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Optimizing *in-situ* char gasification kinetics in reduction zone of pulverized coal air-staged combustion

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ABSTRACT

Reliable kinetics of char gasification are of great importance for accurate prediction of the reductive atmosphere in air-staged combustion of pulverized coal, which is critical in controlling nitrogen and sulfur species for the optimized design and operation of boilers and burners. In this study, a new method of obtaining char gasification kinetics from realistic air-staged combustion experiments is proposed. Firstly, a real combustion atmosphere, including the temperature and concentration fields of air-staged combustion in an actual boiler, is simulated in an electric-heated down-firing furnace by controlling the stoichiometric ratio of air to coal. *In-situ* char gasification is observed by obtaining gas and solid reaction data from staged combustions with stoichiometric ratios in the range of 0.6–0.9 at temperatures of 1200–1400 °C. Secondly, a detailed char combustion/gasification model with emphasis on coupling between the discrete phase and gas phase is developed and verified. The single film model based on *n*th order Arrhenius-type equations is used in the char combustion/gasification model, with consideration of particle boundary layer diffusion. The effect of reduced reactivity of the char at high degrees of conversion is included in the kinetic model. Thirdly, the *in-situ* char gasification kinetics are determined via a CFD-aided rigorous mathematical optimization process. A direct search algorithm is used to accelerate the optimization process. Finally, the determined kinetics are verified at wide ranges of temperatures, residence times, and stoichiometric ratios. Compared with char gasification kinetics from *ex-situ* char gasification experiment using the same coal, it is demonstrated that the kinetics of *in-situ* char gasification are very different from kinetics derived from *ex-situ* char gasification experiment. Therefore, reliable kinetics of *in-situ* gasification are necessary when predicting the fuel conversion and gas phase species in modern air-staged pulverized coal combustion boilers.

Abbreviations

CFD	computational fluid dynamics
DTF	drop tube furnace
E-DFF	electric-heated down firing furnace
EFR	entrained flow reactor
LCV	Low calorific value of coal (J kg^{-1})
OFA	over fired air
RMSE	root mean squared error
TGA	thermo-gravimetric analysis
UDF	user defined function

1. Introduction

The design goal of low-NO_x pulverized coal combustion application is to produce region of fuel rich zone that is depleted in O_2 so that a subset of the formed NO_x can be reduced [1–3]. A proven and widely used technique is air-staged combustion, which divides the furnace into three reaction zones: the main combustion zone, reductive zone, and burnout zone. In the main combustion zone, the supplied air is less than the theoretical amount for coal burnout; thus, the oxygen in the air is consumed rapidly by volatile combustion and char oxidation. In the reductive zone, char oxidation with O_2 is replaced by gasification with CO_2 and H_2O, producing the reductive gases of CO and H_2. This reductive atmosphere has a strong relationship with NO_x reduction [4], H_2S high-temperature corrosion of water-wall [5,6], and slagging [7,8]. Therefore, predicting the reductive gases in air-staged combustion is of huge significance.

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Nomenclature

A_j	pre-exponential factor for reaction j ($kg\ m^{-2}\ s^{-2}\ Pa^{-n}$)
$A_{p,k}$	particle external surface area of particle size k (m^2)
Ash_{coal}	ash fraction of the raw coal (wt%)
Ash_{sample}	ash fraction of the sample (wt%)
$\bar{C}_i$	averaged molar concentration of species i ($mol\ m^{-3}$)
C_0	diffusion constant
c_p	heat capacity of particle ($J\ kg^{-1}$)
$D_{0,i}$	diffusion coefficient of species i
$D_{i,k}$	diffusional reaction rate coefficient of species i of particle size k
$d_{p,k}$	particle diameter of particle size k (m)
$d_{p,0}$	initial coal particle diameter (m)
$d_{p,HTPy}$	particle diameter after high temperature pyrolysis (m)
$d_{p,Com.}$	particle diameter in combustion or gasification (m)
$\bar{d}_{p,HTPy}$	average size of particle after high temperature pyrolysis (m)
$\bar{d}_{p,0}$	average size of initial particle (m)
E	activation energy ($J\ mol^{-1}$)
E_T	total energy (J)
F_{other}	Other interaction forces
$f_{w,0}$	water mass fraction of initial coal particle
f_{min}	objective function
f_p	heat fraction absorbed by particle
H	mass fraction of H in ultimate analysis of coal (wt%, daf)
H_R	reaction heat ($J\ kg^{-1}$)
h_i^0	heat of formation of species i ($J\ mol^{-1}$)
h_i	sensible enthalpy of species i ($J\ mol^{-1}$)
h_k	convection heat transfer coefficient for particle size k ($W\ m^{-2}\ K^{-1}$)
J_i	diffusion flux of species i ($kg\ m^{-2}\ s^{-1}$)
k_{Con}	heat conductivity ($W\ m^{-1}\ K^{-1}$)
$k_{c,k,j}$	chemical reaction rate of char reaction j for particle size k ($kg\ m^{-2}\ s^{-1}\ Pa^{-1}$)
$k_{Surf.}$	surface reaction rate ($kg\ m^{-2}\ s^{-1}$)
k_{Py}	pyrolysis rate ($kg\ kg^{-1}\ s^{-1}$)
k_{Tur}	turbulence kinetic energy
MW_r	molecular weight of reactant ($r=R$) and product ($r=P$) ($kg\ kmol^{-1}$)
m	exponent factor for coal conversion correlation model
mm	exponent factor for particle size model
m_{char}	mass fraction of char in raw coal
$m_{p,k}$	particle mass of particle size k (kg)
nn	exponent factor for particle density model
$dm_{p,k,j}$	Particle mass change due to reaction j (kg)
$m_{p,k,0}$	initial particle mass of size k (kg)
m_{vol}	mass fraction of volatile in raw coal
$n_{i,j}$	reaction order of species i in reaction j
P	pressure (Pa)
$P_{g,i}$	partial pressure of species i in the bulk gas (Pa)
Pr	Prandtl number
$P_{s,i}$	partial pressure of species i on the particle surface (Pa)
R	universal gas constant ($8.314\ J\ mol^{-1}\ K^{-1}$)
Re	Reynolds number
R_i	net rate of production of species i by gas phase reaction ($kg\ m^{-3}\ s^{-1}$)
$R_{CO_2/CO}$	production ratio of CO_2 to CO in char oxidation
$\bar{r}_{j,k}$	averaged gas phase chemical reaction rate of reaction j for particle size k
S	source term for mass (S_m), momentum (S_{mv}), species (S_i), radiation heat (S_{rad}), reaction heat ($S_{h,r}$), and particle heat source (S_h)
SR	stoichiometric ratio of air to coal
SR_1	stoichiometric ratio of air to coal of the main combustion zone
$SR_{r,i}$	stoichiometric ratio in terms of mass for reaction j (drying, pyrolysis, oxidation, gasification) of species i (water, volatile, O_2, CO_2, CO, H_2)
$T_{Exp.}$	experiment temperature (°C)
T_p	particle temperature (K)
T_g	gas temperature (K)
vf	volume fraction
$T_{p,k}$	particle temperature for particle size k (K)
T_r	gas radiation temperature (K)
$u_{p,k}$	particle velocity of particle size k (m/s)
v	velocity ($m\ s^{-1}$)
w_j	mixing rate of reaction j
X_{Char}	char conversion fraction (wt%, daf)
$X_{Coal,k}$	coal conversion fraction for particle size k (wt%, daf)
X_{HTPy}	coal conversion after high temperature pyrolysis (wt%, daf)
x	number of carbon atom in one pseudo volatile species
Y_i	species mass fraction ($kg\ kg^{-1}$)
$Y_{d_{p,k}}$	Volume fraction of particle size larger than $d_{p,\ k}$
$\bar{Y}_r$	averaged species mass fraction ($kg\ kg^{-1}$) (r = R, reactant; r = P, product)
y	number of hydrogen atom in one pseudo volatile species
z	number of oxygen atom in one pseudo volatile species
Δh_x	reaction heat of volatile ($x=vol$), char ($x=char$), CO_2 gasification ($x=CO_2$) and HO gasification ($x=H_2O$) ($J\ kg^{-1}$),
$\Delta m_{p,\ k}$	particle mass change in the calculated cell (kg)
$\Delta m_{p,\ k,\ j}$	particle mass change due to reaction j for particle size k (kg)
$\dot{m}_{p,k,0}$	initial particle mass flow rate at the injection point of particle size k ($kg\ s^{-1}$)
Δt	time step (s)

Greek symbols

α_{HTPy}	coal swelling factor after high temperature pyrolysis
β	temperature exponent
t	time(s)
ρ	gas density ($kg\ m^{-3}$)
$\rho_{p,\ k}$	particle density of size k ($kg\ m^{-3}$)
ε_p	particle emissivity
ε	dissipation rate
σ	Stephan-Boltzmann number ($W\ m^{-2}\ K^{-4}$)
λ	gas thermal conductivity ($W\ m^{-1} K^{-1}$)
μ	fluid viscosity (Pa s)
$\bar{\bar{\tau}}$	stress tensor
υ_i	diffusion volume for species i
υ'_r	stoichiometric constant of reactant r
υ''_r	stoichiometric constant of product r
Φ	mechanical factor
σ_{i,N_2}	binary pair characteristic length