# A THREE DIMENSIONAL COMPUTATIONAL FLUID DYNAMICS MODEL FOR PYROLYSIS OF THERMALLY THICK BIOMASS PARTICLES

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178055B

Degree of Master of Science

Department of Chemical and Process Engineering

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## Declaration

I declare that this is my own work and this thesis does not incorporate without acknowledgement any material previously submitted for a Degree or Diploma in any other University or institute of higher learning and to the best of my knowledge and belief it does not contain any material previously published or written by another person except where the acknowledgement is made in the text.

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

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## Abstract

The solid biomass especially the wood has been used as a source of energy for centuries in the world. However, the present world has started giving it a more value not because it is known for a longer time. But as a renewable energy source it lessens the fossil fuel depletion and be a part of climate change mitigation. Conversion of biomass to energy is done through several methods such as bio-chemical conversion and thermo-chemical conversion. In the present work, the drying and pyrolysis process of a thermally thick single wood particle has been investigated. A novel approach has been introduced considering the two-phase gas and solid inside the particle are not in thermal equilibrium. Mathematical relationship was built to determine distinct temperatures at the boundaries of solid and gas. An unsteady three-dimensional (3D) model is developed and simulated in Computational Fluid Dynamics (CFD) framework. The Euler-Euler approach for modeling of single biomass particle has been succeeded with the help of C++ CFD toolbox in OpenFOAM. The 3D model can simulate the thermochemical conversion process of different particle types, particularly for different shapes to examine the spatial variations during the process. The model was validated by comparing the simulation results with data obtained by experiments conducted using a single particle reactor. Further, the model was applied in torrefaction of single wood particle then expanded to thermochemical conversion in packed bed.

Key words:
Biomass
CFD
Mathematical model
Thermally thick particle
Thermochemical conversion

***Dedicated to my mother and farther***

***for their unconditional love,***

***endless support***

***and encouragement.***

**Acknowledgement**

This work would not have been possible without the opportunity given by the Senate research committee (SRC/ST/2017/06) and the Department of Chemical and Process Engineering, University of Moratuwa. I'm grateful for all the personnel who have provided their valuable support.

I would like to express my sincere gratitude to my supervisor, Prof. M. Narayana, for the continuous support, guidance and being patience throughout this period of study.

My sincere thanks go to the progress review committee for their insightful comments and encouragement to carry out this work successfully.

I would like to thank my fellow lab mates Upuli and Chathuranga for sharing their knowledge and experience. I thank my friends, Wathsala, Gimhani and Imanthi for the stimulating conversations and giving me hand whenever I needed.

Finally, I must express my profound gratitude to my family, for having great faith, giving more strength and motivation to get things done and always showing how proud they are of me.

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| | |
|---|---|
| $\boldsymbol{a}$ | Absorption coefficient ($m^{-1}$) |
| $\boldsymbol{a_i}$ | Fraction of component |
| $\boldsymbol{A}$ | Total specific area of solid phase ($m^{-1}$) |
| $\boldsymbol{A_i}$ | Pre-exponential factor ($s^{-1}$) |
| $\boldsymbol{A_p}$ | Particle surface area ($m^2$) |
| $\boldsymbol{A_{spc}}$ | Specific surface area of char ($m^{-1}$) |
| $\boldsymbol{A_w}$ | Pre-exponential factor for water evaporation ($s^{-1}$) |
| $\boldsymbol{C}$ | Linear anisotropic phase function coefficient |
| $\boldsymbol{C_{eff}}$ | Effective specific heat capacity of the solid (J $kg^{-1}K^{-1}$) |
| $\boldsymbol{C_{p,g}}$ | Specific heat capacity of gas (J $kg^{-1}K^{-1}$) |
| $\boldsymbol{C_{p,w}}$ | Specific heat capacity of water (J $kg^{-1}K^{-1}$) |
| $\boldsymbol{d}$ | Particle diameter (m) |
| $\boldsymbol{D_{i,g}}$ | Gas diffusion coefficient ($m^2$ $s^{-1}$) |
| $\boldsymbol{E_i}$ | Activation energy (J $mol^{-1}$) |
| $\boldsymbol{E_w}$ | Activation energy for water evaporation (J $mol^{-1}$) |
| $\boldsymbol{FSP}$ | Fibre saturation point |
| $\boldsymbol{G}$ | Incident radiation (W $m^{-2}$) |
| $\boldsymbol{h_{rad}}$ | Radiative heat transfer coefficient (W $m^{-2}$ $K^{-1}$) |
| $\boldsymbol{k_g}$ | Thermal conductivity of gas phase (W $m^{-1}$ $K^{-1}$) |
| $\boldsymbol{k_{m,i}}$ | Mass transfer coefficient of species (m $s^{-1}$) |
| $\boldsymbol{L}$ | Characteristic length (m) |

| | |
|---|---|
| $\boldsymbol{LHV_{feed}}$ | Lower heating value of feed |
| $\boldsymbol{LHV_{torrefied}}$ | Lower heating value of torrefied material |
| $\boldsymbol{M_{air}}$ | Molecular weight of air (kg mol$^{-1}$) |
| $\boldsymbol{M_{char}}$ | Char molecular weight (kg mol$^{-1}$) |
| $\boldsymbol{M_{feed}}$ | Mass of feed (kg) |
| $\boldsymbol{M_{i}}$ | Amount of species (kg m$^{-3}$) |
| $\boldsymbol{M_{s}}$ | Molecular weight of specie (kg mol$^{-1}$) |
| $\boldsymbol{M_{solid}}$ | Amount of solid species (kg m$^{-3}$) |
| $\boldsymbol{M_{torrefied}}$ | Mass of torrefied material (kg) |
| $\boldsymbol{n}$ | Refractive index of the medium |
| $\boldsymbol{p}$ | Gas pressure (Pa) |
| $\boldsymbol{Q_{charconversion}}$ | Char conversion source term |
| $\boldsymbol{Q_{drying}}$ | Drying heat (J m$^{-3}$ s$^{-1}$) |
| $\boldsymbol{Q_{gasgeneration}}$ | Total heat interaction during solid to gas conversion (J m$^{-3}$ s$^{-1}$) |
| $\boldsymbol{Q_{pyrolysis}}$ | Pyrolysis heat (J m$^{-3}$ s$^{-1}$) |
| $\boldsymbol{Q_{r}}$ | Radiation flux |
| $\boldsymbol{Q_{radiation}}$ | Radiation source term |
| $\boldsymbol{R}$ | Universal gas constant (J K$^{-1}$mol$^{-1}$) |

| | |
|---|---|
| $\boldsymbol{R_{char,i}}$ | Char reaction rate (kg m$^{-3}$ s$^{-1}$) |
| $\boldsymbol{R_{char,k,i}}$ | Kinetic rate of char reactions (kg m$^{-3}$ s$^{-1}$) |
| $\boldsymbol{R_{char,m,i}}$ | Mass transfer rate of char reactions (kg m$^{-3}$ s$^{-1}$) |
| $\boldsymbol{R_{drying}}$ | Rate of drying (kg m$^{-3}$ s$^{-1}$) |
| $\boldsymbol{R_i}$ | Pyrolysis rate of *i* component (kg m$^{-3}$ s$^{-1}$) |
| $\boldsymbol{R_{pyrolysis}}$ | Total rate of pyrolysis (kg m$^{-3}$ s$^{-1}$) |
| $\boldsymbol{S_{drying}}$ | Drying source term |
| $\boldsymbol{S_{pyrolysis}}$ | Pyrolysis source term |
| $\boldsymbol{S_{charconversion}}$ | Char conversion source term |
| $\boldsymbol{t}$ | Time (s) |
| $\boldsymbol{T_{b,eff}}$ | Effective boundary temperature (K) |
| $\boldsymbol{T_{b,s}}$ | Solid boundary temperature (K) |
| $\boldsymbol{T_{evp}}$ | Boiling pint of water (K) |
| $\boldsymbol{T_g}$ | Gas phase temperature (K) |
| $\boldsymbol{T_i}$ | Initial temperature (K) |
| $\boldsymbol{T_s}$ | Solid phase temperature (K) |
| $\boldsymbol{T_{sg}}$ | Surrounding gas temperature (K) |
| $\boldsymbol{T_w}$ | Reactor wall temperature (K) |
| $\boldsymbol{u_g}$ | Gas phase velocity (m s$^{-1}$) |
| $\boldsymbol{v_i}$ | Stoichiometric coefficient of specie |
| $\boldsymbol{Y_b}$ | Fraction of bound water |

| | |
|---|---|
| $Y_i$ | Mass fraction of gas species |
| $Y_w$ | Mass fraction of wood species |
| $\Delta h_{bw}$ | Evaporation heat of bound water (J kg$^{-1}$) |
| $\Delta h_{char,i}$ | Char reaction heat (J kg$^{-1}$) |
| $\Delta h_{fw}$ | Evaporation heat of free water (J kg$^{-1}$) |
| $\Delta h_{pyrolysis}$ | Heat of pyrolysis (J kg$^{-1}$) |
| $\Delta t$ | Time step (s) |
| $\varepsilon_g$ | Volume fraction of gas porosity |
| $\varepsilon_s$ | Volume fraction of solid porosity |
| $\kappa_c$ | Char permeability |
| $\kappa_w$ | Wood permeability |
| $\epsilon$ | Wall emissivity |
| $\rho_c$ | Mass of char (kg m$^{-3}$) |
| $\rho_{df}$ | Density of dry wood (kg m$^{-3}$) |
| $\rho_g$ | Gas density (kg m$^{-3}$) |
| $\rho_{H_2O,b}$ | Bound water in the wood particle (kg m$^{-3}$) |
| $\rho_{H_2O,f}$ | Free water in the wood particle (kg m$^{-3}$) |
| $\rho_i$ | Density of specie (kg m$^{-3}$) |
| $\rho_{is}$ | Density of specie at the reacting surface (kg m$^{-3}$) |
| $\rho_w$ | Density of moisture (kg m$^{-3}$) |
| $\mu_g$ | Dynamic viscosity (Ns m$^{-2}$) |
| $\sigma$ | Stefan-Boltzmann constant (Wm K$^{-4}$) |

| | |
|---|---|
| $\boldsymbol{\sigma_i}$ | Average collision diameter ($\dot{\mathbf{A}}$) |
| $\boldsymbol{\sigma_s}$ | Scattering coefficient ($m^{-1}$) |
| $\Omega_{\boldsymbol{i}}$ | Diffusion collision integral |
| $\boldsymbol{\Omega_v}$ | Stoichiometric coefficient |
| $\boldsymbol{\delta t}$ | Time step (s) |
| $\lvert\boldsymbol{U}\rvert$ | Magnitude of the velocity through a particular cell |
| $\boldsymbol{\delta x}$ | Cell size in the direction of velocity |