Validation of a numerical approach for simulation of the thermal decomposition behaviour of biomass in grate combustion plants

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The overall objective of the modelling work is to develop CFD aided design tools for optimum grate fired biomass-to-energy (BtE) and waste-to-energy (WtE) plants. An important part of this work has been to develop a flexible detailed transient fuel-bed model taking into account drying, pyrolysis, and char combustion/gasification, for different fuels (i.e. MSW fractions, and softwood and hardwood, including their bark and GROT (branches and treetops)). The fuel-bed model has been implemented in a CFD tool, ANSYS Fluent. The fuel bed consists of a large number of thermally thick particles. In this work, the fuel bed model is made up of representative particles, and the motion of every representative particle is individually tracked (Lagrangian tracking through Fluent's Discrete Phase Model). Thermochemical degradation and conversion of the representative particles are calculated by a thermally thick single particle model (SPM), with boundary conditions obtained from the solutions of the gas phase equations. The SPM model then provides sources to the gas-phase equations. In the modelling approach, the gas phase is solved using the Reynolds Averaged Navier-Stokes (RANS) equations. Under the given conditions, the gas flow in the bed is laminar.

The developed model was validated against detailed experimental results from pyrolysis of dried spruce wood pellets in an electrically heated fixed bed reactor, with varying final pyrolysis temperature (600-800°C), heating rate (5-20 K/min) and purge gas composition (none, 100% N_2 and 90/10% N_2/O_2). The experimental results included transient temperature measurements in different locations in the reactor and inside the pellets bed throughout the thermal decomposition process, as well as gas measurements of permanent gases.

Through the CFD simulations, the main experimental trends could be reproduced, verifying the validity of the detailed modelling approach. This work is a step towards detailed modelling of biomass grate combustion units, to improve their environmental and energetic performance.

1. Introduction

Computational Fluid Dynamics (CFD) based modelling and simulation approaches are among the most powerful tools at hand to achieve a good combustion process and to cope with operational issues connected to the biomass feedstock in grate combustion plants. However, commercial CFD codes do not include the detailed models needed for simulating the thermal decomposition of the fuel bed on a grate. In this work, the focus has been on validating a detailed numerical model applicable for studying the thermal decomposition of biomass in grate combustion plants.

2. Modelling approach

2.1 The single particle model (SPM)

The layer-based single particle model proposed by Ström et al. (2013) and Li et al. (2020), which is based on Thunman's approach (Thunman et al., 2002), is selected to describe the conversion of the thermally thick

particles. In this model, the spherical particle is divided into three distinct layers: wet wood, dry wood, and char, as shown in Figure 1. In the presence of oxygen, or when the temperature is high enough for gasification reactions to be relevant, one may want to include char conversion. A fourth layer, consisting of ash, is then added. The thermal conversion (drying and devolatilization) is assumed to occur at the infinitely thin fronts between the layers. The model can be applied to all particle shapes where the surface area can be expressed as a function of the distance to the particle center. Each layer in the model is assigned a temperature (T_p) and a mass (m_p), and the boundary between layers is assigned a temperature (T_b), which is the reaction or conversion temperature for the particle sub-models. The outermost boundary is the particle surface, and its temperature is determined by a balance between the gas phase and the intra-particle heat transfer process. A more detailed description of the heat and mass transfer model is provided by Zhang et al. (2020).
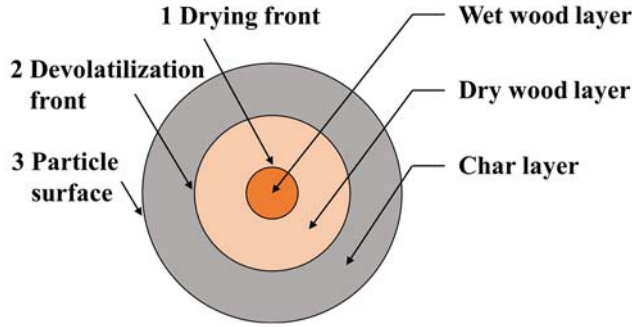

Figure 1: Particle model layout. The three surfaces/fronts are indicated by numbers; 1-drying front, 2-devolatilization front, 3-particle surface

In the literature, one can find two main branches of drying models: thermal and kinetic (Haberle et al., 2017a; Haberle et al., 2017b). In the current work we use a thermal drying model. The rate of drying is then controlled by the heat flux to the drying boundary, such that the reaction rate of the drying layer is given by

$$R_{b0} = Q_{b0}/L_{water}$$

where

$$Q_{b0} = f_{b0}F_{b0}$$

is the total heat that is used to evaporate water, f_{b0} is the total heat flux to the drying boundary and

$$F_{b0} = \frac{10^{8.07131-1730.63/(T_{b0}-39.724)}}{760}$$

is the fraction of that flux that is used for water evaporation. The latent heat of water is given by $L_{water} = 2.26 \times 10^6$ J/kg. Devolatilization of wood is controlled by three parallel reactions giving the yields of gas, tar and char, as presented graphically in Figure 2 (Ström et al., 2013). The Arrhenius parameters for the three reactions are given in Table 1.

Table 1: Arrhenius parameters for the three devolatilization reactions

Reaction	Rate parameter	Pre-exponential factor	Activation energy
Dry wood → gas	k_{d1}	1.3×10^8 s^{-1}	140 kJ/mol
Dry wood → tar	k_{d2}	2.0×10^8 s^{-1}	133 kJ/mol
Dry wood → char	k_{d3}	1.08×10^7 s^{-1}	121 kJ/mol

The composition of the gas is listed in Table 2 while the tar in this work is defined to have the same composition as the gas. Char conversion is not included in these simulations.
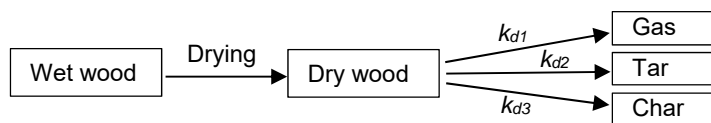

Figure 2: Graphical view of the drying and devolatilization model

2.2 Fuel bed modelling

The fuel bed is made up of representative particles. Every representative particle is individually tracked (through Fluent's DPM model) and evolved (with the SPM) for its entire residence time in the bed. The modelling of the fuel bed is based on the use of user defined functions (UDF). For the fixed bed in this study, the particles are forced to have zero velocity, which means that no particle tracking is required. The main contribution to the UDF is the Single Particle Model (SPM) (Ström et al., 2013; Li et al., 2020; Zhang et al., 2020), which provides a detailed 1-dimensional description of the evolution of a thermally thick particle that exhibits drying and devolatilization. Given the initial particle properties, the inputs to the model are the surrounding gas and radiative temperatures. Based on this, the SPM yields the mass flow rate and temperature of the gaseous yield from individual particles, which are to be considered as sources to the gas-phase equations.

During the drying phase, the released gas will be 100% H_2O. For the devolatilization phase, the gas composition has been optimized towards satisfying available relevant wood pyrolysis gas compositions while maintaining the elemental balances for the solid fuel, dried spruce wood pellets. This means that a mean gas composition is used for the devolatilization stage (Table 2), while the remainder of the carbon in the solid fuel is going into char. Even if the gas composition in reality will vary during the devolatilization stage, the gas composition above the bed will be a mixture from all different stages since the particles in the basket will be at different stages in the process. The thermophysical properties of the gas mixture, such as conductivity and specific heat, are calculated by mass-weighted mixing laws. The ideal gas law is used to calculate the density of the gas phase. For radiation, the P1 model is used.

Table 2: Gas composition during devolatilization of the dry spruce feedstock

Components	Gas composition Mass fraction
CH_4	0.131870
O_2	0
CO	0.342534
CO_2	0.083958
H_2O	0.441638

The fuel bed consists of a large number of particles. Due to CPU restrictions, a simulation cannot handle all these particles individually. Instead, the SPM is solved for representative particles. In Fluent, the concept of parcels was used for the representative particles. The different representative particles can have different radii and composition. This means that each representative particle will represent a certain number of physical particles with the same composition and size.

Hermansson & Thunman (2011) developed a similar bed model as used here, but in their model the solid phase is handled with the Eulerian approach. In their work, the focus is on bed shrinkage, and they present a numerical model that handles both continuous shrinkage and bed collapse. Since the shrinkage model is validated only for char, their simulations do not consider drying and devolatilization.

The effective thermal conductivity in the fuel bed is calculated as

$$k_{eff} = \frac{1}{X_{wood}/k_{wood} + (1 - X_{wood})/k_{gas}}$$

where X_{wood} is the volume fraction of wood (the solid particles) and k_{wood} and k_{gas} are the conductivities of wood and gas, respectively. As the heat conduction in the fuel bed could be higher, also a linear approach was investigated, where the conductivity of wood and gas was scaled with the respective volume fraction, similar to the approach for porous media in ANSYS Fluent, i.e.

$$k_{eff} = X_{wood}k_{wood} + (1 - X_{wood})k_{gas}$$

For cases with large difference in the two conductivities, using the latter approach, the material with the highest conductivity will have a dominant effect on the mixed conductivity. For the case studied here, the model approach had no significant effect on the temperature development in the fuel bed.

In this study, the particle density of the wet wood pellets was set to 1180 kg/m^3 (Obernberger, 2004). Reducing the density by 25% (to 900 kg/m^3) had no significant effect on the simulation results.

3. Results

3.1 Comparison with experiments

Pyrolysis experiments were carried out in an electrically heated fixed bed vertical tube reactor containing a container basket, using dried spruce wood pellets (Skreiberg, 2021). In the batch mode experiments, pyrolysis temperature (873-1073 K (600-800°C)), heating rate (5-20 K/min) and purge gas composition (none, 100% N_2 and 90/10% N_2/O_2) were varied. Temperatures were measured at the reactor wall (3 locations in the vertical direction) and inside the pellets bed (3 locations in the radial direction) throughout the thermal decomposition process. Permanent gases were measured using a GC, while condensables were condensed and collected, in addition to the remaining solids, allowing establishing the mass balance.

A two-dimensional (2D), axis symmetric numerical representation of the reactor tube (500 mm high, 125 mm inner diameter) with the container basket was made for transient simulations. The solid steel walls of the basket were included and meshed, while the solid wall of the reactor was modelled as a boundary condition, using 1400 elements in the entire 2D model. One of the experiments was chosen as the validation base case. This case had the following specifications: the heating rate was set to 10 K/min until the maximum temperature of 873 K (600 °C) was reached, while nitrogen was used as purge gas with a flow rate of 2.2 l/min. The 6 mm diameter pellets were modelled as spherical particles with a diameter of 6 mm. The purge gas inlet temperature was set to 380 K, the emissivity of the reactor wall was set to 0.7 and the emissivity of the basket wall to 0.5. The evolution of the temperature wall boundary condition was set equal to the instantaneous wall temperatures measured during the experiment. The values for the middle wall temperature are shown as the black line in Figure 3. Three thermocouples (T2, T3, T4) were placed inside the pellets bed approximately halfway down into the basket (50 mm from the bottom of the basket), one in the center (T2), one close to the wall (T4) and one in between (T3), approximately 15 mm from the center. The thermocouples measured the fluid temperature at these locations in the void between the particles.

Figure 3 shows that the model prediction of the fluid temperature at the edge and in the center of the fuel bed compare relatively well with the experiments. The temperature profiles at the edge are nearly identical up to 700 K (45 min), then the temperature increase in the experiments becomes slightly steeper than in the simulations, however the deviation is limited. In the center of the bed, the temperature profiles are nearly identical in the first phase (up to 35 min and 470K) and are close after that. The temperatures at different elevations in the fuel bed center presented in Figure 4 shows that in the first period (until 50 min) the heating rate decreases with distance from the bottom of the bed except for the upper part of the bed (compare the results at 61 and 81 mm). The simulated temperature just above the T2 position coincide even better than the simulated T2 with the measured temperature at this position. The hot gas coming into the bed from below is cooled by the particles, and the release of the relatively colder gases during devolatilization from the colder particles to the void where the thermocouples are installed will also lower the fluid temperature. This effect will increase as the distance from the bottom of the bed increases. In the simulations, the maximum gas release is more than 6 times the purge gas flow. This effect might be slightly underestimated in the simulations causing the deviation in the T2 temperature between 35 and 50 min compared to the experimental results. If there is a minor inaccuracy in the thermoelement position in the experiment and it actually is at a slightly higher elevation compared to the simulations, the correspondence will also be improved (ref. Figure 4). The final temperature increases with distance from the bottom of the bed, and the simulated temperature at the highest position (81 mm) coincide best with the measured T2-temperature and the final wall temperature. One reason for this could be that the shrinkage of the bed, moving the bed surface closer to the thermocouples, is not included in the simulations, and this delays the simulated temperature development in the final stage compared to the measurements.
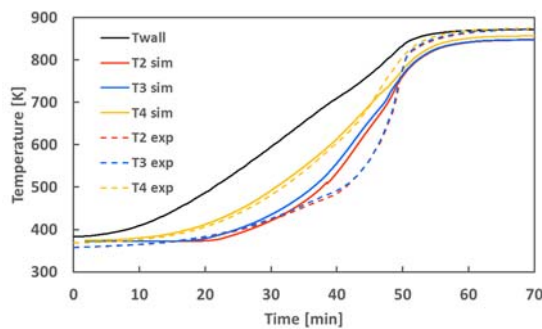

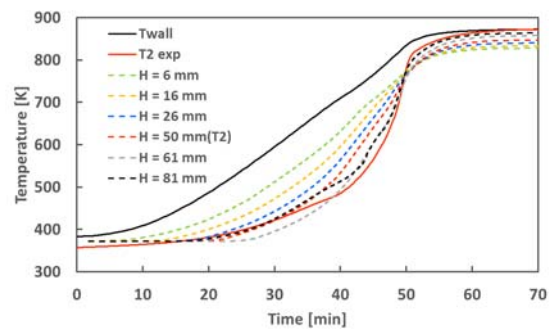*Figure 3 Simulations vs experimental results. Temperatures within the fuel bed*

Figure 4 Simulations results. Fluid temperature in center of fuel bed at different elevations

3.2 Effect of particle size

Variations in particle size do not affect the fluid temperature at the fuel bed edge (Figure 5), this is because the temperature of the fluid at the basket wall is controlled by the heat flux from the reactor wall, through the gap between the reactor wall and basket, and then through the basket wall.

Inside the bed, however, the fluid temperature is affected (Figure 6). This is a result of the hot gas coming into the bed from below and heat conduction from the basket walls. Since the hot gas coming into the bed from below is cooled by the particles in the lower part of the bed, the temperature in the middle of the bed depends on the heat transfer rate between particles and fluid. It is clear that a given solid mass has a larger external surface, and hence a larger heat transfer, if it is divided into many small particles instead of a few large ones. This means that at any given time, the vertical temperature gradient in the bed should be largest for the smallest particles. This is indeed what is seen from Figure 7, where it can be observed that the temperature difference between the different positions in the bed is always (until devolatilization is initiated at around 40 min) larger for the smaller particles.
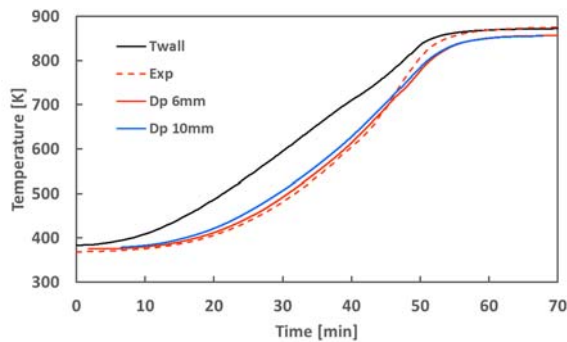

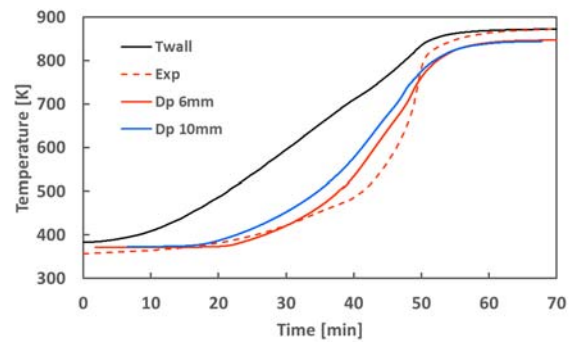Figure 5. Fluid temperature at fuel bed edge at different particle diameters (Dp)

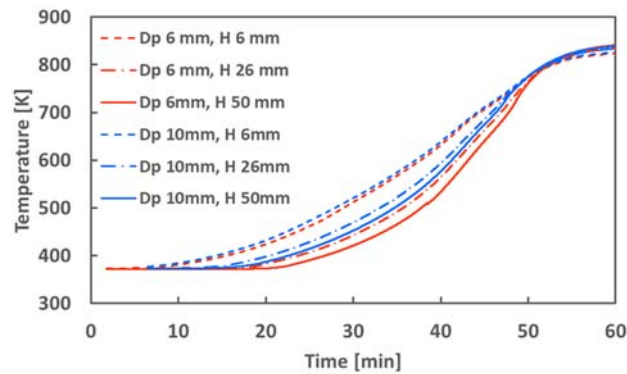Figure 6 Fluid temperature in fuel bed center at different particle diameters (Dp)

Figure 7 Fluid temperature in fuel bed center at different elevations for different particle diameters (Dp). H is distance from bottom of basket

4. Conclusions

In this work a 2D axis symmetrical modelling approach of the transient thermal decomposition process in a fixed bed of pellets was carried out using experimental initial and boundary conditions and was validated against experimental results. The modelling approach enabled reproducing the experimental results relatively well, i.e. the transient temperature profiles at different locations inside the pellets bed. Additional simulations were carried out to investigate the effects of fuel particle size, showing that the vertical temperature gradient inside the pellets bed is largest for the smallest particles, which is a result of the particle external heat transfer area, giving a larger cooling effect on the gas coming into the bed from below for smaller particles.

In the current study, the thermal decomposition under inert conditions involved drying and pyrolysis. For cases with oxygen, the fuel modelling approach will also handle char conversion. The bed model is generic and can be used also for moving grate cases. This work is a step towards detailed modelling of biomass grate combustion units, to improve their environmental and energetic performance.

Acknowledgments

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