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Estimation of gas composition and char conversion in a fluidized bed biomass gasifier

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HIGHLIGHTS

- ▶ The model predicts gas composition and carbon conversion in biomass FB gasifiers.
- ▶ Correction of equilibrium is applied to improve the estimation of the gas composition.
- ▶ Kinetics models are applied to predict char, tar and methane conversion.
- ▶ Fluid-dynamics, entrainment and attrition are accounted for the calculation of char conversion.
- ▶ The model has predictive capability in contrast to available pseudo-equilibrium models.

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ABSTRACT

A method is presented to predict the conversion of biomass in a fluidized bed gasifier. The model calculates the yields of CO, H_2, CO_2, N_2, H_2O, CH_4, tar (represented by one single lump), and char, from fuel properties, reactor geometry and some kinetic data. The equilibrium approach is taken as a frame for the gas-phase calculation, corrected by kinetic models to estimate the deviation of the conversion processes from equilibrium. The yields of char, methane, and other gas species are estimated using devolatilization data from literature. The secondary conversion of methane and tar, as well as the approach to equilibrium of the water–gas-shift reaction, are taken into account by simple kinetic models. Char conversion is calculated accounting for chemical reaction, attrition and elutriation. The model is compared with measurements from a 100 kW_{th} bubbling fluidized bed gasifier, operating with different gasification agents. A sensitivity analysis is conducted to establish the applicability of the model and to underline its advantages compared to existing quasi-equilibrium models.

1. Introduction

Modeling and simulation of fluidized bed biomass gasifier (FBG) is a complex task. Advanced models have been developed for bubbling [1–8] and circulating [9–11] FBG. These models usually require physical and kinetic input, which is difficult to estimate and it is sometimes not available to industrial practitioners. Simple and reliable tools to predict reactor performance with reasonable input are needed to support design and optimization. Besides purely empirical models only valid for specific units, more universal approaches presented up to date have been based on gas phase equilibrium [12].

Equilibrium models (EM) have been widely used because they are simple to apply and independent of gasifier design [13–15]. However, under practical operating conditions in biomass gasification, they overestimate the yields of H_2 and CO, underestimate the yield of CO_2, and predict a gas nearly free from CH_4, tar, and char. Despite these limitations, EM are widely used for preliminary estimation of gas composition in a process flowsheet. However, EM are not accurate enough as tools for design, optimization, and scale-up of FBG units.

Quasi-equilibrium models (QEM) [16–22] improve the accuracy of the prediction of the gas composition. The foundation of the QE approach was given by Gumz [16], who introduced the "quasi-equilibrium temperature", an approach where the equilibrium of the reactions is evaluated at a lower temperature than that of the actual process. The concept was applied for the simulation of a circulating FBG unit in the range of 740–910 °C [17] and for various pilot and commercial coal gasifiers [18]. The approach is still applied, although the method is far from predictive.

Another type of QEM has been developed [14,20–22] for the simulation of biomass and coal gasifiers. The essential idea of this approach was to reduce the input amounts of carbon and

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Nomenclature

A	pre-exponential factor, 1/s
a	decay coefficient, –
c_p	specific heat, J K^{-1} kg^{-1}
c	gas concentration, mol m^{-3}
$C_kH_lO_m$	tar component
d_{ch}	average char particle diameter in the reactor, m
f_{WGSR}	coefficient of approach to WSGR equilibrium, –
E	activation energy, kJ/mol
F_{gp}	gas yield, mol$_{gp}$/kg$_{fuel(daf)}$
$F_{f,daf}$	flowrate of fuel, dry and ash-free (daf), kg/s
h, h_f	specific enthalpy and enthalpy of formation, J/kg,
k	kinetic coefficient, various units
K	equilibrium constant, –
K_{att}	attrition constant, –
L_b, L_{fb}	bed and freeboard heights, m
m	mass, kg
$m_{add,b}$	mass of additive/inert in the reactor, kg
$m_{c,p}$	mass of carbon in a char particle, kg
$m_{c,b}$	mass of carbon in the reactor, kg
$m_{ch,b}$	mass of char (carbon and fuel ash) in the reactor, kg
$m_{ch,b,crit}$	critical value of mass of char in the reactor, kg
$m_{T,b}$	mass of total inventory (additive and char) in the reactor, kg
M	molecular mass, kg kmol^{-1}
k, l, m	atoms in equivalent tar, C, H and O, –
n_1, $n_{2,m}$	fragmentation coefficients in Eq. (29)
p	pressure, Pa
Q_l	specific rate of heat loss, W/kg$_{fuel(daf)}$
R	reaction rate, kmol m^{-3} s^{-1}
R_g	universal constant of gases, J K mol^{-1}
$r_{c,ch}$	overall reactivity of the char, s^{-1}
r_{C+H_2O}	intrinsic reactivity of carbon in char with H_2O, s^{-1}
r_{C+CO_2}	intrinsic reactivity of carbon in char with CO_2, s^{-1}
T	temperature, K
Th	Throughput, kg/(m^2 h)
t	time, s
u_0	superficial gas velocity, m s^{-1}
$x_{i,j}$	mass of compound i in stream j per kg$_{fuel(daf)}$, kg/kg
X_{tar}	conversion of tar
X_{CH_4}	conversion of methane
X_{ch}	conversion of carbon in the char through the reactor
x_{add}	mass of additive fed to the reactor per kg$_{fuel(daf)}$, kg/kg
$x_{ash,da}$	ash (non-carbon) in discharged ash (fly + bottom) per kg$_{fuel(daf)}$, kg/kg
$x_{ch,d}$	mass of char per kg$_{fuel(daf)}$ produced during fuel devolatilization, kg/kg
$x_{ch,2}$	mass of char in the bottom ash discharge (stream 2) per kg$_{fuel(daf)}$, kg/kg
$x_{ch,3}$	mass of char in the bottom fly ash (stream 3) per kg$_{fuel(daf)}$, kg/kg
$x_{c,da}$	mass of carbon in discharged ash (fly + bottom) per kg$_{fuel(daf)}$, kg/kg
$x_{tar,d}$	mass tar per kg$_{fuel(daf)}$ produced during fuel devolatilization, kg/kg
$x_{CH_4,d}$	mass of methane per kg$_{fuel(daf)}$ produced during fuel devolatilization, kg/kg
$x_{H_2O,f}$	moisture (in fuel) per kg$_{fuel(daf)}$, kg/kg
$x_{i,ga}$	mass of i (i=O_2, H_2O, N_2) in the gasification agent per kg$_{fuel(daf)}$, kg/kg
$w_{i,f}$	mass fraction of the i-component (i = C, H, O, N, ash, m(iosture)) in the fuel, kg/kg
$w_{c,b}$	mass fraction of carbon in the reactor, kg/kg
$w_{c,ch,b}$	mass fraction of carbon in the char of the reactor, kg/kg
$w_{c,ch,d}$	mass fraction of carbon in the char after devolatilization, kg/kg
$w_{c,ch,2}$	mass fraction of carbon in the char of bottom ash discharge (stream 2), kg/kg
$w_{c,ch,3}$	mass fraction of carbon in the char of fly ash (stream 3), kg/kg
$w_{ch,b,crit}$	critical value of the char mass fraction in the reactor, kg/kg
y_i	molar fractions of i in the produced gas, kmol/kmol$_{gp}$

Greek symbols

σ	coefficient in Eq. (29), –
τ	residence time, s
τ_2	rate constant of bottom ash discharged, s
τ_3	rate constant of fly ash, s
τ_R	time constant of reaction (the inverse of reactivity of char $\tau_R = 1/r_{c,char}$), s
φ	coefficient in Eq. (29), –

Subscripts

0	standard conditions superficial (velocity)
2, 3	bottom discharge, fly ash
ash	ash
att	attrition
b	bed, reactor
C, H, O, N	carbon, hydrogen, oxygen, nitrogen
c	carbon
daf	dry and ash-free
ch	char
coar	coarse particle fraction
crit	critical value
d	devolatilization
da	discharged ash
df	dry fuel
f	fuel,
fin	fine particle fraction
ga	gasification agent
gp	gas produced
i, *j*	indices
mf	minimum fluidization
k, *l*, *m*	atoms in equivalent (heavy) lumped tar
p	particle
R	reaction
T	total
tar	tar

Abbreviations

av	average
daf	based on dry and ash-free substance
CSTR	continuous stirred tank reactor
EM	equilibrium model
ER	fuel equivalence ratio, –
FBG	fluidized biomass gasification (gasifier)
LHV	lower heating value (lower), J kg^{-1}
na	not available
QEM	quasi equilibrium model
RZ	reduction zone
SBR	steam to biomass ratio
SRMR	steam reforming of methane reaction
WGSR	water–gas-shift reaction

hydrogen, fed to the control volume where the equilibrium is calculated. The underlying reason for the reduction of the C–H–O input is that, under practical operation conditions in a gasifier, the conversion of tar, light hydrocarbons, especially methane, and char