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A homogenization approach

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PATTERN FORMATION IN REVERSE SMOLDERING COMBUSTION: A HOMOGENIZATION APPROACH

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Abstract. The development of fingering char pattern on the surface of porous thin materials has been investigated in the framework of reverse combustion. This macroscopic characteristic feature of combustible media has also been studied experimentally and through the use of phenomenological models. However, much attention has not been given to the behavior of the emerging patterns based on characteristic material properties. Starting from a microscopic description of the combustion process, macroscopic models of reverse combustion that are derived by the application of the homogenization technique are presented. Using proper scaling by means of a small scale parameter, ε, the results of the formal asymptotic procedure are justified by qualitative multiscale numerical simulations at the microscopic and macroscopic levels. We consider two equilibrium models that are based on effective conductivity contrasts, in a simple adiabatic situation, to investigate the formation of unstable fingering patterns on the surface of a charred material. The behavior of the emerging patterns is analyzed using primarily the Péclet number as a control parameter.

Key words. Periodic homogenization; reverse combustion; fingering instability; multiscale modeling

AMS subject classifications. 35B27; 76M50; 35K57; 80A25; 65N99

1. Introduction. Combustion phenomena have been studied extensively over the years, both theoretically and numerically. Due to its vast application especially for industrial and domestic purposes, understanding of combustion mechanisms and flame propagation has attracted the attention of many scientists ranging from combustion engineers, chemists, theoretical physicists and applied mathematicians. Combustion models (see [6, 31] for details) on the other hand, have been developed to account for various physical combustion processes. For instance, in the study of combustion phenomena in premixed gaseous substances, oil shale combustion in fixed beds, combustion process in porous solid fuels etc. The latter that involves a heterogeneous reaction between the interacting gaseous and solid phases has gained much interest in the framework of filtration combustion. Filtration combustion basically involves two configurations which are based on the direction of flow of the inlet gaseous oxidizer and the direction of propagation of thermal and reaction fronts. It is classified as forward filtration combustion when the oxidizer flow and the reaction zone propagates in the same direction. However, when the reaction zone propagates in opposite direction to the direction of propagation of the inlet oxidizer, the process is classified as reverse filtration combustion. Reverse combustion has been studied in detail (see [28, 22] for example) and is known to exhibit certain characteristic features. For instance, in a slow combustion regime referred to as smoldering, the combustion process proceeds in a nonflaming mode [33] in the presence of an oxidizer to produce char, toxic gaseous fumes and the heat that drives the process, without transiting into gaseous flames.

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In addition, the surface of the charred solid fuel develops fingering patterns (see Fig. 1.1) resulting from a destabilizing effect of reactant transport [33]. Such a scenario was investigated by Zik and Moses, who presented experimental results of reverse combustion, in a Hele Shaw cell containing a thin filter paper sample lying between two parallel plates, for the analysis of fingering instability. The major mechanism of their experiments which is most relevant to the present study is the role of oxygen flow velocity (alternatively the Péclet number) in the observed pattern formation on the charred solid fuel.

In porous media, smoldering becomes very complex and involves various chemical reactions and transport processes [7] in the presence of multiple characteristic time and space scales. The reaction site is the surface of the solid fuel, where smoldering initiation requires the supply of heat flux. Consequently, the temperature of the solid is increased, giving rise to its thermal-degradation reactions (endothermic pyrolysis and exothermic oxidation) until the net heat released is high enough to balance the heat required for propagation. The transfer of heat involves transport processes such as conduction, convection and radiation. Common examples of smoldering combustion in porous media include the initiation of upholstered furniture fires by weak heat sources and the flaming combustion of biomass occurring in wild land fires behind the flame front. For details on smoldering, we refer to [27, 25], e.g. Previous theoretical studies in this area include the work of Ohlemiller [25], who presented the most significant mechanisms involved in the smoldering combustion of polymers. Rein [27] presented a 1-D computational study to investigate smoldering ignition and propagation in polyurethane foam. Ikeda and Mimura [16] proposed a coupled reaction-diffusion system for the macroscopic theoretical understanding of pattern formation in smoldering combustion. Their numerical simulations exhibit a good qualitative agreement with the experimental results presented by Zik and Moses [33, 34, 32]. Other theoretical studies include [12, 18, 8], where traveling waves solutions arising from models of smoldering combustion are presented. In [7], a pioneering three-dimensional microscale numerical simulation of smoldering in fixed beds of solid fuels is presented. In a set of 2D and 3D simulations, it was shown, contrary to the predictions of simple macroscopic models, that in some regimes there exist severe thermal disequilibrium in the constituent phases. This is one of the important aspects of the microscale numerical simulation in the detailed microscopic model.
In this paper, we propose a microscopic model of the smoldering combustion of a thin solid fuel—a porous solid with periodic microstructure—by the mathematical concept of periodic homogenization. The theoretical background of the proposed model is partly inspired by a previous macro-geometric model by Kagan et al. [18], which consists of a gas-solid system. We begin with a microscopic description where the solid fuel is assumed to be microscopically dispersed in a homogeneous gas phase. For an illustration of the macro-geometric (reverse flow) configuration, we refer to [18, 33, 12], where the smolder front burns against an incoming gas stream that contains oxygen. In order to reduce the complexity of solving the detailed microscopic model, we consider a macroscopic viewpoint by deriving formally averaged models of reverse combustion via the classical homogenization method. The results of the upscaled models can be rigorously justified, for instance, by the two-scale convergence [2, 14], eventually combined with periodic unfolding (very much in the spirit of [?]). On the other hand, the macroscopic models [19, 28, 13] derived by the volume-averaging method are harder to justify mathematically. The solutions of the upscaled models are illustrated in two dimensional numerical simulations and then compared with solutions obtained from idealized microscopic models to justify their validity within an appropriate parameter space. Using a nondimensional form of the macroscopic models, we investigate in a simple adiabatic case the development of fingering instability on the surface of the charred solid fuel using a range of values of Péclet number as a control parameter.

The remaining part of the paper is organized as follows: section 2 starts with a mathematical description of the microstructure and models for the transport mechanisms. In section 3, we derive the macroscopic models through a formal asymptotic expansion and in section 4, we present a qualitative multiscale numerical simulation and further analyse the macroscopic models for fingering instability. Finally, we conclude in section 5, with remarks on possible directions to the present paper.

2. Formulation of the problem.

2.1. Choice of microstructure. We consider a microscopic description of the macroscopically homogeneous material as illustrated in Fig. 2.1 (left). Based on microscopic evidence, it is observed that the structure of the material consists of complex perforated arrangement of fiber (see Fig. 2.1 (right)). At the scale of the heterogeneity, air permeates the pore scale and interacts with the surface of the fibre. Assuming a typical length at the scale of heterogeneity to be \( \delta \), a reference periodicity cell of length \( \ell \) is identified and is sufficiently large i.e. \( \delta < \ell \) to represent the features at the pore scale. The constituent of the unit volume consists of a spherical structure representative of the solid fibre, which is assumed to be dispersed in a gas matrix (see Fig. 2.2). The heterogeneous medium we have in mind satisfies the following properties:

(i) the typical length \( L \) at the macroscopic scale is in the \( x_1 \) direction
(ii) the period \( \ell \) of the structure representing the scale of heterogeneity is sufficiently small compared to the macroscopic scale
(iii) the length of the region along \( x_3 \)-direction is by far small compared to the lengths in the \( x_1, x_2 \)-directions
(iv) \( x_3 \) has arbitrary periodicity.

From (i)-(ii), the condition of separation of scales applies i.e. \( \varepsilon = \ell / L \ll 1 \), where \( \varepsilon \) is a small scale parameter. By (iii)-(iv), we assume that the size in the \( x_3 \)-direction is the same as period. To be more precise in this construction, we begin with a mathematical
description of the intended medium. The (macroscopic) porous domain

\[ \Omega := \prod_{j=1}^{3} (0, a_j), \]

with \( a_j > 0, j = 1, 2, 3 \) is described with macroscopic (i.e. global) coordinates \( x = (x_1, x_2, x_3) \), and choose in \( \mathbb{R}^3 \), a reference periodicity cell, depicted in Fig. 2.2

\[ Y := \{(y_1, y_2, y_3) | 0 < y_j < 1, j = 1, 2, 3\}, \quad (2.1) \]

with microscopic (i.e. local) coordinates \( y = (y_1, y_2, y_3) \), within which we consider a spherical domain with smooth boundary. We denote this structure as

\[ Y_s := \{(y_1, y_2, y_3) | \sum_{j=1}^{3} (y_j - y_0^j)^2 < R^2 \} \subset Y, \quad (2.2) \]

where \( R \) is the radius and \( y_0^j, j = 1, 2, 3 \), is the centre of the solid structure, (see the solid(pink) as shown in Fig. 2.2), and also the centroid of the reference unit cell, \( Y \). Henceforth, this structure is referred to as the solid part. The solid part is embedded in a pore space \( Y_g := Y \setminus Y_s \), which is referred to as the gas part, so that the reference cell can be written as \( Y = Y_g \cup Y_s \). Let \( \partial Y_s \) represent the interface separating the gas part and the solid part, and \( \partial Y \), the boundaries enclosing the domains in \( Y \), then the cell boundary of \( Y_g \) is represented as \( S_g := \partial Y \). A lattice of copies of \( Y \) is thus generated to span a generic parallelepiped domain \( \Omega \). With the small scale parameter \( \varepsilon \), the periodicity cell as well as its distinct parts and interior boundary are rescaled and translated to cover the macroscopic domain. The structure is thus depicted in Fig. 2.3 and defined viz.
Definition 2.1 (The rescaled periodicity cell). The rescaled periodicity cell can be represented by
\[ Y^\varepsilon := \{(y_1, y_2, y_3) | 0 < y_j < \varepsilon, j = 1, 2, 3\}, \]
\[ Y_s^\varepsilon := \{(y_1, y_2, y_3) | \sum_{j=1}^{3} (y_j - \varepsilon y_j^0)^2 < (\varepsilon R)^2\}, \]
\[ Y_g^\varepsilon := Y^\varepsilon \setminus Y_s^\varepsilon. \] (2.3)

Definition 2.2 (The translated subsets). By definition 2.1, the translation of the rescaled subsets is defined as
\[ Y_k^\varepsilon := \{(\bar{y}_1, \bar{y}_2, \bar{y}_3) | \bar{y}_j = y_j + \varepsilon k_j, j = 1, 2, 3, (y_1, y_2, y_3) \in Y^\varepsilon\}, \]
\[ k = (k_1, k_2, k_3) \in \mathbb{Z}^3. \]

Let the number of cells, with respect to the scaling parameter, \( \varepsilon \), in each coordinate direction be defined as
\[ N_j(\varepsilon) := |a_j|\varepsilon^{-1}, \] (2.4)
then, the total number of cells in the domain \( \Omega \) is
\[ N(\varepsilon) := \prod_{j=1}^{3} N_j(\varepsilon), \] (2.5)

Definition 2.3 (Interconnected matrix and ensemble of inclusions). Let \( Y_{g,k}^\varepsilon := Y_k^\varepsilon \setminus Y_s^\varepsilon \) be any translated gas part according to definition 2.2 with \( Y_{s,k}^\varepsilon \), the corresponding solid part. Then the ensemble of the disconnected solid parts is given by
\[ \Omega_s^\varepsilon := \{(y_1, y_2, y_3) | (y_1, y_2, y_3) \in Y_{s,k}^\varepsilon, k = (k_1, k_2, k_3) \in \mathbb{Z}^3, \]
\[ 0 \leq k_j \leq N_j(\varepsilon), j = 1, 2, 3\} \] (2.6)
such that the matrix of interconnected gas parts can be represented by
\[ \Omega_g^\varepsilon := \Omega \setminus \Omega_s^\varepsilon. \] (2.7)

Further, the interior boundaries may also be denoted, based on periodic translations of the boundaries, \( \partial Y_s \), viz.
\[ \Gamma^\varepsilon := \{(y_1, y_2, y_3) | (y_1, y_2, y_3) \in \partial Y_{s,k}^\varepsilon, k = (k_1, k_2, k_3) \in \mathbb{Z}^3, \]
\[ 0 \leq k_j \leq N_j(\varepsilon), j = 1, 2, 3\}. \] (2.8)
2.2. Mathematical model. In this section, the mathematical model of the combustion process occurring on the surface of the solid structure is described. The full fluid dynamics of the problem posed in the porous material follows a creeping flow, but following [12] regarding the complications that may arise while investigating the full fluid dynamics, we introduce a simplifying assumption that the flow in the porous medium is a constant laminar field \( u \) of pre-heated air in the pore matrix \( \Omega^g \). The key point justifying this approximation is that in the smoldering regime we are considering the mass flow rate is much larger than the mass exchange rate due to combustion, so that \( u \) is not much influenced by the combustion process[12]. In view of the spatially periodic geometry, a spatially periodic flow is also assumed and it is divergence free over the gas domain, \( \Omega_g^x \). This is given by

\[
u(y) = \begin{cases} v, & y \in \Omega_g^x, \\ 0, & y \in \Omega_s^x, \end{cases}
\]  

(2.9)

2.2.1. Mass transport of the gaseous species. For a combustion process, the flowing gas constitute a mixture of gaseous chemical species which are governed by mass conservation equations that are similar in form. In a simplified presentation, however, we do not investigate all the gaseous components in the mixture. In particular, we consider the oxygen flow, which is the major component in the gaseous mixture that takes part in the oxidative combustion process. Thus, we assume that its flow is governed by the following convection-diffusion equation

\[rac{\partial C}{\partial t} + u \cdot \nabla C - \nabla \cdot (D \nabla C) = 0, \quad x \in \Omega_g^x, t > 0,
\]  

(2.10)

where \( C \) is the concentration and \( D \) is the molecular diffusion coefficient, assumed here to be constant.

2.2.2. Heat transport. The transport of heat in the gas part and the subsequent conduction of heat in the solid part follow from the Fourier law of heat conduction. The gas phase heat equation is governed by a convection-conduction equation, whereas the predominant mode of heat transport in the solid phase is governed by a conduction equation. Thus, we have

\[
C_g \frac{\partial T_g}{\partial t} + C_g u \cdot \nabla T_g - \nabla \cdot (\lambda_g \nabla T_g) = 0, \quad x \in \Omega_g^x, t > 0,
\]  

(2.11a)

\[
C_s \frac{\partial T_s}{\partial t} - \nabla \cdot (\lambda_s \nabla T_s) = 0, \quad x \in \Omega_s^x, t > 0,
\]  

(2.11b)

where \( C_i = \rho_i c_i \) is the volumetric heat capacity of phase \( i \), \( \lambda_i \) is the heat conductivity and \( T_i \) is the temperature. Since the reaction between the phases is purely heterogeneous and takes place on the surface of the solid phase, the transport equations are coupled at the pore boundary \( \Gamma^\varepsilon \).

2.2.3. Chemical reactions. The chemical process in the considered combustion regime [33, 22] assumes the following form

\[
\text{Solid fuel} + O_2 \rightarrow \text{solid product} + \text{gas product} + \text{heat.}
\]  

(2.12)

For an oxygen-limited reaction, the reaction rate \( W \) is given by a one-step first order reaction with respect to the deficient gaseous reactant. We also assume that adsorption of the reactant on the solid surface is negligible. The temperature-dependent rate
coefficient $k$ is governed by the Arrhenius’ law, viz.

$$k(T) = A \exp \left( - \frac{T_a}{T} \right).$$  (2.13)

Here, $A$ is the pre-exponential factor, $T_a$ is the activation temperature of the reaction, and $T$ is the interfacial temperature at the gas-solid interface, $\Gamma^e$, satisfying $T = T_g = T_s$. The micro-heterogeneous reaction, localized on the solid-gas interface, induces coupling terms in form of source/sink terms respectively for the oxygen and heat equations where $Q$ is the heat release. The reaction at the surface $\Gamma^e$ is given by the following boundary conditions

2.2.4. Interface conditions.

$$\begin{align*}
& (\lambda_g \nabla T_g - \lambda_s \nabla T_s) \cdot n = Q W(T, C), & x \in \Gamma^e, t > 0, \\
& T_g = T_s, & x \in \Gamma^e, t > 0, \\
& D \nabla C \cdot n = - W(T, C), & x \in \Gamma^e, t > 0,
\end{align*}$$  (2.14a-b-c)

where $n$ is the outward unit normal vector which points in a direction outside $Y_g$, and $W(T, C)$ is given by

$$W(T, C) = A \exp \left( - \frac{T_a}{T} \right).$$  (2.15)

Additionally, the char product, $R$, is given by

$$\frac{\partial R}{\partial t} = W(T, C), \quad x \in \Gamma^e, t > 0.$$  (2.16)

The subscripts $g$ and $s$ are used to denote gas phase and solid phase respectively. So far, the governing equations together with the associated interior coupling conditions have been described. Additionally, the following boundary conditions are prescribed at the exterior boundaries:

Diffusive thermal insulation conditions.

$$n \cdot \nabla T_i = 0, n \cdot \nabla C = 0, \quad \partial \Omega \setminus (\{x = 0\} \cup \{x = a_1\}), t > 0.$$  (2.17)

Upstream/Downstream boundary conditions.

$$\begin{align*}
& T_i = T_u, C = C_u, & \{x = 0\} \cap \partial \Omega, t > 0, \\
& \n \cdot \nabla x T_i = 0, \n \cdot \nabla x C = 0, & \{x = a_1\} \cap \partial \Omega, t > 0.
\end{align*}$$  (2.18a-b)

Here, $u$ denotes the unburnt or initial values, and $i$ represents phase $i = \{g, s\}$. The problem is further supplemented with appropriate initial conditions in order to describe the problem fully.

2.3. Nondimensionalization. We rescale the system of equations derived in the previous section and introduce some dimensionless numbers, which will enable us to consider different problems as well as discuss their upscaling. First, we introduce some characteristic values

$$\begin{align*}
\rho_g &= \rho_g^* \rho_{gc}, & e_g = e_g^* e_{gc}, & \lambda_g = \lambda_g^* \lambda_{gc}, & T_i = T_i^* (T_b - T_u) + T_u, \\
\rho_s &= \rho_s^* \rho_{sc}, & e_s = e_s^* e_{sc}, & \lambda_s = \lambda_s^* \lambda_{sc}, & A = A \alpha^* A^*, & Q = Q c^*, \\
C &= C^* C_c, & R = R^* R_c, & D = D^* D_c, & u = u_c, & \Omega = \Omega^* L_c.
\end{align*}$$  (2.19)
Also, the spatial-temporal variables are rescaled viz.

\[ x = x^* L_c, \quad t = t^* t_c. \]

The dimensionless equations take the following form:

\[
C_g \frac{\partial T_g^*}{\partial t^*} + \rho_g^* C_g^* \frac{u_c t_c}{L_c} \nabla T_g^* - \frac{K_{gc} t_c}{L_c^3} \nabla \cdot (\lambda_g^* \nabla T_g^*) = 0, \\
mC_s^* \frac{\partial T_s^*}{\partial t^*} - \frac{K_{gs} t_c}{L_c^3} \nabla \cdot (\lambda_s^* \nabla T_s^*) = 0,
\]

where \( C_g = \rho_g^* C_g^* \), and \( C_s = \rho_s^* C_s^* \) are respectively the dimensionless heat capacities of the constituents in the gas-phase and solid-phase respectively.

\[
K_{gc} = \frac{\lambda_{gc}}{\rho_g c_g c_g}, \quad \mathcal{P}_T = \frac{K_{gc} t_c}{L_c^3}, \quad m = \frac{\rho_u c_sc_c}{\rho_g c_g c_g}, \quad \mathcal{K} = \frac{\lambda_{sc}}{\lambda_{gc}},
\]

where \( K_{gc} \) is the gas phase thermal diffusivity, \( \mathcal{P}_T \), the ratio of thermal transport to the time scale of the observation. The ratio of heat capacities in the material is denoted as \( m \) and the corresponding ratio of heat conductivities is \( \mathcal{K} \). Further, we define the temperature of combustion product, \( T_b := T_u + Q_c C_c / \rho_g c_g c_g \) and introduce the following global characteristic time scales

\[
t_D := \frac{L_c^2}{D_c}, \quad t_A := \frac{L_c}{u_c}, \quad t_G := \frac{L_c}{A_c}, \quad t_R := \frac{R_c}{C_c A_c},
\]

where \( t_D \) is the characteristic global diffusion time scale, \( t_A \) is the characteristic global advection time scale, \( t_G \) and \( t_R \) are respectively the characteristic time of gas reaction and the characteristic time of combustion product. We introduce also the following characteristic dimensionless numbers

\[
\mathcal{P}_e := \frac{L_c u_c}{D_c}, \quad \mathcal{L}_e := \frac{K_{gc} t_c}{D_c}, \quad \mathcal{D}_a := \frac{L_c A_c}{D_c} = \frac{t_D}{t_G},
\]

We take the time of diffusion in the subdomain, \( \Omega^*_g \), as the characteristic time of the observation at the macroscopic scale, i.e. \( t_c = t_D \).

\[
C_g \frac{\partial T_g^*}{\partial t^*} + C_g \mathcal{P}_e L_c u_c \nabla T_g^* - \mathcal{L}_e \nabla \cdot (\lambda_g^* \nabla T_g^*) = 0 \quad (2.20a) \\
mC_s^* \frac{\partial T_s^*}{\partial t^*} - \mathcal{K} \mathcal{L}_e \nabla \cdot (\lambda_s^* \nabla T_s^*) = 0 \quad (2.20b)
\]

After introducing some simplifications, the corresponding boundary conditions to (2.20a)-(2.20b) are

\[
n \cdot (\mathcal{L}_e \lambda_g^* \nabla T_g^* - \mathcal{K} \mathcal{L}_e \lambda_s^* \nabla T_s^*) = \mathcal{D}_a Q^* W^* (T^*, C^*), \quad (2.21a) \\
T_g^* = T_s^*, \quad (2.21b)
\]
with
\[
W^*(T^*, C^*) = A^*C^* \exp \left( -\frac{T_u}{T^*(T_b - T_u)} \right).
\]
(2.22)

Similarly, the mass concentration of oxygen in dimensionless form is viz.
\[
\frac{L_c^2}{D_c t_c} \frac{\partial C^*}{\partial t^*} + \frac{u_c L_c}{D_c} v \cdot \nabla C^* - \nabla \cdot (D^* \nabla C^*) = 0,
\]
(2.23)

where
\[
\mathcal{P}_C = \frac{L_c^2}{D_c t_c}, \text{ the ratio of global characteristic transport times.}
\]

With the choice of characteristic time of diffusion $t_D$, we introduce the Péclet number in (2.23),
\[
\mathcal{P}_C \frac{\partial C^*}{\partial t^*} + \mathcal{P}_E L v \cdot \nabla C^* - \nabla \cdot (D^* \nabla C^*) = 0.
\]
(2.24)

The boundary condition corresponding to (2.24) is
\[
D^* \nabla C^* \cdot n = -D a W^*(T^*, C^*).
\]
(2.25)

The solid char product is given in dimensionless form as
\[
\frac{\partial R^*}{\partial t^*} = \frac{t_c A_c C_c}{R_c} W^*(T^*, C^*) = \frac{t_D}{t_R} W^*(T^*, C^*).
\]
(2.26)

Finally, the system is completed with the following rescaled initial and boundary conditions:
\[
T_i^* = 0, C^* = 1, R^* = 0, \quad x \in \Omega, t = 0.
\]
(2.27)

\[
T_i^* = 0, C^* = 1, \quad \{x = 0\} \cap \partial \Omega, t > 0,
\]
\[
n \cdot \nabla T_i^* = 0, n \cdot \nabla C^* = 0, \quad \{x = a_1\} \cap \partial \Omega, t > 0.
\]

3. Homogenization method.

3.1. General averaging strategy. We describe formally the passage to a macroscopic limit whose form is in general different from that of the microscopic model presented in the previous sections. We do this by applying the mathematical theory of periodic homogenization. For a detailed description of the homogenization techniques, we refer to [5, 30, 29].

In this technique, the micro-model is replaced by a particular limit model which is usually referred to as the macro-model. The idea of the method is to consider a sequence of problems in a periodically repeating structure of which the length has dimension $\varepsilon$ and being increasingly small, goes to zero.

An advantage of this approach, despite its complexity, is that one obtains a much simpler and numerically well-conditioned problem with effective constant coefficients. This is in contrast to the difficulty involved in the direct numerical solution of the
micro-model with periodic microstructure when $\varepsilon$ is by far small. The premise of the micro-model is as follows: we assume periodicity with respect to the physical fields and material coefficients of the micro-model. Majority of the physical situation involving a medium under thermal stress usually leads to deformation of the medium. However, to be consistent with the method at hand, we assume that the medium is structurally undeformed. This means basically that the porosity is taken to be constant. Since our interest is to study a bi-composite medium, we denote the volume porosity by

$$\phi := \frac{|Y_g|}{|Y|},$$

(3.1)

for the gas-phase and by $(1 - \phi)$, the solid-phase porosity. The surface porosity is denoted by

$$\phi^s := \frac{\partial Y_s}{|Y|}.$$  

(3.2)

In (3.1) and (3.2), $|Y|$ is the Lebesgue measure for the volume of $Y$, with $|Y_g|$ and $|Y_s|$, the corresponding volume fractions in the gas and solid parts respectively. We also denote the volume average of a generic field $\varphi_i$ over $Y_i$ by

$$\langle \varphi_i \rangle := \frac{1}{|Y|} \int_{Y_i} \varphi_i dY.$$ 

(3.3)

The oscillatory behavior of the coefficients in the period $Y^\varepsilon$ implies for example $\lambda^\varepsilon(x) = \lambda\left(\frac{x}{\varepsilon}\right) = \lambda(y)$, where $y = x/\varepsilon$. We assume that the material coefficients all belong to the space $L^\infty(\Omega)$, and in particular, the diffusion coefficients are symmetric and positive definite i.e. for a positive constant $\gamma$, and any choice of vector $\xi = (\xi_1, \xi_2, \xi_3), 1 \leq i,j \leq 3$, we have e.g. $\lambda_{ij} = \lambda_{ji}, \lambda_{ij}\xi_i \xi_j \geq \gamma \xi_i \xi_j$. In addition, the coefficients are also taken to be isotropic tensors, i.e. $\lambda = \lambda_o I$ and $D = D_o I$, where for instance, $\lambda_o$ is defined as

$$\lambda_o(y) = \begin{cases} 
\lambda_g, & y \in Y_g, \\
\lambda_s, & y \in Y_s,
\end{cases}$$ 

(3.4)

with $I \in \mathbb{R}^{3 \times 3}$, being the identity matrix.

### 3.2. Asymptotic Homogenization

The main idea of the (formal) asymptotic homogenization procedure is to assume a solution to the microscopically derived models, in a form of an asymptotic expansion involving the macro variable, $x$, and the micro variable, $y = x/\varepsilon$ i.e. we consider an expansion of the form

$$\varphi^\varepsilon(x,t) = \sum_{j=1}^{\infty} \varepsilon^j \varphi^j(x,x/\varepsilon, t).$$ 

(3.5)

Next, we introduce (3.5) into, for example, (2.11a)-(2.11b), identifying problems at the same powers of $\varepsilon$, and finally solving a succession of $\varepsilon$ order local boundary value problems in the $Y$ periodicity cell. The existence and uniqueness of auxiliary solutions can be rigorous justified by the Lax-Milgram lemma. We omit this here and focus on the main aspects of the homogenization procedure.
3.2.1. Comparable material coefficients and transport parameters. We analyse the microscopic model described in previous sections for the heat equations. Here, we consider a problem where the material thermal coefficients in the phases as well as the transport parameters are comparable at the macroscopic level. In the context of the discussion here and all subsequent sections, we refer to this model as the comparable conductivity (CC) model. Thus, the following parameter regimes is considered.

**Case I:** \( K = \mathcal{O}(1) \), \( \mathcal{P}C_L = \mathcal{O}(1) \), \( \mathcal{L}c_p = \mathcal{O}(1) \), \( \mathcal{D}a = \mathcal{O}(\varepsilon) \). Here, the orders of magnitude describe the importance (or the dominance) of a particular physical phenomena (or material coefficient) over another. Our interest in the considered case is to derive particularly a macroscopic model that relates the conductivities of the two phases. By choosing the scaling \( K = \mathcal{O}(1) \), we derive a model where the effect of thermal conductivities of the phases is comparable. Comparability here means that there exist no large contrast (i.e. a low contrast case) of material parameters and the connectivity of the media does not influence the form of the model. Other features of the expected macroscopic limit problem with respect to the choice of scalings include comparable effect of convection to molecular diffusion and a diffusion controlled regime as expressed by \( \mathcal{D}a \). Here and in subsequent cases, the ratio of heat capacities, \( m \), is assumed to be of order \( \mathcal{O}(1) \) for simplicity.

As pointed out earlier, the first step is to assume that solutions to the unknown fields in (3.6a)-(3.6d) follow a formal asymptotic expansion, namely:

\[
\begin{align*}
C_y \frac{\partial T_y}{\partial t} + C_y v \cdot \nabla T_y - \nabla \cdot (\lambda_y \nabla T_y) &= 0, & x \in \Omega_y, t > 0, \\
C_s \frac{\partial T_s}{\partial t} - \nabla \cdot (\lambda_s \nabla T_s) &= 0, & x \in \Omega_s, t > 0, \\
T_y &= T_s, & x \in \Gamma^y, t > 0, \\
n \cdot (\lambda_y \nabla T_y - \lambda_s \nabla T_s) &= \varepsilon QW(T,C), & x \in \Gamma^y, t > 0. 
\end{align*}
\]

As pointed out earlier, the first step is to assume that solutions to the unknown fields in (3.6a)-(3.6d) follow a formal asymptotic expansion, namely:

\[
T_i(x,t) = T_i^{(0)}(x,y,t) + \varepsilon T_i^{(1)}(x,y,t) + \varepsilon^2 T_i^{(2)}(x,y,t) + \mathcal{O}(\varepsilon^3),
\]

\[
C(x,t) = C^{(0)}(x,y,t) + \varepsilon C^{(1)}(x,y,t) + \varepsilon^2 C^{(2)}(x,y,t) + \mathcal{O}(\varepsilon^3),
\]

where \( T_i^{(n)} \) and \( C^{(n)}, n = 1, 2, \ldots, i = \{ g, s \} \) are \( Y \) periodic in \( y \) with \( y = x/\varepsilon \), and describes in multiple scales, solutions in \( \Omega \times Y \). Due to the scale separation, the unknowns in (3.7a) and (3.7b) are functions of three variables: \( x, y \) and \( t \), and consequently, we transform the derivatives through chain rule:

\[
\nabla_x = \nabla_x + \frac{1}{\varepsilon} \nabla_y.
\]

Applying expansions (3.7a)-(3.7b), using (3.8) and collecting terms in powers of \( \varepsilon \), we obtain the following succession of problems:

**Boundary value problem for** \( T_y^{(0)} \) **and** \( T_s^{(0)} \):

\[
\begin{align*}
-\nabla_y \cdot (\lambda_y \nabla_y T_y^{(0)}) &= 0, & y \in Y_g, \\
-\nabla_y \cdot (\lambda_s \nabla_y T_s^{(0)}) &= 0, & y \in Y_s, \\
T_y^{(0)} &= T_s^{(0)}, & y \in \partial Y_s, \\
(\lambda_y \nabla_y T_y^{(0)} - \lambda_s \nabla_y T_s^{(0)}) \cdot n &= 0, & y \in \partial Y_s, \\
T_y^{(0)} \text{ and } T_s^{(0)} \text{ are } Y \text{ periodic.}
\end{align*}
\]
By introducing in (3.9), the following form
\[ T^{(n)}(x, y, t) = T_g^{(n)}(x) + T_s^{(n)}(y), \]
\[ \lambda = \lambda_g(y) + \lambda_s(y), \tag{3.10} \]
we can rewrite (3.9) as
\[ \begin{cases} \nabla_y \cdot (\lambda \nabla_y T^{(0)}) = 0, & y \in Y, \\ [T^{(0)}]_{\partial Y_s} = 0, & y \in \partial Y_s, \\ [\lambda \nabla_y T^{(0)}]_{\partial Y_s} \cdot n = 0, & y \in \partial Y_s, \end{cases} \tag{3.11} \]
where \([ \cdot ]_{\partial Y_s}\) represents the jump \(T_g - T_s\) across the interface \(\partial Y_s\). Problem (3.11) involves only derivatives in \(y\), while \(x\) and \(t\) are present as parameters. The only periodic solution satisfying (3.11) for the local heat problem is that \(T^{(0)}(x, y, t)\) must be a constant, i.e.
\[ T^{(0)}(x, y, t) = T^0(x, t). \tag{3.12} \]
By using (3.10), we write the following boundary value problem for \(T^{(1)}\):
\[ \text{Boundary value problem for } T^{(j)}_g \text{ and } T^{(j)}_s : \]
\[ \begin{cases} \nabla_y \cdot (\lambda \nabla_y T^{(j)} + \nabla_x T^{(0)}) = 0, & y \in Y, \\ [T^{(j)}]_{\partial Y_s} = 0, & y \in \partial Y_s, \\ [\lambda \nabla_y T^{(j)} + \nabla_x T^{(0)}]_{\partial Y_s} \cdot n = 0, & y \in \partial Y_s, \end{cases} \tag{3.13} \]
The linearity of (3.13) makes it possible to consider the following cell problems for the components of the vector, \(\mathcal{M} = (\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3)\), each problem corresponding to a unit macroscopic gradient \(\nabla_x T^{(0)} = e_j, j = 1, 2, 3\), where \(e_j\) is the canonical orthonormal basis in \(\mathbb{R}^3\)
\[ \begin{cases} \nabla_y \cdot (\lambda \nabla_y \mathcal{M} + 1) = 0, & y \in Y, \\ [\mathcal{M}]_{\partial Y_s} = 0, & y \in \partial Y_s, \\ [\lambda \nabla_y \mathcal{M} + 1]_{\partial Y_s} \cdot n = 0, & y \in \partial Y_s, \end{cases} \tag{3.14} \]
Therefore, the solution to the initial problem (3.13) can be written as
\[ T^{(1)}(x, y, t) = \mathcal{M}(y) \cdot \nabla_x T^{(0)}(x, t) + \bar{T}^{(1)}(x, t). \tag{3.15} \]
In (3.15), \(\mathcal{M}\) is the vector satisfying (3.14) and \(\bar{T}^{(1)}(x, t)\) is basically the mean over \(T^{(1)}(x, y, t)\). Again, using the compact form (3.10), the boundary value problem for \(T^{(2)}_g\) and \(T^{(2)}_s\) is given viz.
\[ \text{Boundary value problem for } T^{(2)}_g \text{ and } T^{(2)}_s : \]
\[ \begin{cases} (C_g + C_s) \partial_t T^{(0)} - \nabla_y \cdot (\lambda \nabla_y T^{(2)} + \nabla_x T^{(1)}) - \nabla_x \cdot (\lambda \nabla_y T^{(1)} + \nabla_x T^{(0)}) + C_g v \cdot \nabla_x T^{(0)} = 0, & y \in Y, \\ [T^{(2)}]_{\partial Y_s} = 0, & y \in \partial Y_s, \\ [\lambda \nabla_y T^{(2)} + \nabla_x T^{(1)}]_{\partial Y_s} \cdot n = QW(T^{(0)}, C^{(0)}), & y \in \partial Y_s, \tag{3.16} \end{cases} \]
\(T^{(2)}\) is \(Y\) periodic.
The existence of $T^{(2)}$ enforces a compatibility condition that involves taking the mean of (3.16), applying the divergence theorem and using the prescribed conditions on $\partial Y_s$, i.e.

$$
- \frac{1}{|Y|} \int_Y \nabla_y \cdot (\lambda (\nabla_y T^{(2)} + \nabla_x T^{(1)})) dY = \cdots \\
\frac{1}{|Y|} \int_{S_y} \lambda (\nabla_y T^{(2)} + \nabla_x T^{(1)}) \cdot ndS - \frac{1}{|Y|} \int_{\partial Y_s} \lambda (\nabla_y T^{(2)} + \nabla_x T^{(1)}) \cdot ndS
$$

(3.17)

The first integral at the right-hand side of (3.17) vanishes due to periodicity in $Y$ and the second integral leads to

$$
\frac{1}{|Y|} \int_{\partial Y_s} -QW(T^{(0)},C^{(0)}) dS = -\frac{|\partial Y_s|}{|Y|} QW(T^{(0)},C^{(0)})
$$

(3.18)

Also, we obtain the following averages:

$$
\frac{\partial T^{(0)}}{\partial t} \left[ \frac{1}{|Y|} \int_Y (C_g + C_s) dY \right] = \langle C \rangle^{\text{eff}} \frac{\partial T^{(0)}}{\partial t},
$$

(3.19)

$$
v \cdot \nabla_x T^{(0)} \frac{1}{|Y|} \int_Y C_g dY = \phi C_g v \cdot \nabla_x T^{(0)}.
$$

(3.20)

Further, we see, by using (3.15), that

$$
\nabla_y T^{(1)} + \nabla_x T^{(0)} = (\nabla_y M + I) \nabla_x T^{(0)}
$$

(3.21)

With (3.21), it follows from (3.16), by noting that the integration with respect to $y$ commutes with derivative with respect to $x$

$$
\int_Y \nabla_x \cdot (\lambda (\nabla_y T^{(1)} + \nabla_x T^{(0)})) dY = \nabla_x \left( \left( \frac{1}{|Y|} \int_Y \lambda (\nabla_y M + I) dY \right) \nabla_x T^{(0)} \right)
$$

(3.22)

Finally, the macroscopic description is viz.

$$
\langle C \rangle^{\text{eff}} \frac{\partial T^{(0)}}{\partial t} - \nabla_x \cdot (\langle \lambda \rangle^{\text{eff}} \nabla_x T^{(0)}) + \phi C_g v \cdot \nabla_x T^{(0)} = \phi^{\ast} QW(T^{(0)},C^{(0)}),
$$

(3.23)

with

$$
\langle C \rangle^{\text{eff}} = \frac{1}{|Y|} \int_{Y_s} C_g dY + \int_{Y} C_s dY
$$

(3.24)

$$
\langle C \rangle^{\text{eff}} = \frac{1}{|Y|} \int_{Y_s} C_g dY + \int_{Y} C_s dY
$$

$$
= \phi C_g + (1 - \phi) C_s.
$$

### 3.2.2. Effect of high contrasts in thermal conductivities.

We discuss the upscaling of the derived microscopic heat model in a framework of high contrasts in thermal conductivities of the components of the medium. As pointed out in [26], an important mode of heat transfer for smolder propagation is solid-phase conduction. Thus, we investigate the effect of a high thermal conductivity, by considering the following parameter regime:
Case II: $\mathcal{K} = \mathcal{O}(\varepsilon^{-1}), \mathcal{P}e_L = \mathcal{O}(1), \mathcal{L}e_g = \mathcal{O}(1), \mathcal{D}a = \mathcal{O}(\varepsilon)$. In this case, the objective is to derive a macroscopic model based on the contrast $\mathcal{K} = \mathcal{O}(\varepsilon^{-1})$ in the conductivity of the phases. A similar consideration in the context of a double porosity soil model was presented in [20, 21]. In our case, the contrast $\mathcal{K}$ describes a situation where the conductivity of the solid inclusion is high compared to the gas phase conductivity. Thus, we refer to this model as the high conductivity (HC) model here and in subsequent considerations.

We now solve the following succession of boundary value problems corresponding to the $\varepsilon^{-1}$ term.

**Boundary value problem for $T_s^{(0)}$ and $T_g^{(0)}$**

\[
\begin{align*}
\nabla_y (\lambda_s \nabla_y T_s^{(0)}) &= 0, & y &\in Y_s, \\
\lambda_s \nabla_y T_s^{(0)} \cdot n &= 0, & y &\in \partial Y_s,
\end{align*}
\]

(3.26)

of which the solution has the form

\[
T_s^{(0)}(x, y) = T_s^{(0)}(x),
\]

(3.27)

and for the problem posed in $Y_g$

\[
\begin{align*}
\nabla_y (\lambda_g \nabla_y T_g^{(0)}) &= 0, & y &\in Y_g, \\
T_g^{(0)} &= T_s^{(0)}(x), & y &\in \partial Y_s,
\end{align*}
\]

(3.28)

we obtain the following solution:

\[
T_s^{(0)}(x, y) = T_s^{(0)}(x) = T^{(0)}(x).
\]

(3.29)

Since $T_s^{(0)}$ and $T_g^{(0)}$ are $y$-independent, all subsequent spatial derivatives in $y$ vanishes.

The next problem uses the $\varepsilon^{-1}$ term of $T_s^{(0)}$ and the $\varepsilon^0$ term of the interface condition:

**Boundary value problem for $T_s^{(1)}$**

\[
\begin{align*}
\nabla_y (\lambda_s (\nabla_y T^{(1)} + \nabla_x T^{(0)})) &= 0, & y &\in Y_s, \\
\lambda_s (\nabla_y T^{(1)} + \nabla_x T^{(0)}) \cdot n &= 0, & y &\in \partial Y_s.
\end{align*}
\]

(3.30)

The problem (3.30) is different from the problems considered earlier. We multiply the terms in (3.30) by $y \cdot \nabla_x T^{(0)} + T_s^{(1)}$, integrating by parts over $Y_s$, and using the prescribed condition on $\partial Y_s$

\[
\int_{Y_s} \nabla_y (\lambda_s (\nabla_y T^{(1)} + \nabla_x T^{(0)})) (y \cdot \nabla_x T^{(0)} + T_s^{(1)}) dY
\]

\[
= \int_{Y_s} \lambda_s (\nabla_y T^{(1)} + \nabla_x T^{(0)})^2 dY - \int_{\partial Y_s} n \cdot \lambda_s (\nabla_y T^{(1)} + \nabla_x T^{(0)}) (y \cdot \nabla_x T^{(0)} + T_s^{(1)}) dS
\]

\[
= \int_{Y_s} \lambda_s (\nabla_y T^{(1)} + \nabla_x T^{(0)})^2 dY = 0.
\]

(3.31)
The positivity of $\lambda_s$ implies that $\nabla_y T_s^{(1)} + \nabla_x T_s^{(0)} = 0$. Thus, we obtain

$$T_s^{(1)}(x, y) = -y \cdot \nabla_x T_s^{(0)} + \nabla_y T_s^{(1)}(x). \tag{3.32}$$

**Boundary value problem for $T_g^{(1)}$**

$$\begin{cases}
\nabla_y \cdot (\lambda_g (\nabla_y T_g^{(1)} + \nabla_x T_g^{(0)})) = 0, & y \in Y_g \\
T_g^{(1)} = -y \cdot \nabla_x T_g^{(0)} + \nabla_y T_g^{(1)}(x), & y \in \partial Y_g,
\end{cases} \tag{3.33}$$

where $\nabla_x T_g^{(0)}$ and $\nabla_y T_g^{(1)}(x)$ are taken as forcing terms. The solution of (3.33) can be written in the form:

$$T_g^{(1)}(x, y) = \mathcal{N}(y) \cdot \nabla_x T_g^{(0)} + \nabla_y T_g^{(1)}(x), \tag{3.34}$$

where the vector $\mathcal{N}(y)$ is the solution of the following boundary value problem

$$\begin{cases}
\nabla_y \cdot (\lambda_g (\nabla_y \mathcal{N} + \mathbf{I})) = 0, & y \in Y_g \\
\mathcal{N} + y = 0, & y \in \partial Y_g.
\end{cases} \tag{3.35}$$

For the macroscopic equations, we look at the $\epsilon^0$ term from $T_g^{(2)}$ and the $\epsilon^1$ term from $T_s^{(3)}$, i.e.

$$\begin{align*}
C_g \frac{\partial T_g^{(0)}}{\partial t} &= \nabla_y \cdot (\lambda_g (\nabla_y T_g^{(2)} + \nabla_x T_g^{(1)})) + \\
\nabla_x \cdot (\lambda_g (\nabla_y T_g^{(1)} + \nabla_x T_g^{(0)})) - C_g v \cdot \nabla_x T_g^{(0)}, & y \in Y_g,
\end{align*} \tag{3.36}$$

Averaging (3.36) over $Y_g$ and $Y_s$, and using the prescribed boundary condition:

$$\begin{align*}
(1 - \phi)C_s + \phi C_g \frac{\partial T_s^{(0)}}{\partial t} + \phi C_g v \cdot \nabla_x T_s^{(0)} &= \frac{1}{|Y|} \nabla_x \left( \int_{Y_g} \lambda_g (\nabla_y T_g^{(1)} + \nabla_x T_g^{(0)}) dY \right) + \\
\frac{1}{|Y|} \nabla_x \left( \int_{Y_s} \lambda_s (\nabla_y T_s^{(2)} + \nabla_x T_s^{(1)}) dY \right) + \phi \epsilon QW(T^{(0)}, C^{(0)}) \tag{3.37}
\end{align*}$$

Since $T_s^{(2)}$ is unknown, we transform the integrals by identifying the heat fluxes in each constituent viz [20]:

$$\begin{align*}
q_g &= \lambda_g (\nabla_y T_g^{(1)} + \nabla_x T_g^{(0)}), \tag{3.38a} \\
q_s &= \lambda_s (\nabla_y T_s^{(2)} + \nabla_x T_s^{(1)}). \tag{3.38b}
\end{align*}$$

The flux in (3.38a) satisfy the following dyadic product identity

$$q_{ik} = \frac{\partial}{\partial y_j} (y_k q_{ij}), \quad \text{where} \ q_i = \nabla_y \cdot (y \otimes q_i), i = \{g,s\}.$$
Since the solid inclusions are completely embedded in the matrix, it makes sense to apply the divergence theorem to the integrals in (3.37), i.e.

\[ \int_{Y} q_{g} dY = \int_{\partial Y_{s}} (y \otimes q_{g}) \cdot ndS + \int_{S_{g}} (y \otimes q_{g}) \cdot ndS \]  
\[ \int_{Y} q_{s} dY = -\int_{\partial Y_{s}} (y \otimes q_{s}) \cdot ndS, \]

(3.39a)

(3.39b)

(3.39c)

Substituting (3.39a) and (3.39b) for the integrals in (3.37) and making use of the condition of flux continuity (i.e. the boundary condition corresponding to the $\varepsilon^1$ term) over $\partial Y_{s}$, we obtain:

\[ \langle C \rangle_{\text{eff}} \frac{\partial T^{(0)}}{\partial t} + \phi C_{g} v \cdot \nabla_{x} = \nabla_{x} \cdot (\hat{\lambda}_{\text{eff}} \nabla_{x} T^{(0)}) + \phi^{*} Q W(T^{(0)}, C^{(0)}), \]  

(3.40)

where the effective conductivity tensor, $\hat{\lambda}_{\text{eff}}$, is given by the following surface integral:

\[ \hat{\lambda}_{k}^{ij} = \frac{1}{|S_{g}|} \int_{S_{g}} \lambda_{g}^{ij} \left( \frac{\partial N_{k}}{\partial y_{l}} + I_{kj} \right) y_{k} n_{l} dS. \]  

(3.41)

From (3.41), we see that the effective conductivity is evaluated over the cross-sectional surface of $Y$, orthogonal to the $k$th-direction.

We point out that the heat models (3.23) and (3.40) derived based on the conductivity parameter regime $K = \lambda_{sc}/\lambda_{gc} = O(\varepsilon^{\alpha})$ can be grouped into three categories in terms of the value of $\alpha$. We treated two cases of $\alpha$ in the present paper. A third case applies, for example, when $\alpha = 2$. In this case, the conductivity of the solid inclusion is very low compared to the gas phase conductivity. This model is similar in form to the distributed microstructure models presented in [15, 11, ?]. Generally, such problems exhibit memory effects in the limit problem due to the time retardation that is introduced by the solid phase conductivity.

### 3.2.3. Homogenization of the concentration model.

As in the case of the temperature model, we derive macroscopic model for the concentration of the oxidizer based on the following parameter regime.

\[ P_{eL} = O(1), P_{C} = O(1), D_{a} = O(\varepsilon). \]

\[ \frac{\partial C}{\partial t} + v \cdot \nabla C = \nabla \cdot (D \nabla C) = 0, \quad x \in \Omega^{x}, t > 0, \]  

(3.42a)

\[ -D \nabla C \cdot n = \varepsilon W(T, C), \quad x \in \Gamma^{x}, t > 0. \]  

(3.42b)

We introduce in (3.42a) and (3.42b) the expansions (3.7a) and (3.7b), and identify powers of $\varepsilon$. From these expansions, we are led to a few local boundary value problems:

**Boundary value problem for $C^{(0)}$**:

\[
\begin{align*}
-\nabla_{y} \cdot (D \nabla_{y} C^{(0)}) = 0, & \quad y \in Y_{g}, \\
-D \nabla_{y} C^{(0)} \cdot n = 0, & \quad y \in \partial Y_{s}, \\
C^{(0)} & \text{ is $Y$ periodic.}
\end{align*}
\]  

(3.43)

As seen earlier, any solution of (3.43) is unique up to an additive function of $x$ and $t$, where $x$ and $t$ are parameters. Thus, the solution to (3.43) is

\[ C^{(0)}(x, y, t) = C^{(0)}(x, t). \]  

(3.44)
Pattern formation in reverse combustion

(3.44) implies that the concentration \( C^{(0)} \) is a constant over the period.

**Boundary value problem for \( C^{(1)} \):**

\[
\begin{align*}
- \nabla_y \cdot (D(\nabla_y C^{(1)} + \nabla_x C^{(0)})) &= 0, \quad y \in Y_g, \\
- D(\nabla_y C^{(1)} + \nabla_x C^{(0)}) \cdot n &= 0, \quad y \in \partial Y_s, \\
C^{(1)} &= \text{Y periodic}.
\end{align*}
\]  

(3.45)

Here, the gradient, \( \nabla_x C^{(0)} \), is only present as a source term in (3.44). Due to linearity and the fact that spatial derivatives are only in \( y \), it makes sense to consider the following local problem for the periodic vector \( \mathcal{N} = (N_1, N_2, N_3) \), with a mean of zero over \( Y_g \) i.e.

\[
\begin{align*}
\nabla_y \cdot (D(\nabla_y \mathcal{N} + \mathbf{I})) &= 0, \quad y \in Y_g, \\
D(\nabla_y \mathcal{N} + \mathbf{I}) \cdot n &= 0, \quad y \in \partial Y_s, \\
\langle \mathcal{N} \rangle &= 0, \mathcal{N} \text{ is Y periodic},
\end{align*}
\]  

(3.46)

where the solution to (3.45) can be written in the form

\[ C^{(1)}(x, y, t) = \mathcal{N}(y) \cdot \nabla_x C^{(0)} + \overline{C}^{(1)}(x, t), \]

(3.47)

and \( \overline{C}^{(1)}(x, t) \) is only an arbitrary function of \( x \) and \( t \). With the results obtained in (3.44) and (3.47), we write the boundary value problem for \( C^{(2)} \) as

**Boundary value problem for \( C^{(2)} \):**

\[
\begin{align*}
\partial_t C^{(0)} - \nabla_y \cdot (D(\nabla_y C^{(2)} + \nabla_x C^{(1)})) - \nabla_x \cdot (D(\nabla_y C^{(1)} + \nabla_x C^{(0)})) + \\
v \cdot \nabla_x C^{(0)} &= 0, \quad y \in Y_g, \\
- D(\nabla_y C^{(2)} + \nabla_x C^{(1)}) \cdot n &= W(T^{(0)}, C^{(0)}), \quad y \in \partial Y_s, \\
C^{(2)} &= \text{Y periodic}.
\end{align*}
\]  

(3.48)

Applying the compatibility condition for the existence of \( C^{(2)} \), and using the expressions for \( C^{(0)} \) and \( C^{(1)} \), respectively in (3.48), we obtain

\[
\begin{align*}
- \frac{1}{|Y|} \int_{Y_g} \nabla_y \cdot (D(\nabla_y C^{(2)} + \nabla_x C^{(1)}))dY &= \cdots \\
- \frac{1}{|Y|} \int_{S_g} (D(\nabla_y C^{(2)} + \nabla_x C^{(1)})) \cdot ndS - \frac{1}{|Y|} \int_{\partial Y_s} (D(\nabla_y C^{(2)} + \nabla_x C^{(1)})) \cdot ndS.
\end{align*}
\]  

(3.49)

The first integral at the right-hand side of (3.49) vanishes due to periodicity condition in \( Y \) and the second integral yields

\[ \frac{1}{|Y|} \int_{\partial Y_s} W(T^{(0)}, C^{(0)})dS = \phi^* W(T^{(0)}, C^{(0)}) \]  

(3.50)

The average of the remaining terms in (3.49) is viz.

\[ \phi \frac{\partial C^{(0)}}{\partial t} + \phi v \cdot \nabla_x C^{(0)} - \nabla_x \left( \frac{1}{|Y|} \int_{Y_g} D(\nabla_y \mathcal{N}(y) + \mathbf{I})dY \right) \nabla_x C^{(0)} \]  

(3.51)
Collecting the terms together, the macro-model can be written as

\[ \phi \frac{\partial C^{(0)}}{\partial t} + \phi v \cdot \nabla_x C^{(0)} - \nabla_x \cdot ((D)^{eff} \nabla_x C^{(0)}) = -\phi s W(T^{(0)}, C^{(0)}), \quad (3.52) \]

where the effective diffusion tensor \( D^{eff} \) is defined as:

\[ D^{eff}_{ij} = \frac{1}{|Y|} \int_Y g D(I_{ij} + \frac{\partial N_j}{\partial y_i}) dY. \quad (3.53) \]

4. Multiscale numerical experiments. We consider now the derived macroscopic models posed in a two-dimensional \( x_1, x_2 \)-plane along the direction of the prescribed flow field. The problem is posed in a domain with dimensions \( 0 \leq x_1 \leq 5 \text{ cm}, \ 0 \leq x_2 \leq 3 \text{ cm} \), which consists of a periodic arrangement of circular solid disks within a matrix of gas phase. The two subdomains are spatially homogeneous as depicted in the geometry of the unit (periodicity) cell in Fig. 4.1. The geometry represents a theoretical representation of the microstructure, chosen for computational simplicity. Other more realistic geometries are also possible. The first step to obtaining a solution to the homogenized models is to calculate the solutions to corresponding cell problems arising in the heat and concentration equations, and then use the solutions to calculate respectively the effective conductivity and diffusivity tensors.

4.0.4. Computation of the effective coefficients. For the two dimensional macroscopic flow, the contributions of (3.14)-(3.46) to the effective conductivity and diffusivity tensors are dependent only on the canonical \( e_1 \) and \( e_2 \) directions i.e. the local boundary value problems are solved for \( M_j(y_1, y_2) \) and \( N_j(y_1, y_2) \), \( j = 1, 2 \) respectively. The problems must be supplemented with periodic boundary conditions, namely

\[ M_j(y_1 = 0, y_2) = M_j(y_1 = 1, y_2), \quad (4.1a) \]

\[ M_j(y_1, y_2 = 0) = M_j(y_1, y_2 = 1), \quad (4.1b) \]

for \( j = 1, 2 \). The solutions to (3.14) are computed on the unit structure as depicted in Fig. 4.1 and implemented with COMSOL Multiphysics ®. However, the computation of the solution to (3.46) is restricted only to the gas part, \( Y_g \), of the unit structure (see Fig. 4.1). The coefficient values used in the numerical experiment are given in Table 4.1. For the implementation, the coefficients must satisfy the scalings implied in the problem.
Table 4.1

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<td>J g$^{-1}$ K$^{-1}$</td>
<td>1.142[1]</td>
<td>1.27[10]</td>
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<tr>
<td>$\rho$</td>
<td>g cm$^{-3}$</td>
<td>1.376 $\times$ 10$^{-3}$[33]</td>
<td>0.54[33]</td>
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<tr>
<td>$D$</td>
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<tr>
<td>$\lambda$</td>
<td>J cm$^{-1}$ s$^{-1}$ K$^{-1}$</td>
<td>2.38 $\times$ 10$^{-4}$</td>
<td>7 $\times$ 10$^{-4}$[10]</td>
</tr>
<tr>
<td>$T_a$</td>
<td>K</td>
<td>-</td>
<td>-</td>
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<td>$T_u$</td>
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</tr>
<tr>
<td>$Q$</td>
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<td>-</td>
</tr>
<tr>
<td>$A$</td>
<td>cm s$^{-1}$</td>
<td>-</td>
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Fig. 4.2. Solutions to the local cell problems. Dimensionless temperatures $M_1$ (top left) and $M_2$ (top right) (3.14). Dimensionless concentrations $N_1$ (bottom left) and $N_2$ (bottom right) (3.46).

The solutions to the vector valued functions $M(y_1, y_2)$ and $N(y_1, y_2)$ are illustrated in Fig. 4.2, while the corresponding effective coefficients are computed respectively from the formula (3.24) and (3.53) viz.

\[
\langle \lambda \rangle_{\text{eff}} = \begin{pmatrix} 3.9562 \cdot 10^{-4} & 1.476 \cdot 10^{-14} \\ 1.476 \cdot 10^{-14} & 3.9562 \cdot 10^{-4} \end{pmatrix}, \quad D_{\text{eff}} = \begin{pmatrix} 0.080523 & -4.4 \cdot 10^{-12} \\ -4.4 \cdot 10^{-12} & 0.080523 \end{pmatrix}
\]

4.0.5. Computation of the homogenized solution. Having computed the values of the effective tensors, we proceed to the problem of numerically evaluating the homogenized models (3.23)-(3.52). We use the streamline diffusion method (see [17] for details) for the computation of the homogenized model. Following the same procedure as described above, we also obtain solutions for the HC model. The normalization [20, 4] of the problem with the orders of magnitude in $\varepsilon$ must be reflected on the choice of coefficient values. In the HC model, for example, the contrast in the thermal conductivities is satisfied by considering the following scaling in the inclusion: $\lambda_s = \varepsilon^{-1} \lambda_g$. For this case, we have e.g. $\lambda_g = 0.0238 \times 10^{-2}$, $\lambda_s = \varepsilon^{-1} \lambda_g$, for $\varepsilon = 0.04$. Subsequently, after solving the local boundary value problem (3.11) the solutions to
the effective conductivity tensor is calculated by the formula (3.41) as

\[
\langle \lambda \rangle_{eff} = \begin{pmatrix}
7.39 \cdot 10^{-4} & 0.00 \\
0.00 & 7.39 \cdot 10^{-4}
\end{pmatrix}.
\]  (4.2)

We point out that the implication of the high contrast in the inclusion is such that the same result (4.2) is obtained, even for \( \lambda_s \to \infty \).

4.1. Results and discussion. The solutions to the homogenized problems (3.23)-(3.52), together with the microscopic problem are studied in their dimensional form. We demonstrate the solutions to the two models by prescribing an inlet velocity of 0.005 cm s\(^{-1}\) at the left boundary and using the base parameters given in Table 4.1. The main focus in this section is to carry out a comparative numerical simulation for
the upscaled models approximating an idealized microscopic model. The temperature distribution for the model problems is illustrated in Fig. 4.3. For the HC model, we see that there is an overall temperature drop in the vicinity of the reaction region. This is due to the high conductivity of the solid phase i.e. the solid conducts heat faster leading to a decrease in temperature at the reaction region. The bump approximately 2cm at the spatial axis of the temperature profile indicates the location of the reaction region.

4.1.1. Effect of geometric properties. The volume fractions in the solid and gas parts are modified to investigate the effect of porosity and solid volume fractions on the effective tensors and on the model problems in general. It can be seen in Fig. 4.5 that the value of the conductivity tensor decreases with increasing porosity whereas that of the diffusion tensor increases with porosity. However, the converse is the case when we consider the effect of the solid volume fraction, c, on the material tensors.

4.2. Analysis of macroscopic system. The macroscopic systems are considered in their two dimensional forms along the plane of propagation. We are particularly interested in investigating interfacial front instabilities exhibited by the effective one-temperature combustion system. For a simple case of isotropic effective material coefficients and geometric properties of the microstructure, the following system of equations is considered:

\[
\begin{align*}
C_{eff} \frac{\partial T}{\partial t} - \lambda_{eff} \nabla^2 T + \phi C_g v \cdot \nabla T &= \phi Q W(T, C), \\
\phi \frac{\partial C}{\partial t} - D_{eff} \nabla^2 T + \phi v \cdot \nabla C &= -\phi W(T, C), \\
\frac{\partial R}{\partial t} &= W(T, C).
\end{align*}
\]

System (4.3) is analyzed in its nondimensional form by introducing some characteristic units based on the effective equations and the typical values given in Table 4.1.

\[
\begin{align*}
\tilde{C} &= \frac{C}{C_0}, \tilde{R} = \frac{R}{R_0}, \tilde{T} = \frac{T}{T_b}, \tau = \frac{t \alpha}{l_{th}}, \tilde{x} = \frac{x}{l_{th}}, \\
N &= \frac{T_a}{T_b}, \tilde{A} = \frac{\phi A \alpha}{U^2 N c^N}, \tilde{W} = \frac{W \alpha}{U^2}, l_{th} = \frac{\alpha}{U}.
\end{align*}
\]
where $C_0$ and $R_0$ are respectively the initial unburnt concentrations of the deficient oxidizer and the fuel sample. $\alpha$ is the effective thermal diffusivity defined as $\alpha := \frac{\lambda_{eff}}{C_{eff}}$ and $T_b := \frac{QC_0}{C_{eff}}$ is the temperature of combustion product, $U$ is a virtual velocity of a uniformly propagating plane reaction front. $N$ is a nondimensional activation temperature, $\tilde{W}$ is a nondimensional reaction rate and the parameter $\tilde{A}$ is introduced to normalize the virtual velocity of normal propagation to one [24]. In terms of the quantities introduced, the nondimensional system is given by

$$
\frac{\partial \tilde{T}}{\partial \tau} - \nabla^2 \tilde{T} + \Lambda Pe \nabla \tilde{T} = W(\tilde{T}, \tilde{C}),
$$

$$
\phi \frac{\partial \tilde{C}}{\partial \tau} + \phi Pe \nabla \tilde{C} - \frac{1}{Le} \nabla^2 \tilde{C} = -W(\tilde{T}, \tilde{C}),
$$

$$
\frac{\partial \tilde{R}}{\partial \tau} = H_{R}W(\tilde{T}, \tilde{C}),
$$

where

$$W = \tilde{A}N\tilde{C}e^{N(1-\frac{1}{\tilde{T}})}.$$

In (4.4), $\Lambda = \phi C_g/C_{eff}$, whereas $Pe = v l_{th}/\alpha$ and $Le = \alpha/D$ are respectively the effective Péclet number and Lewis number and $H_{R} = C_{0}/\phi^{\prime} R_{0}$. System (4.4) is solved numerically using the Streamline Upstream Petrov–Garlekin (SUPG) scheme. The time integration was performed using an implicit BDF solver.

4.3. Numerical results. The nondimensional system (4.4) was solved using the typical values in Table 4.1. A feature of the numerical results presented here lies in the chosen characteristic length and range of chosen Péclet numbers. The nondimensional spatial coordinates were expressed in units of $l_{th} = \alpha/U$, the thermal length of the smolder front, where $U$ is a fixed virtual velocity. The inlet gas velocity $v$, was chosen in the range $[2.5 \times 10^{-4} - 2.5 \times 10^{-1}]cm/s$ such that the Péclet number lies within the interval $0.05 \leq Pe \leq 50$.

Fig. 4.6. Spatial profiles of temperature, char, concentration and heat release rate for the HC model (Pe = 34).

The value of $\tilde{A}$ was chosen within the range $[2.5 \times 10^{3} - 10^{4}]$. In the numerical simulations, all other parameters correspond to the typical values given in Table 4.1.
Pattern formation in reverse combustion

Fig. 4.7. Spatial profiles of char pattern for the CC (left) and HC (right) models for $Pe = 1$. Ignition is initiated from bottom, front propagation is from bottom to top and gas inlet is directed downwards from top. (a)-(b) show elongated fingers with low conversion depth.

We point out that in all cases considered, the combustion process is incomplete. In Fig. 4.6, the location in space of the flame can be identified at the reaction region which is delineated within a limited vicinity of the tips of the fingers. This region is traced by dark shades as shown in Fig. 4.6 (d), where oxygen is fully consumed as the front advances. Behind (or along) the fragmented advancing flame front, there is no reaction but only a trace of the heterogeneous charred region (see Fig. 4.6(b)).

Fig. 4.8. Spatial profiles of char pattern for the CC (left) and HC (right) models for $Pe = 17$. Fingering with tip-splitting and increase in conversion depth.

The emerging fingering instability is controlled through the Péclet number $Pe$, which is akin to those studied in [33, 22]. At a relatively low blowing rate i.e. for $Pe = 1$, the char pattern emerged as elongated fingers that strictly avoid each other (Fig. 4.7). Also, the pattern shows a low contrast in the spatially heterogeneous conversion depth. The conversion depth describes the intensity of conversion of the solid fuel to char. The dark shades in Fig. 4.7 represent the regions of the char pattern with high conversion intensity. A further increase in the Péclet number, i.e. $Pe = 17$ increases the contrast in the conversion depth and the fingers tip-split (Fig.
4.8). We describe the mechanism of tip-splitting later on in this discussion. As before, the uncharred area of the pattern represents the quenched parts of the fragmented reaction zone and smoldering is only intensified at the tips of the fingers where the oxidant is fully consumed.

From our understanding of adiabatic smoldering [22, 18], the absence of heat losses is a factor that can prevent the patterns from being clearly visible. It can be seen (Fig. 4.8) that from bottom section to some points midway the char propagation, the patterns are not so visible. At $Pe = 40$, the fingering pattern is fully developed with the characteristic feature of tip-splitting, increase in conversion depth and bifurcation (Fig. 4.9). Bifurcation of the fingers describes the splitting of a single finger into multiple branches. Besides the fact that there is an overall drop in temperature in the vicinity of the reaction zone for the HC model due to the high contrast in thermal conductivity, a disparity in the two models considered lies in the fact that the HC model exhibited enhanced finger patterns and bifurcation.

4.4. Effect of Lewis number. The macroscopic models describe, in an effective sense, a one temperature gas-solid system for the coupled two temperature microscopic model. However, the effects arising from the gas phase and solid phase Lewis numbers can be investigated via the nondimensional Lewis number, $Le$. The numerical simulations presented in the preceding section were based on the typical effective values $Le = 0.01422$ and $Le = 0.026563$ i.e. $Le \ll 1$ which corresponds respectively to the CC and HC models. According to Ronney [26], Lewis number effects are not the controlling transport mechanism for a fingering behavior. However, we point out particularly in the models discussed here that there presence introduces some characteristic features. As it is known, the Lewis number relates heat transport to mass transport. It is based on this knowledge that we describe the following effects arising from the Lewis number.

At a very low blowing rate, the effective oxygen mass transport is dominant and thus the Lewis number is close to a value which is much smaller than unity ($Le \ll 1$). However, at large flows the gas heat transport dominates and corresponds to a Lewis number close to unity (i.e. $Le = 1$) for gases. Results of numerical simulations with $Le = 1$ show a stable planar front that advances without fragmentation. That is, the finger patterns combine together into an unbroken front and hence no visible pattern
is observed in a range of chosen Péclet numbers. This case is illustrated in Fig. 4.10. Further, a moderate flow is considered, e.g. $Le = 0.1$. In this case, the development of fingering patterns is enhanced with an increase in the density of fingers that leads to a decrease in distance between fingers, as the value of $Pe$ is increased from left to right Fig. 4.11(a)-(c) and Fig. 4.12(a)-(c). It can be clearly seen at this point that some regions of the pattern also exhibited shielding effect [33, 22]. Such shielding of fingers by adjacent fingers that are close to the oxygen source causes the shielded fingers to stop growing and the tips of the shielding fingers split.

5. Conclusion. We have described, in a simple adiabatic case, the smoldering combustion model of a thin solid fuel that assumes a periodic distribution in its microstructure. We considered also in the present paper two different models of smoldering combustion that are particularly based on the conductivities in the constituent phases. The form of the homogenized model in both cases resembles the one-temperature model of filtration combustion [22, 23, 9] and are indeed similar to most other models obtained by the volume averaging method [13, 28]. The numerical simulations show that the results of the upscaled models are comparable to the predictions of the mesoscopic models, thereby justifying the classical homog-
enization technique. However, one difficulty that was encountered in the comparative tests is that the presence of (strong) chemical reaction terms lead to a contradiction of the classical homogenization approach. A possible remedy to this problem would be to seek for solutions to the microscopic problem in a moving frame. This approach was recently presented in [3].

Within the limit of theoretical assumptions in the problem formulation, we have observed in a set of macroscopic numerical simulations that the proposed models of reverse combustion capture the basic physics underlying the experimental observations of Zik and Moses [33, 34, 32] and Olson et. al [26]. In spite of the fact that the approach explored in this paper is quite different from those reported in other literatures [33, 18, 22], the results of the numerical simulations were in agreement with the mechanism of the emerging patterns. While the effect of heat losses has not been considered in the present paper, we expect that its inclusion in a future review of the present study will extend the theory closer to a real-life situation and further to capture other forms of patterns that were not observed in this study.

The developed models are in general for the qualitative treatment of the development of patterns in a reverse combustion in porous media. Nevertheless, the results of the homogenization technique presents an effective way of integrating material microstructural properties in a macroscopic system describing real life processes. Thus, it can serve as a paradigm for further investigation of combustion processes in a rigorous mathematical treatment.

6. Acknowledgement. This work is jointly supported by the Meiji University Global Center of Excellence (GCOE) Program and the Japanese Government (Monbukagakusho:MEXT). A. M. thanks Prof. Willi Jäeger (Heidelberg) for having drawn his attention to the application of homogenization methods to combustion in porous media.

REFERENCES

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