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A two dimensional Euler–Lagrangian model of wood gasification in a charcoal bed – Part I: model description and base scenario

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HIGHLIGHTS

- Steady state results of a two dimensional Euler–Lagrangian model for wood gasification are shown.
- A complex reactive Euler–Lagrangian model in the dense particle regime is used for long time simulations.
- Comparison with experimental results indicate reasonable agreement.

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ABSTRACT

In this article we present a parameter study for an Euler–Lagrangian model with application to wood gasification in fluidized beds. The bed material consists of charcoal and wood only. The detailed model involves processes of heat up, drying, particle shrinkage, primary and secondary pyrolysis, gasification, and tar decomposition. Initially we introduce a bidisperse mixture of 12,000 charcoal particles idealised as perfect spheres. The collision model is based on a linear discrete element method (DEM) and allows to account for multiple particle–particle contacts and collisions. This first part of the study gives a detailed description of the model with all submodels and assumptions. The base scenario mimics experimental conditions of a lab-scale fluidized bed reactor. The base scenario will be used in the second part of the study as the base of comparison for a comprehensive parameter study. The data shown for the base scenario include temporal data for the reactor outlet temperature and species concentrations (including tars) as well as barycenter data for the solid phases. The data gained from the simulation is also compared to available experimental data.

1. Introduction

The usage of biomass as a resource for future energy supply is promoted by public grants in various countries either due the installation of an energy infrastructure in the developing countries or as part of a reorganisation of the energy infrastructure in developed countries. This enforced development has several reasons like the limited availability of fossil fuels, the problem of the climate change through the emission of greenhouse gases or simply by the need of developing countries for first-time installations of an infrastructure for energy supply. The local character of biomass usage may avoid the installation of elaborate electrical networks and may locally tie a bigger part of the financial earnings than for conventional energy supply. Biomass conversion has additional benefits like the ability of supporting the base load supply and the missing need of an intermediate energy storage. The competing situation between food and energy supply is solved in case of second and third generations of biofuels, due to the usage of biomasses which are based on non-food crops or the residues from food crops.

The thermo-chemical biomass conversion has further advantages like the opportunity to use bigger parts of the biomass than bio-chemical conversion. Especially the usage of lignin as a main component of several biomasses is a feature most other techniques are lacking. Furthermore, thermo-chemical biomass conversion allows also for the non-energetic usage of the biomass, e.g., for a base process of a future chemical industry.

Although charcoal as a medium to conserve and utilise energy has long traditions reaching back several hundred years there is still a fundamental lack of understanding the involved processes in detail. Problems in modelling the overall process of wood gasification in fluidised beds arise on one hand from the natural origin of the fuel (wood and/or charcoal). The fuel is therefore a complex mixture of several components with strong variations in composition which make the chemical modelling more challenging than for

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Nomenclature

A	frequency factor of Arrhenius kinetic rate expression (1/s K^a)
a	power of temperature of Arrhenius kinetic rate expression (–)
α	overall heat exchange coefficient (kg/s^3 K)
α_{Newton}	Newtonian heat exchange coefficient (kg/s^3 K)
A_p	particles outer surface (m^2)
$c_{p,\alpha}$	heat capacity of species α at constant pressure (m^2/K s^2)
$c_{p,p}$	particles overall heat capacity at constant pressure (m^2/s^2 K)
$c_{p,cc}$	heat capacity of charcoal at constant pressure (m^2/s^2 K)
$c_{p,w}$	heat capacity of wood at constant pressure (m^2/s^2 K)
$c_{p,water}$	heat capacity of water at constant pressure (m^2/s^2 K)
c_t	constant of the Smagorinsky model (–)
Δ	spatial averaged grid size (m)
Δh_α^0	standard heat of formation of species α (m^2/s^2)
$\Delta h_{evap.}$	constant heat of evaporation (m^2/s^2)
d_P	particles diameter (m)
E	activation energy of Arrhenius kinetic rate expression (kg m^2/s^2 mol)
ε	gaseous volume fraction (–)
η	linear conversion factor between wood and charcoal (1)
$\mathbf{F}_i$	force i acting on particle (kg m/s^2)
$\mathbf{F}_s$	momentum source term (kg/s^2 m^2)
h	total enthalpy (m^2/s^2)
h_α	total enthalpy of species α (m^2/s^2)
I_p	particles moment of inertia (kg m^2)
λ_{cc}	charcoal heat conductivity (kg m/s^3 K)
λ_P	particles overall heat conductivity (kg m/s^3 K)
λ_w	heat conductivity of wood (kg m/s^3 K)
M_0	initial charcoal mass (kg)
M_C	molar mass of carbon (kg/kmol)
m_{cc}	charcoal mass of particle (kg)
M_i	molar mass of species i (kg/kmol)
M_∞	final charcoal mass (kg)
m_p	particles overall mass (kg)
μ_{eff}	effective dynamic viscosity (kg/s m)
μ_{lam}	laminar dynamic viscosity (kg/s m)
μ_{turb}	turbulent dynamic viscosity (kg/s m)
m_w	wood mass of a particle (kg)
$m_{w,0}$	initial wood mass of particle (kg)
m_{water}	water mass of particle (kg)
Nu	Nusselt number (–)
ν_g	gaseous kinematic viscosity (m^2/s)
$\nu_{i,j}$	stoichiometric coefficient of species i in reaction j (–)
$\boldsymbol{\omega}_p$	particles rotational velocity (1/s)
p	dynamic pressure (kg/s^2 m)
Pr	Prandtl number (–)
$\mathbf{q}$	heat flow (kg/s^3)
$\dot{Q}_s$	enthalpy source term from solid phase (kg/m s^3)
R	universal gas constant (kg m^2/s^2 mol K)
$\dot{r}_{CO_2}$	production rate of charcoal with CO_2 caused by heterogeneous reactions (1/s)
$\dot{r}_{cc}$	production rate of charcoal from wood caused by primary pyrolysis (1/s)
$\dot{r}_{evap,H_2O}$	particles evaporation rate of water (kg s)
$\dot{r}_{H_2O}$	production rate of charcoal with H_2O caused by heterogeneous reactions (1/s)
$\dot{r}_{O_2}$	production rate of charcoal with O_2 caused by heterogeneous reactions (1/s)
$\dot{r}_{tar(g)}$	production rate of tar from wood caused by primary pyrolysis (1/s)
$\dot{r}_{w,gas}$	production rate of gaseous species from wood caused by primary pyrolysis (1/s)
Re_P	particle Reynolds number (–)
ρ_g	gaseous density (kg/m^3)
$\mathbf{S}$	symmetric part of the stress tensor (1/s)
T	temperature (K)
t	time (s)
τ	stress tensor (kg/s^2 m)
T_{evap}	constant temperature at which water evaporation occurs (K)
T_g	gaseous temperature at particle position (K)
$\mathbf{T}_i$	torque i acting on particle (kg m^2/s^2)
T_p	particle temperature (K)
$\mathbf{u}_g$	gaseous velocity (m/s)
$\mathbf{u}_p$	particles velocity (m/s)
V_p	particles volume (m^3)
V_{p,w_0}	initial volume of particle (m^3)
$\dot{w}_{\alpha,g}$	rate of production of gaseous species α from gaseous phase (kg/s m^3)
$\dot{w}_{\alpha,s}$	rate of production of gaseous species α from solid phase (kg/s m^3)
X	charcoal conversion state of particle (–)
$\mathbf{x}_p$	particles position (m)
Y_α	mass fraction of species α (–)

common fuels like diesel or natural gas, which are usually well defined mixtures of well known species. The modelling of reactive multiphase processes on the other hand is a computationally challenging problem requiring many simplifications in the modelling process in order to calculate the overall process.

The possible range of models to numerically investigate the gasification process varies from simple cell or zone models based on empirical correlations to time consuming models like direct numerical simulations. Typical representatives of the first class [1–9] allow for the optimisation of industry scale facilities but they are limited to the validity range of the used empirical correlations and cannot be regarded as predictive. Direct numerical simulations (DNS) (see e.g. [10]) are based on first principles, e.g., no modelling of turbulence, and resolve every process involved in the model. Resolving all processes demands huge computational resources and is even in our times not feasible for most non-reacting multiphase flows.

Among the most advanced computational models used today are multi-fluid and Euler–Lagrangian models. The first type considers all phases involved – solid and gaseous – as continua. The continuum assumptions for fluids is for most common situations a well justified way to model fluid flow problems. However, the continuum assumption for solid phases in multi-fluid models is non-trivial because the character of the solid phases differs significantly from real fluids. Representatives of the multi-fluid type of modelling are [11–22]. In Euler–Lagrangian models a continuum approach is used for the fluid phase while the particulate phase is modelled by tracking individual particles (or particles representing a whole particle cloud) by their Newtonian equations of motion. Examples in this area are include [23–34]. Multi-fluid type of models are often considered to be more feasible for larger industrial facilities than Euler–Lagrangian models but this may not be the case for polydisperse flows requiring a large number of solid phases for a realistic modelling.