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CFD modeling of sawdust gasification in a lab-scale entrained flow reactor based on char intrinsic kinetics. Part 1: Model development

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ABSTRACT

The heterogeneous reactions between char and gases are crucial for the whole biomass gasification process due to their slow reaction rates. In this study, the intrinsic kinetics of birch wood chars react with CO_2 and O_2were investigated through thermogravimetric analysis (TGA) experiments. For char-CO_2 reaction, the pre-exponential factor, activation energy and reaction order were 2.130×10^2 1/s Pa^m, 160.01 kJ/mol, and 0.525, respectively. For char-O_2 reaction, the intrinsic kinetic parameters were 0.570 1/s Pa^m (pre-exponential factor), 134.15 kJ/mol (activation energy), and 1.796 (reaction order). Biomass gasification model was then built based on the Euler-Lagrange approach, and the intrinsic kinetic parameters were adopted in the char-gas reaction submodel to calculate the heterogeneous reaction rates with consideration of mass diffusion limitation and chemical reaction. Sawdust-air gasification in an entrained flow reactor under different equivalence ratios (ERs) and temperatures were simulated. The relative errors for produced gas compositions were mainly less than 20%, and the relative errors for gasification performances were 9.65–23.33% (gas heating value), 1.17–5.95% (gas production), and 9.76–16.57% (carbon conversion efficiency), respectively. The model based on intrinsic kinetics can therefore be employed to predict the biomass gasification performances.

1. Introduction

Being eco-friendly and widely available, the renewable biomass is a potential resource to replace the fossil fuels for all energy productions [1–4]. Pyrolysis, gasification and combustion are three typical thermochemical techniques to utilize biomass for energy production [2,5,6], and gasification is a key solution to the generation of biogas due to the advantages of minimum waste products, low gas emissions, high recycling rates as well as high energy efficiency [7–9]. A typical biomass gasification process experiences the sequential steps of drying, devolatilization, partial combustion, and gasification. Compared with the other steps, the heterogeneous reactions between particles and gases (char-gas reactions) are much slower, thus they are regarded as the controlling step during the whole gasification process [10,11].

The kinetics of char-gas reactions are extremely significant for designing and modeling of biomass gasification process [12]. The effects of carbon source, char property, reaction conditions, etc., on the char-gas reaction kinetics have been widely studied [12–15]. Yuan et al. [13] studied the impacts of biomass type and pyrolysis condition on the char-CO_2 reaction rates and revealed the order of gasification reactivity of different biomass chars. Trubetskaya et al. [14] addressed a comparison study to investigate the relationship between the inorganic matter and char-O_2 reaction rate. The experiments of steam gasification of refuse derived fuel char were conducted by Le and Kolaczkowsk [15] to study the effects of reaction temperature and steam partial pressure on the apparent reactivity. The intrinsic reaction rate, measured in chemical controlled regime, is of great use for the design and development of biomass gasification, since the combination of intrinsic kinetics with heat and mass transfer physics can provide detailed process information [16,17]. However, the kinetics studies emphasizing the intrinsic kinetics of biomass char-gas reactions are relatively few [12,17].

A computational fluid dynamics (CFD) model for biomass gasification is able to predict the spatial and temporal distributions of temperature, pressure, concentration, as well as other parameters inside a reactor, therefore, it's highly effective in parametric analysis and optimal study of gasification process [18,19]. Euler–Euler method and Euler-Lagrange method are two typical approaches to model the gas-

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Nomenclature

A	pre-exponential factor (1/s·Pa^m); Magnussen constant for reactant
B	Magnussen constant for product
C	model constant, molar concentration (kmol/m^3)
C_D	drag coefficient
c_p	heat capacity (J/kg K)
D_e	effective diffusion coefficient (m^2/s)
D_i	molecular diffusion coefficient of gas component i (m^2/s)
$D_{k,i}$	Knudsen diffusion coefficient of gas species i (m^2/s)
$D_{T,i}$	thermal diffusion coefficient of gas species i (m^2/s)
D_t	turbulent diffusion coefficient (m^2/s)
d	diameter (m)
E	activation energy (kJ/mol)
$F(X)$	surface function
f_v, f_w	volatile fraction and moisture fraction of biomass particle
$\vec{g}$	gravitational acceleration (9.8 m/s^2)
G_k	turbulent kinetic energy generation
H_{rec}	reaction heat (J/kg)
h	specific enthalpy of gas phase (J/kg) and convective heat transfer coefficient (W/m K)
h_{fg}	latent heat (J/kg)
K_r	equilibrium constant
k	turbulence kinetic energy (m^2/s^2)
k_g	mass transfer coefficient between water vapor and bulk gases (m/s)
k_{gp}	mass transfer coefficient between gases and particles (m/s)
k_r	reaction kinetic rate constant
M_j	molecular weight (kg/kmol)
m	mass (kg)
P	pressure (Pa, atm)
R	universal gas constant (J/kmol·K) and reaction rate
$\bar{r}_{pore}$	mean pore radius (m)
S_m, S_F, S_h	source terms for mass, momentum and energy equations
Sc	Schmidt number
T	temperature (K)
t	reaction time (s)
$\vec{u}$	gas phase velocity (m/s)
$\vec{v}$	velocity of particle phase (m/s)
v_g	stoichiometric ratio of gas moles to carbon moles
X	carbon conversion degree
Y	mass fraction

Greek letters

ε	dissipation rate (m^2/s^3)
ε_p	particle emissivity
η	effectiveness factor
θ	porosity
θ_R	radiation temperature (K)
λ	thermal conductivity coefficient (W/m K)
μ	gas phase viscosity (kg/m·s)
ρ	density (kg/m^3)
σ	Stefan-Boltzmann constant (5.67×10^{-8} W/m^2 K^4)
σ_k, σ_ε	turbulent Prandtl numbers for turbulent kinetic energy and dispasstion rate
φ	Thiele modulus
τ	pore tortuosity
$\bar{\bar{\tau}}$	the turbulent Reynolds stress
ν_i', ν_i''	stoichiometric coefficients of reactant i

Subscript

ash	ash
b	backward
f	forward
g	gas phase
int	intrinsic
m	mean
P	product
p	particle phase
R	reactant
r	reference
s	particle surface
t	turbulence
t	at t moment
w	water
0	initial

particle flow in various gasifiers. Euler–Euler method treating both gas and particles as continuous phases is unable to recognize the particle characteristics, e.g. non-uniform particle size [20]. While it is easy to track the particle features by using Euler-Lagrange method, where the particles are treated as discrete phases. Xie et al. [21] employed Euler-Lagrange approach to investigate the wood gasification in a fluidized bed with the particle contact force calculated based on a discrete particle method. Oevermann et al. [22] built a CFD model for biomass gasification in a fluidized bed based on Euler-Lagrange method, and the solid phase was simulated by discrete element method to consider the particle collisions. Ku et al. [20] combined multiphase dynamic with reaction models to validate the Euler-Lagrange model of biomass entrained flow gasification. In most of the numerical studies on biomass gasification, the process of char-gas reactions is often simplified into a rate expression with the citation of kinetic parameters from coal chars or different biomass chars, although it is the rate-determining step in gasification. As the reactivities of biomass chars are much different from coal chars [12], the simulation is more likely to cause errors.

Therefore, the main aim of the present study was to establish and verify a CFD model for biomass gasification based on the kinetic study on char reactions. The specific objectives were: (a) to study the intrinsic kinetics for char-gas reactions according to thermogravimetric analysis (TGA) results, (b) to couple the char intrinsic kinetics into the CFD model, and (c) to test the reliability of the developed gasification model.

2. Materials and methods

2.1. Materials

The sawdust of birch wood was supplied by a furniture factory in Harbin, China. The received sawdust particles were ground and sieved to a cut-size range of 75–400 μm. The proximate and ultimate analyses are listed in Table 1.

2.2. TGA measurements

The devolatilization of birch wood particles was carried out in a micro pyrolysis system. In order to obtain biomass char derived from fast pyrolysis, the wood granules were pyrolyzed at 800 °C in a high pure N_2 flow (99.999%).

For the study of intrinsic gasification and oxidation kinetics of wood char, isothermal experiments were performed in a TGA apparatus (TGA/DSC1, Mettler-Toledo AG, Switzerland). At the beginning of each