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Delay of biomass pyrolysis by gas–particle interaction

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ABSTRACT

We apply a biomass pyrolysis model, based on the model developed by Haseli et al. [4], which can be used in combination with Direct Numerical Simulation. The pyrolysis model is combined with a model for particle tracking to simulate 3D turbulent particle-laden channel flow with biomass particles undergoing pyrolysis in nitrogen. Transfer of momentum, heat and mass between gas and particles are fully taken into account. The effects of this transfer are analyzed and quantified in terms of the delay in the conversion or pyrolysis time. The delay is shown to depend on the initial volume fraction (number of particles) and on the size of the particles. The two-way coupling effects are relevant at volume fractions $>10^{-5}$. For a fixed volume fraction, gas–particle interaction induces a delay in the devolatilization, decreasing with increasing particle size. Using this model, we also performed simulations of realistic biomass particle size distributions in order to compare two-way and one-way coupling.

1. Introduction

Biomass has the attention of researchers and industrial companies because it is believed to play an important role in the future since, unlike other renewable energies, it is available in large quantities in many regions of our planet [1]. Secondly, but of equal importance, biomass research is important in view of increasing concerns about the environmental impact of most other methods of energy conversion. For instance, the target of reducing CO_2 emissions from coal-fired power plants can be accomplished with co-firing at high biomass fraction and high oxygen concentration [2,3].

During the pyrolysis of biomass, virgin biomass is converted into char and volatiles are released. The volatile composition, concentration and thermal properties depend on the fuel type, temperature, pressure, heating rate and reaction time [4]. Various models of a single biomass particle undergoing pyrolysis are available in literature. Haseli has presented an overview of the available models in [5]. These models are able to capture the variation of important particle quantities during pyrolysis. However, the complexity of these models requires a computational cost which is unfeasible when dealing with a large number of particles undergoing thermo-chemical conversion and interacting with the surrounding turbulent gas flow. In some applications, like the design of combustors or gasifiers, only a few parameters are of interest; for example, the mean temperature or surface temperature of the particles, the amount of volatiles released during pyrolysis and the ignition time or the conversion time of the particles. For simulating biomass pyrolysis with a large number of particles, a simplified biomass pyrolysis model is necessary. Here, we present a biomass pyrolysis model based on the model developed by Haseli et al. [5,6], which has the advantage to be suitable in combination with Direct Numerical Simulation (DNS). We combined the pyrolysis model with a model for particle tracking to simulate 3D turbulent particle-laden channel flow with particles consisting of biomass undergoing pyrolysis and interacting with nitrogen. The turbulent gas flow is solved in an Eulerian framework and the particles in a Lagrangian way. To the best of our knowledge, this is the first 3D Euler–Lagrange formulation of biomass pyrolysis.

The presence of particles in a turbulent gas requires that the flow around each particle is solved. Despite the enormous progress in computing power, it is still impossible to simulate millions of particles interacting with a turbulent flow up to all details of the flow [7–9]. Therefore, in case of turbulent flow with large numbers of particles with sizes smaller than the Kolmogorov scale η, it is common practice to adopt a point-particle approach to keep the computational cost at acceptable levels [10,11]. This approach allows numerical simulations with millions of particles [12] and has been used to perform direct numerical simulations (DNS) as well as large-eddy simulations (LES) in many applications [13–16]. By employing Haseli's pyrolysis model, we extend this approach to

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Nomenclature

α_B	thermal diffusivity of virgin biomass (m^2/s)
α_C	thermal diffusivity of char (m^2/s)
Δh_p	specific heat of pyrolysis (J/kg)
Δt	time step (s)
$\dot{q}$	heat flux applied to particle surface (W/m^2)
ϵ	emissivity of particle
μ_g	dynamic viscosity of gas (kg/(m s))
ν	kinematic viscosity of gas (m^2/s)
ϕ	particle volume fraction
Re_τ	frictional Reynolds number
ρ_p	particle mass density (kg/m^3)
σ	Stefan–Boltzmann constant ($W/(m^2 K^4)$)
τ_p	particle relaxation time (s)
τ_w	wall shear stress ($kg/(m s^2)$)
$\mathbf{u}$	velocity (m/s)
$\mathbf{v}_i$	particle velocity (m/s)
$\mathbf{x}_i$	particle position (m)
C_c	specific heat capacity of char (J/(kg K))
C_{vol}	specific heat capacity of volatiles (J/(kg K))
d_p	particle diameter (m)
h	heat transfer coefficient ($W/(m^2 K)$)
k_g	thermal conductivity of gas (W/(m K))
m_i	particle mass (kg)
R	particle radius (m)
r	radial coordinate (m)
r_c	char front (m)
r_t	thermal front (m)
T	temperature (K)
t	time (s)
T_0	initial particle temperature (K)
T_p	pyrolysis temperature (K)
T_s	particle surface temperature (K)
T_w	wall temperature (K)
u_τ	friction velocity (m/s)
v_c	velocity of char front (m/s)
Re_p	particle Reynolds number
H	half the channel height (m)

biomass pyrolysis including the heat and mass exchange between gas and particle. Usually, this approach implies uniform temperature of the particle, whereas in the model presented here, the thermal diffusion inside the particle is taken into account although the particle is modeled as a point.

In this paper the steps necessary to obtain the ordinary differential equations from the work of Haseli et al. [6] and to describe the pyrolysis coupled to the flow and the subsequent steps to enable the coupling of the model to DNS of turbulent gas flow are described. The flow regime in burners is typically turbulent to enhance mixing and, therefore, the combustion efficiency. We test the biomass pyrolysis model in a turbulent channel flow. A real burner geometry was used by Ghenai and Janajreh [17], who performed a 2D simulation of co-firing biomass with coal. Ghenai and Janajreh [17] did not solve the turbulent fluctuations directly but used the RANS equations adopting the k-ϵ turbulence model and a stochastic tracking model to predict particle dispersion. In our formulation the particle–gas interactions are modeled in detail. We restrict to the pyrolysis phase, whose prediction, in case of biomass, is very important for a good prediction of the subsequent combustion phase. Implementation of combustion will be a future extension of this research.

An important parameter in the pyrolysis of biomass is the conversion time, i.e., the time biomass particles need to fully convert to char. Due to the very high content of volatiles in biomass, the concentration of volatiles influences the combustion process. With our model we can compute the volatiles concentration at any time and take into account the effects of particle–gas interactions as well. We focus on the pyrolysis conversion or volatilization and in particular analyze the effect of the two-way coupling on the volatilization. We also simulate the mass loss of a realistic biomass particle size distribution to compare the differences between a two-way and a one-way coupling formulation and investigate under which conditions gas–particle interaction considerably delays biomass pyrolysis.

The structure of the paper is as follows. In the next section Haseli's model is introduced and the steps to make the model suitable for implementation in DNS are described. In Section 3, the gas model is introduced. Then, the numerical methods used to perform the simulations and the simulation set up are described in Sections 4 and 5, respectively. Section 6 is dedicated to the presentation and discussion of the results.

2. Biomass particle model

In this section, we present the pyrolysis model used to derive the equations for the particle temperature during pyrolysis. Then, the equation of motion used for tracking each single particle in the system is presented.

The biomass type considered in this work is torrefied wood. Torrefaction or drying is a thermo chemical treatment of biomass at 200 to 320 °C. During this process, carried out in the absence of oxygen, the water contained in the biomass is released obtaining dry biomass. The torrefaction helps to produce much better fuel quality for combustion and gasification applications. It improves the grindability and the hydrophobicity, very important to store the biomass outside. The energy required for torrefaction is partly compensated by the energy reduction for grinding torrefied wood compared to raw wood. The energy requirement for grinding biomass chips is about 1/6 of the heating value. The torrefaction can reduce this energy up to 90% [18].

After milling, two of the main differences between wood and torrefied wood are the smaller size and the more spherical shape of the torrefied biomass particle [19]. The biomass particle model presented here is based on the assumption of spherical shape of the particle, which is a better assumption for torrefied wood than for the raw material.

2.1. The mathematical model of biomass particle pyrolysis

The biomass pyrolysis model of Haseli et al. [5,6] consists of several phases for modeling the overall process. The pyrolysis process is only one of these phases, which are described in the following.

Consider a spherical particle with a uniform initial temperature. When a positive heat flux $\dot{q}$ is applied to its surface, the surface temperature starts to rise and, due to the thermal conductivity of the particle, the temperature profile inside the particle starts to change. Theoretically, the velocity at which the thermal disturbance propagates through the particle is infinite. However, following Haseli et al. [5,6], immediately after the heat flux is applied, the particle is divided into two regions, the outer region closer to the surface, in which the temperature has changed, and the inner region around the center of the particle, in which the temperature is still unchanged (Fig. 1(a)). The surface which separates these two regions is called *thermal front* and moves from the particle surface towards the particle center. Although the thermal front is assumed to move with a finite velocity, the model has been demonstrated to predict results which agree well with a full thermal model. This method of introducing a thermal moving front is