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Lattice Monte Carlo simulation of single coal char particle combustion under oxy–fuel conditions

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HIGHLIGHTS

- Model for single char particle combustion in air and oxy conditions was developed.
- Model is based on lattice percolation, random walkers and Monte Carlo simulation.
- Model points out char structure influence on randomness of the combustion process.
- Model was verified by comparison with experimental data from single particle reactor.
- Special care was given to the CO_2 gasification reaction influence on char combustion.

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ABSTRACT

A descriptive model for isolated char particle combustion under conventional and oxy–fuel conditions was developed. Suggested model is based on the percolation theory and Monte Carlo simulation technique. Char particle was modeled as a square lattice consisting of a large number of small sites. Sites correspond either to fixed carbon, ash, or pore, and they were distributed randomly inside char lattice using percolation concept, at the start of simulation. Random walk model was used to represent gaseous species diffusion through particle pores. Char combustion was modeled using power law Arrhenius model which assumes that reaction rate depends of particle temperature and oxygen partial pressure on particle surface. The main aim of the proposed model was to take into account influence of heterogeneous char particle structure to randomness of the char combustion process. The suggested model's behavior was validated by qualitative comparison with experimental data obtained in single particle reactor. It was found that simulated combustion time, char burnout and particle temperature values are in good agreement with experimentally determined data. Special emphasis was given to the CO_2 gasification reaction influence on char conversion and particle temperature values. Further development of the proposed model with appropriate simplifications would enable its inclusion in comprehensive CFD codes.

1. Introduction

CO_2 emissions contribute to about 75% of total greenhouse gases emissions [1]. Closely to 40% of CO_2 emitted into atmosphere is generated in thermal power plants which use coal as a main fuel. It is expected that coal consumption, and consequently CO_2 emissions, will increase in a foreseeable future [2,3]. Because of this, different carbon capture and storage (CCS) technologies for possible continued coal utilization are under constant development and investigation. Among different possible CCS technologies oxy–fuel combustion (combustion in a mixture of O_2 and recycled CO_2 rich flue gas) is especially attractive, mainly due to its potential to be implemented to existing power plants' boilers, and due to a fact that current technology level makes its implementation technically feasible [4]. However, switching from conventional to oxy/fuel combustion brings significant changes in all phases of combustion process: devolatilisation, ignition time delay, ignition mechanism, char combustion [4]. Char combustion phase is especially important due to its dominant influence on overall coal particle burnout, and subsequently due to its influence on power plant thermal efficiency [5]. Thus, investigation of char combustion mechanism, which is the main motivation for the presented work, is of paramount importance in overall oxy–fuel combustion process understanding.

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Nomenclature

Symbols

A	pre-exponential factor ($kg_{char}\ m^{-2}\ s^{-1}\ Pa^{-n}$)
C	average molar concentration of the gases (mol/K)
c_p	specific heat capacity ($J\ kg^{-1}\ K^{-1}$)
c_0	morphological coefficient (= 0.2) (–)
D_j	mass diffusivity of O_2 in CO_2 or of O_2 in N_2
$D_{0,O_2\text{-}N_2}$	mass diffusivity of O_2 in N_2 at 1373 (K)
Ea	apparent activation energy ($J\ kmol^{-1}$)
$\Delta H_{P,j}$	enthalpy of char particle reaction ($J\ kg^{-1}$)
h_j	convective heat transfer coefficient of gaseous mixture ($Wm^{-2}\ K^{-1}$)
i	reaction or reactant number (1 – O_2, 2 – CO_2) (–)
j	combustion atmosphere (O_2–CO_2 or O_2–N_2) (–)
k	surface reaction rate coefficient ($kg_{char}\ m^{-2}\ s^{-1}\ Pa^{-n}$)
L	lattice size (m)
l	site size (m)
m	mass (kg)
$\dot{m}$	char mass consumed by heterogeneous reaction (kg/s)
MW	molecular weight (kg/kmol)
N	number of lattice site on random walker path (–)
$\dot{N}$	species molar flux ($kmol\ m^{-2}\ s^{-1}$)
n	apparent reaction order (–)
nm_i	number of reactant occupied sites necessary to burn out char site (–)
OF	oxidizer to fuel ratio (–)
$prob$	percolation probability (–)
$prob_t$	percolation threshold (–)
$p_{S,i}$	partial pressure of reactant i at particle surface (Pa)
$p_{S,i,\infty}$	partial pressure of reactant i in a bulk flow (Pa)
p_0	normal pressure (=1.013e+05) (Pa)
R	gas constant (=8.314) ($J\ mol^{-1}\ K^{-1}$)
S	area (m^2)
T	temperature (K)
t	time (s)
t_{cr}	chemical reaction time (s)
$t_{D,j}$	reactant diffusion time to pass N sites (s)
$\Delta t_{D,j}$	reactant time to pass form N-1 to N site (s)
X	molar fraction (–)

Greek

γ	Stefan flow factor (–)
v	stoichiometric coefficient (–)
ψ	carbon fraction that becomes CO_2 (–)

Subscripts

0	beginning or initial stage
∞	bulk phase
mix	gaseous mixture

The main differences between char combustion characteristics during conventional and oxy–fuel combustion come from different properties of dominant gases: N_2 in case of conventional and CO_2 in case of oxy–fuel combustion. The lower diffusivity of O_2 in CO_2 than in N_2 may influence char oxidation rate [6,7]. Approximately 1.6 times higher CO_2 specific heat capacity compared with N_2 specific heat capacity influences adiabatic flame temperature [8]. CO_2 and H_2O gasification reactions affect both char conversion time and char particle temperature [9].

Number of different models, which aim to incorporate above described phenomena and to quantify its influence on char combustion properties under oxy/fuel conditions were reported in scientific literature during past several years. These models are usually validated against experimental data obtained from single particle or laminar flow reactors.

Murphy, and Shaddix, measured the combustion rates of two different pulverized coal chars both in conventional and oxygen-enhanced conditions inside entrained flow reactor [10]. The obtained results showed that pulverized coal chars combust in increasing kinetic regime in elevated O_2 amounts. Authors developed single-film model which represents char particle as spherical, homogeneous, reactive medium surrounded by chemically inactive boundary layer. Conductive and radiative heat transfer was taken into account as well as effects of thermal inertia and Stefan flow. Numerical single-film model for instantaneous char burning rates with incorporated both nth-order Arrhenius and an nth-order Langmuir–Hinshelwood kinetic equations showed satisfying fits to the experimental data.

Molina and Shaddix performed investigation on ignition and devolatilisation behavior of single bituminous coal particles in O_2/N_2 and O_2/CO_2 mixtures. It was shown that CO_2 presence delays particle ignition, but does not have significant influence on volatile combustion time. Moreover, increase of O_2 amounts both in O_2/N_2 and O_2/CO_2 mixtures accelerates coal particle ignition [11].

Murphy, and Shaddix, in the study [12] improved single-film char burnout model assuming that total char burning rate is a sum of an external burning rate and an internal burning rate. These two burning rates were than correlated with an intrinsic char burning rate, assuming that the external burning rate is dependent on carbon amount present in a particle. Also, the rate used for intrinsic char consumption took into account effects of reactivity loss due to ash displacement on the particle surface ("ash dilution"). Model results were compared with the experimental data from their previous work [10] and pointed out that the use of a simple expression for "ash dilution" together with a single-film nth-order Arrhenius char combustion model has no major effect on char conversion, but greatly affects the apparent reaction order of char combustion. Model showed that the apparent reaction order is initially lowered, depending on initial ash content in coal, and continues to slowly fall up to 70% of char conversion, after which even more rapid reaction order decrease occurs leading to negative apparent reaction order values.

Extended single-film model was extensively used to describe combustion behavior of single char particles in different oxidizer compositions (O_2/N_2 and O_2 CO_2) in last few years. Geier and coauthors showed the development and application of extended single-film reaction model optimized for oxy–fuel combustion simulations [13]. Geier et al. in their study [14] proposed a novel mechanistic char oxidation model based on a single-film model which treats char particle as spherical, reactive, homogeneous media. Kim and coauthors proposed a variation of a single-film model which accounts for char oxidation and char gasification (with CO_2) reactions and includes Stefan flow effects on mass and energy transfer [15]. Yu and coworkers presented modification of single-film model which assumes continuous-film model in contrast with commonly accepted infinitesimally thin film model [7].

Significant efforts and advancement were recently made in the modeling of single char particle combustion under oxy–fuel conditions, as it is shown in previous paragraphs. However, it is important to emphasize that all described single particle models treat char particles as a continuum with homogeneous properties, while char oxidation (and gasification) is treated as continuous and deterministic process. However, experimentally obtained values of single particle burnout time histories showed that randomness