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Multi-physics modelling of packed bed biomass combustion

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HIGHLIGHTS

• A transient 3D model was developed to simulate fuel bed and freeboard of biomass grate furnaces.

• The intra-particle gradients, the bed shrinkage and variations of the bed porosity are considered.

• Detailed kinetic mechanisms are used for the homogeneous gas phase reactions.

• The results are in a good agreement with experimental data.

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ABSTRACT

A transient 3D model for two main zones, namely the fuel bed and the freeboard, of biomass packed bed combustion systems was developed. It integrates the models for the biomass conversion sub-processes and solves the governing equations for the gas and solid phase and their interactions. The intra-particle gradients are included by considering the biomass particles as thermally thick particles. The shrinkage of the packed bed and the variations of the bed porosity due to the uneven consumption of the fuel are taken into account. Detailed kinetic mechanisms are used for the simulation of homogeneous gas phase reactions. To verify the model and to increase the understanding of packed bed combustion, laboratory-scale fixed-bed batch experiments have been performed in a reactor with 9.5 cm diameter and 10 cm length. The model performance was extensively validated with gas phase measurements (CO, CO₂, CH₄, H₂, H₂O and O₂) above the fuel bed, temperatures at different heights in the bed and in the freeboard, and the propagation rate of reaction front. The simulation results are in a good agreement with the measured values.

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1. Introduction

Among the applied biomass combustion technologies grate-firing is one of the most widely spread, because it can handle a wide range of fuels of varying quality and moisture contents and requires less fuel pretreatment. However, the bed inhomogeneity due to the inhomogeneity of the biomass fuel and insufficient mixing in the fuel bed, causes non-uniform combustion on the grate. This may reduce the efficiency of the plant and increase the emissions. Dealing with these deficiencies requires an improved understanding of the combustion processes in the fuel bed.

Due to the limited accessibility and inhomogeneity inside the packed bed, it is difficult and complex to obtain information by measurements about the conversion processes in the packed bed. As a result, there are few experimental investigations on packed

* Corresponding author at: Institute for Process and Particle Engineering, Graz University of Technology, Inffeldgasse 21b, 8010 Graz, Austria. Tel.: +43 (0) 316 8739232; fax: +43 (0) 316 8739202. bed biomass furnaces which include a complete set of measurements. Ryu et al. [1] measured temperatures, species and mass loss profiles of four different biomass types in a fixed bed under fuelrich conditions. The combustion of straw in a fixed bed was experimentally investigated by van der Lans et al. [2]. They measured temperatures in the packed bed at different heights and species concentrations above the bed. Porteiro et al. [3,4] measured the propagation rates of the reaction front in a fixed bed combustor.

The review of elaborations on packed bed modelling published in literature shows a broad variety of different model approaches to describe entire packed bed systems. The main distinctive features are homogeneous and heterogeneous models. The difference between them lies in the calculation of the energy equation. In homogeneous models the temperature of the gas and of the solid phase are assumed to be equal and one overall energy balance equation is applied [5,2]. The physical properties which appear as constants in the energy equation are described by their effective values over the entire bed. In heterogeneous models the gas phase and the solid phase have individual energy equations [6–8]. They





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Nomenclature

Α	pre-exponential factor (s ⁻¹)
a_{p_i}	acceleration of particle i (m s ⁻²)
Ci	biomass pseudo-component contributions (–)
C_1	permeability (m ²)
<i>C</i> ₂	inertial loss coefficient (m^{-1})
\mathcal{D}	diffusivity $(m^2 s^{-1})$
Ε	activation energy (kJ mol ⁻¹)
F	view factor
ġ	gravity (m s ⁻²)
h	heat transfer coefficient (W m ⁻² K ⁻¹)
h_m	mass transfer coefficient (m s $^{-1}$)
k	kinetic rate constant (s ⁻¹)
k_c	reaction rate constants, char conversion (m s $^{-1}$)
т	mass (kg)
M_c	molecular weight of carbon (kg kmol ^{-1})
п	mole (–)
NC	number of cells
NP	number of particles
Nu	Nusselt number (–)
р	pressure (Pa)
Pr	Prandtl number (–)
q	heat flux (W m^{-2})
r	reaction rate (kg s ⁻¹)
R	universal gas constant (kJ mol ^{-1} K ^{-1})
Re	Reynolds number (–)
S	surface area (m ²)
Scon	source term in continuity equation $(\text{kg m}^{-3} \text{ s}^{-1})$
$\underline{S}_{s,i}$	species <i>i</i> source term $(\text{kg m}^{-3} \text{ s}^{-1})$
S _m	momentum source term (kg $m^{-2} s^{-2}$)
S_q	energy source term (J m ⁻³ s ⁻¹)
t	time (s)
Т	temperature (K)
и	velocity (m s ⁻¹)

have different temperatures, and heat and mass transfer between the two phases are described by means of Nusselt and Sherwood correlations. When the temperature difference between the gas and solid is not negligible, which is the case for packed bed combustion, heterogeneous modelling is recommended.

Based on the treatment of the solid phase in the heterogeneous models, they can be classified into continuous models [9–12] and discrete particle models [13–16]. Continuous heterogeneous models treat both phases as if they are distributed continuously over the whole spacial domain. At each point in space both phases exist with distinguished properties. The common restriction of continuous packed bed models is that the intra-particle effects cannot be described sufficiently. Additionally, it is very difficult to model the inter-particle interactions in the packed bed with continuous models. The discrete particle models enhance the packed bed modelling by considering the packed bed as an ensemble of representative particles, where each of these particles undergoes thermal conversion processes. In this way the inter-particle effects, e.g. momentum and energy exchanges, can be fully described.

However, there is a limitation in almost all existing models, with the exception of [11], that they consider the packed bed and the freeboard separately, although there is a strong interaction between them. The conversion of the packed bed provides the temperatures and species as inlet conditions for gas phase modelling. Additionally, the published models are validated only to a certain extent, typically using either propagation rates of the reaction front or species profiles. This can be attributed to the fact that experimental data which include complete sets of measurements

X_{∞} molar concentration of gas species at bulk flow (kmol m⁻³)

Greek	symbols
α_i	conversion of each biomass pseudo-component (–)
δ	distance (m)
δ_{ash}	thickness of ash layer (m)
ϵ	emissivity (–)
ϕ	porosity (–)
ή	tortuosity (–)
μ	viscosity (kg m ^{-1} s ^{-1})
v	stoichiometric coefficient mass basis (-)
ρ	density (kg m ^{-3})
σ	Stefan–Boltzmann constant (W m ⁻² K ⁻⁴)
$\tilde{\tau}$	stress tensor (Pa)
ω	mass fraction (–)
Ω	stoichiometric ratio of moles of carbon per mole of o
	dising/gasifying agent in corresponding reaction (-)
ψ	number of particles per volume (m^{-3})
Subscr	ipts
0	initial condition
ch	char
dry	drying
e	effective
f	final condition
g	gas
lam	laminar
р	particle
pyr	pyrolysis
rad	radiation
turb	turbulent
θ	radiation control volume

with a detailed information about the boundary conditions are scarce.

The objectives of this paper are to present a fully coupled threedimensional model for the combustion of biomass packed beds which includes both the freeboard and the packed bed as well as detailed experimental data for model validation. A validated comprehensive single particle model [17] for the combustion of thermally thick biomass particles is applied to model the conversion of particles in the packed bed. The size and the position as well as the conversion state of each particle is determined at every time step. The packed bed shrinkage and local porosity of the bed are calculated in each time step. The interaction between the gas phase and particles is considered by an iterative procedure. The radiative heat transfer between the particles and the walls is updated at the beginning of each time step. With these results, the conservation equations of the entire bed are integrated. The homogeneous gas phase reactions are modelled with a detailed kinetic mechanism, instead of applying global reactions. To validate the coupled packed bed/gas phase model, an experimental setup under known conditions has been simulated and the temperature profiles at different heights in the packed bed and in the freeboard, several species concentrations above the fuel bed as well as the propagation of the reaction front are compared with measurements.

2. Experimental setup

The laboratory-scale reactor is a discontinuously operated pot furnace, see Fig. 1. It consists of a cylindrical retort (height

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