Fuel 132 (2014) 107–115

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Modeling biomass char gasification kinetics for improving prediction of carbon conversion in a fluidized bed gasifier

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HIGHLIGHTS

- A novel conversion rate equation for biomass char gasification based on TGA data.
- TGA experiments conducted to simulate conditions in a fluidized bed gasifier.
- A fluidized bed gasifier model using the newly developed conversion rate expression.
- Comparison of reactor modeling results against pilot plant measurements.

ARTICLE INFO

Article history:
Received 28 January 2014
Received in revised form 1 April 2014
Accepted 6 April 2014
Available online 24 April 2014

Keywords:
Biomass
Gasification
Reaction kinetics
Modeling
Fluidized bed

ABSTRACT

Gasification of biomass in a fluidized bed (FB) was modeled based on kinetic data obtained from previously conducted thermogravimetric analysis. The thermogravimetric analysis experiments were designed to closely resemble conditions in a real FB gasifier by using high sample heating rates, in situ devolatilization and gas atmospheres of H_2O/H_2 and CO_2/CO mixtures. Several char kinetic models were evaluated based on their ability to predict char conversion based on the thermogravimetric data. A modified version of the random pore model was shown to provide good fitting of the char reactivity and suitability for use in a reactor model. An updated FB reactor model which incorporates the newly developed char kinetic expression and a submodel for the estimation of char residence time is presented and results from simulations were compared against pilot scale gasification data of pine sawdust. The reactor model showed good ability for predicting char conversion and product gas composition.

1. Introduction

Gasification of biomass has become a topic of increasing interest as a potentially renewable method of electricity, heat and liquid fuel production. The gasification process can be divided into a number of steps, of which char gasification is often the slowest. As a result, char gasification tends to represent a rate controlling step of the overall thermo-chemical conversion process. Char can contain 25% of the energy content of the biomass fuel [1] and the total char conversion can significantly influence the composition of the product gas as well as the overall efficiency of the gasification process. As a result, accurate prediction of char conversion is a key factor to optimize a biomass gasifier.

Mathematical models for fluidized bed gasification (FBG) can be used in all stages of the gasifier design and operation. The models can vary significantly in terms of complexity and scope, where the two extremes are often considered to be thermodynamic equilibrium models for simplicity and computation fluid dynamical models for complexity [2]. For all modeling approaches obtaining experimental data for model validation is a widely acknowledged challenge.

This work presents a method for predicting the reactivity of biomass char as a function of conversion, temperature and pressure based on experimental data obtained from dedicated thermogravimetric analysis, where operating conditions are applied to closely resemble conditions in a FBG. Various char reactivity models were examined for their ability to predict the experimental conversion rate and suitability for use in a FBG model. One of these char reactivity models was implemented into a FBG model and the modeling results were compared against

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http://dx.doi.org/10.1016/j.fuel.2014.04.014
0016-2361/

Nomenclature

Abbreviations

DAF	dry ash-free fuel
FB	fluidized bed
FBG	fluidized bed gasifier
HRPM	hybrid random pore model
MRPM	modified random pore model
PPW	proposed in present work
RPM	random pore model
TGA	thermogravimetric analysis
UCM	uniform conversion model

Symbols

α	kinetic parameter for hybrid models (–)
ψ	random pore model surface parameter (–)
τ	char residence time (s)
τ_2	time constant for bottom ash removal (s)
τ_3	time constant for fly ash removal (s)
τ_R	char conversion time (s)
ξ	catalytic deactivation coefficient (–)
c	modified random pore model parameter (–)
E	activation energy (J/mol)
k_0	frequency factor for Arrhenius terms (1/s)
k_3	Arrhenius term of K_r (1/s)
K_r	kinetic coefficient (1/s)
k_{1b}	Arrhenius term of K_r (1/s)
k_{1f}	Arrhenius term of K_r (1/s)
$k_{ccg,1}$	three parallel reaction model rate coefficient (1/s)
$k_{ccg,2}$	three parallel reaction model rate coefficient (1/s)
k_{ncg}	three parallel reaction model rate coefficient (1/s)
m_0	initial char mass (g)
N	number of reactor sections in FBG model (–)
$n_{c,fix}$	char carbon flow from devolatilization stage (mols/s)
$N_{C,tot}$	total carbon inventory in the reactor bed (mol)
$n_{CO_2,eq,(i)}$	equilibrium adjusted CO_2 flow leaving reactor section i (mol/s)
$n_{H_2O,eq,(i)}$	equilibrium adjusted steam flow leaving reactor section i (mol/s)
p	modified random pore model parameter (–)
p_i	partial pressure of gas i (bar)
r	conversion rate (1/s)
r''	instantaneous reaction rate (1/s)
$r^*_{(i)}$	apparent instantaneous reactivity in ith section of gasifier model (1/s)
T	temperature (°C)
$W_{b,tot}$	total bed inventory (kg)
$w_{c,ch,b}$	weight percentage of carbon in char in the bed (–)
$w_{c,ch,d}$	weight percentage of carbon in char from devolatilization (–)
X_{ch}	char conversion (–)
X_c	overall fuel carbon conversion (–)
$X_{g,(i)}$	fractional molar conversion of reactant gas in section i of FBG reactor model (–)

measured char conversion and product gas composition from a pilot scale gasifier. The focus of the model is to examine the effects of char reactivity on the performance of FBGs. The model is intentionally simple in that the required inputs are easily obtained experimental characterization of the fuel and basic reactor operating conditions.

2. Theory and methods

This section presents the approach followed in this work to model a FBG from thermogravimetric analysis (TGA) measurements. Four different aspects are discussed: (i) definitions of char reactivity and reaction rates; (ii) how to calculate these quantities from TGA measurements in which the whole conversion of the sample occurs, including devolatilization and char gasification; (iii) selection of a model to represent the effects of temperature, gas composition and carbon conversion in the form of a kinetics equation; (iv) development of a FBG model where the char reactivity model is implemented together with devolatilization and reactor considerations (e.g. input flow rate of biomass fuel, ash bed inventory, reactor size).

2.1. Definitions

Char conversion of a fuel sample being converted at uniform and constant temperature and gas composition is defined as,

$$X_{ch} = \frac{m_0 - m_t}{m_0} \tag{1}$$

where m_0 and m_t are, respectively, the ash-free mass of the sample at the start of gasification and time t.

The conversion rate is defined as,

$$r = \frac{dX_{ch}}{dt}, \tag{2}$$

and the instantaneous reactivity is calculated by normalizing the conversion rate by the mass of the sample at time t,

$$r'' = -\frac{1}{m_t}\frac{dm_t}{dt} = \frac{1}{1 - X_{ch}}\frac{dX_{ch}}{dt}. \tag{3}$$

2.2. Measuring char reactivity for FBG from thermogravimetric measurements

As the purpose of this work is to model gasification of biomass in FBGs, the TGA experiments were designed to mimic the conditions of those gasifiers as closely as possible. The experimental setup and data used in the present work has been described in detail elsewhere [3]. In the experiments the sample is lowered into the preheated reactor chamber causing devolatilization and gasification reactions to begin immediately. This way of operation closely simulates the char generation in a FBG in a number of key ways: high heating rates during devolatilization, devolatilization occurs in the presence of the gasification agent, and, most importantly, the sample is not cooled between devolatilization and char gasification.

The tests were carried out in isothermal conditions on pine sawdust samples at 750 °C and 850 °C using atmospheres containing mixtures of either H_2O/H_2 or CO_2/CO. Proximate and ultimate analysis of the fuel samples have been published previously by Moilanen and Saviharju [4]. The volume fraction of each gas component in the atmosphere during each TGA test was varied to observe the inhibiting effects of H_2 and CO on the char reactivity. Table 1 summarizes the operating conditions for the TGA tests [4].

While this setup more accurately resembles a fuel particle being injected into a hot fluidized bed, it adds the complication of separating the devolatilization and gasification stages in order to correctly model only the char gasification. The approach used in this work to define the initial char conversion is based on the