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A two dimensional Euler-Lagrangian model of wood gasification in a charcoal bed — Particle histories

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ABSTRACT

An Euler-Lagrangian simulation applied to wood gasification in a fluidized bed is used to investigate individual particle histories and to provide a statistical analysis for temperature, apparent density as well as radial and axial positions of charcoal and dry wood particles. The model and several parameter variations have been discussed in detail in previous articles [1–3]. Based on simulation results we find much higher particle heating rates than typically used to measure kinetic data for, e.g., pyrolysis models. Although we presented a rather complex interplay of particle heating rate, biomass decomposition, particle shrinkage and particle fluidization the simulation results emphasize the importance of the usage of realistic particle size distributions for the initial bed as well as the fuel inlet. Furthermore, particle shrinkage data in combination with mass decomposition data appear to be crucial for realistic simulations.

1. Introduction

The present article completes the data presentation of our two dimensional Euler-Lagrangian simulations of wood gasification in a charcoal bed. The model used for the simulation and a detailed parameter variation were presented in Refs. [1–3] and features comprehensive extensions of an earlier model [4]. The detailed parameter description as well as the broad parameter variation and discussion allows for a comprehensive evaluation of the shortcomings and benefits of our model in order to switch to more demanding three dimensional simulations on the base of a numerically cheaper two dimensional study. Besides the Euler-Lagrangian modeling approach used here for the simulation of wood gasification in fluidized beds, we also apply multi-fluid models [5] which allows a comparative view on those two model approaches.

There are many references discussing the pros and cons of Euler-Lagrangian vs. multi-fluid models (see e.g. Refs. [6,7]) but there are just a few references reporting data for the scale which is only accessible in Euler-Lagrangian models: the single particle scale. This lack of data is even more existent for dense reactive flows such as the one discussed here.

In a series of papers, Papadikis et al. [8–15] report such particle data. They used FLUENT 6.2 together with user defined functions (UDF) for the particle drag law in order to couple the Lagrangian calculation of single char or biomass particles to an Eulerian system consisting of one solid phase made up of sand particles and a gaseous phase fluidizing the sand bed. The article series starts with two articles introducing the model [8,9] and first results for one single biomass particle and a total simulation time of 3 s (first second is without the biomass particle). The lab-scale reactor used for the studies has a diameter of 40 mm and a height of 260 mm, while the bed height is 80 mm. Data concerning the used mesh was not reported.

The Eulerian model used by Papadikis et al. [8,9] is a standard single solid phase model coupled to a standard gas phase modeling approach. The Eulerian sand phase consists of mono-disperse particles with a diameter of 440 μm (Geldart type B). The movement of the Lagrangian particles considers standard expressions for drag, gravity, buoyancy, and virtual mass for free particles. In order to use these expressions in the dense regime, the authors use effective continuous properties for material properties such as the density and the dynamic viscosity. The precise calculation of these effective properties is not reported. The theory behind this ansatz relies on three phase flow ideas (liquid-gas-solid particle) taken from Ref. [16] for particles which are free in the mixture flow of gas and liquid. This theory is adapted such that the liquid phase in Ref. [16] is replaced by

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the solid Eulerian phase, even though the sand and biomass particle are of almost same size. There is no consideration of particle-particle and particle-wall collisions in the equation of motion for the single biomass particle. The validity to adopt the theory – which was developed for a different kind of multiphase flow [16] – is not discussed in Refs. [8,9].

The results of Ref. [8] include 2d/3d comparative data for velocity components of gas, sand, and the one Lagrangian particle as well as local volume fractions, temporal evolutions of drag, and virtual mass forces. Some qualitative pictures documenting the general flow regime are presented. The one single particle in the first study is chemically and thermally not coupled to any phase. The difference of the 2d and 3d data was used to pronounce the asymmetric flow pattern in the 3d case compared to the 2d case.

In the second part of the article series, Papadikis et al. [9] investigate the pyrolytic decomposition of a single biomass particle in the identical reactor as in the first part [8] . Compared to Ref. [8] there are no documented model changes for the Eulerian model for the gaseous and solid phases while the model for the single biomass particle is complemented by an one dimensional transient heat equation in spherical coordinates which accounts for heat conduction and the heat of reaction of the biomass decomposition reaction. The effective heat capacity and thermal conductivity are mixture values of the char and wood properties which are linearly dependent on the grade of decomposition (which is a standard assumption in these kind of models; see e.g. Ref. [17]).

The biomass decomposition model consists of two steps: the first step decomposes the biomass in three competing reactions into char, gaseous components, and tar and the second step decomposes the tar further to char and gaseous components. There is no information on the kind of energy and species balances for the gaseous phase as well as the energy balance of the solid continuous phase which makes it difficult to evaluate these parts of the model. Papadikis et al. [10] document an energy balance but no species balance.

The overall simulation duration reported in Ref. [9] is 3.5 s and the single biomass particle is again introduced after 1 s of simulation time. The authors present qualitative data about the flow regime. Furthermore, particle data for the temporal evolution of the density and velocity components are pictured. The one dimensional particle model allows the authors to present plots of particle temperature as well as charcoal, wood, gaseous components, and tar mass percentage data over time and the radial coordinate of the single particle. Because of the small size of the particle there are fairly smooth gradients inside the particle. Data for the local heat exchange coefficients of the particle are shown as a function of time.

The following articles of Papadikis et al. [11–15] further investigate the influence of particle size and sphericity on char entrainment [12,14], particle size on heat transfer coefficient [13] and effect of biomass shrinkage [11]. Additionally, Ref. [15] investigates the special case of a cellulose particle under consideration of two different heat exchange models. The simulated time ranges and the number of particles do not change significantly (up to three particles and 5 s simulation time) in the later part of the series [11–15].

Although the article series by Papadikis et al. highlights the importance of detailed particle resolved data for a better understanding of the chemical and physical processes governing gasification and pyrolysis, one shortfall of the series lies in the short simulation times and the usage of only up to three particles. The limited particle number results in data which are not representative but exemplary. From the fluid dynamical point of view, it is questionable if the data calculated without the biomass particle results in bed properties which are close to steady state. The reactive part of the simulation does certainly not reach steady state while no data at the reactor outlet are given. Furthermore, the description of several numerical parameters (e.g. the mesh in use for continuous as well as single particle itself) is not documented, which hinders a detailed model evaluation.

Another shorter article series on reactive particles in fluidized beds is given by Zhou et al. [18,19]. The authors report data based on a two dimensional Euler-Lagrangian model for a coal fired fluidized bed reactor under usage of a large-eddy simulation (LES) approach. The particle phase collisions are handled by a Discrete Element Method (DEM). The bed consists of 1400 sand particles (diameter 1 mm) and 20 coal particles (diameter 0.8 mm, 1.5 mm and 2 mm). The simulation duration is 2 s. The first part of the series documents the gas phase model as well as data for particle velocity distribution (over particle number), particle-particle and particle-wall collisions, temporal snapshots of the gas particle moment and turbulent energy distributions, and plots for the gas and particle velocity, turbulent intensity (both components), and Reynolds stresses over the bed width. Furthermore, the authors shortly present comparison of five cases with variations on the inlet gas temperature, coal particle diameter, and inlet gas velocity with an inert case.

In the second part, Zhou et al. [19] discuss the coal combustion on the particle level. First, they document the considered gas phase reactions, gaseous species and energy balances. The particle energy balance is written with the help of submodels for the heat exchange caused by convection and radiation between gas and particles as well as heat conduction in the particle phase and heat of combustion for the coal particles. Furthermore, they present data for the particle heating rate over the particle diameter, the power exchange rates of the terms involved in the particle energy balance, the pyrolysis rate, particles excess temperature as well as species data at the reactor outlet and snapshots of species concentration in the bed. The particle heating rates reported range from approx. 432 $^{K}/_{s}$ (for 2 mm particles) to 1627 $^{K}/_{s}$ (for 0.8 mm particles) and heating histories of individual particle differ greatly depending on particles bed position. The particle excess temperature are found to be much higher than the average bed temperatures.

A further contribution results from the work of Bruchmüller et al. [20]. The authors simulate a lab-scale reactor in 3d and compare with experimental data. The reactor is filled with approx. 0.8 million sand and biomass particles (red oak). The biomass enters the reactor with a massflow of 100 $^{g}/_{h}$ in batches of 318 particle which results in approx. 37,000 biomass particles per second. The particle model is a zero dimensional approach accounting for particle heat-up, drying and biomass pyrolysis. The pyrolysis model is based on the work of Miller et al. [21] and assumes biomass to consist of three components (cellulose, hemicellulose and lignin) degrading to an intermediate activated biomass state. A further degrading in two competing reactions to either gas and char or tar follows the first step. The ratio of gas and char yields is fixed per component. No further homogeneous or heterogeneous reactions are considered. The authors argue that tar decomposition can be neglected through the chosen reactor conditions. Shrinkage is considered to be mass proportional during pyrolysis and neglected during the drying process. The drying process and the moist content of the particle in general seem to be of minor importance — certainly connected to the chosen reactor conditions like temperature and biomass particle diameter and the neglected heterogeneous and homogeneous reactions.

The simulated time period consists of a 5 s initial fluidization period and another 5 s of reactive biomass conversation period. The biomass particles of 500 μm diameter enter the reactor bed consisting of sand particles with a mean diameter of 520 μm.

The authors show several qualitative figures picturing the fluidization regime for different inlet velocities and the inlet flow conditions which are varied between a plug flow inlet and a perforated distributor inlet. Differences for the inlet flow conditions are found to be of minor importance while the inlet flow velocity is significant. Further pictures are shown for exemplary particle trajectories. Particle yield results are compared with experimental