Fuel 135 (2014) 443–458

Contents lists available at ScienceDirect

Fuel

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

Computational modeling of autothermal combustion of mechanically-activated micronized coal

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HIGHLIGHTS

- Computational modeling of autothermal combustion of mechanically-activated coal.
- Verification of applicability of comprehensive combustion model to microground coal.
- Improved modeling of heat transfer and reactivity of micronized coal.
- Prospects for computational design and optimization of new coal-dust burners.

ARTICLE INFO

Article history:
Received 8 April 2014
Received in revised form 19 June 2014
Accepted 24 June 2014
Available online 12 July 2014

Keywords:
Pulverised/micronized coal combustion
Autothermal regime
Computational modeling

ABSTRACT

Burdukov et al. [6] showed experimentally that enhancement of coal reactivity when micronized in a high-impact disintegrator mill makes it possible to attain self-igniting and self-sustaining (autothermal) compact-flame combustion in a cold environment, akin to that of heavy oil. We present computational modeling of autothermal combustion of mechanically-activated microground coal in a 5 MW pilot-scale combustor that complements the experiments of Burdukov et al. [7]. The aim was to verify the applicability of the comprehensive model of pulverized coal combustion to microground coal and to validate the submodel of the coal reactivity enhancement. The modeling follows the standard RANS approach to computing two-phase (reactive dispersed particles in gaseous medium) multi-component system, but with several new modifications related to particle heat transfer and their reactions. For reference, the study includes also the case with non-activated coal of the same granulation micronized in a vibrocentrifugal mill. The computations showed good agreement with the measurements and observations confirming that the model can reproduce the autothermal combustion of activated micronized coal and, thus, be employed with credible certainty to the computational design and optimization of new combustion (and gasification) devices fired with mechanically activated coal dust.

1. Introduction

Computational modeling of pulverized coal combustion has matured over the past 30 years and it is currently being used more and more as a tool in the design and optimization of various combustion installations, for improving the existing devices or for feasibility studies of new concepts of methods. Comprehensive overviews of methods and models can be found in e.g. Backreedy et al. [2], Williams et al. [32], Eaton et al. [11], Peters and Weber [26], K. Hanjalić et al [16] and others. Various improvements of specific submodels have also been proposed over the years, among which we mention some recent developments such as e.g. the tabulated-devolatilization-process (TDP) model [17], "transient group" modeling [35] or accounting for temperature fluctuations [33]. These works have been complemented by numerous experimental studies at the laboratory and pilot scales, aimed at better understanding of still many pertaining issues, especially in thermochemistry, radiation, interactions with and effects of turbulence.

The numerical study here reported focuses on modeling combustion of mechanically-activated micro-grinded coal. The study was aimed first at reproducing the main experimental results

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http://dx.doi.org/10.1016/j.fuel.2014.06.052
0016-2361/

Nomenclature

a	absorption coefficient
a	thermal diffusivity
A	prefactor in Arrhenius equations
A_p	particle effective surface area (m^2)
B_{CO2}^{CO}	stoichiometric coefficient
c_p	specific heat (J/(kg K))
C_D	particle drag coefficient
d_p	particle diameter (m)
D	mass diffusion coefficient (m^2/s)
D	burner and furnace diameter (m)
E	activation energy (J/mol)
E_r	radiation flux density
f_i	mass fraction of ith component (kg/kg)
$\mathbf{F}$	body force per unit volume
$\mathbf{g}$	gravitation vector (m/s^2)
h	enthalpy (J/kg)
k	reaction rate constants
k	turbulent kinetic energy (m^2/s^2)
K_{comb}	empirical coefficient
l, L	turbulence length scale (m)
$\dot{m}$	mass flow rate (kg/s)
$\dot{m}_{char}$	char oxidation rate (kg/s)
m_p	mass of a single particle (kg)
$\dot{m}_p$	mass flow rate of particles (kg/s)
M	molecular mass (kg/kmol)
Nu	Nusselt number
p	pressure (N/m^2)
Pe	Peclet number
Q	calorific value (J/kg)
r	radius, radial coordinate
R	gas constant (kJ/(kg K)
R	reaction rate (kg/s m^3)
Re	Reynolds number
S	source terms
Sc_i	turbulent Schmidt number
t	time (s)
T	temperature (K, °C)
$\mathbf{v}$	velocity vector (m/s)
w	release rate of reaction products (m/s)
V	control volume (m^3)
V_{TGA}^{daf}	proximate volatile matter
V_{ht}^{daf}	actual volatile yield
$x_{r,i}$	mass concentration of ith reactant (kg/kg)
x, y, z	longitudinal, wall-normal and tangential coordinates
Z_a	number of particles release pints
Z_b	mass fraction of particles size-class b

Greek symbols

α	convective heat transfer coefficient (W/(m^2 K))
β	temperature exponent in Arrhenius equation
γ_p	particle dispersion coefficient
χ	fraction of char heat absorbed by gas (relative to particles)
ε	rate of dissipation of turbulence kinetic energy (m^2/s^3)
ε_p	particle radiation emissivity
μ	fluid dynamic viscosity
$\mu_{r,i}$	molecular mass of ith component
$\nu_{r,I}$	stoichiometric coefficient of $x_{r,i}$
ρ	density (kg/m^3)
σ	Stefan–Bolzman constant
ξ	coefficient of scattering anisotropy
ξ_G	random number
τ	turbulence time scale
τ_p	particle relaxation time scale
$\boldsymbol{\tau}$	stress tensor
Δ	difference

Suffices and superscripts

+	variables normalized with the inner-wall scales (friction velocity and viscosity)
0	initial, reference
a	particle position index
b	initial particle diameter index
char	char
C	carbon
conv	convection
devol	devolatilization
diff	diffusion (regime)
eb	eddy breakup
i	ith component in the mixture
in	conditions at the inlet
kin	kinetic (regime)
out	conditions at the outlet
p	particle
r	reagent
start	starting conditions
vol	volatiles

reported in Burdukov et al. [7]. The main goal was to verify the computational model and its suitability for subsequent application to computational design and optimization of a possible new concept of coal combustion and gasification using activated pulverized coal. Most model segments ("submodels"), tested earlier on predicting the conventional dust-coal combustion, have been taken from the literature. However, some modifications are introduced in the models of particle heating, devolatilization and char burning following the earlier extensive, but relatively unknown work (published in Russian) of Babiey and Kuvaev [1], which were recently reported to improve the predictions of burnout of a single particle of a hard coal in a drop tube [9]. Another novelty is the implementation and testing of the experimentally obtained information on the enhanced coal activation – primarily through the activation energy and the prefactor in the Arhenius expressions – into the comprehensive model of pulverized coal combustion.

It is recalled that a comprehensive ("complete") model of pulverized coal combustion in a realistic configuration consists of a number of submodels of various phenomena and processes encountered in coal combustion, most of which – in the original or modified forms – have in the present paper been adopted from the literature. However, for each of these submodels a number of options are available and a judicious choice is a challenge on its own. One of the important criteria for choosing various submodels is to achieve a balanced level of approximation. Adopting a highly sophisticated submodel for some phenomena (e.g. turbulence model) and a crude submodel of others (e.g. of chemical reaction or particle dispersion) or vice versa, makes obviously no sense as the advantages of using advanced model(s) for some processes will be annulled by the crudeness and empiricism of the other model elements. Moreover, as most of submodels are to a large degree empirical, they contain a number of empirical parameters that need to be chosen depending on the type of coal and its features, burner configuration, operating conditions and other factors. In cases where no reliable information are available, the only option for making a rational choice is a sensitivity analysis of the response