CHEMICAL ENGINEERING TRANSACTIONS Volume 21, 2010
Editor J. J. Klemeš, H. L. Lam, P. S. Varbanov
 ISBN 978-88-95608-05-1 ISSN 1974-9791
DOI: 10.3303/CET1021185

Mathematical Modelling of Biomass Combustion: Packing Conditions Issues

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This article follows the authors' previous works on numerical simulations of biomass drying and devolatilization (Juřena et al., 2009a-b), in which a packed bed of solid fuel particles is treated as a continuous porous medium. The bed model consists of several sub-models describing individual combustion processes. Since packing conditions change markedly during the processes, a proper description of all the phenomena related to it must be included as well.
A mathematical model of wheat straw combustion in 1D experimental fixed-bed reactor is implemented into a computer program GRATECAL and effects of bed porosity change and particle volume shrinkage as two important packing conditions parameters are studied. The combustion includes drying, devolatilization and char oxidation. Results from simulations are shown and discussed.

1. Introduction

Numerous mathematical models of combustion in packed beds have been developed during the last 50 years, from simple ones with many simplifying assumptions to very sophisticated models with detailed description of combustion-related phenomena (Würzenberger, 2001). A typical detailed numerical model describes fluid flow through a densely packed bed, heat and mass transfer within the bed during drying, devolatilization and combustion of fixed-carbon and gaseous species. These phenomena are influenced by several factors, one of which, the so called packing conditions, refers to a set of parameters defining certain physical properties of the bed such as porosity, fuel particle shape and size, bulk density and bed volume. On the other hand, the structure of the bed and so the packing conditions change due to mass loss as particular combustion processes proceed. Thus, there is coupling between changes of packing conditions and heat and mass transfer and fluid flow and it should be considered in modelling of combustion in packed beds. In this work, effects of particle size as well as bed porosity on combustion of wheat straw are investigated through a series of numerical simulations.
It has been concluded from both experimental and theoretical studies that the bed porosity has impact on ignition and burning rates (Zhou et al., 2005, Yang et al., 2005c). It is defined as the fraction of bed volume occupied by the gas phase. However, it is

Please cite this article as: Juřena T. and Hájek J., (2010), Mathematical modelling of biomass combustion: packing conditions issues, Chemical Engineering Transactions, 21, 1105-1110 DOI: 10.3303/CET1021185

important to distinguish between porosity of the bed and particle porosity referred to as internal pores. While generation of internal pores is caused by mass loss of particles during individual combustion stages, bed porosity is determined from volumetric shrinkage of the particle (Yang et al., 2004). For example, during drying, mass of particles is decreased about 10 % depending on the initial moisture content, but there is only a little change in the size of the particle, thus the bed porosity remains unchanged. The volumetric shrinkage can lead both to an increase in the bed porosity and decrease of the bed height based on experimental observations. Nevertheless, inconsistencies can be found in the literature concerning combustion of wheat straw. The volume reduction was neglected in (Zhou et al., 2005), while a local volume shrinkage was assumed in (Yang et al., 2007). The effect of bed porosity on ignition flame front rate was shown to be significant in (Zhou et al., 2005), but neither decrease of bed height nor change of bed porosity were taken into account in their mathematical model.

Effects of fuel particle size on combustion were studied e.g. by Yang et al. (2005a). Smaller particles produce higher moisture evaporation and char burning rates due to higher volumetric surface. Also temperature profile inside sufficiently small particles is uniform allowing us to treat the fuel bed as a continuous porous medium. If particle size is very small, there is small difference between gas and solid phase temperatures (Thunman et al., 2005). On the other hand, particles with diameter larger than 35 mm can develop very steep inner temperature gradients (Yang et al., 2005b). In such cases, a particle-resolved model of the bed is more appropriate. The temperature distribution inside a particle also affects particular process rates (Yang et al., 2005a).

2. Bed modelling

A simple thermally insulated laboratory-scale experimental furnace of a cylindrical shape is considered. Fuel bed is treated as a continuous porous medium which consists of solid and gas phases. The model and modelling assumptions are adopted mainly from (Zhou et al., 2005). Although the model was developed for combustion of straw, it can be applied to various kinds of fuels with a few modifications of physical and chemical properties of the fuel and setup (design and operating conditions) of the furnace. This model is briefly described in the following text. Modifications related to boundary conditions and changes of packing conditions that generalize the model of Zhou et al. (2005) are highlighted.

2.1 Mathematical model

Biomass combustion in a packed bed of the experimental furnace is described by a system of transient one-dimensional partial differential equations. The system includes equations governing heat and mass transfer of both gas and solid phase. The solid phase consists of moisture, volatile matter, fixed-carbon and ash. Gas is in plug flow and can be described as incompressible ideal gas. The gas-phase species are H_2O, CO_2, CO, H_2, O_2, N_2, light hydrocarbon and tar represented by CH_4 and CH_2O, respectively. It is assumed that the radiative heat transfer inside the bed can be modelled by effective thermal conductivity, which is broadly supposed to depend mainly on solid temperature, particle size and bed porosity (Yang et al. 2007, Zhou et al., 2005).

Furthermore, the combustion process is divided into four sub-processes: evaporation of moisture from the fuel, volatile release/char formation, combustion of volatiles and

combustion of char. Homogeneous chemical reactions in the gas phase are not considered here. It is assumed that the fuel is ignited at the top of the bed by radiation and individual reaction fronts travel down the bed towards the grate.
Moisture evaporation and devolatilization have been described in detail in (Juřena et al. 2009a, 2009b). The diffusion-limited rate and first-order kinetic rate models are used for prediction of drying and devolatilization stages, respectively. The rate of char combustion is limited both by diffusion of oxygen through a boundary layer around a fuel particle and kinetics of surface reaction of oxygen with fixed carbon. Parameters and kinetic constants for this model are taken from (Kær, 2001).
As mentioned above, the packing conditions change markedly as particular processes proceed. According to Zhou et al. (2005), the fuel layer of wheat straw keeps its bulk volume. However, bed porosity must change due to particle shrinkage. In this respect, the change of bed porosity is calculated using the relation (Yang et al., 2005a)

$$\epsilon = \epsilon_0 + (1 - \epsilon_0) \cdot \sum_i f_i \left(w_{i,0} - w_i\right), \tag{1}$$

where ϵ_0 is initial bed porosity, $w_{i,0}$ is initial mass fraction of the *i*-th solid component and f_i is a shrinkage factor, which, for the two extreme cases, if $f_i = 0$,, then the mass loss of the *i*-th solid component does not cause increase of bed porosity, if $f_i = 1$, then the bed porosity increases by the entire volume of the *i*-th solid component removed. Modelling of the growth of internal particle pores is not considered in the present work.
Bed porosity in turn affects particle volumetric surface, which is an important parameter in heat and mass transfer between gas and solid phases. For the sake of simplicity, solid particles are modelled as spheres (different shapes can be taken into account by introducing the sphericity parameter). For the case of spheres, the bed volumetric surface can be expressed as

$$S = 6(1 - \epsilon)/d_\mathrm{p}, \tag{2}$$

where d_p is particle diameter.

Boundary conditions for the gas phase at the grate are set according to operating conditions of the furnace, whereas zero gradients (homogeneous Neumann boundary condition) are assumed for the solid phase. At the top of the bed, a radiative heat flux from a heating device placed above the bed is given for the solid phase (the temperature of the radiation source is 1173 K), while zero gradients are prescribed for the gas phase (an outflow boundary condition). However, for better accuracy the boundary condition for the gas phase is placed a few centimetres above the bed top.

2.2 Solution technique

The mathematical model has been implemented into a computer program GRATECAL developed in the Matlab® environment. The governing equations are solved numerically by the finite volume method. The whole computational domain is divided into 1250 control volumes (50 cells are used above the bed top) and time solutions of gas velocity and both gas and solid temperatures and species are sought in each cell using techniques described in (Patankar, 1980). The convergence of iterations at each time step is judged by scaled residuals (Fluent 6.3.26., 2006). Due to convergence problems that slowed down the solution procedure, an adaptive time stepping has been employed as well.

3. Discussion on results from simulations

In order to assess the approach for modelling the change of bed porosity and particle size during wheat straw combustion, a number of simulations has been performed, three of which are discussed in more detail in this section. Initial and operating conditions of these simulations are the same and are listed in Table 1. The difference between the simulations is in the initial size of particles and in the dynamic change of bed porosity (included or not). Discussion of results from simulations is based on physical reasoning and qualitative comparison to both theoretical and experimental results of other authors.

Yang et al. (2005c) studied the effects of porosity on burning rate with respect to the primary air flow rate. At low air flow rates (around 0.1 kg/m^2/s), the burning rate decreases as the bed porosity increases. A similar trend was obtained from the model of van der Lans et al. (2000). As for the particle size, larger fuel particles cause lower burning rate, thicker reaction zone and higher bed temperature.

Table 1 – Initial and operating conditions

Property	*Value*
Bed height [m]	0.5
Bed diameter [m]	0.2
Primary air-flow rate [kg·m^{-2} s^{-1}]	0.1
Initial (ambient) and primary air temperature [K]	298.15
Initial moisture in fuel [wt%] (dry basis)	10
Initial volatile matter in fuel [wt%] (dry basis)	79.28
Initial char in fuel [wt%] (dry basis)	16.03
Initial bulk density of straw [kg·m^{-3}]	130
Initial bed porosity [-]	0.58
Shrinkage factors for individual processes [-]	0-drying, 1-devol. and char comb.
Particle diameter [mm]	4 or 20

Figure 1 illustrates propagation of char combustion fronts for the case of a bed of particles with diameter $d_{\mathrm{p}} = 4\ \mathrm{mm}$ as calculated during simulations with constant porosity (solid line) and variable porosity (dash-dotted line). It is important to note that burning rate is different from char combustion reaction rate. Burning rate is defined as mass of solid fuel that is converted into gas phase per unit time and unit cross-sectional area of the bed (van Kuijk, 2008). However, mass loss is proportional to the sum of reaction rates. Since drying and devolatilization fronts advance through the bed before the char combustion reaction front, the propagation of the latter can be used as an indicator of the burning rate. It can be seen in the figure 1, that the reaction front as predicted by the model with variable bed porosity moves downward the bed with lower velocity than the reaction front in case of the constant porosity model. This partially corresponds with the aforementioned results of other authors, because the bed porosity increases during straw combustion. But particle shrinkage should lead to lower bed volume and thus to higher surface density and higher reaction rate. The problem should be resolved by including the internal particle porosity into the model.

The value of the char combustion reaction rate predicted with the variable-porosity is however lower than the value obtained with the constant-porosity, because volumetric surface of particles in the present model decreases with increasing porosity. Figure 2 shows propagation of reaction front in the bed of particles with $d_p = 20\ \mathrm{mm}$. The variable-porosity model has been used. The reaction front travels down with considerably lower speed than in the bed of 4-mm particles. A thicker reaction zone can be seen as well. This corresponds well with experimental results (Yang et al., 2005a, 2005c). However, a thicker reaction zone can also be seen in the case of 4-mm particles for the variable-porosity compared to the reaction zone from the simulation with the constant-porosity model (figure 1). This unexpected behaviour was caused by lower volumetric surface of particles, which in turn has impacted interphase heat transfer.

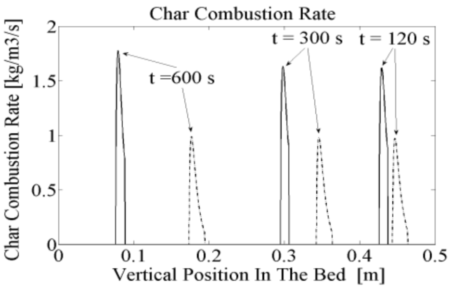

Figure 1 – Propagation of char combustion reaction front in the bed of 4-mm particles. Variable-porosity model (dash-dotted line), Constant-porosity model (solid line).

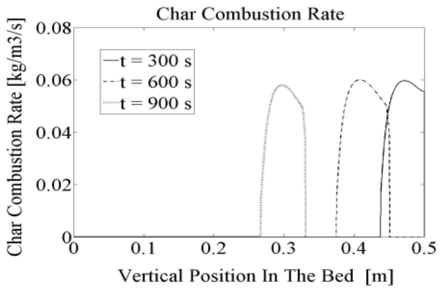

Figure 2 – Propagation of char combustion reaction front in the bed of 20-mm particles. Variable-porosity model.

4. Conclusions

Bed porosity and particle size belong to a set of parameters that define bed packing conditions, which have impact on heat and mass transfer, propagation and thickness of reaction front in the bed. The propagation of char combustion fronts during wheat straw combustion has been compared for two cases – a constant-porosity bed model and variable-porosity bed model. Results from simulations qualitatively match experimental and theoretical results of other researchers to a certain extent, i.e. at low primary air flow rates, the burning rate decreases with increasing porosity. However, the variable-porosity model produced larger reaction zone than the constant-porosity model, which is in contradiction with the fact that volume of particles shrinks. To remedy this effect, internal particle porosity should be considered.

5. Acknowledgements

The authors gratefully acknowledge financial support of the Ministry of Education, Youth and Sports of the Czech Republic within the framework of project No. 2B08048 "Waste as raw material and energy source", research plan No. MSM 0021630502 "Waste and Biomass Utilization focused on Environment Protection and Energy

Generation" and within the framework of Operational Programme “Research and Development for Innovations” – “NETME Centre – New Technologies for Mechanical Engineering”. Tomáš Juřena gratefully acknowledges financial support of statutory city of Brno within the framework of programme "Scholarship for Talented PhD students".

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