



# Gas phase combustion in the vicinity of a biomass particle during devolatilization – Model development and experimental verification

Hesameddin Fatehi<sup>a,\*</sup>, Florian M. Schmidt<sup>b</sup>, Xue-Song Bai<sup>a</sup>

<sup>a</sup> Department of Energy Sciences, Lund University, 221 00 Lund, Sweden

<sup>b</sup> Thermochemical Energy Conversion Laboratory, Department of Applied Physics and Electronics, Umeå University, Umeå SE-90187, Sweden

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## ABSTRACT

A numerical and experimental study on the devolatilization of a large biomass particle is carried out to quantify the effect of homogeneous volatile combustion on the conversion of the particle and on the temperature and species distribution at the particle vicinity. A global chemical kinetic mechanism and a detailed reaction mechanism are considered in a one dimensional numerical model that takes into account preferential diffusivity and a detailed composition of tar species. An adaptive moving mesh is employed to capture the changes in the domain due to particle shrinkage. The effect of gas phase reactions on pyrolysis time, temperature and species distribution close to the particle is studied and compared to experiments. Online in situ measurements of average H<sub>2</sub>O mole fraction and gas temperature above a softwood pellet are conducted in a reactor using tunable diode laser absorption spectroscopy (TDLAS) while recording the particle mass loss. The results show that the volatile combustion plays an important role in the prediction of biomass conversion during the devolatilization stage. It is shown that the global reaction mechanism predicts a thin flame front in the vicinity of the particle deviating from the measured temperature and H<sub>2</sub>O distribution over different heights above the particle. A better agreement between numerical and experimental results is obtained using the detailed reaction mechanism, which predicts a wider reaction zone.

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## 1. Introduction

Increased demands for energy sustainability and concerns over global warming have led to an increased interest in sustainable and renewable sources of energy. The EU's Renewable Energy Road Map proposes creating a new legislative framework to enhance the promotion and use of renewable energy and sets a mandatory target of 20% energy consumption through renewable energy and a mandatory minimum target of 10% for biofuels by 2020 [1]. As a sustainable and renewable source of energy, biomass has great potential in generating heat and power via thermochemical conversion.

Thermochemical conversion of biomass can be done in three main systems, fixed or moving beds, fluidized beds and entrained flow reactors. There are plenty of literature studying different aspects of these systems [2,3], however, there are still challenges such as efficiency, pollutant emissions, ash deposition and corrosion as well as fuel flexibility that need to be addressed. A thorough understanding of the processes occurring during the

thermochemical conversion of biomass is essential for the proper design and optimization of biomass combustion and gasification systems. Important parameters at reactor level, such as distribution of temperature and species and overall conversion rate of biomass are strongly dependent on the processes involved in the particle scale. A detailed resolved numerical simulation of a single particle is useful for improving the understanding of the interaction between transport, chemical kinetics and morphological transformation at particle scale.

The conversion of a biomass particle can be divided into the processes occurring inside the solid structure of the particle and processes occurring in the particle boundary layer, where chemical reactions and heat and mass transfer between the particle and the surrounding take place. Homogeneous reactions in the particle boundary can affect the concentration of species and temperature and alter the heat and mass transfer rate to the particle. For fine coal particles, such as pulverized coals, there have been extensive studies on the effect of homogeneous reactions in the vicinity of the particle. For instance, Timothy et al. [4] developed a simplified model for the location and temperature of the volatile flame envelope around a coal particle. The model showed reasonable agreement compared with the experimental data for the volatile

\* Corresponding author.

E-mail address: [Hesameddin.fatehi@energy.lth.se](mailto:Hesameddin.fatehi@energy.lth.se) (H. Fatehi).

burn-out time and was in partial agreement with the particle burn-out time. In another study [5], the volatile combustion was modeled by global reactions and it was concluded that the flame may extend to several particle diameters, questioning the validity of the flame sheet models during devolatilization. Comparing detailed chemistry and an infinitely-fast (flame-sheet) chemistry model, it was reported that for flame stand-off distance around a coal particle, the results are less sensitivity to the gas phase chemistry compared with the devolatilization model [6]. However, the shape of the flame stand-off PDF (Probability Density Function) was shown to be altered by the flame-sheet assumption.

Most of the available models on the homogeneous reactions around the particle are developed for coal particles in pulverized size range. Compared with coal, biomass has a lower energy density and much higher volatile content and can produce a considerably stronger flame during the devolatilization stage. Moreover, the wide range of biomass sources can result in different conversion characteristics. For instance, a recent experimental study on different pulverized biomass sources showed diverse burning characteristic of the various biomass particles due to different thermochemical properties [7].

Validation of particle conversion models is challenging, since it is difficult to directly measure what happens inside the particle during thermochemical conversion. If the gaseous devolatilization products are predicted, or if homogeneous reactions are to be studied, measurements of gases in the surroundings of the particle can be used for model validation. Experimental studies of volatile release and the gas-phase composition around particles have been conducted in laboratory furnaces or flat flame burners using various laser-based analytical techniques, such as laser-induced breakdown spectroscopy (LIBS) [8,9], laser-induced fluorescence (LIF) [10] and tunable diode laser absorption spectroscopy (TDLAS) [11,12], but also with inductively coupled plasma mass spectrometer (ICP-MS) [13].

The effect of homogeneous reactions on the conversion of large biomass particles during pyrolysis is not well investigated; the gas phase reaction is usually neglected in modeling biomass particle conversion [14–17] or an effective gas temperature is used to include the effect of homogeneous reactions in the model [18]. The homogeneous reactions can substantially alter the temperature and species fields around the particle and affect the formation of unwanted emissions such as  $\text{NO}_x$ , soot and trace species like alkali and chlorine compounds [9,19].

In this paper, a joined numerical and experimental study is presented aimed at investigating the effect of homogeneous reactions in the boundary layer of a biomass pellet on the thermochemical conversion of the particle. A 1D detailed numerical model consisting of a particle and its boundary layer is developed for the biomass conversion. Different chemical kinetic mechanisms for reaction of pyrolysis products are employed. Gas temperature and  $\text{H}_2\text{O}$  concentration in the vicinity of the particle as well as particle mass loss are experimentally obtained using TDLAS and thermogravimetric analysis, respectively, and compared with the model results during the devolatilization stage. Since tar species are the main product of the devolatilization stage, the composition of tar is calculated based on a detailed pyrolysis mechanism. An adaptive moving mesh method is employed to capture the effect of the particle shrinkage. The effect of preferential diffusion on the heat release rate and species profile is discussed and the differences in the heat release rate from global and detailed reaction mechanisms are outlined.

## 2. Numerical model

Thermochemical conversion of biomass is a complex, multi-phase and multi-scale problem. This process involves strong in-

teraction between the heat and mass transport phenomenon and chemical reactions. The convective, conductive and radiative heat transfer inside the particle as well as heat and mass transfer between the particle and the surrounding gas result in gradients of species and temperature inside the particle, which is specially important for particles with a Biot number greater than unity ( $Bi = Nu k_{gas}/k_{solid} > 1$ ;  $Nu$  being the Nusselt number). For biomass particles, a particle of roughly 200  $\mu\text{m}$  size or larger has a Biot number greater than unity, indicating that for most practical applications the temperature and species gradients inside the particles are significant. The conservation of gaseous species, mass and energy inside the particle and in its surrounding are as follows:

$$\frac{\partial}{\partial t}(\varepsilon \rho_g Y_i) + \frac{1}{r^n} \frac{\partial}{\partial r}(r^n \varepsilon \rho_g u_g Y_i) = + \frac{1}{r^n} \frac{\partial}{\partial r} \left( r^n \rho_g D_{i,m} \frac{\partial Y_i}{\partial r} \right) + \sum_j \vartheta_{i,j} \mathfrak{R}_j, \quad (1)$$

$$\frac{\partial}{\partial t}(\varepsilon \rho_g) + \frac{1}{r^n} \frac{\partial}{\partial r}(r^n \varepsilon \rho_g u_g) = \sum_i \sum_j \vartheta_{i,j} \mathfrak{R}_j, \quad (2)$$

$$\left( \rho_m c_{p,m} + \rho_{bm} c_{p,bm} + \rho_c c_{p,c} + \rho_g \sum_{i=1}^N Y_i c_{p,i} \right) \frac{\partial T}{\partial t} + \varepsilon \rho_g u_g \sum_{i=1}^N Y_i c_{p,i} \frac{\partial T}{\partial r} = \frac{1}{r^n} \frac{\partial}{\partial r} \left( r^n k_{eff} \frac{\partial T}{\partial r} \right) + \mathfrak{R}_{Heat}, \quad (3)$$

where  $\rho_g$  is the gas density,  $u_g$  is the gas velocity,  $D_{i,m}$  is the effective diffusion coefficient of species  $i$  into the mixture,  $\mathfrak{R}$  is the mass release rate source term due to chemical reactions and moisture evaporation and  $\varepsilon$  is the void fraction inside the particle and is equal to unity in the gas phase around the particle.  $Y_i$  and  $\vartheta_{i,j}$  are the mass fraction of species  $i$  and the stoichiometric coefficient of species  $i$  in reaction  $j$ , respectively. This system of equations is valid for an arbitrarily shaped particle within a one dimensional framework. Therefore,  $r$  is the distance from the particle center and  $n$  is the Lamé coefficient accounting for a non-Cartesian coordinates system:  $n = 2$  for spherical,  $n = 1$  for cylindrical and  $n = 0$  for large slab plate shaped particles.  $\mathfrak{R}_{Heat}$ , the heat source term in energy equation, includes the heat of reaction of different processes and the changes in sensible enthalpy.

Transport and evaporation of moisture inside the particle is governed by following equation;

$$\frac{\partial \rho_m}{\partial t} = \frac{1}{r^n} \frac{\partial}{\partial r} \left( r^n D_{eff,m} \frac{\partial \rho_m}{\partial r} \right) + \mathfrak{R}_m, \quad (4)$$

The evaporation source term is based on the equilibrium model, which is shown to perform well at different conditions [16]. The model can be presented as,

$$\mathfrak{R}_m = h_{m,vap} S_p (\rho_{w,sat} - \rho_{H_2O,\infty}), \quad (5)$$

where  $\rho_{w,sat}$  is the saturation vapor density calculated based on the Clausius–Clapeyron relation for the saturation pressure and  $\rho_{H_2O,\infty}$  is the partial density of water vapor in the pores of the particle.  $S_p$  is the specific surface area of the particle available for moisture and vapor diffusion.  $h_{m,vap}$  is the mass transfer coefficient of vapor in the pores of the particle, which can be determined using empirical equations [14,16].

The mass degradation of biomass particle based on the selected pyrolysis mechanism is presented as follows,

$$\frac{\partial \rho_{bm}}{\partial t} = -\rho_{bm} \sum_j k_j = \mathfrak{R}_{pyr}, \quad (6)$$

where  $k_j$  is the rate of reaction  $j$  in Arrhenius form.

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