_{L^2(\hat{\Omega})}^2 + \frac{1}{\delta^2} \|\nabla_w T^\delta(t)\|_{L^2(\hat{\Omega})}^2 \leq c. \quad (42)$$

Proof. The proof is similar to the one of Lemma 4.2. We omit to repeat the arguments. It is worth noting this statement enforces the fact that $\|\nabla_w C^\delta(t)\|_{L^2(\hat{\Omega})}$ and $\|\nabla_w T^\delta(t)\|_{L^2(\hat{\Omega})}$ are of order of $\mathcal{O}(\delta)$. This fact will be essential to the success of Step 4. \square

Lemma 6.4. *Assume Assumptions (B). Then there exist $(C^0, T^0, \mathcal{R}^0)$ and a subsequence still labeled with δ converging to zero such that*

- (i) $C^\delta \rightarrow C^0$, $\nabla_X C^\delta \rightarrow \nabla_X C^0$ and $\partial_t C^\delta \rightarrow \partial_t C$ in $L^2((0, T); L^2(\hat{\Omega}))$.
- (ii) $T^\delta \rightarrow T^0$, $\nabla_X T^\delta \rightarrow \nabla_X T^0$ and $\partial_t T^\delta \rightarrow \partial_t T$ in $L^2((0, T); L^2(\hat{\Omega}))$.
- (iii) $\langle R^\delta \rangle \rightarrow \mathcal{R}^0$ in $L^2((0, T), L^2(\hat{\Omega}))$, $\partial_t \langle R^\delta \rangle \rightarrow \partial_t \mathcal{R}^0$ in $L^\infty((0, T), L^\infty(\hat{\Omega}))$.
- (iv) $W(T^\delta, C^\delta) \rightarrow W(T^0, C^0)$ in $L^2((0, T), L^2(\hat{\Omega}))$.

Proof. (i)-(iii) The proof of these estimates follows the same line of the proof of Lemma 4.2 and Lemma 4.6. We omit to show it here. The statement (iv) follows by the strong convergence $C^\delta \rightarrow C^0$ in $L^2((0, T); L^2(\hat{\Omega}))$ and the fact that $f(T^\delta) \rightarrow f(T^0)$ in $L^2((0, T); L^2(\hat{\Omega}))$. This concludes that $W(T^\delta, C^\delta) \rightarrow W(T^0, C^0)$ in $L^2((0, T), L^2(\hat{\Omega}))$. Compare Lemma 5.5 (d). \square

Lemma 6.5. *Under the assumptions of Lemma 6.4, the following statements hold true:*

- (i) *For any $\varphi \in H_\Gamma^1(\hat{\Omega})$, the functions $t \rightarrow \int_{\hat{\Omega}} C^\delta \varphi dx$ and $t \rightarrow \int_{\hat{\Omega}} C^0 \varphi dx$ belong to $H^1(0, T)$ and for the same subsequence we have*

$$\int_{\hat{\Omega}} C^\delta \varphi dx \rightarrow \int_{\hat{\Omega}} C^0 \varphi dx \text{ in } L^2(0, T) \text{ and in } C([0, T])$$

and

$$\int_{\hat{\Omega}} C^\delta \varphi dx \rightharpoonup \int_{\hat{\Omega}} C^0 \varphi dx \text{ in } H^1(0, T).$$

- (ii) *For any $\phi \in H_\Gamma^1(\hat{\Omega})$, the functions $t \rightarrow \int_{\hat{\Omega}} T^\delta \phi dx$ and $t \rightarrow \int_{\hat{\Omega}} T^0 \phi dx$ belong to $H^1(0, T)$ and for the same subsequence we have*

$$\int_{\hat{\Omega}} T^\delta \phi dx \rightarrow \int_{\hat{\Omega}} T^0 \phi dx \text{ in } L^2(0, T) \text{ and in } C([0, T])$$

and

$$\int_{\hat{\Omega}} T^\delta \phi dx \rightharpoonup \int_{\hat{\Omega}} T^0 \phi dx \text{ in } H^1(0, T).$$

Proof. The proof follows the lines of Lemma 3.3 in [11]. \square

Step 2. *(Recovering the weak and strong formulations of problem (\mathcal{P}^{00})).* This step is more delicate and its success strongly depends on the regularity constraints from Assumptions (B). We skip here the proof and refer the reader to [11], where a scalar case has been treated in full details. To recover the ordinary differential equation for R^0 , one proves first that the sequence (R^δ) is a Cauchy sequence in a

suitable functions space. Section 5.1 from [19] provides the insight needed to show this property.

Step 3. (*Uniqueness of weak solutions to problem (\mathcal{P}^{00})*). Since the system is semi-linear, the globally Lipschitz non-linearity of the production term by chemical reaction ensures the desired uniqueness of (weak) solutions.

Step 4. (*Removing the w -dependency. Projection on Ω*). Integrating the PDE system over the w -variable reduces the formulation of the model posed on $\hat{\Omega}$ to a formulation posed on the “plate” Ω . Integrating over the reaction term does not commute with the nonlinearity. This requires a proof of a corrector estimate of the type claimed in (43), viz.

Claim 6.6. *The inequality*

$$\left| \int_0^1 W(T^\delta, C^\delta) dw - W\left(\int_0^1 T^\delta dw, \int_0^1 C^\delta dw\right) \right| \leq C\delta \quad (43)$$

holds true for an appropriate constant C independent of the choice of δ .

Proof. (of Claim 6.6) We prove the result (43) by inserting the δ -depending estimates from Lemma 6.3 into the inequality given by the following auxiliary Lemma.

Lemma 6.7. *Let $\alpha, \beta \in H^1(\hat{\Omega}) \cap L^\infty(\hat{\Omega})$. Then for any $w^* \in [0, 1]$ and a.e. $X \in \Omega$, it exists a constant $c > 0$ such that*

$$\begin{aligned} & \left\| \alpha(X, w^*) \beta(X, w^*) - \int_0^1 \alpha(X, w) \beta(X, w) dw \right\|_{L^2(\Omega)}^2 \\ & \leq c \left(\|\nabla_w \alpha\|_{L^2(\Omega)}^2 + \|\nabla_w \beta\|_{L^2(\Omega)}^2 \right). \end{aligned} \quad (44)$$

Proof. (of Lemma 6.7) For all $(X, w) \in \hat{\Omega}$, denote $\Psi(x, w) := \alpha(X, w^*) \beta(X, w)$ and $\Phi(X) := \int_0^1 \Psi(x, w) dw$.

We have

$$\begin{aligned} \|\Psi(X, 1) - \Phi\|_{L^2(\Omega)}^2 &= \int_{\Omega} \left(\Psi(X, w^*) - \int_0^1 \Psi(X, w) dw \right)^2 dX \\ &= \int_{\Omega} \left(\int_0^1 (\Psi(X, w^*) - \Psi(X, w)) dw \right)^2 dX \\ &= \int_{\Omega} \left[\int_0^1 \left[\int_w^{w^*} \nabla_{\rho} \Psi(X, \rho) d\rho \right] dw \right] dX \\ &\leq \|\nabla_w \Psi\|_{L^2(\Omega)}^2 \leq c \left(\|\nabla_w \alpha\|_{L^2(\Omega)}^2 + \|\nabla_w \beta\|_{L^2(\Omega)}^2 \right). \end{aligned} \quad (45)$$

The last inequality follows by Minkowski’s inequality. \square

Now, take in (45) $\alpha := C^\delta$ and $\beta := T^\delta$ and note that by Lemma 6.3 we have that $\|\nabla_w \alpha\|_{L^2(\Omega)}$ and $\|\nabla_w \beta\|_{L^2(\Omega)}$ are of order of $\mathcal{O}(\delta)$. This concludes the proof of the Claim. \square

Note that a corrector estimate related to (43) has been proven in Lemma 4.5 from [48]. Putting now together the information from Step 1 – Step 4 leads to the statement of Theorem 6.2. \square

7. Numerical illustration of the fingering instability. The case $\delta > \varepsilon > 0$, $\delta = \mathcal{O}(1)$. One application of the model derived in the previous sections is the investigation of a problem of smoldering combustion under microgravity. The pertinent problem of fingering instability arises under microgravity conditions when a porous sample burns against a gaseous oxidizer air, i.e. when the direction of flow of the oxidizer is opposite to the direction of propagation of the smolder front. In this sense, the transport of the gaseous oxidizer exerts a destabilizing effect on an emerging smolder front. For a detailed report on the fingering instability, we refer the interested reader to [51, 39]. The pattern-forming dynamics described here resembles those occurring in low Lewis number premixed [17, 29] and non-premixed [9, 42, 50, 30] flames. Thus, to maintain adequate precautions regarding fire hazards, particularly in a microgravity spacecraft [39], the fingering phenomenon becomes fundamentally insightful to understanding the mechanism of smolder spread in such environments. In this section, we simply illustrate an application of the macroscopic equations with effective diffusion constants recovered via two-scale convergence for the typical case $\delta > \varepsilon > 0$, $\delta = \mathcal{O}(1)$. For this scenario, we consider a simple two-dimensional unit cell $Y = [0, 1]^2$ containing a circular open set (solid part), Y_s , with a smooth boundary Γ . The physical parameters used in the numerical simulation have been taken from [25]. The numerical method for the results depicted in Figure 6 and 7 are based on a quadratic finite elements algorithm on an unstructured triangular mesh. In Figure 7, a stabilized Streamline-Upwind Petrov-Galerkin (SUPG) method, implemented in COMSOL Multiphysics®, was used. The time-stepping was performed using a Backward Differentiation Formula (BDF). The time step of the computation is $dt = 0.012$. The gaseous part is denoted

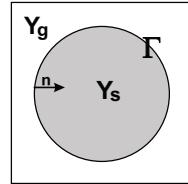


FIGURE 5. Unit cell used in the current simulations.

by $Y_g := Y \setminus \bar{Y}_s$, as depicted in Figure 5. The steps of our numerical multiscale homogenization procedure are as follows:

1. Solve the cell problems in each of the canonical e_j directions for the temperature and concentration fields;
2. Calculate the effective thermal conductivity and diffusion tensors using the solutions of the cell problems;
3. Solve the coupled system of homogenized problems for the temperature T^0 and concentration C^0 fields.

In Figure 6, we illustrate the solutions to the cell problems for the temperature and concentration fields. The cell functions ω_j allow to compute the effective diffusion matrices depicted in (46). The numerical results in Figure 6 were obtained on a unit domain with periodic boundary conditions. In Figure 6(c)-(d), the computation was restricted on the gas part, Y_g , of the domain. Since the geometry of the problem is symmetric, the effective thermal conductivity and diffusion constants are isotropic,

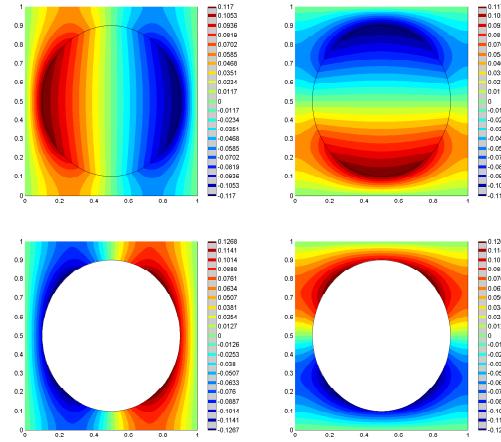


FIGURE 6. Solutions to the cell problems. For the temperature field, see top left: ω_1 ; and right: ω_2 . For the concentration field, see bottom left: ω_1 and right: ω_2

and the calculated values are given viz.

$$\lambda^{\text{eff}} = \begin{pmatrix} 3.96 \cdot 10^{-4} & 0.00 \\ 0.00 & 3.96 \cdot 10^{-4} \end{pmatrix} \quad D^{\text{eff}} = \begin{pmatrix} 0.080523 & 0.00 \\ 0.00 & 0.080523 \end{pmatrix}. \quad (46)$$

In the next step, the effective diffusion constants are used together with the upscaled equations in order to verify our homogenization process. The macroscopic system of equations is used to verify the development of fingering instability of the thin porous sample described in Section 2. The macroscopic behavior of the captured flame structure is illustrated in Figure 7, where \mathcal{R}^0 is the char pattern on the surface of the sample. T^0 is the macroscopic temperature field, C^0 the concentration and W is the nonlinear heat released rate. It should be pointed out that the fingering instability depicted in Figure 7 results from the thermal-diffusive instability (cf. [9, 50, 42, 30]) of the competing transport processes. In the model, the instability manifested at small values of the Lewis number. For the computation, we have used a value of $Le = 0.09$. The structure of the nonlinearity is also important, since it provides the desired coupling between heat and mass transport. In Figure 7(b)

8. Discussion. We keep as further work the case $\delta = \mathcal{O}(\varepsilon)$, when δ vanishes uniformly (in space). Since the diagram of taking the limits $\varepsilon \rightarrow 0$ and $\delta \rightarrow 0$ seems to be commutative, we expect that the concept of thin heterogeneous convergence cf. [36] can be applied to $(\mathcal{P}^{\delta\varepsilon})$ in a rather straightforward way. The derivation of corrector estimates in terms of $\mathcal{O}(\varepsilon, \delta)$ is open; this fact makes unavailable rigorous MsFEM approximations for this multiscale problem. Particularly critical is how to proceed in the fast convection case $u^\varepsilon = \mathcal{O}(\frac{1}{\varepsilon^\alpha})$ and/or in the fast reaction case $A = \mathcal{O}(\frac{1}{\varepsilon^\beta})$, with $\alpha > 0, \beta > 0$ (or in suitable combinations of both).

For a non-uniform shrinking of the layer (see Figure 8 for an illustration of the case $\delta(x) \rightarrow 0$), we expect that a convergence in measures is needed to describe how the “mass” and the “energy” distribute on the flat supporting surface as the volume of the layer vanishes; see [41] for a related context. Both cases $\delta(x) = \mathcal{O}(1)$ and $\delta(x) = \mathcal{O}(\varepsilon)$ are for the moment open.

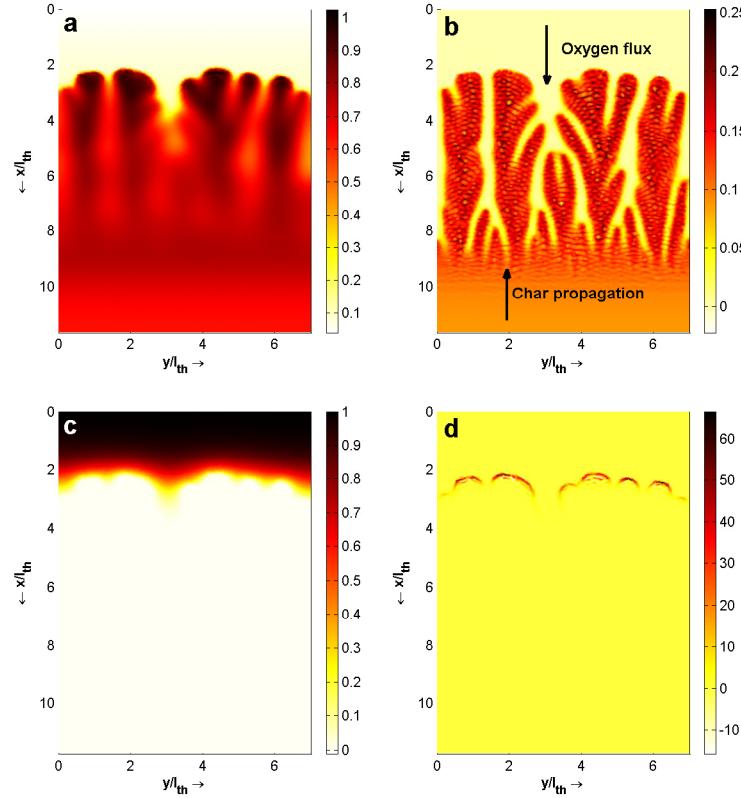


FIGURE 7. Macroscopic profiles of the spatial structure of the flame front: (a) Temperature T^0 , (b) Reaction product \mathcal{R}^0 , (c) Active concentration C^0 , (d) Heat released rate $W(C^0, T^0)$. The macroscopic model was rescaled according to [25, 24], which introduces some dimensionless parameters. Ignition is initiated at the bottom and oxidizer gas is passed from the top. The char propagation is from bottom of the domain to top. The simulation corresponds to $Le = 0.09$ and $Pe = 10$.

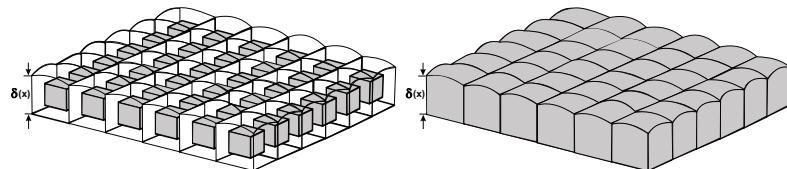


FIGURE 8. Heterogeneous thin layer of height of order of $\mathcal{O}(\delta(x))$: Microscopic view (left) and macroscopic view (right).

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