A detailed one-dimensional model of combustion of a woody biomass particle

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ABSTRACT

A detailed one-dimensional model for combustion of a single biomass particle is presented. It accounts for particle heating up, pyrolysis, char gasification and oxidation and gas phase reactions within and in the vicinity of the particle. The biomass pyrolysis is assumed to take place through three competing reactions yielding char, light gas and tar. The model is validated using different sets of experiments reported in the literature. Special emphasis is placed on examination of the effects of pyrolysis kinetic constants and gas phase reactions on the combustion process which have not been thoroughly discussed in previous works. It is shown that depending on the process condition and reactor temperature, correct selection of the pyrolysis kinetic data is a necessary step for simulation of biomass particle conversion. The computer program developed for the purpose of this study enables one to get a deeper insight into the biomass particle combustion process.

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1. Introduction

An emerging challenge of the 21st century is to seek alternative fuels to combat concerns over scarcity of fossil fuels and the increasing amount of greenhouse gases. In recent years, these issues have motivated both industry and academic sectors to examine feasibility of utilization of renewable fuels through large scale national and international projects. Biomass, among various alternatives, has become an attractive renewable energy source. The research and development on thermochemical conversion of biomass have been continuously attracting researchers across the globe.

Tang et al. (2011) conducted experiments of the combustion of microalgae and municipal solid waste under N_2/O_2 and CO_2/O_2 atmospheres using a thermogravimetric apparatus. They measured the temperature of volatile release, maximum rate of weight loss, and the temperature at the maximal peak. They concluded that blending with microalgae would improve combustion of solid waste. Qian et al. (2011) studied the combustion of rice husk, corn, and soybean in a pilot scale fluidized bed combustor at different nitrogen contents, and measured NO emission. They found that the most nitric oxide was formed at just above the bed surface. For biomass with high nitrogen content, NO emission decreased with excess air, but it increased with bed temperature.

One novel idea to reduce CO_2 emission is to co-fire biomass at oxy-fuel conditions in the furnaces of coal fired power plants which significantly contribute to carbon dioxide emissions. The combination of oxy-fuel combustion and co-firing biomass and coal leads to a low flow of flue gas with high concentration of CO_2, thereby resulting in an efficient CO_2 capture. Because of the existing infrastructure of coal fired power stations, the extra investment costs for co-firing biomass takes advantage of the high efficiencies obtainable in large coal fired power plants.

Gil et al. (2010) studied the co-combustion of coal/sawdust pine in a non-isothermal thermogravimetric method. The combustion process of coal consisted of one reaction, whereas in the case of the biomass and coal/biomass blends, this process consisted of two and three reactions, respectively. Their results showed the first order reaction is the most effective mechanism for the first step of biomass oxidation and for coal combustion. However, diffusion mechanisms were found to be responsible for the second step of biomass combustion. Muthuraman et al. (2010) investigated the co-combustion of wood and municipal solid waste (MSW) with Indian coal using the thermogravimetric analysis. They found that blending of both wood and MSW would improve devolatilization of coal. Significant interaction was detected between wood and coal, and the reactivity of coal was improved upon blending with wood. MSW showed a good interaction with coal leading to significant reduction in ignition temperature of coal.

To be able to fully understand thermochemical characteristics of biomass conversion at operational conditions relevant to those found in real furnaces, fundamental research needs to be conducted at various scales by performing experiments and numerical simulations. The present work aims at describing a detailed model of biomass particle combustion by accounting for various physical and chemical processes involved in the particle conversion process. The primary idea is to get a deeper insight into single woody biomass particle combustion through observing time and space evolution of key parameters such as virgin biomass and char densities.

The thermochemical conversion of biomass includes virgin biomass heating up (and drying in case of a wet particle), pyrolysis

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Nomenclature

A	pre-exponential or frequency factor, 1/s		R_g	universal gas constant, kJ/mol.K
A_v	specific inner surface, 1/m		r	radial (sphere and cylinder), axial (slab) distance, m
c_P	specific heat, J/kg K		r	reaction rate, 1/s
D	diffusivity coefficient, m^2/s		S	source term in Eqs. (6) and (15), kg/m^3 s
E	activation energy, kJ/mol		T	temperature, K
e	surface emissivity		t	time, s
h	convective heat transfer coefficient, W/m^2 K		u	superficial gas velocity, m/s
k^*	effective thermal conductivity, W/m K		Y	mass fraction
M	molecular weight, kmol/kg		**Greek letters**	
$\dot{m}_C''$	char oxidation rate per surface area, g/cm^2 s		ε	porosity
Nu	Nusselt number		ρ	density, kg/m^3
n	shape factor		σ	Stephan–Boltzmann constant
n_{sto}	stoichiometry coefficient		v	mass fraction of gaseous species in light gas
P	pressure, atm		**Subscripts**	
Pr	Prandle number		∞	surrounding condition
$\tilde{Q}$	source term in energy equation, kJ/m^3 s		B	biomass
R	particle radius, m		C	char
Re	Reynolds number		g	gas phase (tar + light gases)

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through which the virgin material decomposes to volatiles and char, char gasification and combustion, homogenous gas phase reactions, heat transfer via conduction, convection and radiation mechanisms, migration of gaseous species through the pores of the solid matrix via diffusion and convection mechanisms, pressure build-up, variation of thermo-physical properties with composition and temperature, structural changes and particle shrinkage.

A literature review reveals that unlike biomass pyrolysis which has been extensively investigated numerically and experimentally by a large number of researchers, limited work has been carried out with a focus on comprehensive modeling of biomass particle combustion. Most of these works carried out in recent years have simulated particle combustion through one-dimensional models. Wurzenberger et al. (2002) presented a combined transient single particle and fuel-bed model. Primary pyrolysis was described by independent parallel reactions. Secondary tar cracking, homogenous gas reactions and heterogeneous char reactions were modeled using kinetic data obtained from literature. The validation of the particle combustion model was performed using experimental data of conversion of spherical beech wood particles. Porteiro et al. (2006) reported a mathematical model to describe thermal conversion of biomass particles. The pyrolysis of biomass was modeled using three competitive reactions yielding light gases, tar and char. Additional kinetics considered in their work were combustion of char yielding carbon monoxide and carbon dioxide, and combustion of hydrogen at the surface of the particle. They validated the model using measured mass loss histories of cylindrical Spanish briquettes.

Further comprehensive modeling studies of biomass particle combustion appeared quite recently in the literature are those reported by Lu et al. (2008) and Yang et al. (2008). The particle model presented by Lu et al. (2008) accounts for drying, devolatilization, char oxidation and gasification, and gas phase combustion. The kinetic scheme of Shafizadeh and Chin (1977), which assumes biomass decomposes to light gases, tar and char through three parallel reactions and tar undergoes further reactions yielding additional char and gas, was adapted to describe particle pyrolysis. Heterogeneous reactions were modeled by accounting for char oxidation and gasification with water vapor and carbon dioxide. The gas phase reactions considered were oxidation of hydrogen, carbon monoxide and a lumped hydrocarbon species represented by the empirical formula $C_6H_{6.2}O_{0.2}$. As will be discussed in the upcoming section, this empirical formula does not represent accurately the

hydrocarbons and tar released from biomass pyrolysis. To validate their combustion model, the predicted mass loss history and center temperature of spherical poplar particles were compared with measured values.

Yang et al. (2008) conducted a two-dimensional simulation of a cylindrical wood particle. The sub-processes considered in the model were very much similar to those employed in the study of Lu et al. (2008), but different schemes were implemented for describing the chemistry of the particle conversion. The pyrolysis scheme employed by Yang et al. (2008) assumes that biomass decomposes to volatiles and char through a global one-step reaction. They also applied a different kinetic scheme for gas phase combustion. The volatiles were characterized by the empirical formula $C_mH_nO_l$ whose combustion produced hydrogen and carbon monoxide. These gaseous species also reacted with oxygen. The only heterogeneous reaction considered in the work of Yang et al. (2008) was char combustion. Given that they investigated the effect of particle size ranging from 0.5 to 20 mm in diameter, no validation of the model was reported.

More recently, Yin et al. (2010) have presented a computational fluid dynamics modeling of co-firing wheat straw with coal in a 150 kW swirl-stabilized dual-feed reactor. The particle conversion was simulated using a 1-D particle model by assuming that the sub-processes take place sequentially. The model allowed predicting the mass, temperature, density and size of the particles along their trajectories.

In contrast to these past works outlined above, this paper is intended to develop a detailed model to describe combustion of a woody biomass particle, and to examine its accuracy at different process conditions. It is an extension of the biomass particle pyrolysis model presented previously by the authors (Haseli et al., 2011a,b). Special emphasis is given to identify the role of pyrolysis and gas phase combustion during particle conversion process, which has not been thoroughly studied in previous works. The modeling methodology will be described in the subsequent section.

2. Modeling approach

The problem under study is a dry woody biomass particle initially at room temperature that is exposed to an oxidative hot environment. The particle may be of three common shapes: sphere, cylinder or slab. The main physical and chemical processes which