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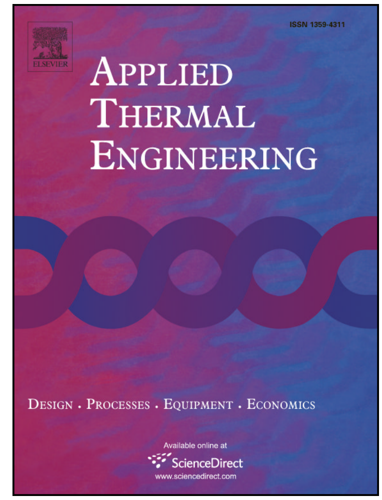

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Numerical modelling of unsteady transport and entropy generation in oxy-combustion of single coal particles with varying flow velocities and oxygen concentrations

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Abstract

Unsteady generation of entropy and transfer of heat and chemical species in the transient oxy-combustion of a single coal particle are investigated numerically. The burning process takes place in oxygen and nitrogen atmospheres with varying chemical compositions and under either quiescent or active flows. The combustion simulations are validated against the existing experimental data on a single coal particle burning in a drop-tube reactor. The spatio-temporal evolutions of the gas-phase temperature and major gaseous species concentration fields as well as that of entropy generation are investigated for the two types of gas flow. It is shown that the rates of production and transport of chemical species reach their maximum level during the homogenous combustion of volatiles and decay subsequently. Yet, the transient transfer of heat of combustion continues for a relatively long time after the termination of particle life time. This results in the generation of a large amount of thermal entropy at post-combustion stage. The analyses further indicate that the entropy generated by the chemical reactions is the most significant source of unsteady irreversibilities. Most importantly, it is demonstrated that a slight oxygenation of the atmosphere leads to major increases in the total chemical entropy generation and, thus it significantly intensifies the global irreversibilities of the process. However, upon exceeding a certain mole fraction of oxygen in the atmosphere, further addition of oxygen only causes minor increases in entropy generation. This trend is observed consistently in both quiescent and active flow cases.

Keywords: Transient heat and mass transfer; Unsteady entropy generation; Coal particle combustion; Spatio-temporal evolution; Oxy-combustion; Varying oxygen concentration.

Nomenclature

A	pre-exponential factor	$\vec{s}$	entropy flux vector
A_p	particle surface area, m^2	s	specific entropy, $J/kmol \cdot K$
a_1, a_2, a_3	constants	s_b	Stefan-Boltzmann constant $5.67032 \times 10^{-8}\ W/m^2 \cdot K^4$
C_D	drag coefficient	T	temperature, K
C	Concentration, $kmol/m^3$	t	time, s
c_p	specific heat capacity, $J/kg \cdot K$	t_t	effective time of entropy generation, s
D_{ij}	binary diffusion coefficient for the $i-j$ species pair, m^2/s	u	velocity, m/s
$D_{T,i}$	thermal diffusion coefficient for the i^{th} species, m^2/s	$\vec{u}$	velocity vector
D_{im}	effective diffusion coefficient of species i, m^2/s	$\vec{V}$	diffusion velocity of the i^{th} species
d	diameter, m	X	mole fraction
F_d	drag force, N	Y	mass fraction
f_h	fraction of heat absorbed by the particle		
$\vec{f_\iota}$	body force per unit mass	*Greek Symbols*	
H	enthalpy, $J/kmol$	α	distribution coefficient of volatile in coal
$H_{reac_{cr}}$	enthalpy of reaction cr, $J/kmol$	μ_m	viscosity, $kg/m \cdot s$
h	specific enthalpy, $J/kmol$	μ_c	specific chemical potential, J/kg

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