DEVELOPMENT OF A SOLID-GAS COUPLED MODEL FOR THERMALLY THICK BIOMASS COMBUSTION IN PACKED BEDS

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Thesis submitted in fulfillment of the requirement for the Degree Doctor of Philosophy of Engineering in Chemical and Process Engineering

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DECLARATION

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The above candidate has carried out research for the PhD thesis under my supervision.

Name of the supervisor: Prof. Mahinsasa Narayana

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Abstract

The aim of this research is to model the moving grate combustion process by Computational Fluid Dynamics (CFD) method by OpenFOAM software. Kinetic data for heterogeneous reactions, specific to local fuel types is essential. Therefore, pyrolysis kinetics of Rubber and Gliricidia was evaluated by two methods; the sequential approach for Kissinger method and Miura and Maki approach for Ditributed Activation Energy Model (DAEM). The activation energy values obtained by the sequential spproach for Kissinger method are 107.9 kJmol⁻¹ for Gliricidia and 83.44 kJmol⁻¹ for Rubber wood. Obtained activation energy by Miura and Maki approach for DAEM, varies between 190.57 kJmol⁻¹ and 230.58 kJmol⁻¹ for Gliricidia and between 111.52 kJmol⁻¹ and 179.07 kJmol⁻¹ for Rubber wood.

A CFD model was developed which describes the wood combustion in fixed grate type packed bed furnaces. Linear rate of mass loss observed in batch type simulations can be used to describe the steady state burning characteristics of a continuously operated furnace which has a feeding rate equal to burning rate. This mass loss rate was used to evaluate Equivalence Ratio (ER) variation for different particle sizes of wood. A sensitivity analysis was conducted to find the effect of moisture content and particle size on ER. It was found that moisture content of wood has more significant effect on ER than the particle size. The optimum equivalence ratio was studied based on the maximum outlet gas temperature with minimum CO fraction for different particle sizes of wood. The optimum ER values obtained were 0.28 for 25 mm sized particles, 0.13 for 38 mm sized particles and 0.18 for 63 mm sized particles.

The model was elaborated to simulate wood combustion in moving grate type furnaces. This heterogeneous model developed within Eulerian framework, includes the grate movement through boundary conditions, which can solve both bed and free board region simultaneously.

Keywords: Computational Fluid Dynamics, packed beds, combustion, moving grate furnaces

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LIST OF ABBREVIATIONS

Abbreviation Description

CFD Computational Fluid Dynamics

DAEM Distributed Activation Energy Method

DNS Direct Numerical Simulation

DOM Discrete Ordinates Model

DPM Discrete Particles Models

DTM Discrete Transfer Method

ER Equivalence Ratio

FVM Finite Volume Method

FWO Flynn-Wall-Ozawa

KAS Kissinger–Akahira–Sunose

LES Large Eddy Simulation

RANS Reynolds Averaged Navier-Stokes

RTE Radiative Transfer Equation

TGA Thermo Gravimetric Analysis

LIST OF NOMECLATURE

Symbol Description

A pre-exponential factor (s⁻¹)

A_{spec} volume specific surface area (m⁻¹)

A_p projected area (m²)

 $a_{\rm g}$ absorption coefficient of gas $(m^{\text{-}1})$

a_s absorption coefficient of solid (m⁻¹)

C_i concentration of gases (molm⁻³)

 C_1, C_2 constants used in standard k-epsilon equation

 C_{pg} specific heat capacity of gas (Jkg⁻¹K⁻¹) C_{ps} specific heat capacity of solid (Jkg⁻¹K⁻¹)

D_{a.I} effective diffusivity of species i through ash layer (m²s⁻¹)

 $\begin{array}{ll} D_i & \text{binary diffusivity of species i in air (m^2s^{-1})} \\ D_{k,i} & \text{Knudsen diffusivity of species i} & (m^2s^{-1}) \end{array}$

D_{eff,i} effective diffusivity of species i (m²s⁻¹)

d_p particle diameter (m)

d_{p,o} initial particle diameter (m)

d_{pore} pore diameter (m)

E activation energy (Jmol⁻¹K⁻¹)

E_p radiation emission from particles (Wm⁻³)

G radiation intensity (Wm⁻²)

e emissivity

H_{g,i} heat of reactions gas phase reactions (Jkg⁻¹)

H_m heat of evaporation (Jkg⁻¹)

 $H_{s,i}$ heat of reactions solid phase reactions (Jkg⁻¹) h convective heat transfer coefficient (Wm⁻²K⁻¹)

 $h_{m.a.i}$ mass transfer coefficient of i^{th} gaseous component through ash layer

 (ms^{-1})

 $h_{mi} \qquad \qquad \text{mass transfer coefficient of i^{th} gaseous species in boundary layer (ms^{-1})}$

h_{mi,eff} effective mass transfer coefficient (ms⁻¹)

k turbulent kinetic energy (m²s⁻²)

ki kinetic reaction rate of char with ith gaseous component (ms⁻¹)

k_{i,eff} effective reaction rate (ms⁻¹)

l_a ash layer thickness (m)

M_{air} air molar weight (kgmol⁻¹)

M_c carbon molar weight (kgmol⁻¹)

M_i species molar weight (kgmol⁻¹)

m₀ initial mass of sample (kg)

m_f final mass of sample (kg)

m_{s,i} mass of solid phase constituents in a computational cell (kgm⁻³)

m_{s,w} mass of water in a computational cell (kgm⁻³)

m mass (kg)

n reaction order /refractive index

Nu Nusselt number
P pressure (Pa)

Pr Prandtl number

Q_{rad,g} radiation heat source term (Jm⁻³s⁻¹) R universal gas constant (kJK⁻¹mol⁻¹)

Re Reynolds number

 $R_{g,i}$ gas phase reaction rate ith species (kgm⁻³s⁻¹)

 R_{ki} gas phase kinetic reaction rate of i^{th} species (kgm⁻³s⁻¹)

 $R_{mix,i}$ gas phase mixing rate i^{th} species $(kgm^{-3}s^{-1})$

 $R_{s,i}$ solid phase reaction rate $(kgm^{-3}s^{-1})$

 $R_{s,w}$ rate of drying $(kgm^{-3}s^{-1})$

S_{g,i} summed production rate of ith gas species in gas phase reactions (kgm⁻

 $^{3}s^{-1}$)

Sh Sherwood number

S_{ij} turbulent stress tensor (Pa)

S_m momentum resistance source term (kgm⁻²s⁻²)

 $S_{s,i}$ summed production rate of i^{th} gas species in solid phase reactions (kgm⁻

 $^{3}s^{-1}$)

 T_{evap} evaporation temperature (K)

 T_g gas phase temperature (K)

T_s solid phase temperature (K)

t time (s)

u velocity (ms⁻¹)

 $\begin{array}{ll} u_{bed} & bed \ velocity \ (ms^{\text{-}1}) \\ \\ u_{grate} & grate \ velocity \ (ms^{\text{-}1}) \\ \\ V_{cell} & volume \ of \ cells \ (m^3) \end{array}$

X_a mass fraction of ash

x conversion

Y_i mass fraction of gas species i

Y_b mass fraction of bound water in solid phase

Y_w mass fraction of water in solid phase

Greek symbols

α mass fraction

β heating rate in pyrolysis kinetic determination/solid cell identification

factor shrinkage model

γ factor of bed height change

ε turbulent dissipation rate

 λ_g thermal conductivity of gas (Wm⁻¹K⁻¹)

 λ_s thermal conductivity of solid (Wm⁻¹K⁻¹)

μ viscosity (kgm⁻¹s⁻¹)

 μ_t turbulent viscosity (kgm⁻¹s⁻¹)

 ρ_a ash density (kgm⁻³)

 ρ_g gas density (kgm⁻³)

 ρ_s solid density (kgm⁻³)

σ Steffan Boltzmann constant (Wm⁻²K⁻⁴)

 $\sigma_{i,air}$ collision diameter (A)

 σ_{ϵ} , σ_{k} model constants in standard k-epsilon equation

 $\sigma_{\rm s}$ scattering coefficient

 τ stress tensor (Nm⁻²)

 $\begin{array}{lll} \varphi & porosity \\ \\ \varphi_a & ash \ layer \ porosity \\ \\ \Omega_{c,i} & stoichiometric \ coefficient \ of \ i^{th} \ heterogeneous \ reaction \\ \\ \Omega_{g,i} & stoichiometric \ coefficient \ of \ i^{th} \ gas \ phase \ reactions \\ \\ \Omega_{c,o} & stoichiometric \ coefficient \ of \ char \ oxidation \ reactions \\ \\ \Omega_{g,i,o} & stoichiometric \ coefficient \ of \ i^{th} \ gas \ phase \ oxidation \ reaction \\ \\ \Omega_{i,air} & collisional \ integral \end{array}$

LIST OF APPENDICES

Appendix A OpenFoam programme for packed bed combustion

Appendix B OpenFoam programme for moving grate combustion

Appendix C List of papers