

Direct Numerical Simulation of biomass pyrolysis and combustion with gas phase reactions

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Abstract. We present Direct Numerical Simulation of biomass pyrolysis and combustion in a turbulent channel flow. The model includes simplified models for biomass pyrolysis and char combustion along with a model for particle tracking. The gas phase is modelled as a mixture of reacting gas species. The gas-particle interactions for mass, momentum, and energy exchange are included by two-way coupling terms. The effect of two-way coupling on the conversion time of biomass particles is found noticeable for particle volume fractions $> 10^{-5}$. We also observe that at constant volume fraction the effect of two-way coupling increases as the particle size is reduced, due to the higher total heat exchange area in case of smaller particles. The inclusion of gas phase homogeneous reactions in the DNS model decreases the biomass pyrolysis time due to higher gas temperatures. In contrast, including gas phase reactions increases the combustion time of biomass due to the lower concentration of oxygen at the particle surface.

1. Introduction

Biomass co-firing with coal is one of the main methods to achieve the objectives of sustainable and clean energy production. In order to improve our understanding of the biomass energy conversion process, researchers have studied single particle biomass pyrolysis, combustion and gasification [1] [2]. A better understanding of the interaction between the biomass particles and the surrounding turbulent gas flow would enable efficient design of the process units. Our aim is to develop a DNS model for biomass conversion in a turbulent gas flow, which can help in better understanding of the process inside a furnace. In this paper, the framework for the development of such a DNS model, involving the two-way interactions of chemically reacting particles with the gas, is presented.

In order to model the thermo-chemical conversion and interaction of biomass particles in the surrounding turbulent gas flow, the DNS model needs to be coupled with single particle chemistry models of biomass. To simulate biomass pyrolysis and combustion with a large number of particles, simplified models are required to reduce the computation time. Haseli [1] [2] developed simplified models based on some key parameters of interest such as the surface temperature of particles, the amount of volatiles released, and the conversion time of particles during pyrolysis and combustion. Russo et al. [3] combined Haseli et al.'s [1] pyrolysis model



with a model for particle tracking and simulated 3D turbulent particle-laden channel flow by accounting for two-way interactions with the gas phase. In this work, we extend Russo et al.'s [3] model by adding solid-gas heterogeneous combustion reactions and gas-phase homogeneous reactions.

2. Gas model

The model is based on an Eulerian-Lagrangian approach in which gas and particle phases are treated in different ways. Owing to the wide range of temperatures involved in the process which results in significant variations in mass density, the gas phase is described by the compressible Navier-Stokes equations. The governing equations are based on conservation of mass, momentum, total energy, and species mass; and this conservation property is retained in the numerical model by application of a finite-volume method. The governing equations for the gas can be written as the volume integral of conservation laws over an arbitrary volume V with boundary S :

$$\int_V \frac{\partial \mathbf{w}}{\partial t} dV + \int_{\partial V} \hat{n} \cdot f_c dS = \int_{\partial V} \hat{n} \cdot f_v dS + \int_V L_{2way} dV + \int_V F dV \quad (1)$$

with $\mathbf{w}(\mathbf{x}, t) = [\rho u, \rho v, \rho w, \rho, e, \rho_{O_2}, \rho_{CO_2}, \rho_{CO}]^T$ the vector of dependent variables. Here, ρ is the total mass density of the gas; u , v , and w are the Cartesian components of the velocity vector; e is the total energy density; $[\rho_{O_2}, \rho_{CO_2}, \rho_{CO}]$ are the mass densities of individual gas species, t denotes the time, and $\mathbf{x} = [x, y, z]^T$ is the vector of Cartesian co-ordinates. These governing equations express that the rate of change of \mathbf{w} in the volume V is due to the convective fluxes (f_c), the diffusive fluxes (f_v), and the two-way coupling terms (L_{2way}) which account for the presence of the particles. For channel flow, a driving force, F , is added to the streamwise momentum equation in such a way that the total mass flow rate in the streamwise direction is kept exactly constant.

The two-way coupling terms in the governing equations for the gas phase account for the transfer of mass, momentum and energy between the gas and the particles. It should be noted, that these terms do not change the total mass, total momentum, and total energy of the system but rather account for the transfer between the discrete and the continuous phases of the model. The assumption is that all these two-way coupling terms act as point sources in the conservation laws for the gas phase. The control volume in which a particle is located can be identified from the coordinates of the centre of the particle. The coupling terms stemming from this particle will be included in the gas equations of this control volume only.

The reactions between the gas species are modelled using kinetic rate laws which contribute as source terms to the gas species balance equations. Presently, the model includes 6 gas species - O_2 , CO_2 , CO , H_2O , H_2 , and N_2 . The homogeneous gas phase reactions include the combustion of CO and H_2 along with the water-gas shift reaction. To model the interaction between the gas and chemically reacting particles, single particle models for pyrolysis and combustion are developed, which are presented in the next section.

3. Biomass particle model

Each particle is modeled as a point particle. Figure 1 shows the sequence of steps in the biomass conversion process. To model the process of biomass particle pyrolysis a simplified model as developed by Haseli et al. [1] and modified for time-dependent surrounding gas temperature by Russo et al. [3] is used. In this model a set of equations for the char front and temperature profile inside the particles is solved.

After the pyrolysis has finished, the next stage is the combustion of char. In the present model, pyrolysis and combustion reactions take place in sequence and not simultaneously, i.e.,

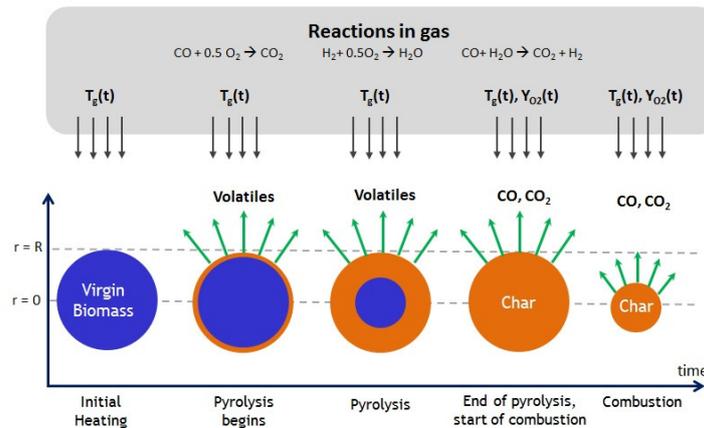
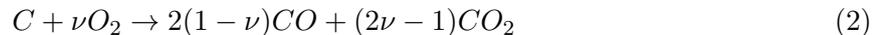


Figure 1. Stages of the biomass conversion process - pyrolysis and combustion; T_g and Y_{O_2} are the bulk gas temperature and bulk gas oxygen concentration respectively; R is the radius of the biomass particle

pyrolysis is followed by combustion. For simplicity, the char obtained after pyrolysis is treated as pure carbon. To keep the computational costs limited, we adopt the simplified single particle combustion model of Haseli et al. [2]. We consider the two most relevant heterogeneous reactions in the model - char oxidation and char gasification with carbon dioxide.



The stoichiometric coefficient (ν) of O_2 in the oxy-combustion reaction (2) depends on particle surface temperature based on an Arrhenius type equation. The reactions rates for (2) and (3) are described by kinetic rate laws [2]. The model is formulated based on a conventional shrinking core approximation. This implies that the char-gas reaction front, where reaction (2) and (3) take place, starts at the surface of the particle and then moves towards the center as the combustion proceeds. This results in a decreasing particle size. The density of the shrinking core remains unchanged throughout the conversion process.

For particle tracking, a Lagrangian formulation is used. We use the Schiller-Naumann drag correlation, valid for particle Reynolds numbers between 0 and 1000, for calculating the drag force on the particles which are assumed to be spherical. The small size and very short residence time of particles inside the combustor motivate to neglect the effects of gravity.

4. Numerical method

All equations for the gas and the particles are non-dimensionalized using appropriate reference values. The particle equations are in the form of ordinary differential equations. The gas equations assume this form after spatial discretization based on a second-order accurate finite volume method.

Boundary conditions in the streamwise and spanwise directions are periodic. In the wall-normal direction the walls of the channel coincide with the boundaries of the cells neighbouring the walls. No-slip boundary conditions are applied at the walls for all three velocity components. An isothermal wall condition is applied to the energy conservation equation with a constant temperature for both the upper and the lower wall. A zero-flux condition is applied to the species conservation equations by setting the gradients of gas species concentrations to zero at

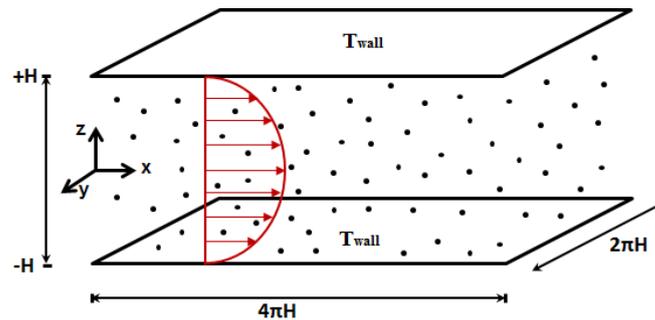


Figure 2. Geometry of the channel with randomly distributed particles, z is the wall-normal direction

Table 1. Virgin biomass and char properties used in the simulations [3]

	Mass density (kg/m^3)	Thermal conductivity ($\text{W}/\text{m}/\text{K}$)	Specific heat capacity ($\text{J}/\text{kg}/\text{K}$)
Biomass	650	0.25	2500
Char	190	0.1	1100

the walls. The wall is also considered to be inert and all solid-gas reactions take place only at the biomass particle surface.

For time-integration, Russo et al. [3] used a low-storage second-order explicit Runge-Kutta scheme to simulate the process of biomass pyrolysis. However, it is observed that the process of combustion is quite fast in comparison to pyrolysis. The fast nature of the combustion process presents itself in the form of stiffness of the system of equations. This renders the explicit Runge-Kutta scheme (as could be used during pyrolysis) inefficient for solving the particle model equations, as a large number of small time steps is required to achieve stability. To resolve this problem, a hybrid implicit-explicit method [4] is used here. As the stiffness is due to the combustion model, the implicit scheme is used only during this stage of the particle conversion. To keep the simulation time low and reduce the complexity of the numerical algorithm, the explicit part of the hybrid scheme is used for the gas phase equations and particle tracking, and during particle pyrolysis.

5. Setup of simulations

We consider the gas-particle system inside a channel, bounded by two parallel horizontal plates (Figure 2). The domain size is $4\pi H$ in streamwise direction and $2\pi H$ in spanwise direction, where H is half the channel height. Simulations are performed with frictional Reynolds number approximately equal to $Re_\tau = 150$, which is based on friction velocity $u_\tau = \sqrt{\tau_w/\rho_g}$ and half the channel height. Here, τ_w is the wall shear stress based on the mean streamwise velocity component, averaged over the two homogeneous directions and time. In the simulations, we vary the volume fraction of particles, keeping it always smaller than $O(10^{-3})$, so that particle-particle collisions can be neglected [5].

The domain is divided into 128^3 control volumes. The grid spacing is uniform in streamwise and spanwise directions, whereas it is non-uniform in the wall-normal direction with clustering of grid points near the walls. Bukhvostova et al. [6] report that this grid resolution is fine enough

to capture the flow characteristics without the need for any turbulence model in the DNS of droplet-laden turbulent channel flow for the same Re_τ values as in this paper. In the channel flow the Kolmogorov length varies along the wall-normal direction from a minimum value of 1.6 near the wall to a maximum value of 3.6 in wall units at the centerline [7].

The flow is initialized with a turbulent velocity field in the statistically steady state obtained from a simulation without particles. The initial oxygen mole fraction is $X_{O_2} = 0.1$ with nitrogen the remainder. The initial gas temperature is set equal to 1400 K, and the particles are initialized with a temperature of 300 K which is constant within the particle. The walls of the channel are maintained at a temperature of 1400 K. Initially, the particles are randomly, and uniformly, distributed over the channel and the particle velocity is equal to the gas velocity at the location of the particle. With these initial conditions we simulate the pyrolysis and combustion of biomass particles in a turbulent channel flow.

The properties of virgin biomass used in the simulations and the properties of char formed after biomass pyrolysis are presented in Table 1. The difference between biomass and char mass density is important as it is an indicator of mass loss in the form of volatile gases from the particles during pyrolysis.

6. Results

We present the results of the DNS model for biomass pyrolysis and combustion in a turbulent channel flow. One of the key parameters in designing a combustor is the conversion time of the fuel particles. For biomass particles, the total conversion time (t_{conv}) is the sum of the time required for the virgin biomass to get converted into char during the pyrolysis stage (t_{pyro}) and the time required by the char particle to burn in the combustion stage (t_{comb}). In this paper, we analyze the effect of two-way coupling, particle size, and gas phase reactions on the conversion time of biomass particles.

6.1. Effect of two-way coupling

If the particle concentration is large, the conversion times for particles are different from those obtained from a single-particle biomass conversion model. The two-way interaction of the particles with the gas affects the surrounding gas temperature and the gas species concentrations, which in turn affect the particle conversion process. The DNS model presented here was used to analyze the effect of two-way coupling between the gas and particles on the conversion time. Figure 3 shows the effect of two-way coupling on the time taken for biomass pyrolysis.

For one-way coupling there is no feedback from the particles to the gas and the gas temperature is not affected by the particle conversion process. Thus, there is no change in the pyrolysis time either. On the other hand, with two-way coupling, the presence of particles affects the gas temperature. We analyze two cases for two-way coupling - with and without the gas phase reactions in the DNS model. For the case of two-way coupling without gas phase reactions it can be seen that two-way coupling effects are noticeable at volume fractions $\phi > 10^{-5}$. At higher volume fractions ($\phi > 5 \times 10^{-4}$), the conversion time for two-way coupling is significantly higher (around 1.8 times) compared to the one-way coupling case.

However, when the gas phase reactions are included in the model, the difference in the pyrolysis time between one-way and two-way coupling is reduced. This can be explained as the effect of two competing phenomena. During pyrolysis, the particles withdraw heat from the gas thus decreasing the gas temperature. But during pyrolysis the particles also release volatile combustible gases which react with oxygen in bulk gas to produce heat. These gas combustion reactions result in higher gas temperatures as compared to the case of two-way coupling when gas reactions are excluded from the DNS model. The higher gas temperatures thus result in a lower biomass pyrolysis time, as can be seen in figure 3.

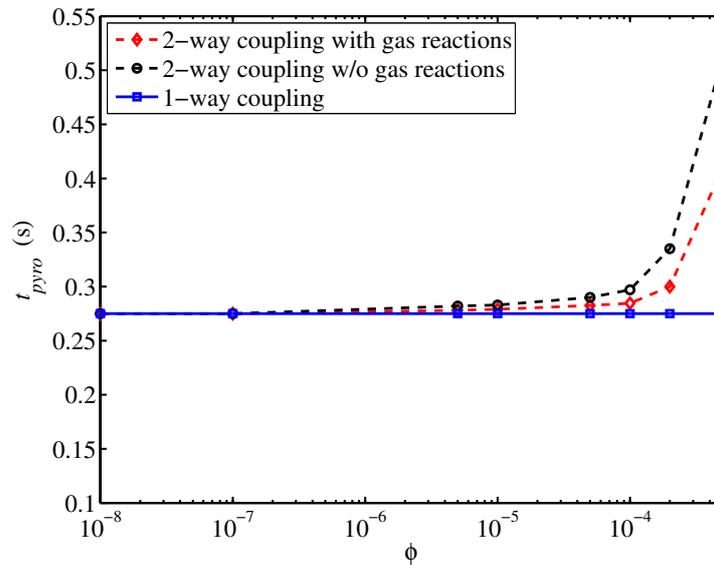


Figure 3. Pyrolysis time (t_{pyro}) at different volume fractions ϕ with particle diameter 0.7 mm, for one-way and two-way coupling with and without gas reactions

6.2. Effect of particle size

Figure 4 presents the variation of t_{pyro} and t_{comb} with particle size (d_p) on a log-log scale along with the corresponding one-way coupling results. All the cases in Figure 4 are for particle volume fraction $\phi = 2 \times 10^{-4}$ and with gas reactions. It can be seen that both for the pyrolysis and for the combustion, the difference between two-way and one-way coupling is larger at smaller particle sizes. This is because as the particle size increases at constant volume fraction, the total surface area available for heat exchange between the gas and the particles decreases. This reduces the total interphase convective heat exchange for larger particles as compared to the smaller particles and hence a closer agreement between one-way and two-way coupling is observed for larger particles.

During pyrolysis, for smaller particles, the higher convective heat exchange between the gas and the particles increases the pyrolysis time as particles withdraw more heat from the gas which decreases the temperature of the gas. In contrast, during the combustion stage more heat is transferred to the gas because of the larger interphase surface area thus reducing the particle temperature compared to larger particles. This reduced temperature decreases the kinetic rate of surface reactions, thereby increasing the combustion time. In Figure 4, we also present the corresponding values for the combustion time as calculated from a single-particle model. The single-particle model has a constant surrounding gas temperature and constant oxygen mass fraction. As seen in the figure, the conversion times from the single-particle model are the lowest. The relative difference in the combustion times for the two-way coupling, one-way coupling and the single-particle model highlights the importance of two-way coupling for the combustion stage.

6.3. Effect of gas phase reactions

We observe that the inclusion of gas phase reactions in the DNS model has an opposite effect on the pyrolysis and combustion stages of biomass conversion. During pyrolysis, the volatile gas combustion increases the gas temperature thus decreasing the pyrolysis time. Figure 5 presents the pyrolysis time of biomass particles for varying particle sizes for cases with and without gas reactions. It can be seen that the effect of gas phase reactions on the pyrolysis time is higher for

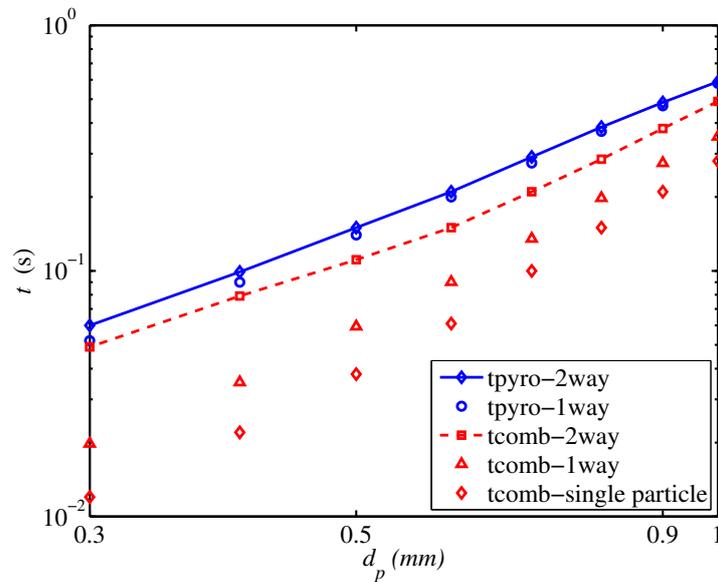


Figure 4. Pyrolysis time (t_{pyro}) and combustion time (t_{comb}) vs particle diameter (d_p) for one-way and two-way coupling

smaller particles. This is because pyrolysis is governed by the heat transferred from the gas to the particles. For smaller particles the higher total heat exchange area implies that more heat will be transferred to the particles. This reduces the pyrolysis time. It can be seen that for larger particles, the effect of including gas phase reactions is very small.

In contrast to its effect on the pyrolysis, including gas phase reactions increases the combustion time of biomass particles. As volatile gases react with oxygen in the gas phase, they consume a part of the total oxygen available to the solid particle for char combustion. This decreases the oxygen concentration at the particle surface which results in a higher combustion time for the particles. In Figure 6, we present the combustion times for varying particle sizes. It can be seen that, unlike during pyrolysis, the effect of gas phase reactions is higher for larger particles. This is due to the longer duration of the combustion process for the larger particles. It should be noted that at the oxygen concentration and temperature conditions in the simulations presented in this paper, the rates of char combustion reaction are much larger than homogeneous gas phase combustion reactions. The longer duration of the char combustion process causes a higher fraction of oxygen to be consumed in the gas phase reactions. Hence, the effect of including gas phase reactions is higher for larger particles.

7. Conclusion and future work

In this paper, we have extended the DNS model of biomass pyrolysis of Russo et al. [3] by including heterogeneous particle combustion and homogeneous gas phase reactions. We use Haseli's [1] [2] simplified model for biomass combustion which is suitable for DNS implementation in case of simulations with a large number of point particles. The interactions between gas and particles are modelled by two-way coupling terms. We observe that the effect of two-way coupling on particle conversion time increases with increasing particle volume fractions (ϕ) with the effect being noticeable at $\phi > 10^{-5}$. At constant values of ϕ , the effect of two-way coupling is higher for smaller particles due to higher total heat exchange area.

We also study the effect of including gas phase reactions and find that it has an opposite effect on the pyrolysis and combustion stages of the particle conversion. The inclusion of gas phase

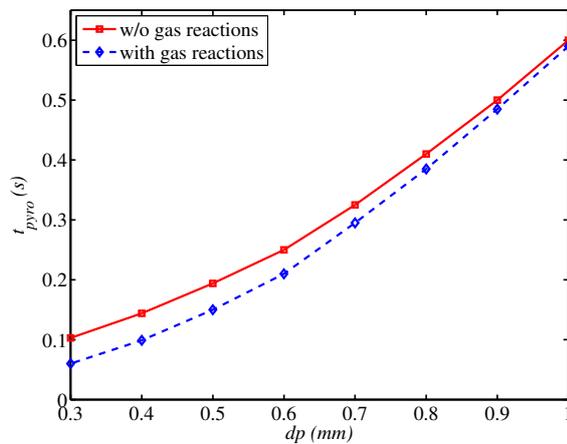


Figure 5. Pyrolysis time (t_{pyro}) vs. particle diameter (d_p) for cases with and without gas phase reactions

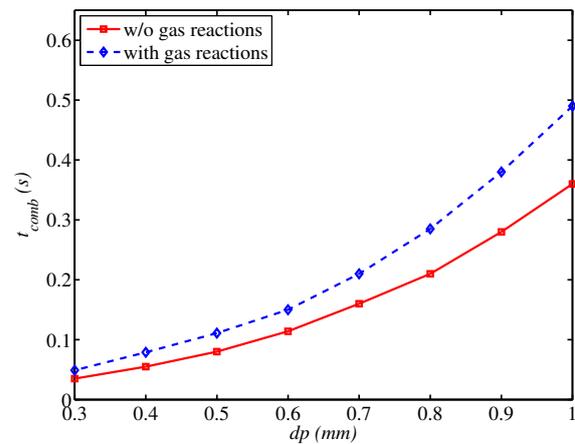


Figure 6. Combustion time (t_{comb}) vs. particle diameter (d_p) for cases with and without gas phase reactions

reactions in the DNS model decreases the biomass pyrolysis time due to higher gas temperatures. In contrast, including gas phase reactions increases the combustion time of biomass due to the lower availability of oxygen at the particle surface. We also find that the effect of gas phase reactions on pyrolysis is higher for smaller particles due to the higher heat exchange area. However, for combustion the effect is higher for larger particles due to the longer duration of the combustion process which results in more oxygen getting consumed in the gas phase reactions, thereby decreasing the oxygen available for char combustion.

Future research is devoted to the inclusion of coal particles in the DNS model for simulating the co-firing of biomass and coal. Particle-particle interactions in terms of radiative heat exchange between the particles is also an area of future research.

8. Acknowledgments

This work is part of the Industrial Partnership Programme (IPP) 'Computational sciences for energy research' of the Foundation for Fundamental Research on Matter (FOM), which is part of the Netherlands Organisation for Scientific Research (NWO). This research programme is co-financed by Shell Global Solutions International B.V.

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