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On the modeling of oxy-coal combustion in a fluidized bed

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HIGHLIGHTS

- A model has been developed to predict oxy-coal combustion in fluidized beds.
- Model comprises fluid-dynamics, coal combustion, sulfur capture and heat transfer.
- Validation is accomplished for three coals, under a variety of operating conditions.
- Pressure, temperature and emissions patterns are simulated.

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ABSTRACT

This paper addresses the modeling of oxy-coal combustion and its validation for a 90 kW fluidized bed unit. The one-dimensional model is based on semi-empirical approaches, which assumptions are presented and discussed in the paper. Model predictions comprise fluid dynamics, combustion and heat transfer rates under oxy-coal combustion conditions. The model is experimentally fitted to the fired coals, and validation is accomplished by comparing simulations with experimental measurements, when firing three different coals for a wide range of O_2 concentrations. Results demonstrate that the model is able to adequately simulate the phenomena occurring in the reactor, showing good agreements and well capturing all the trends observed during the experiments. The model can then be used to analyze the facility performance in a reliable and inexpensive way.

1. Introduction

Carbon Capture and Storage (CCS) comprises a set of bridging technologies favoring the use of fossil fuels in a more sustainable way, moving forward a lower carbon-based energy future. The IEA Energy Technology Perspectives Report 2010 [1] remarks the decarbonisation of the power sector as a key point to achieve a low-intensity carbon scenario; CCS applied to conventional power plants could reduce CO_2 emissions to the atmosphere by 80–90% compared to a plant without CCS. Among the different technologic alternatives to get carbon capture in solid-fired power plants, oxy-coal combustion in fluidized bed boilers arises as a quite promising solution. Fluidized bed combustion offers outstanding advantages in comparison to pulverized coal combustion, like wider fuel/operation flexibility and larger control of SO_2 and NOx emissions.

Initially, most of oxy-fuel research was devoted to gas and pulverized-coal combustion, but now the focus is being increasingly turned to fluidized bed combustion. Different issues are addressed in the literature: pollutant emissions under oxy-fuel conditions [2,3], fuel conversion rates [4–6], combustion efficiency dependency on O_2 concentration [7], or characterization of ashes and sulfur capture processes [8]. Nevertheless, there are still scarce publications reporting coal models specifically developed to predict the performance of oxy-fuel combustion fluidized bed units. It is clear the need of mathematical models to support the design of new facilities and the diagnosis of existing units.

At the Czestochowa University of Technology, a model has been designed to characterize emissions in a fluidized bed [9], but no details are reported about a global coal conversion model. They have also modeled a large-scale oxy-CFB boiler (670 t/h lignite), simulating different O_2/N_2 and O_2/CO_2 atmospheres and confirming higher heat transfer rates to furnace walls when increasing O_2 concentration at the inlet [10]. Seddighi et al. [11] have presented 1.5- and 3-dimensional models able to describe fluid dynamics, chemistry conversion and heat transfer in the furnace of a 5 MW_{th} fluidized bed boiler. Saastamoinen et al. [12] and Bolea et al. [13] have suggested some re-design concepts for new oxy-fuel CFB boilers, based on semi-empirical simulations of heat transfer rates. Under a quite different approach, Zhou et al. [14] completed a CFD model of a 50 kW_{th} oxy-fuel CFB rig, although the results are only validated under air conditions and the kinetics are not modified accounting for the different combustion atmospheres.

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Nomenclature

A	bed area (m^2)
A_{int}	intrinsic specific area (m^2/m^3)
a	thermal diffusivity (m^2/s)
C	molar concentration (mol/m^3)
c	specific heat (J/kg K)
c_p	specific heat at constant pressure (J/kg K)
D	diameter (m)
$D_{eff,i}$	effective molecular diffusivity of species i in a mixture of gases (m^2/s)
D_{ij}	molecular diffusivity of species i in species j (m^2/s)
E	energy of activation (J/mol)
f_b	fraction of bubbles
h_{conv}	convective heat transfer coefficient (W/K m^2)
$h_{m,i}$	mass transfer coefficient in species i (m/s)
h_{rad}	radiative heat transfer coefficient (W/K m^2)
LHV	low heating value (J/kg)
H	heating value (J/kg)
H_m	heat of vaporization (J/kg)
K_{be}	exchange coefficient between bubble and emulsion (1/s)
k	thermal conductivity (W/K m)
k_{rc}	rate for char conversion (m/s)
$k_{rc,eff}$	effective kinetic rate for char conversion (m/s)
k_s	rate for sulfatation (m/s)
k_t	elutriation constant (kg/m^2 s)
k_v	pre-exponential factor for coal devolatilization (1/s)
M_i	molecular weight of species i (kg/mol)
m	mass (kg)
N_{or}	number of orifices in the distributor
n	number of cells in reactor discretization
P	pressure (Pa)
Q	heat rate (W)
R	ideal gas constant (J/mol K)
R_i	rate of char conversion with species i (mol/m^3 s)
r	radius (m)
S	sensitive coefficient
T	temperature (K)
TDH	Transport Disengaging Height (m)
t	time (s)
u	velocity (m/s)
u_t	terminal velocity (m/s)
X	conversion rate
Y	mass fraction
z	height (m)

Subscripts

av	average
b	bubble
c	char
dev	devolatilization
e	emulsion
eff	effective
eq	equilibrium
g	gas phase
gen	generated
i	inert; index counter
in	inlet
m	moisture
max	maximum
mf	minimum fluidization
out	outlet
p	particle
R	reactor
res	residence
v	volatile
0	initial value
∞	surrounding ambient

Greek symbols

α	dimensionless parameter in Eq. (13)
β	dimensionless parameter in Eq. (14)
ε	emissivity; porosity
γ	calcium to sulfur ratio
ϕ	spherecity
η	efficiency
λ	excess oxygen
μ	dynamic viscosity (Pa s)
Ω	stoichiometric coefficient
ρ	density (kg/m^3)
σ	Stefan–Boltzmann constant (W/m^2 K^4)

Dimensionless numbers

Ar	Archimedes number, $gD_p^3\rho_g(\rho_p-\rho_g)/\mu_g^2$
Bi_t	thermal Biot number, $h_{eff}D_p/k_p$
Nu	Nusselt number, $h_{conv}D_p/k_g$
Pr	Prandtl number, $c_{pg}\mu_g/k_g$
Re	Reynolds number, $\rho_g u_g D/\mu_g$
Sc	Schmidt number, $\mu_g/\rho_g D_{ij}$
Sh	Sherwood number, $h_m D_p/D_{ij}$

Harris and Davidson [15] classified fluidized bed models into three categories: semi-empirical models focusing on axial variations only, semi-empirical models addressing both axial and radial variations depending on the reactor region, and fundamental models (CFD-oriented) solving governing equations of the two phase flow structure. The latter solve transport equations in a fine discretization grid, yielding a more rigorous and detailed solution. Solid phase treatment is done by different methodologies depending on the fluid-dynamic regime, from a discrete particle modeling to a continuous medium consideration (Eulerian approach). On the other hand, semi-empirical models are not so accurate but can reasonably predict the macroscopic performance based on empirical correlations, without demanding long computational times. Application of semi-empirical approaches [16,17] and findings on fundamental modeling [18,19] can be both found in recent literature.

In the case-study of this paper, a semi-empirical 1D model is applied, which is a typical approach for small-scale facilities. Since a global description of the process is pursued, a lot of computations are required –covering different fuels, unit loads and fluidizing atmospheres – and only limited instrumentation is available, a simplified approximation can be considered a suitable option. Despite the model simplicity, it takes into account specific issues related to the conditions arising during oxy-combustion, as explained along the paper. Aside from the variation of fluid-dynamics and heat transfer rates due to the different gas composition, main differences from conventional air combustion concern particles conversion in the bed: weakening of diffusion rates in the gas phase, increase of heterogeneous oxidation rates, enhancement of gasification reactions and modification of sulfation mechanism.

Validation is carried out for a 90 kW fluidized bed reactor [20]. Fundamentals of the model are streamlined in the paper, and predictions are validated with experimental values gathered during the execution of oxy-firing tests for three coals of very different