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Numerical modeling of self-heating and self-ignition in a packed-bed of biomass using XDEM

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ABSTRACT

In a packed bed of biomass, spontaneous ignition might occur due to oxidation of volatiles and causes a serious and unforeseen risk. On the other hand self-ignition may be useful in gasifiers and combustors if it occurs at the expected location and time. Therefore self-ignition can be categorized as a favorable or an unfavorable process, which can be controlled by managing some parameters such as gas velocity and temperature. However, spontaneous ignition originates from a complex combination of physiochemical processes such as gas flow through the void space of the bed, heat and mass transfer between two phases, drying, devolatilization, gas phase reaction and char combustion and gasification. The main aim of this work is to investigate the characteristics of self-heating and self-ignition in a packed bed using XDEM as an Euler–Lagrange model. The influence of different parameters such as gas velocity, gas temperature, particle size and moisture content will be studied and discussed in details. The numerical model is validated with experimental data. Good agreements were achieved between predicted results and measurements. The results show that ignition delay increases with fuel properties such as moisture content and particle size, while it decreases with process conditions such as gas velocity and temperature. However ignition height shows an increase with gas velocity and a decrease with gas temperature and moisture content.

1. Introduction

Fossil fuels are a traditional and convenient source of energy, and they comply the energy demands effectively. However fossil fuel resources are finite and not renewable. Moreover, due to global warming, it is necessary to reduce human-made greenhouse gas emissions. Therefore, the last two decades, demand for using biomass as a CO_2-neutral fuel and renewable source of energy is increasing dramatically.

In order to improve the efficiency and to reduce the gas emissions, the optimization of biomass furnaces has become of great importance in recent years. Therefore, it is very important to know detailed information about the conversion process in the reactor. However conversion of biomass to heat or other forms of energy is a very complex phenomenon because of the numerous involved physical and chemical processes (e.g. heating up, drying, pyrolysis, oxidation of pyrolysis product, char oxidation and gasification).

Combustion of biomass has been investigated experimentally on different operating conditions [1–6]; however, experimental study of biomass combustion in a packed bed is usually difficult to carry out due to limited access into the bed. Therefore it demands cost-intensive setups to capture all the processes and measure detailed information. An alternative and promising way is numerical modeling, which is remarkably used in the recent years [7–14].

Lu et al. [9] proposed a numerical model to simulate the combustion of a single wood particle. They compared the results of combustion of cylindrical wood particles with measurements and obtained a good agreement. Haseli et al. [10] investigated the effects of pyrolysis kinetic constants on the combustion process. Their results showed, in the model, the pyrolysis kinetic data should be selected based on the process condition and reactor temperature. Mehrabian et al. [12] divided the particle into four layers corresponding to the main stages of biomass thermal conversion, and solved energy and mass conservation for each layer. By comparing the results with measurements, they conclude their layer model is accurate and fast enough to be applied to grate furnace simulations.

In general, models representing the combustion in the fixed beds can be classified into two groups: 1D models [7,15,16] and 3D

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Nomenclature

A	pre-exponential factor
C	concentration
c_p	specific heat capacity at constant pressure, J/kg K
d	diameter, m
D	diffusion coefficient, m^2/s
E	activation energy, J/mol
h	enthalpy, J/kg
H_k	heat of reaction, evaporation, J/kg
K^*	permeability, m^2
K	reaction rate
$\dot{m}'''$	mass source, kg/m^3 s
p	pressure, Pa
$\dot{q}''$	heat flux, W/m^2
$\dot{q}'''$	heat source, W/m^3
r	radius; radial coordinate, m
R	radius, m
S_a	specific surface area, m^{-1}
t	time, s
T	temperature, K
v	velocity, m/s
$\dot{\omega}$	mass source, kg/m^3 s

Greek symbols

α	heat transfer coefficient, W/m^2 K
β	mass transfer coefficient, m/s
ϵ	porosity, dimensionless
λ	heat conductivity, W/m K
μ	dynamic viscosity, kg/m s
ρ	density, kg/m^3
ν	mass fraction, dimensionless

Subscripts

f	fluid
g	gas
p	particle
s	solid
∞	ambient

models [11,14]. Di Blasi [7] proposed a one-dimensional transient model for prediction of biomass gasification in a stratified downdraft reactor. Together with the pyrolysis and char combustion/gasification, they also considered combustion of pyrolysis product and secondary cracking of tar. However, they have neglected the intra-particle temperature and species gradients. Later, Di Blasi and Branca [16] used the same model to study the effect of secondary air entry on the gasification process. Based on the assumption that the gradient along the grate is negligible, Wurzenberger et al. [15] presented a transient 1D–1D model to predict conversion of biomass on a moving bed furnace.

Collazo et al. [11] introduced a three dimensional model (both in solid and gas phases) for simulation of the combustion in the fixed bed. In this model, they neglected movement of bed due to shrinkage of particle during char conversion. In a study performed previously by the authors [14], an Euler–Lagrange model (XDEM) was used in which the fluid phase was a continuous phase but each particle was tracked with a Lagrangian approach. The model included a three-dimensional approach for the gas phase and one-dimensional approach for the solid particles. Since in this proposed model, the motion of particles was taken into account, they could predict the change in the bed height, which was caused by particle shrinkage. High level of agreement between predicted results and measurements proved that XDEM is a reliable tool to predict and obtain detailed information about conversion of biomass in a packed bed [17–19].

Packed bed dryer is one of the most common types of industrial dryers, in which hot air flows through the bed and evaporates the moisture content of the particles. However, spontaneous ignition might occur due to the oxidation of volatiles and causes a serious and unforeseen risk. On the other hand, the self-ignition can be useful in gasifiers if it occurs at the expected location and time. Therefore, self-ignition can be categorized as a favorable or an unfavorable processes. This can be controlled by managing some parameters such as gas velocity and temperature [20].

Different experimental investigations have been conducted on self-ignition of various materials such as coal, RDF and sewage sludge [21–23]. Moreover, ignition time and temperature for different types of wood samples were measured by Shi et al. [24]. Anez et al. [25] analyzed the emitted gases of various fuel samples and found that it is possible to detect incipient spontaneous combustion processes using measurements of CO and CO_2 emissions during heating process. Torrent et al. [26] studied the influence of some factors (such as chemical composition, physical treatments and flammability characteristics) on self-ignition of biomass fuel. They reported that the chemical composition of the biomass has an overriding role in characterizing the self-ignition tendency. Yafei et al. [27] investigated the altitude effects on spontaneous ignition characteristics of wood. The results showed that mass loss rate of wood at high altitudes (3650 m) was higher than the one at low altitudes (50 m), while ignition delay time of the sample at high altitude was shorter.

Ejlali et al. [28] studied numerically the self-ignition of a wet coal stockpile. They developed a correlation to estimate the time that a typical coal stockpile can be kept safe as well as the maximum temperature inside the pile. Gao et al. [29] proposed an analytical model based on the principle that the spontaneous ignition is determined by the combination of convective heat transfer between the gas flow and the particles and the heat generated by the oxidation reactions. Blijderveen et al. [30] used a similar model to predict the ignition temperature and ignition delay for different types of fuel. Although the analytical model can predict the ignition temperature well, it is not able to calculate ignition delay. This is due to the fact that the effect of the heat released by particles upstream on particles downstream in the bed is neglected. As a results, the position where ignition starts cannot be calculated.

The above literature survey indicates that there are few works investigating the parameters involved in spontaneous ignition of biomass fixed-bed. More knowledge about self-ignition allows designers to control this process either as a favorable or unfavorable phenomena. Therefore, the objective of this work is to use a comprehensive and precise numerical model (XDEM [14]) to predict self-ignition in a packed-bed of biomass at different operating conditions. The effect of different parameters such as gas velocity, gas temperature, particle size and moisture content on self-ignition will be investigated; in each case the ignition delay and ignition position will be calculated. Prediction of the position that ignition starts is one of the most challenging part of the work and to the best knowledge of the authors, no related study has been yet reported in the literature in this regard.

In this study, a map is presented which related gas temperature, gas velocity, ignition delay and ignition position together. This results provide a guidance for design and operation of packed bed dryers or gasifiers. Moreover, to examine the accuracy of the model, the predicted results are compared with experimental data.

2. Mathematical model

The eXtended Discrete Element Method (XDEM) is an advanced multiphysics and numerical model framework in which the dynamics of granular material or particles described by the classical discrete element method (DEM) is extended by additional properties such as the thermodynamic state for each particle (Peters [31,32], Mahmoudi