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Gas-phase transport and entropy generation during transient combustion of single biomass particle in varying oxygen and nitrogen atmospheres

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ABSTRACT

Transient combustion of a single biomass particle in preheated oxygen and nitrogen atmospheres with varying concentration of oxygen is investigated numerically. The simulations are rigorously validated against the existing experimental data. The unsteady temperature and species concentration fields are calculated in the course of transient burning process and the subsequent diffusion of the combustion products into the surrounding gases. These numerical results are further post processed to reveal the temporal rates of unsteady entropy generation by chemical and transport mechanisms in the gaseous phase of the reactive system. The spatio-temporal evolutions of the temperature, major chemical species including CO, CO₂, O₂, H₂ and H₂O, and also the local entropy generations are presented. It is shown that the homogenous combustion of the products of devolatilisation process dominates the temperature and chemical species fields at low concentrations of oxygen. Yet, by oxygen enriching of the atmosphere the post-ignition heterogeneous reactions become increasingly more influential. Analysis of the total entropy generation shows that the chemical entropy is the most significant source of irreversibility and is generated chiefly by the ignition of volatiles. However, thermal entropy continues to be produced well after termination of the particle life time through diffusion of the hot gases. It also indicates that increasing the molar concentration of oxygen above 21% results in considerable increase in the chemical and thermal entropy generation. Nonetheless, further oxygen enrichment has only modest effects upon the thermodynamic irreversibilities of the system.

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Introduction

It is well-established that combustion is, by far, the most irreversible process taking place in thermal power stations

[1,2]. Recent studies of coal fired power stations showed that the exergy efficiency of circulating fluidised bed boiler can be lower than 30% [3,4]. This figure clearly reflects the significant role of combustion process in exergetic losses of thermal power generation. Thus, future improvements in power

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| Nomenclature | | R _i | net rate of production of species i due to chemical |
|--------------------------------------|---|------------------------|--|
| А | pre-exponential factor, unit vary | | reactions, kg/m³·s |
| Ap | particle surface area, m ² | R _{i,cr} | chemical production rate for species i, kmol/m ³ ·s |
| | a3 constants | SE | effective area of entropy generation, m ² |
| C _D | drag coefficient | S | entropy flux vector |
| c | concentration, kmol/m ³ | S | specific entropy, J/kmol•K |
| - | specific heat capacity, J/kg·K | s _b | Stefan-Boltzmann constant, 5.67032 $	imes$ |
| с _р Du | binary diffusion coefficient for the $i - j$ species | | $10^{-8} \text{ W/m}^2 \cdot \text{K}^4$ |
| D _{ij} | pair, m ² /s | Т | temperature, K |
| л | | T ⁰ | reference temperature, K |
| $D_{T,i}$ | thermal diffusion coefficient for the <i>i</i> th species, | t | time, s |
| D | m^2/s | tt | effective time of entropy generation, s |
| Di | diffusion coefficient of species i, m ² /s | и | velocity, m/s |
| d | diameter, m | ù | velocity vector |
| e | specific internal energy, J | $\overrightarrow{V_i}$ | diffusion velocity of the i th species |
| Е | entropy generation rate, W/K | V' _{i,cr} | stoichiometric coefficients of the reactants of |
| Ea | active energy, J/kmol | 1,Cr | species i in reaction cr |
| E _h | rate of entropy generation due to heat transfer, | $V'_{i,cr}$ | stoichiometric coefficients of the products of |
| | W/K | • 1,Cr | species i in reaction cr |
| Em | rate of entropy generation due to mass transfer, | Х | mole fraction |
| | W/K | Y | mass fraction |
| Er | rate of entropy generation duo to chemical | 1 | |
| | reactions, W/K | Greek S | Symbols |
| E′ | average entropy generation rate, W/K | α | distribution coefficient of volatile in biomass |
| F _d | drag force, N | μ | viscosity, kg/m·s |
| f_{h} | fraction of heat absorbed by the particle | μ_{c} | specific chemical potential, J/kg |
| $\frac{f_h}{f_i}$ | body force per unit mass | $\overline{\mu_{c}}$ | Molar chemical potential, J/mol |
| H _{reac_{cr}} | enthalpy of reaction cr, J/kmol | μ_m | molecular viscosity, kg/m∙s |
| h | specific enthalpy, J/kmol | λ | thermal conductivity, W/m·K |
| h_{fg} | latent heat of devolatilization, J/kg | ρ | density, kg/m ³ |
| h′ | enthalpy of mixture, J/kmol | ω_{i} | rate of species i mass production per unit volume |
| g _x | acceleration gravity, m/s ² | ε_p | particle emissivity |
| J _{i,j} | molecular mass flux, kg/m³•s | $\theta_{\rm R}$ | radiation temperature, K |
| K | reaction rate, $\text{kmol}^{1-(d+e)}/(\text{m}^3)^{1-(d+e)} \cdot s$ | σ | Rate of entropy generation per unit volume, W/ |
| ka | rate constant of char combustion reactions, | 0 | m ³ K |
| ĸu | kmol/m ³ ·s | Φ | viscous dissipation |
| k _c | thermal conductivity, K•m/W | Ŧ | viscous dissipation |
| k _{cr} | rate constant of reaction cr, kmol/m ³ ·s | Subscri | ipts |
| k _d | kinetic rate of devolatilization reaction, s^{-1} | cr | chemical reaction number |
| | Lewis number | cr' | char reaction number |
| Le | | i | i th species |
| M | molecular weight, kg/kmol | j | indices: 1,2,,N |
| M | average molecular weight, kg/kmol | g | gas |
| m | mass, kg | р | particle |
| Ν | number of chemical species | rg | gaseous reactants |
| n _{cr} | number of chemical reactions | X | composition of chemical element H |
| Nu | Nusselt number | Y | composition of chemical element O |
| р | pressure, Pa | x,r | coordinates |
| p^0 | reference pressure, Pa | Λ,Ι | corumates |
| Qr | internal production rate for thermal energy, J/s | Supers | cripts |
| | energy flux | a _{i,cr} | reaction order of species i in reaction cr |
| $\stackrel{q_j}{\overrightarrow{q}}$ | heat-flux vector | b | temperature exponent |
| $\overrightarrow{q_R}$ | radiant heat-flux vector | d | reaction order of related gaseous reactants |
| Re | Reynolds number | е | reaction order of oxygen |
| Ru | universal gas constant, kg/kmol | | |
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