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# Upscaling of mass and thermal transports in porous media with heterogeneous combustion reactions

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ABSTRACT

The present paper aims at an upscaled description of coupled heat and mass processes during solid–fluid combustion in porous media using volume-averaging theory (VAT). The fluid flows through the pores in a porous medium where a heterogeneous chemical reaction occurs at the fluid–solid interface. The chemical model is simplified into a single reaction step with Arrhenius kinetic law, but no assumption of local thermal equilibrium is made. An array of horizontal channels is chosen for the microstructure. The corresponding effective properties are obtained by solving analytically the closure problems over a representative unit cell. For a range of Péclet and $\Delta$ numbers, the results of the upscaled model are compared with microscale computations found in the literature. The results show that, under the same circumstances, the upscaled model is capable of predicting the combustion front velocity within an acceptable discrepancy, smaller than 1% when compared to the analytical solution. Furthermore, it has been found that for the Péclet and $\Delta$ numbers considered in this study, the fluid concentration and temperature profiles that stem from the present upscaled model are in accordance with those obtained using a microscale model.



## 1. Introduction

The propagation of combustion fronts in reactive porous media, which is usually referred to as smouldering or filtration combustion (FC), is a subject of interest for many applications. These include oil recovery using *in situ* combustion, coal gasification, fire safety, and foam combustion in a variety of situations. A broad review of all these domains is provided by Rein [1]. In all cases, an oxidation reaction is involved between an immobile fuel and an oxidizer, conveyed by a gas flow through the pore space.

Many contributions referring to this topic have been published in the past 40 years, such as the pioneer work of Aldushin et al. [2] where the structure of the filtration combustion wave was analyzed in one-dimensional geometries, followed by a series of papers using asymptotic methods for rapid, diffusive, co-current or counter-current filtration combustion waves [3–6]. All these contributions investigated the macroscale behaviors and the structure of solutions in effective porous media. More complex multicomponent, multiphysical, reactive problems were studied in this framework. For instance, Moallemi et al. [7] studied the smouldering in a two-dimensional scale solid material. They assumed a global single-step combustion reaction, and the associated transport problem was formulated via conservation equations for mass, species, linear momentum, and energy on the Darcy scale. Limits of flammability were compared to experimental tests. Rostami et al. [8] investigated the combustion of a porous biomass fuel, with a transient two-dimensional model without thermal equilibrium hypothesis and a complex multi-step chemistry. They showed the existence of a steady combustion regime depending on the ratio of oxygen to fuel contents. Rein et al. [9] studied the propagation of combustion fronts using a simplified transport model and complex chemistry of gas and solid components. Lapene et al. [10] developed a coupled simplified-transport model with chemistry to determine, by an optimization procedure, the effective multi-step reaction scheme of heavy-oil combustion in porous media. Fadaei et al. [11] investigated the combustion of reactive carbon in carbonate reservoirs by varying several parameters (flow rates, fraction of carbon and fraction of carbonates). No explicit link was made between local-scale phenomena and the heuristic macroscale model.

Local-scale solid–gas combustion was described in the review paper of Ohlemiller [12]. The structure and couplings were explained in detail, with a realistic description of a porous medium. The chemical coupling, the local-scale effects — i.e., local scale temperature effects — were addressed. According to Ohlemiller [12], all

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**Nomenclature**

| | |
|---|---|
| $a_V$ | interfacial surface area per unit cell volume ($m^{-1}$) |
| $A_0$ | pre-exponential factor ($m\ s^{-1}$) |
| $A_{fm}$ | interfacial surface area between the fluid and solid phases ($m^2$) |
| **b** | closure variable |
| $c_p$ | specific thermal capacity at constant pressure ($J\ kg^{-1}\ K^{-1}$) |
| $C_{f,in}$ | concentration of oxidizer at the inlet ($mol/m^3$) |
| $C_{f,out}$ | concentration of oxidizer at the outlet ($mol/m^3$) |
| $\Delta C_f$ | difference of oxidizer concentration between inlet and outlet ($mol/m^3$) |
| $C_{c,in}$ | concentration of fuel at the inlet ($mol/m^3$) |
| $C_{c,int}$ | concentration of fuel at the interface ($mol/m^2$) |
| $C_{c,out}$ | concentration of fuel at the inlet ($mol/m^3$) |
| $\Delta C_c$ | difference of fuel concentration between inlet and outlet ($mol/m^3$) |
| $C$ | concentration ($mol\ m^{-3}$) |
| $D_f$ | mass diffusivity of fluid phase ($m^2\ s^{-1}$) |
| $\mathbf{D}_{eff}$ | effective mass diffusivity tensor of fluid phase ($m^2\ s^{-1}$) |
| $E$ | activation energy ($J\ mol^{-1}$) |
| $F$ | arbitrary function of Taylor series |
| $h$ | heat transfer coefficient ($J\ m^{-2}\ s^{-1}\ K^{-1}$) |
| $H$ | heterogeneous reaction heat ($kJ\ mol^{-1}$) |
| $H_c$ | heaviside step function accounting for the fuel exhaustion |
| $\langle H_c \rangle$ | average step function |
| $H_{\langle c \rangle}$ | binary function describing the presence or not of carbon at the macroscale |
| **i**, **j** | unit base vectors |
| **I** | unit matrix |
| $k$ | thermal conductivity ($W\ K^{-1}\ m^{-1}$) |
| **K** | effective thermal conductivity tensor ($W\ K^{-1}\ m^{-1}$) |
| $\mathbf{K}_f$ | effective permeability tensor ($m^2$) |
| $l$ | microscopic characteristic length (m) |
| $L$ | length of channel (m) |
| $n_{fm}$ | normal unit vector from the fluid phase to the solid phase |
| $p_f$ | pressure (Pa) |
| $Pe_D$ | cell Péclet number based on the mass diffusivity |
| $Pe_T$ | cell Péclet number based on the thermal diffusivity |
| $Pe_{F,s}$ | thermal Péclet number based on solid thermal diffusivity and front speed velocity |
| $q$ | heat generation ($kJ\ m^{-3}\ s^{-1}$) |
| $r$ | special closure variable for the heterogeneous chemical reaction case |
| $r_0$ | characteristic length associated with averaging volume |
| $R$ | universal gas constant ($J\ mol^{-1}\ K^{-1}$) |
| $s$ | closure variable |
| $s_{rxn}$ | heterogeneous reaction rate ($mol\ m^{-2}\ s^{-1}$) |
| $t$ | time (s) |
| $T$ | temperature (K) |
| $T_{-\infty}$ | reference upstream temperature (K) |
| $T_{+\infty}$ | reference downstream temperature (K) |
| **u** | transport coefficient ($m\ s^{-1}$ or $W\ K^{-1}\ m^{-2}$) |
| $U_F$ | combustion front velocity ($m\ s^{-1}$) |
| $\mathbf{v}_f$ | velocity vector ($m\ s^{-1}$) |
| $V$ | unit cell volume ($m^3$) |
| $W$ | height of channel (m) |
| $x$, $y$ | Cartesian coordinates (m) |

*Greek letters*

| | |
|---|---|
| $\varepsilon$ | porosity |
| $\mu$ | dynamic viscosity ($kg\ m^{-1}\ s^{-1}$) |
| $\rho$ | density ($kg\ m^{-3}$) |
| $\psi$ | arbitrary variable |
| $\varsigma$ | arbitrary function of closure problem |
| $\xi$ | heat distribution coefficient |
| $\varphi$ | cell Thiele modulus |
| $\sigma$ | Stephan–Boltzman constant ($W\ m^{-2}\ K^{-4}$) |

*Subscripts and superscripts*

| | |
|---|---|
| *ad* | adiabatic |
| *c* | concentration |
| *f* | fluid phase |
| *F* | combustion front |
| *in* | inlet |
| *int* | interface |
| *out* | outlet |
| *m* | solid phase |
| *p* | plateau |

*Special symbols*

| | |
|---|---|
| $\tilde{\phi}$ | deviation from intrinsic average |
| $\langle \phi \rangle$ | Darcian average |
| $\langle \phi \rangle^{f,m}$ | intrinsic average |

of the existing models in the literature were overly simplified and while they could be used for obtaining trends in front-velocity estimates and maximum-temperature approximations, for instance, they could not be predictive because of the lack of details in the description. Few references of studies on this scale can be found in the literature. Microscale or pore-scale studies are usually done to investigate the details of all the phenomena and to determine local effects, local thermal non-equilibrium, reaction shape, and speed, depending on the local properties. For example, based on a dual lattice, Lu and Yortos [13] developed a pore-network model to investigate the dynamics of forward filtration combustion in porous media. The pore-scale results showed that the overall macroscopic behavior of this process strongly depends on microscopic features, such as heterogeneity. Debenest et al. [14,15] performed 3D numerical calculations of smouldering processes in a detailed discretized image of porous medium, to demonstrate the ability of a numerical model proposed by Debenest et al. [16] to handle a variety of situations. Since combustion in porous media with heterogeneous chemical reactions is a complex phenomenon, which involves the transports of mass and heat as well as various chemical reactions, the numerical computations based on microscale structure are challenging. Upscaling approaches that treat a porous medium as an equivalent continuum have proved useful to overcome these limitations.

The published upscaling studies of reactive transport in porous media mainly focus on the mass or heat transfer. In an important reference paper, Oliveira and Kaviany [17] identified the length and time scales involved in heat and mass transports during combustion in porous media and determining the conditions for local equilibrium. Yet, they did not upscale the local-scale system of equations. Akkutlu and Yortsos [18] addressed theoretically *in situ* combustion and the explicit coupling between heat and mass transports with Arrhenius-type functions. Using a non-dimensional system, they obtained solutions for forward-filtration combustion and determined the effect of heat losses on the stability of the process. The link between the local-scale system of equations and the one pertaining to the macroscale has been addressed in detail in the pioneering works of Ryan [19] and Whitaker [20] on mass transfer