A One-Grid Framework for Anisotropic Reacting Porous Media: Application to Biomass Pyrolysis

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Abstract
This study presents a new computational framework for modelling thermochemical conversion of porous media at the particle scale with a special focus on biomass pyrolysis. The model integrates conservation equations of mass, momentum and energy, with the Volume-Of-Fluid approach, which tracks the interface between the particle and the gaseous environment. Including internal and external transport phenomena, the model enables accurate prediction of the species and temperature profiles inside the porous particle and in the surrounding environment. One of the most significant advancements of this approach is that it can directly resolve the gas phase boundary layer under various flow conditions without relying on sub-grid-scale correlations. The performance of the model is tested against experimental data, demonstrating its accuracy and effectiveness as a tool for designing and optimizing biomass conversion processes.

Introduction
As the need for sustainable chemicals and energy has steadily increased over the last 25 years, biomasses have emerged as possible candidates to tackle these challenges. Due to their wide distribution, easy access and relatively cheap prices, bio-sources conversion processes have been widely studied and investigated. The experimental observation of biomass particles pyrolysis is hindered by the difficulty of measuring the reaction products, and the complex deformation of the porous structure. In this context, numerical models are valuable tools which can drive and integrate the experimental measurements. For this reason, many mathematical models have emerged in the literature to describe the biomass pyrolysis both at the chemical and at the particle scale. At the particle scale, the literature models focus either on the deformation and the porosity changes of the biomass particle [1], or on the dynamics of the external environment [2]. With this work, we propose a general framework which can combine these two complementary problems, tracking the evolution of an arbitrary particle shape, the porosity distribution, and the dynamics of the surrounding environment.

Numerical Model
The governing equations are integrated on a control volume which comprises two immiscible phases: a solid phase *s* and a fluid phase *f*. The mathematical model is

derived from the conservation laws of mass, momentum, and energy for the system. These equations consider the gas-solid system by including the information about the porosity. By doing so, we avoid a sharp description of the pore interface, and we consider a whole pseudo-phase which includes both solid and fluid. Following [3], we define the porosity ϵ as the volume fraction occupied by the fluid phase over the total volume of the domain. We can then describe the system through the subsequent system of equations:

$$\frac{\partial}{\partial t}\left[(1-\epsilon)\rho_s\right] + \nabla\cdot\left(\boldsymbol{u}_s(1-\epsilon)\rho_s\right) = -(1-\epsilon)\sum_{i=1}^{NR}\Omega_i \quad (1)$$

$$\frac{\partial}{\partial t}\left[\epsilon\rho_f\right] + \nabla\cdot\left(\left(\boldsymbol{u}_f\epsilon + \boldsymbol{u}_s\right)\rho_f\right) = (1-\epsilon)\sum_{i=1}^{NR}\Omega_i \quad (2)$$

$$\left[\frac{\partial}{\partial t}\left(\epsilon\boldsymbol{u}_f\right) + \nabla\cdot\left(\epsilon\boldsymbol{u}_f\boldsymbol{u}_f\right)\right] = -\nabla\left(\epsilon p_f\right) + \mu_f\nabla^2(\epsilon\boldsymbol{u}_f) - \left[\frac{\mu_f\epsilon^2\boldsymbol{u}_f}{K} + \rho_f\frac{F\epsilon^3|\boldsymbol{u}_f|\boldsymbol{u}_f}{\sqrt{K}}\right] \quad (3)$$

$$\left(\rho C_p\right)_m\frac{\partial T}{\partial t} + \left(\rho C_p\right)_f\left(\epsilon\boldsymbol{u}_f + \boldsymbol{u}_s\right)\nabla T = \nabla\cdot\left(\lambda_m\nabla T\right) + \dot{Q}_r + \dot{Q}_\Gamma\delta_\Gamma \quad (4)$$

Local thermal equilibrium is assumed between the fluid and solid inside the pseudo-phase. The chemical reactions and initial biomass surrogate composition are computed as proposed by Debiagi et al [4]. The interface between the pseudo-phase and the external gas phase is tracked using the Volume-Of-Fluid (VOF) approach [5], by solving an additional transport equation which advances the position of the pseudo-phase. The interface regression velocity is calculated form the solid phase mass balance under the approximation of potential flow.

Results

The presented model was implemented within the open-source software Basilisk [6]. We compare the prediction of the proposed model with experimental measurements from Gautier et al. [7] of a centimeter scale cylindrical pellet, considering the anisotropic distribution of the thermal conductivity, which is typical of wood. Results in terms of mass loss, axial and radial shrinking factors are reported in Figure 1. Good agreement with the experimental points is found for the mass profile, whereas during the early stages of pyrolysis the models fail to predict the initial sharp shrinking of the particle. Nonetheless, good agreement is found with intermediate and steady state measurements. Small discrepancies could be explained with the strong uncertainties in the characterization of the feedstock, the estimation of its physical properties and the non-uniformity of the medium.

Conclusions

This work has successfully developed and implemented a novel computational framework for modeling thermochemical conversion of porous media at the particle scale, specifically focusing on biomass pyrolysis. The proposed model accurately

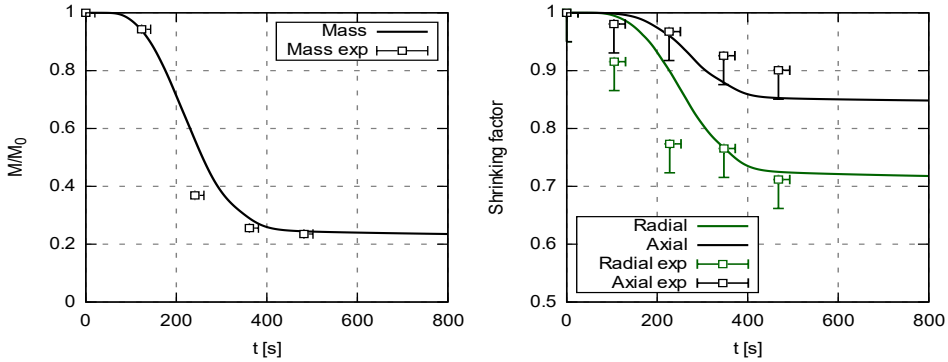

Figure 1: Mass loss (left) and shrinking factor for the two main directions (right). Model comparison with experimental data

captures the evolution of the particle shape and the porosity distribution. Additionally, it advances the state-of-the-art by simultaneously resolving the surrounding environment, addressing limitations in the existing approaches. The framework provides a valuable tool for understanding the complex interplay between heat transfer, mass transfer, and chemical reactions during biomass pyrolysis, enabling more efficient design of sustainable energy and chemical production processes.

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