# PROCESS PARAMETER OPTIMIZATION OF URBAN BIOWASTE CARBONIZATION

Sinhara Mudalige Hasitha Dhananjana Perera (159261R)

Dissertation submitted in partial fulfillment of the requirements for the degree Master of Science

Department of Chemical and Process Engineering

University of Moratuwa Sri Lanka

January 2020

#### DECLARATION

I declare that this is my own work and this dissertation does not incorporate without acknowledgment 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 acknowledgment is made in the text.

Also, I hereby grant to University of Moratuwa the non-exclusive right to reproduce and distribute my dissertation, in whole or in part in print, electronic or other medium. I retain the right to use this content in whole or part in future works (such as articles or books).

Signature

Date

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

.....

.....

Date

Signature of the supervisor

Prof. Mahinsasa Narayana Department of Chemical and Process Engineering, University of Moratuwa.

#### ABSTRACT

About 75% of Municipal solid waste (MSW) collected around the country is organic biomass which mainly includes food waste, wood, paper, saw dust and paddy husk. Urban councils in Colombo city and nearby suburbs collect biowaste separately which has created a huge potential in converting urban biowaste into value-added component like biochar, thus resolving the problems associated with MSW management and mitigating socio-economic and environmental issues related to MSW. In this study, torrefaction is identified as the most viable technology available for the conversion of organic MSW into biochar and the study mainly focuses on developing a three dimensional computational fluid dynamics (CFD) model of a continuous packed-bed torrefaction reactor for organic MSW and then optimizing the process variables and the geometry. A mathematical model including all heat, mass and energy transfers, and heterogeneous & homogeneous reactions is firstly developed and then converted to a numerical model and simulated using OpenFOAM for an insulated cylindrical reactor in which hot gas at elevated temperatures (473 - 623K) is provided from the bottom while solid at ambient conditions is fed from the top. The torrefaction reactor is optimized for gas inlet temperature and residence time and then the geometry of the reactor is optimized for the optimum gas inlet temperature and residence time. Four reaction zones are identified in the reactor domain; i.e. drying, softening & depolymerization, limited devolatilization & carbonization and extensive devolatilization and carbonization. The optimum inlet gas temperature, residence time and D/L ratio are 573K, 13000s and 0.24 respectively. For the optimum conditions, biochar yield is 55.7% while ash content is 19.1%. Further In dry basis, 95.9% of biomass is decomposed and the total weight loss based on the initial wet biomass is 86.6%.

**Keywords:** Urban biowaste; Biochar; Torrefaction; Computational fluid dynamic; Continuous packed-bed; numerical model

#### ACKNOWLEDGMENT

I owe my deepest gratitude to the people mentioned below without whom the successful completion of this research would not have been possible. The support received in numerous ways is invaluable and beyond description.

First and foremost, I would like to express my heartfelt gratitude to my supervisor Prof. Mahinsasa Narayana for the immense support and the technical guidance provided throughout the course of conduction of this research. His immense knowledge and vast experience in the field of modeling and simulation helped me tremendously whenever I had come across with problems. Also I am very much grateful for the inspiration and motivation given by him to accelerate the research activities whenever I was lagging behind the schedule.

It is with great pleasure that I acknowledge Mr. Chathuranga Wikramasinghe for the tremendous support given throughout the research. I am indebted to him for the assistance provided during the learning process of C++ language and OpenFOAM software. Also I owe my gratitude to him for the support given in finding resource materials.

I gratefully acknowledge all the lecturers of Department of Chemical and Process Engineering, University of Moratuwa. Also I would like to extend my gratitude to non-academic staff of Department of Chemical and Process Engineering, University of Moratuwa. Further I would like to specially thank Mr. Sunil Dayananda of Process Control Laboratory of Department of Chemical and Process Engineering for facilitating laboratory resources.

All the colleagues supported me during the course of conduction of this research are earnestly remembered for their numerous support. Finally I would like to express my heartfelt gratitude to my beloved family for motivating me to complete this research successfully.

### **TABLE OF CONTENTS**

DECLA	RATIONi
ABSTR	ACTii
ACKNO	OWLEDGMENTiii
LIST O	F FIGURES vi
LIST O	F TABLES
LIST O	F ABBREVIATIONS x
LIST O	F APPENDICES x
NOMEN	NCLATURE
1. IN	TRODUCTION1
1.1	Biomass1
1.2	Potential of biomass in waste management
1.3	Context of municipal solid waste in Sri Lanka5
1.4	Organic waste processing technologies7
1.4	.1 Gasification7
1.4	.2 Pyrolysis, Torrefaction and Incineration
1.4	.3 Fermentation, Anaerobic digestion and Hydrothermal carbonization 8
1.5	Background of the research
1.6	Research problem
1.6	.1 Modelling and simulation of organic waste torrefaction using CFD14
1.6	.2 Introduction to OpenFOAM
1.7	Scope of the research
1.8	Research objectives
1.9	Thesis outline
2. LIT	TERATURE REVIEW

	2.1	Tor	refaction process	. 18
	2.	1.1	Introduction to biomass torrefaction	18
	2.	1.2	Principal and mechanism of torrefaction	18
	2.	1.3	Effect of process parameters on torrefaction	22
	2.2	Bio	char and its applications	24
	2.3	Che	emical Kinetics of Torrefaction	25
	2.	3.1	Thermal decomposition of cellulose, hemicellulose and lignin	25
	2.	3.2	Solid-phase and gas-phase heterogeneous reactions	27
	2.	3.3	Gas phase homogeneous reactions	28
	2.4	CFI	D approach to heat, mass and momentum transfer modeling	29
	2.4	4.1	Navier-Stokes equations	29
	2.4	4.2	Equations of state	. 31
	2.4	4.3	Finite volume method	. 31
3.	ST	ΓUDY	METHODOLOGY	36
	3.1	Pro	cess selection	36
	3.2	Phy	vsical model	37
	3.3	Ma	thematical Model	40
	3.	3.1	Governing equations	40
	3.	3.2	Reaction sub models	42
	3.	3.3	Heat transfer sub models	48
	3.	3.4	Modeling of physical properties	52
	3.	3.5	Assumptions	53
	3.4	Ope	enFOAM simulation	55
	3.4	4.1	Mesh generation	55
	3.4	4.2	OpenFOAM simulation Parameters	58
	3.4	4.3	Initial and boundary conditions	59

	3.4	.4 Optimization of residence time and temperature	61
	3.4	.5 Optimization of reactor geometry	61
4.	RE	SULTS & DISCUSSION	
4	4.1	Optimization of temperature and residence time	
4	4.2	Analysis of results	
4	4.3	Optimization of geometry	91
4	1.4	Biochar quality and suitability for an industrial application	
4	4.5	Model validation	
5.	CO	NCLUSIONS	
	5.1	Drawbacks of the model and suggestions for future works	
RE	FER	ENCES	
AP	PEN	DICES	
1	Appe	ndix A	

## LIST OF FIGURES

Figure 1-1: Gross final energy consumption globally in 2016 [3]	. 2
Figure 1-2: Total primary energy supply of all renewables in 2014 [3]	. 2
Figure 1-3: Total MSW disposed of worldwide [4]	. 3
Figure 1-4: Global solid waste composition [4]	.4
Figure 1-5: Biowaste processing technologies	.7
Figure 1-6: Organic waste torrefaction	11
Figure 1-7: Experimental approach in optimization	12
Figure 1-8: Computer aided simulation and optimization	13

Figure 2-1: TGA and DTG curves of thermal degradation of cellulose, hemicellulose
and lignin [18]19
Figure 2-2: van Krevelen diagram [19]
Figure 2-3: Schematic representation of different torrefaction stages [19]
Figure 2-4: Comparison of non-torrefied and torrefied biomass characteristics [21] 22
Figure 2-5: Physico-chemical phenomena during the torrefaction [21]
Figure 2-6: Three steps of finite volume method
Figure 2-7: Schematic representation of grid generation for a one dimensional case
[16]
Figure 2- 8: Matrix solution techniques in CFD
Figure 3-1: Process flow diagram of the torrefaction process
Figure 0-2: Schematic representation of porous biomass particles in an exemplary
computational domain [40]
Figure 3-3: Schematic representation of solution algorithm
Figure 3-4: 3D grid developed for the solution domain
Figure 4-1: Reaction zones in the solution domain
Figure 4.2: Gas velocity profile at $14000s$ for 573K inlet gas temperature 84
Figure 4-2. Gas velocity prome at 14000s for 575K linet gas temperature
Figure 4-3: Char yield percentage in outlet
Figure 4-4: Ash percentage in outlet
Figure 4-5: Unreacted lignocellulose percentage in outlet
Figure 4-6: Moisture content profiles over the time for the optimized case (573K.
14000s)
1 10000/

Figure 4-7: Profiles of unreacted lignocellulose per unit volume over the time span
for the optimized case (573K, 13000s)90
Figure 4-8: Solid temperature profiles for different D/L ratios at optimized conditions
Figure 4-9: Char yield profiles for different D/L ratios at optimized conditions92
Figure 4-10: Unreacted lignocellulose composition profiles for different D/L ratios at
optimized conditions
Figure 4-11: Ash content per unit volume profiles for different D/L ratios at
optimized conditions
Figure 4-12: Char percentage in the outlet with respect to D/L ratio
Figure 4-13: Ash percentage in the outlet with respect to D/L ratio96
Figure 4-14: Simulation and experimental temperature profiles after 2700s

## LIST OF TABLES

Table 1-1: Average solid waste generation in Sri Lankan local government councils
[5]5
Table 1-2: Average composition of MSW collected in Sri Lanka [5]
Table 2-1: Thermal decomposition temperatures of cellulose, hemicellulose and
lignin19
Table 2-2: Proximate analysis results of different torrefied biomass sources [25] [26]
Table 2-3: Chemical kinetic data for drying and lignocellulose decomposition
reactions

Table 2-4: Kinetics of heterogeneous reactions 28
Table 2-5: Reaction kinetics of gas-phase homogeneous reactions
Table 3-1: Proximate analysis results for dry composted organic MSW
Table 3- 2: Discretisation schemes 58
Table 3-3: Matrix solvers 58
Table 3-4: Control parameters of the simulations
Table 3-5: Initial and boundary condition of the model 60
Table 4- 1 Solid temperature (Ts) profiles
Table 4- 2: Char formation $(kg/m^3)$
Table 4- 3: Lignocellulose per unit volume (kg/m <sup>3</sup> )73
Table 4- 4: Ash generation (kg/m <sup>3</sup> )
Table 4- 5: Char yield percentage in outlet
Table 4- 6: Ash percentage in outlet
Table 4- 7: Unreacted lignocellulose percentage in outlet
Table 4- 8: Char, ash and unreacted lignocellulose percentages in the outlet with   respect to D/L ratio
Table 4- 9: Gas composition at the gas outlet for the optimum conditions    96
Table 4-10: Solid composition at the solid outlet for the optimum conditions97
Table 4- 11: Operating parameters of the experimental reactor
Table 4- 12: Operating parameters of the experimental reactor
Table A-1: Gas-phase temperature (Tg) profiles

#### LIST OF ABBREVIATIONS

Abbreviation	Description
CFD	Computational Fluid Dynamics
MSW	Municipal Solid Waste

## LIST OF APPENDICES

Appendix	Description	Page
Appendix A	Gas-phase temperature (Tg) profiles	108

#### NOMENCLATURE

- $\rho_g$  Density of gas phase (kg m<sup>-3</sup>)
- $\epsilon_g$  Volume fraction of gas phase

 $U_q$  - Velocity of gas phase (m s<sup>-1</sup>)

- $\mu$  Dynamic viscosity (Pa s)
- *p* Pressure (Pa)
- k Turbulent kinetic energy (m<sup>2</sup> s<sup>-2</sup>)
- I Second order identity tensor
- d Particle size (m)
- $T_g$  Gas phase temperature (K)
- T<sub>s</sub> Solid phase temperature (K)
- $\rho_s$  Density of solid phase (kg m<sup>-3</sup>)
- $\epsilon_{s}$  Volume fraction of solid phase

 $C_{v,q}$  - Specific heat capacity of gas phase (J kg<sup>-1</sup> K<sup>-1</sup>)

- $C_s$  Specific heat capacity of solid phase (J kg<sup>-1</sup> K<sup>-1</sup>)
- $k_g$  Thermal conductivity of gas phase (W m<sup>-1</sup> K<sup>-1</sup>)
- $k_s$  Thermal conductivity of solid phase (W m<sup>-1</sup> K<sup>-1</sup>)
- $R_{i,hetero}$  Rate of heterogeneous reaction i (kg m<sup>-3</sup> s<sup>-1</sup>)
- $R_{i,homo}$  Rate of homogeneous reaction i (kg m<sup>-3</sup> s<sup>-1</sup>)
- $Q_R$  Radiation heat (W)
- h Heat transfer coefficient (W m<sup>-2</sup> K<sup>-1</sup>)
- A Specific surface area of bed  $(m^{-1})$
- $\Delta H_i$  Enthalpy of the reaction i (J kg<sup>-1</sup>)
- $Y_{g,i}$  Mass fraction of i in the gas phase
- $Y_{s,i}$  Mass fraction of i in the solid phase
- $D_{q,i}$  Diffusion coefficient of i in the gas phase (m<sup>2</sup> s<sup>-1</sup>)
- $D_{s,i}$  Diffusion coefficient of i in the solid phase (m<sup>2</sup> s<sup>-1</sup>)
- $r_{cel}$  Degradation rate of cellulose (kg m<sup>-3</sup> s<sup>-1</sup>)
- $r_{hem}$  Degradation rate of hemicellulose (kg m<sup>-3</sup> s<sup>-1</sup>)
- $r_{lig}$  Degradation rate of lignin (kg m<sup>-3</sup> s<sup>-1</sup>)

 $f_{cel}$  - Pre-exponential factor of cellulose decomposition (s<sup>-1</sup>)

 $f_{hem}$  - Pre-exponential factor of hemicellulose decomposition (s<sup>-1</sup>)

 $f_{lig}$  - Pre-exponential factor of lignin decomposition (s<sup>-1</sup>)

 $E_{cel}$  - Activation energy of cellulose decomposition (kJ mol<sup>-1</sup>)

 $E_{hem}$  - Activation energy of hemicellulose decomposition (kJ mol<sup>-1</sup>)

 $E_{lig}$  - Activation energy of lignin decomposition (kJ mol<sup>-1</sup>)

 $Y_{cel}$  - Mass fraction of cellulose

 $Y_{hem}$  - Mass fraction of hemicellulose

 $Y_{lig}$  - Mass fraction of lignin

 $r_{k,O2}$ ,  $r_{k,CO2}$  and  $r_{k,H2O}$  - Kinetic reaction rate of char combustion, char CO<sub>2</sub> gasification and char H<sub>2</sub>O gasification respectively (kg m<sup>-3</sup> s<sup>-1</sup>)

 $f_{O2}$ ,  $f_{CO2}$  and  $f_{H2O}$  - Pre-exponential factor of char combustion, char CO<sub>2</sub> gasification and char H<sub>2</sub>O gasification respectively (m s<sup>-1</sup> K<sup>-1</sup>)

 $E_{O2}$ ,  $E_{CO2}$  and  $E_{H2O}$  - Activation energy of char combustion, char CO<sub>2</sub> gasification and char H<sub>2</sub>O gasification respectively (kJ mol<sup>-1</sup>)

 $M_c$ ,  $M_{O2}$ ,  $M_{CO2}$  and  $M_{H2O}$  - Molar mass of char, O<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O respectively (kg mol<sup>-1</sup>)

 $v_{O2}$ ,  $v_{CO2}$  and  $v_{H2O}$  - Stoichiometric coefficient of O<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O in char combustion, char CO<sub>2</sub> gasification and char H<sub>2</sub>O gasification reactions respectively

 $\rho_{O2}$ ,  $\rho_{CO2}$  and  $\rho_{H2O}$  - Density of O<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O in the gas phase respectively (kg m<sup>-3</sup>)

 $m_{char}$  - Mass of char per unit volume (kg m<sup>-3</sup>)

 $m_{biomass}$  - Initial mass of biomass per unit volume (kg m<sup>-3</sup>)

a - Average stoichiometric coefficient of char in the degradation reactions

 $A_{ss}$  - Total specific surface area of solid phase (m<sup>2</sup>)

 $r_{m,O2}$ ,  $r_{m,CO2}$  and  $r_{m,H2O}$  - Mass transfer rate of O<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O (kg m<sup>-3</sup> s<sup>-1</sup>)

 $\rho_{O2,s}$ ,  $\rho_{CO2,s}$  and  $\rho_{H2O,s}$  - Density of O<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O in the solid surface respectively (kg m<sup>-3</sup>)

 $k_{m,O2}$ ,  $k_{m,CO2}$  and  $k_{m,H2O}$  - Mass transfer coefficient of O<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O respectively (m s<sup>-1</sup>)

 $Sh_i$  - Sherwood number of i<sup>th</sup> gas

 $Sc_i$  - Schmidt number of i<sup>th</sup> gas

 $D_{i,q}$  - Diffusion coefficient of i<sup>th</sup> gas (m<sup>2</sup> s<sup>-1</sup>)

Re - Reynolds number

 $r_{k,i}$  - Kinetic reaction rate of i<sup>th</sup> equation (kmol m<sup>-3</sup> s<sup>-1</sup>)

 $f_i$  - Pre-exponential factor of i<sup>th</sup> equation

 $E_i$  - Activation energy of i<sup>th</sup> equation (kJ mol<sup>-1</sup>)

[H<sub>2</sub>], [O<sub>2</sub>], [CO], [H<sub>2</sub>O], [CO<sub>2</sub>] and [CH<sub>4</sub>] - Concentration of H<sub>2</sub>, O<sub>2</sub>, CO, H<sub>2</sub>O, CO<sub>2</sub>

and  $CH_4$  in the gas phase (kmol m<sup>-3</sup>)

 $r_{t,i}$  - Turbulent mixing limited reaction rate (kmol m<sup>-3</sup> s<sup>-1</sup>)

 $\rho_q$  - Density of gas (kg m<sup>-3</sup>)

k - Turbulent kinetic energy (m<sup>2</sup> s<sup>-2</sup>)

 $\in$  - Turbulent dissipation rate (m<sup>2</sup> s<sup>-3</sup>)

 $Y_j$  and  $Y_k$  - Mass fraction of reactants of reaction i

 $v_j$  and  $v_k$  - Stoichiometric metric coefficient of reactants of reaction i

 $M_j$  and  $M_k$  - Molar mass of reactants of reaction i (kg kmol<sup>-1</sup>)

 $Q_{sg}$  - Interphase convective heat transfer rate (W)

A - Specific surface area of solid  $(m^{-1})$ 

Nu - Nusselt number

Re - Reynolds' number

Pr - Prandtl number

G - Incident intensity (W m<sup>-2</sup>)

*a* - Absorption coefficient of gas phase  $(m^{-1})$ 

 $a_p$  - Absorption coefficient of solid phase (m<sup>-1</sup>)

n - Refractive index of gas phase

 $\sigma$  - Stefan constant (W m<sup>-2</sup> K<sup>-4</sup>)

 $E_p$  - Equivalent emission of particles

 $A_r$  - Specific surface area available for radiation (m<sup>-1</sup>)

 $\varepsilon$  - Emissivity of solid particles

 $H_{evp}$  - Heat of evaporation (kJ kg<sup>-1</sup> m<sup>-3</sup>)

 $Y_{moisture}$  - Mass fraction of moisture

 $r_d$  - Drying rate (kg m<sup>-3</sup> s<sup>-1</sup>)

 $E_{tor}$  - Torrefaction heat (kJ m<sup>-3</sup>)

 $C_{\nu,g}$  - Specific heat of gas (kJ K<sup>-1</sup> kg<sup>-1</sup>)

 $R_{biomass}$  - Decomposition rate of biomass (kg m<sup>-3</sup> s<sup>-1</sup>)

 $E_{Ri}$  - Energy released or absorbed due to the reaction i (kJ m<sup>-3</sup>)

 $r_i$  - Rate of the reaction i (kmol m<sup>-3</sup> s<sup>-1</sup>)

 $H_i$  - Enthalpy of the reaction I (kJ mol<sup>-1</sup>)