

# One Dimensional Mathematical Model for Packed Bed Biomass Combustion Using MATLAB

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Dr. M. Narayana  
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## **Abstract**

Packed bed biomass combustion is widely used thermal conversion process which contributes major portion of energy fulfillment around the globe. This process is usually involving higher operation cost due to low efficiency and high emissions. Hence there is a huge room for improvements in the process and needs to be optimized as well as modernized. This thesis presents two-phase one-dimensional mathematical model with MATLAB solver which can be used for diagnosis and optimization of packed bed combustion process under low computing resources and less cost. The mathematical model uses the discretized equations to develop the ordinary differential equations which are solved using implicit method. Free-board region is not taken into account. Only the biomass bed is considered here to solve the combustion system by applying conservation equations into gas and solid phase separately. The main model is consisting with different sub models with subjected to four stages of combustion as drying, pyrolysis, Char oxidization and char combustion. The biomass batch is initially ignited by continuous preheated gas inlet and higher gas flow rate. Radiation heat transfer is assumed to be negligible due to high temperature gas flow at the inlet. Combustion is occurred in batch wise. Particle diameter and bed porosity is considered with a mean value for the simplicity of the model. The developed model is used to find the solid temperature profile and generation of CO<sub>2</sub> and CO gases. By using walking column approach, industrial moving grate furnace was represented and required optimum grater length for a particular mass flow rate can be calculated with the fixed bed simulation results.

***Keywords—Biomass combustion, Mathematical model, Layer-lumped model, MATLAB simulation***

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## Nomenclature

$A$	Specific surface area of packed bed ( $\text{m}^{-1}$ )
$A_p$	Specific surface area of particle ( $\text{m}^{-1}$ )
$A_w$	pre exponential factor ( $\text{s}^{-1}$ )
$C_g$	Heat Capacity of gas phase ( $\text{J kg}^{-1} \text{K}^{-1}$ )
$C_s$	Heat Capacity of solid phase ( $\text{J kg}^{-1} \text{K}^{-1}$ )
$D_{g,i}$	Diffusion coefficient of gas species $i$ ( $\text{m}^2 \text{s}^{-1}$ )
$d_p$	Particle Diameter (m)
$E_w$	Activation Energy (J/mol)
$H$	Heat transfer coefficient ( $\text{W m}^{-2} \text{K}^{-1}$ )
$k_g$	Thermal Conductivity of gas phase ( $\text{W m}^{-1} \text{K}^{-1}$ )
$k_s$	Thermal Conductivity of solid phase ( $\text{W m}^{-1} \text{K}^{-1}$ )
$M_i$	Molecular weight of species $i$ ( $\text{kg mol}^{-1}$ )
$Nu$	Nusselt number
$P$	Pressure (Pa)
$Pr$	Prandtl Number
$Q_{s,g}$	Convective Heat transfer rate ( $\text{W m}^{-3}$ )
$Re$	Reynolds Number
$R_{Drying}$	Rate of Drying reaction $i$ ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$R_{pyr}$	Rate of pyrolysis reaction $i$ ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$R_{g,pyro}$	Rate of release of pyrolytic volatiles ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$r_{char}$	Rate of char combustion reaction $i$ ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$r_i$	Rate of reaction $i$ ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$r_{i,hetero}$	Rate of heterogeneous reaction $i$ ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$r_{i,homo}$	Rate of homogeneous reaction $i$ ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$r_{t,i}$	Rate of turbulent mixing limitation in reaction $i$ ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$r_{out}$	Reactor outer radius (m)
$S_{sg}$	Heterogeneous reaction rates involving for mass transfer ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$T_g$	Gas phase temperature (K)
$T_s$	Solid Phase temperature (K)
$U_g$	Gas phase velocity ( $\text{m s}^{-1}$ )
$U_s$	Shrinkage Velocity ( $\text{m s}^{-1}$ )
$Y_{g,i}$	Mole fraction of gas species $i$
$Y_{i,s}$	Mass fraction of solid species $i$
$\varepsilon_b$	Bed porosity
$\rho_g$	Gas Density ( $\text{kg m}^{-3}$ )
$\rho_s$	Solid Density ( $\text{kg m}^{-3}$ )
$\Phi$	Stoichiometric ratio
$\mu$	Kinematic Viscosity (Pa S)
$\sigma_{i,air}$	Average Collision diameter (A)
$\Omega_{i,air}$	Diffusion collision integral
$\Delta H_i$	Enthalpy of reaction $i$ ( $\text{J kg}^{-1}$ )



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# 1. Introduction

Among leading renewable energy trends in the twenty first century, biomass will play a significant role in the world energy supply while it is being adopted in many countries due to several factors. Ranging from agricultural/wood residuals to municipal solid waste, this is one of the largely untapped resource available while being carbon neutral energy source. It is identified as the fourth largest energy source after coal, oil and natural gas (Figure 1-1) and largest renewable energy option in the present. [1] According to the International Energy Agency (IEA), biomass contribution will increase by 10% by year 2050. It will affect for a significant drop of emissions which is forecast to be peak in year 2030.[2].

Though biomass energy is identified as zero emission energy source, the usage has been limited due to feedstock availability issues, lack of dedicated biomass plants, and lower electrical efficiency compared to other energy sources. [2] To recover the feedstock availability many countries are moving to grow dedicated biomass plants to increase the efficacy of using biomass as per the fulfillment of their energy needs. Unless byproducts from major crops in the world wide such as wheat/rice straw, rice husk and saw dust can be used to produce bio-energy without compromising existing forests, which is tend to reduce carbon footprint in energy production.

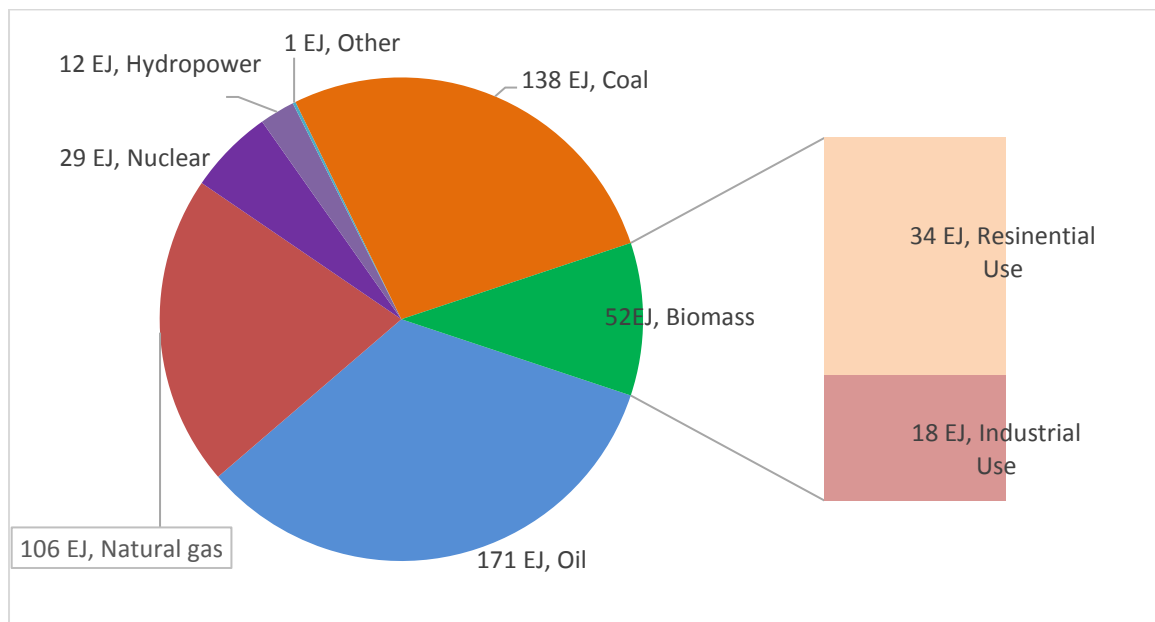


Figure 1-1 Global Energy Picture [3]

In contrast to the other renewable energy sources, capital cost for biomass thermal conversion processes is significantly lower.[3] However, the operating process tends to be less economically viable due to lower efficiency as technological advancement is in its early stages.

This implies the study of biomass thermo-chemical conversion methods are highly required to increase the system efficiency and process optimization while maintaining lower operating cost as it will help to reduce future energy crisis due to depletion of non-renewable energy sources.

There are several types of bio-energy systems are available in the present energy sector like thermo-chemical-(Combustion, Pyrolysis, Gasification and Liquefaction), Biochemical- (Digestion and Fermentation) and Mechanical- (etherification and transesterification). Among those technologies combustion is one of the major processes of thermal conversion of biomass into energy. It is a complex system involving heat and mass transfer in two phases and involved both heterogeneous and homogeneous reactions. Therefore, the process optimization is still in the developing stage and several studies have been conducted in order to develop mathematical models for this purpose. But most of the studies are based on high tech computer programming like Computational Fluid Dynamics (CFD) which is highly time consuming and complex solver and hardly affordable to small scale industries.

This study is focused on developing a numerical model for the packed bed combustion and solved using MATLAB which is commonly available and possible to simulate under below medium scale computing power with lower computational cost.

## **1.1 Biomass Combustion**

Combustion is a thermal conversion process which biomass is fully oxidized with excess air flow and produce heat. In many industries this process is used for combined heat and power plants (CHP). After supplying initial ignition source, biomass undergoes four main stages (Figure 1-2) as drying, Pyrolysis, Char oxidation and Char Combustion. It involves both heterogeneous and homogeneous reactions as listed in table (1-1). These reactions are exothermic and supply the heat to precede the other reactions. After completion of these reactions, only ash will remain. [4]

<b>Heterogeneous Reactions</b>	
Drying	$Wet\ Biomass \rightarrow Dry\ Biomass + (H_2O)_g$
Pyrolysis of biomass	$Biomass \rightarrow C + Volatiles + Ash$
Char Combustion	$char + \alpha O_2 \rightarrow 2(1 - \alpha)CO + (2\alpha - 1)CO_2$
<b>Homogeneous reactions</b>	
Formation of Water	$H_2 + 0.5O_2 \rightarrow H_2O$
Methane Oxidization	$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$
Carbon monoxide Oxidization	$CO + 0.5O_2 \rightarrow CO_2$

Table 1-1: Reactions involving Biomass Combustion

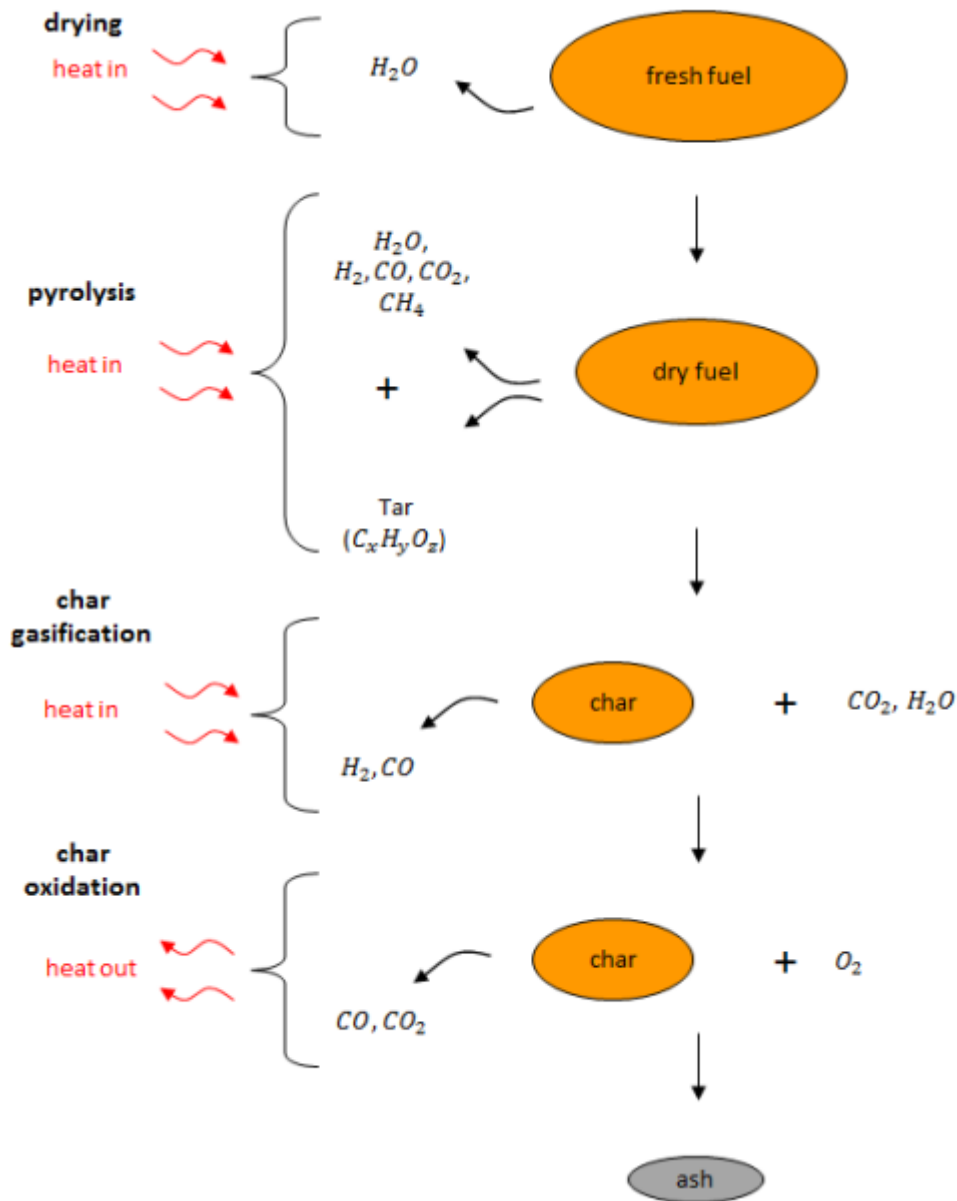


Figure 1-2: Different stages in biomass combustion[4]

## 1.2 Biomass Combustion Technologies

There are three main technologies used in biomass combustion as fixed bed, Fluidized bed and Pulverized bed. All the related technologies have been categorized as (Figure 1-3)

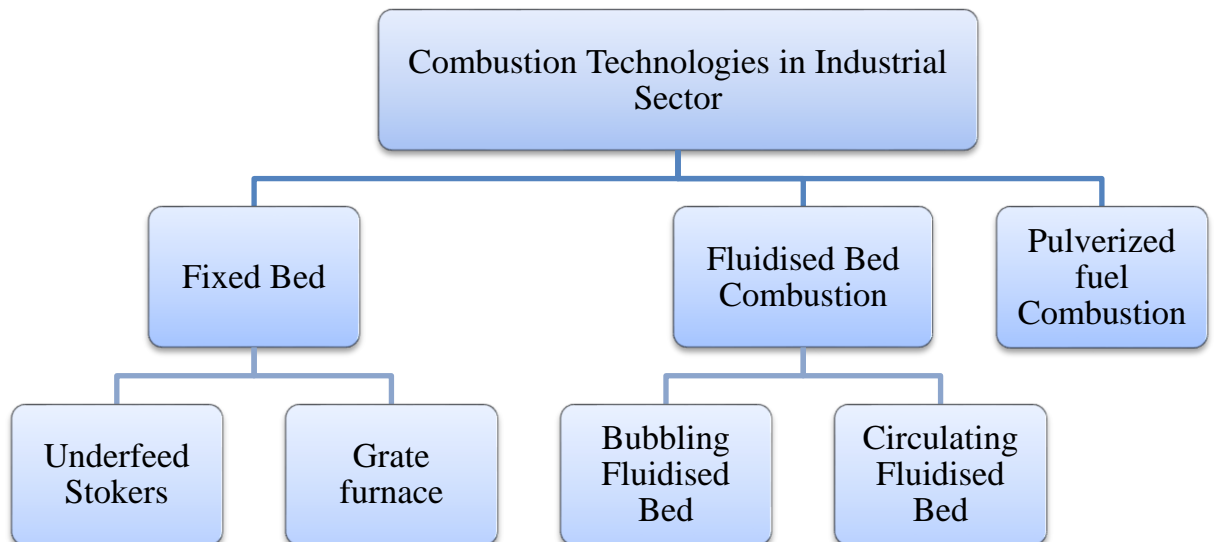


Figure 1-3: Biomass Combustion Technologies

### 1.2.1 Fixed bed biomass Combustion

Fixed beds are also known as grate furnaces, is the simplest and most common thermal conversion method which is highly used in small scale applications. Grate furnaces and underfeed stokers are main two types of fixed bed systems. In the industrial scale there are variety of grate furnaces are available such as fixed grates, moving grates, traveling grates, rotating grates and vibrating grates. Solid fuel with various characteristics can be burnt in this type of furnaces.

There are two types of fixed bed furnaces; co-current and counter current conversion as shown in (Figure 1-4)

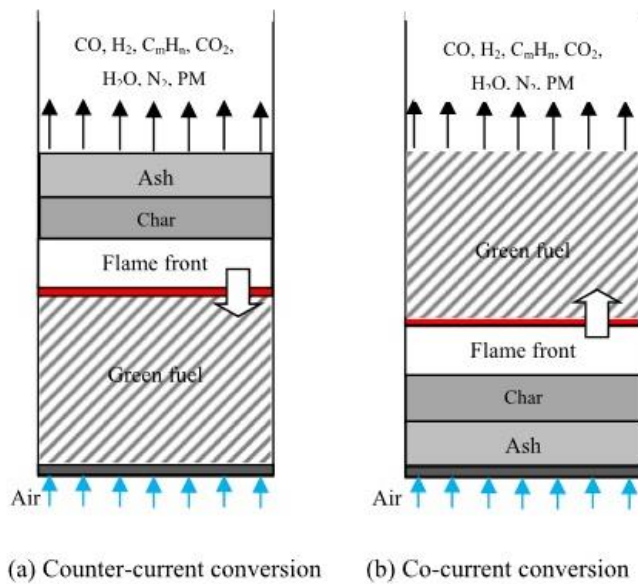


Figure 1-4 Fixed bed configurations[5]

In co-current configuration, the flame propagate upward with the direction of gas flow. The radiation and the diffusion of heat flows are relatively smaller because combustion starts at the bottom. Therefore the convective heat and mass flow in the co-current fixed bed is dominant.[5] High flue gas temperature, ease of implementation and high conversion rate are the advantages of this type whilst incorporated high cost due to installing complex initial ignition at the bottom and high level of tar deposition on the walls are the disadvantages.

In counter-current configuration ignition starts at the bed top, and propagates downwards which is opposite to the gas flow. This generate lower particulate matter and incorporate low cost in comparison with co-current packed beds.

### 1.2.2 Fluidized bed biomass Combustion

Biomass fuel is burnt in a self-mixing suspension of gas and solid bed material, in the fluidized bed. Fuel is mixed with an inert material such as sand. The primary air enters through the perforated plate at the bottom of fluidizes the bed and therefore it becomes a bubbling mass of particles and bubbles. The bed material represents 90-98% of the mixture of fuel and bed material and air flow must be sufficient enough to bed materials to be suspended and making the entire solid phase as a fluid. These furnaces are applicable for burning low quality, high moisture fuels.

This fluidized bed mechanism can be divided to sub categories in accordance with different gas flow patterns (Figure 1-5).

- **Bubbling Fluidized bed** – Air speed is high enough to cause fluidization of the fuel, but low enough to prevent solid particles from escaping the bed.
- **Circulating Fluidized bed** – operate with higher speed than bubbling fluidized bed to elutriation of smaller unburnt particles from the bed, hence cyclone is required in the downstream.

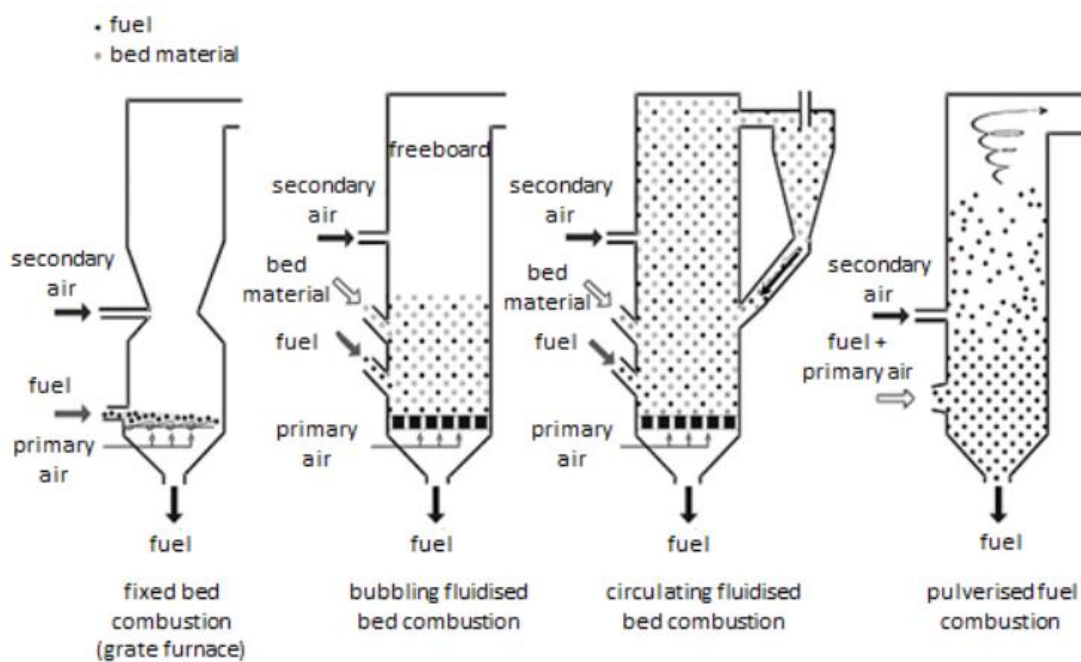


Figure 1-5: Principle combustion technologies for Biomass[4]

### 1.2.3 Pulverized Fuel Combustion

This is applicable for small size biomass particles. In pulverized combustion saw dust and fine wood particles are injected pneumatically into the furnace, while the transportation air is used as primary air which should be sufficient enough to entrain the particles. Fuel moisture contains should be less than 20% and should be maintain maximum fuel particle size between 10-20 mm range. Initial ignition introduced by an auxiliary burner and then transferred to the biomass. Fuel quality should be kept constant and the fuel injection to the system has to be carefully controlled due the explosion like behavior of biomass particles entering to the system. Since fuel gasification and charcoal burning occur simultaneously, quick load changes and efficient load control can be achieved.

### 1.3 Background

In accordance with Sri Lanka energy balance report 2007, the total primary energy requirement of the country is fulfilled by biomass, petroleum and hydropower. (Figure 1-6). But most of the secondary energy needs are driven by oil burning and hydropower which are non-renewable. As the primary energy, majority of bio-thermal energy is used in rural household sector as firewood. But there is a high potential to use biomass as the major energy source for power generation instead of non-renewable energy sources like coal or crude oil. Agricultural by products like rice husk, straw, saw dust and woods from Rubber and Gliricidia are highly available all over the country. Therefore bio-thermal conversion processes are very much applicable in the cost wise as well as environmental and renewable perspective as long term.

As the secondary energy, most of the power requirements for the industrial sector are fulfilled from the main coal power generation system. Presently biomass is widely using in the industries like tea, rubber, ceramic and textile manufacturing. Majority of them are moving towards biomass to fulfill their thermal and power requirements. Biomass energy can be adopted to the CHP systems if it is carefully optimized and efficiently designs to overcome present limitations and drawbacks in the industrial processes.

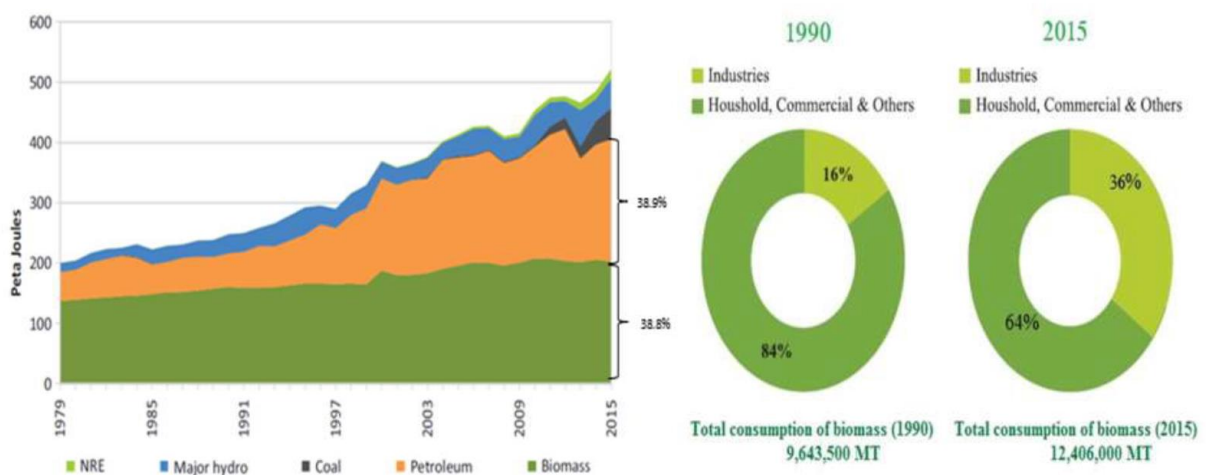


Figure 1-6: Primary Energy Supply of Sri Lanka & Biomass Utilization [6]



## 1.4 Objectives of Present Research

This research is focusing on two main objectives,

- Study the thermo-chemical processes in packed bed combustion
- Develop one dimensional mathematical model for two phase and solve using MATLAB and introduce simple layer lumped model for process simulation purpose

## 1.5 Summary of the thesis

**Chapter 1:** It gives brief introduction about world energy picture, biomass combustion, and its conversion technologies and Sri Lankan Background. In addition, there is a brief description about research objectives and summary of the thesis.

**Chapter 2:** In this section, Theory and literature review is presented about overview of biomass combustion and mathematical models and Solvers

**Chapter 3:** Mathematical model is explained in this chapter.

**Chapter 4:** In here Discretization method and MATLAB solver is described.

**Chapter 5:** This is consisting with results and discussion, how to present moving grate technology with walking column approach.

**Chapter 6:** Conclusion of the research work and future potentials are described here.

## 2. Literature Review

### 2.1 Overview of Fixed Bed Combustion

Numerous packed bed combustion models are available in the literature from zero dimensional to three dimensional analyses which has various forms depending on the configurations of combustors. The review of elaborations on packed bed modeling has broader due to its complexity and different fuel types. Basically there are homogeneous and heterogeneous models. There the difference lies in energy calculation procedure. In homogeneous models the temperature of gas and solid phase are assumed to be equal and single energy balance equation is applied. [7]-[9] In heterogeneous models the gas and solid phase has separate energy equations with two different temperatures in each phases.[10] - [12] They have considered heat and mass transfer between two phases by means of Nusselt and Sherwood Number correlations. In real the temperature difference between gas and solid phases is significant and should be taken into account. Therefore heterogeneous models are recommended for the detail analysis of the process.

Based on literature data heterogeneous models can be categorized into continuous models and discrete models. In continuous models, both phases are considered as distributed continuously over the whole spatial domain as macro scale. Inter particle effects are neglected and it is difficult to describe the bed shrinkage by using continuous models. To overcome these limitations discrete particle models are developed by considering intra-particle effects with momentum and energy exchange in micro scale.[13]-[15] In discrete models there is high calculation time with compared to continuous models.

During last two decades different types of fixed beds combustion models have been developed for several categories of solid fuels. Kinetics of burning char particles is investigated in several studies. [16] And there are numerous investigations are available for the packed bed combustion of solid waste materials. [17][18]

In addition most of the packed bed combustion models are developed for its steady state behavior. [19]

## 2.2 Mathematical Models

Biomass combustion study is a complicate process due to its large variation and physical structures. There are many parameters requires to analyze one particular system. Hence collecting parameters experimentally is difficult. For this reason, mathematical models use to analyze the process in wide range and use to optimize the combustion process. Advantage of using model-based simulations is, it can be used to study the process in detail by combining lower number of experimental data in a different way to analyze the whole system varying parameters. In this research works MATLAB is introduced as a solver for the mathematical simulation tool which is not been used in fixed bed combustion systems.

Most of the recent investigations based on the computational fluid dynamics (CFD) or Aspen plus which are complex solvers and need high computer facility to run the solver and highly time consuming. Therefore, those tools are not affordable for small scale industrial applications which have high potential to use fixed bed combustion applications.

CFD packed bed models are highly available in literature from varying different parameters. Mainly the studies have focused on both solid bed and free board. [20][12][4]. Free board modeling with CFD is highly investigating area during last two decades, because it is very much helpful to analyze the initial ignition and propagation of flame in the reactor.

One-Dimensional Pseudo-Homogeneous packed bed reactor modeling with NO-CO kinetics was investigated with MATLAB solver by Anad Srinivasan. [21] There finite difference method has been used for the modeling of species and energy equations while forward time center space (FTCS) method has been used to temperature modeling.

Since MATLAB is easily available and can be run with lower computer facility, this investigation fully focused on how to use MATLAB in transient one-dimensional fixed bed combustion system as a tool of model simulation.

### 3. Mathematical Model

A two phase, one dimensional, transient biomass packed bed combustion model was developed in this study to analyze the thermal properties of the general packed bed combustion reactor. Simple layer lumped modeling approach is being used in order to solve the correlations in MATLAB.

Mass, energy and species conservation has been applied for each solid and gas phase separately. Since uniform gas temperature was assumed in the bed for the simplicity of the model, energy equation for the gas is not applied.

#### 1-D transient governing equations for gas phase

Mass balance,

$$\frac{\partial(\varepsilon_b \rho_g)}{\partial t} + \frac{\partial(\rho_g U_g \varepsilon_b)}{\partial y} = S_{sg} \quad (3.1)$$

Where;

- $S_{sg}$  Heterogeneous reaction rates involving for mass transfer ( $\text{kg m}^{-3} \text{s}^{-1}$ )
- $\varepsilon_b$  Bed porosity
- $\rho_g$  Gas Density ( $\text{kg m}^{-3}$ )
- $U_g$  Gas phase velocity ( $\text{m s}^{-1}$ )

Energy balance;

$$\begin{aligned} \frac{\partial \varepsilon_b \rho_g C_{v,g} T_g}{\partial t} + \frac{\partial \varepsilon_b \rho_g U_g C_{v,g} T_g}{\partial y} \\ = \frac{\partial}{\partial y} \left( \varepsilon_b k_g \frac{\partial T_g}{\partial y} \right) + hA(T_s - T_g) + \sum_i r_{i,homo} \\ + R_{pyr} C_{v,g} (T_s - T_g) \end{aligned} \quad (3.2)$$

Where;

- $h$  Heat transfer coefficient ( $\text{W m}^{-2} \text{K}^{-1}$ )
- $k_g$  Thermal Conductivity of gas phase ( $\text{W m}^{-1} \text{K}^{-1}$ )
- $r_{i,homo}$  Rate of homogeneous reaction  $i$  ( $\text{kg m}^{-3} \text{s}^{-1}$ )
- $A$  Specific surface area of packed bed ( $\text{m}^{-1}$ )
- $C_{v,g}$  Heat Capacity of gas phase ( $\text{J kg}^{-1} \text{K}^{-1}$ )

Species balance;

$$\frac{\partial(\varepsilon_b \rho_g Y_{g,i})}{\partial t} + \frac{\partial(\varepsilon_b \rho_g U_g Y_{g,i})}{\partial y} = \frac{\partial}{\partial y} \left( \varepsilon_b \rho_g D_{g,i} \frac{\partial Y_{g,i}}{\partial y} \right) + r_i + \sum_j r_{i,homo} + \sum_i r_{i,hetero} \quad (3.3)$$

Where;

$Y_{g,i}$	Mole fraction of gas species i
$D_{g,i}$	Diffusion coefficient of gas species i ( $\text{m}^2 \text{s}^{-1}$ )
$r_{i,homo}$	Rate of homogeneous reaction i ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$r_i$	Rate of reaction i ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$r_{i,hetero}$	Rate of heterogeneous reaction i ( $\text{kg m}^{-3} \text{s}^{-1}$ )

### **1-D transient governing equations for solid phase**

Mass balance,

$$\frac{\partial(\varepsilon_b \rho_s)}{\partial t} + \nabla \cdot (\varepsilon_b \rho_s u_s) = -S_{sg} \quad (3.4)$$

Where;

$S_{sg}$	Heterogeneous reaction rates involving for mass transfer ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$\varepsilon_b$	Bed porosity
$\rho_s$	Solid Density ( $\text{kg m}^{-3}$ )
$U_s$	Shrinkage Velocity ( $\text{m s}^{-1}$ )

Energy balance;

$$\begin{aligned} \frac{\partial(1 - \varepsilon_b) \rho_s C_s T_s}{\partial t} + \frac{\partial(1 - \varepsilon_b) \rho_s C_s T_s U_s}{\partial y} \\ = \frac{\partial}{\partial y} \left( (1 - \varepsilon_b) k_s \frac{\partial T_s}{\partial y} \right) - hA(T_s - T_g) - \sum_i \Delta H_i r_{i,hetero} \end{aligned} \quad (3.5)$$

Where;

$h$	Heat transfer coefficient ( $\text{W m}^{-2} \text{K}^{-1}$ )
$k_s$	Thermal Conductivity of solid phase ( $\text{W m}^{-1} \text{K}^{-1}$ )
$r_{i,hetero}$	Rate of heterogeneous reaction i ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$A$	Specific surface area of packed bed ( $\text{m}^{-1}$ )
$C_s$	Heat Capacity of solid phase ( $\text{J kg}^{-1} \text{K}^{-1}$ )

Species balance;

$$\frac{\partial((1 - \varepsilon_b)\rho_s Y_{i,s})}{\partial t} + \frac{\partial((1 - \varepsilon_b)\rho_s U_s Y_{i,s})}{\partial y} - \frac{\partial((1 - \varepsilon_b)D_{i,s}U_s Y_{i,s})}{\partial y} = \sum_i r_{i,hetero} \quad (3.6)$$

- $Y_{i,s}$  Mass fraction of solid species i  
 $D_{g,i}$  Diffusion coefficient of solid species i ( $\text{m}^2 \text{s}^{-1}$ )  
 $r_{i,hetero}$  Rate of heterogeneous reaction i ( $\text{kg m}^{-3} \text{s}^{-1}$ )

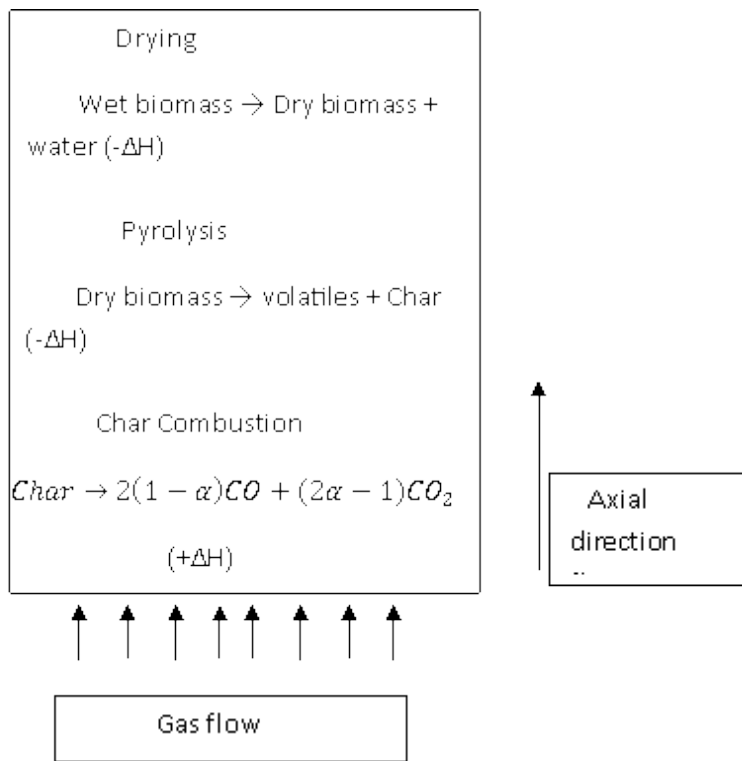


Figure 3-1: Fixed bed Combustion system

In the combustion process the main steps of solid conversion process-drying, devolatilization and char generation are controlled thermally while char combustion can be controlled both kinetically and diffusionally.

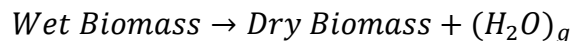
Model was developed by using below assumptions,

## Assumptions

- Biomass bed can be considered as a solid and gas phase reacting system.
- Free board is not considered for the Model
- Bed is assumed to be one dimensional- i.e. variations of temperatures and other parameters with the horizontal direction are neglected.
- Uniform high temperature gas flux is introduced with a high flow rate to initiate and propagate the reactions. (Therefore, assumed that radiation heat transfer is negligible)
- Layer lumped model is assumed by dividing the bed into six sections with 0.05m per each section.
- No heat is transferred through the walls of the packed bed.
- The biomass bed is considered as a porous zone with gas and solid phases with a mean porosity value
- The solid phase is proposed as a homogenous medium
- A thermally thin particle is used; no intra-particle temperature gradients are considered.
- Major constituents of biomass are water moisture, volatiles, char and ash
- Gas flow is incompressible and the fuel and gases are idealized as a plug flow
- Pressure drop along the bed is neglected
- The combustion gas is a mixture of species represented by  $H_2O_g$ ,  $O_2$ ,  $CO_2$ ,  $CO$ ,  $H_2$ ,  $N_2$ , and  $CH_4$

### **3.1 Drying Model**

Moisture content in the biomass is divided into two categories as free water which exists as liquid and vapour in the cell cavities and bound water in the cell walls.



In literature there are three different categories of models [4] to calculate the drying rate as thermal models, equilibrium models and kinetic rate models. Equilibrium models are applicable for low temperature drying processes while thermal models are using with the assumption of drying occurs at the fixed boiling temperature (373.15). In packed bed combustion drying occurs at high temperature range. Therefore the kinetic rate model is considered here and used the Arrhenius rate equation to calculate the drying rate.

$$R_{drying} = A_w \times \exp\left(\frac{-E_w}{RT_s}\right) \times \rho_s Y_{H_2O} \quad (3.7)$$

Where,

$Y_{H_2O}$  = Moisture fraction in biomass

$\rho_s$  = Solid phase density (kg/m<sup>3</sup>)

$A_w$  = pre exponential factor (s<sup>-1</sup>)

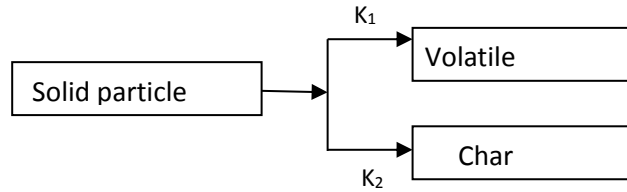
$E_w$  = Activation Energy (J/mol)

$R$  = Universal gas constant (J/mol.K)

$T_s$  = Solid Temperature (K)

### 3.2 Pyrolysis Model

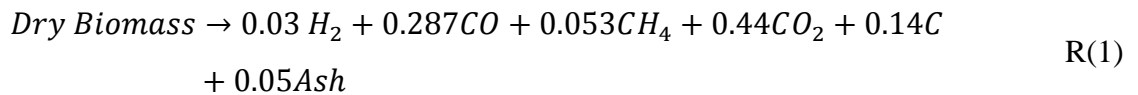
Analyzing this process involves series of complex steps and different models have been developed based on several conditions. During this study, single step pyrolysis is considered, where biomass is decomposed and produce volatiles and char.



$$r_{pyr,i} = 7 \times 10^4 \exp\left(-\frac{9977}{T_s}\right) (1 - \varepsilon_b) \rho_s Y_{Drywood} \quad (3.8)$$

#### 3.2.1 Composition of volatile matters

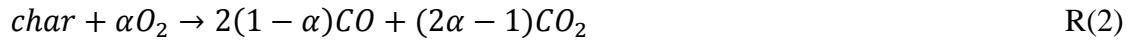
During the biomass pyrolysis process, CO, CO<sub>2</sub>, H<sub>2</sub>, CH<sub>4</sub>, carbon, ash and some light hydrocarbons are released. In this model, devolatilization reaction is considered as given below. The stoichiometric coefficients are taken from the literature. [22]





### 3.3 Char combustion Model

Here, overall heterogeneous char combustion is considered. [2]



$$r_{\text{char}} = A_p \left( \frac{[O_2]}{\frac{1}{K_t} + \frac{1}{K_d}} \right) \quad (3.9)$$

The terms are defined as below. [23]

$$k_t = 8620 \exp\left(-\frac{15900}{T_s}\right) \quad (3.10)$$

$$k_d = 2.53 \times 10^{-7} T_s^{0.75} / r_{\text{out}} \quad (3.11)$$

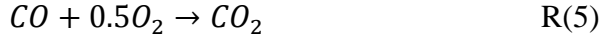
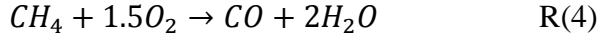
$$K_{\text{char}} = \frac{r_{CO}}{r_{CO_2}} = 33 \exp\left(-\frac{4700}{T_s}\right) \quad (3.12)$$

Therefore;

$$\alpha = \frac{2 + K_{\text{char}}}{2(1 + K_{\text{char}})} \quad (3.13)$$

### 3.4 Homogeneous reactions

Following homogeneous reactions were considered for this study.



The kinetic rate reactions are listed in table (3-1)[10]

Reaction	Reaction rate
$H_2 + 0.5O_2 \rightarrow H_2O$	$RH2 = 5.18 \times T_g^{1.5} \exp\left(\frac{-3420}{T_g}\right) C_{H_2}^{1.5} C_{O_2}$
$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$	$RCH4 = 1.6 \times 10^{10} \times \exp\left(\frac{-24157}{T_g}\right) C_{CH_4}^{0.7} C_{O_2}^{0.8}$
$CO + 0.5O_2 \rightarrow CO_2$	$RCO = 3.25 \times 10^7 \times \exp\left(\frac{-15098}{T_g}\right) C_{CO}^{0.5} C_{O_2}^{0.5}$

Table 3-1: Kinetic Reaction Rates

The kinetic reaction rate is limited by turbulent mixing rate of gas species, which can be calculated by using Eddy dissipation model. [24]

$$r_{t,i} = 4\rho_g \frac{\varepsilon}{k_g} \min\left(\frac{Y_j}{\phi_j M_j}, \frac{Y_k}{\phi_k M_k}\right) \quad (3.14)$$

Where,

j and k represent the reactants of reaction (i)

$\Phi$  is the stoichiometric ratio.

As the reaction rate of the homogeneous reaction is taken to be equal to the minimum value of kinetic rate and turbulent mixing rate. [24]

### 3.5 Heat and Mass transfer

In the biomass bed, gas and solid phases involve two main processes for interphase heat transfer,

- Convective heat transfer between two phases as a result of temperature difference
- Energy flow from solid to gas via hot volatile gases generated within the porous structure of biomass during pyrolysis process.

Overall Convective heat transfer coefficient is used here to develop the model;

$$Q_s^{conv} = -Q_g^{conv} = hA_p(T_g - T_s) \quad (3.15)$$

Where;

$$A_p - \text{specific surface area of biomass} = \frac{6 \times (1 - \varepsilon_b)}{d_p} \quad (3.16)$$

$$h = \frac{\varepsilon_b k_g Nu}{d_p} \quad (3.17)$$

$$Nu = 2 + 0.1Pr^{1/3}Re^{0.6} [5] \quad (3.18)$$

$$Pr = (C_{p,g}\mu)/k_g \quad (3.19)$$

In the pyrolysis process dry biomass is converted into gas products with creating energy transferring flow from solid phase to gas phase. It is assumed that these gasses are at the temperature of the solid phase. The release of these gas products are added additional energy transfer term in the gas phase energy equation;

$$H_{pyr} = R_{pyr}C_{v,g}(T_s - T_g) \quad (3.20)$$

#### 3.5.1 Initial ignition source

Gas is preheated to higher temperature and introduce to the packed bed at the bottom grate to initiate the combustion process. This flow is introduced continuously throughout the process to supply heat for the reactions since radiation heat is omitted for the simplicity of the model.

### 3.6 Physical Properties

Gas phase and solid phase thermal conductivity is evaluated by using below mentioned correlations [24]

$$k_g = 4.8 \times 10^{-4} T_g^{0.717} \quad (3.21)$$

$$k_s = 0.8k_g + 0.5RePrk_g \quad (3.22)$$

Heat capacities of solid and gas phase are assumed to be vary according to the relations given in equations ( 3.23) and (3.24) [24]

$$C_s = 420 + 2.09T_s + 6.85 \times 10^4 T_s^{-2} \quad (3.23)$$

$$C_g = 990 + 0.122T_g - 5680 \times 10^3 T_g^{-2} \quad (3.24)$$

The binary diffusion coefficients based on diffusion of a specific component in air, are calculated using equation (3.25) [25][26]

$$D_{i,air} = 0.0018583 \sqrt{T_g^3 \left( \frac{1}{M_i} + \frac{1}{M_{air}} \right) \frac{1}{p \sigma_{i,air}^2 \Omega_{i,air}}} \quad (3.25)$$

Where;

$\sigma_{i,air}$	Average Collision diameter (A)
$\Omega_{i,air}$	Diffusion collision integral
$M_i$	Molecular weight of species i (kg mol <sup>-1</sup> )
$M_{air}$	Molecular weight of air(kg mol <sup>-1</sup> )

## 4. Numerical Solution for the packed bed Model

### 4.1 Procedure

1. Define initial conditions
2. Assumed layer lumped model and apply conversion equations to both gas and solid phases separately.
3. Solve continuity equation for the gas phase
4. Apply mass balance for the solid phase
5. Solve discretized species balance equation for gas phase
6. Solve the discretized energy equations with the MATLAB for solid temperature
7. Take solved TS as the initial conditions and repeat the above procedure with time step  $t=1s$  and spacious step  $by=0.05 m$

### 4.2 Discretization

Gas phase species balance:

$$\frac{\partial(\varepsilon_b \rho_g Y_{g,i})}{\partial t} + \frac{\partial(\varepsilon_b \rho_g U_g Y_{g,i})}{\partial y} = \frac{\partial}{\partial y} \left( \varepsilon_b D_{g,i} \frac{\partial Y_{g,i}}{\partial y} \right) + \sum_j r_{i,homo} + \sum_i r_{i,hetero}$$

This is discretized as follows.

Assuming all the calculated variables n point;

$$\begin{aligned} \frac{\partial(Y_{g,i})}{\partial t} = & \left( \frac{1}{\varepsilon_b \rho_g} \right) (\varepsilon_b D_{g,i} \frac{\partial}{\partial y} \left( \frac{\partial Y_{g,i}}{\partial y} \right) - \varepsilon_b \rho_g U_g \frac{\partial(Y_{g,i})}{\partial y} \\ & + \sum_j r_{i,homo} + \sum_i r_{i,hetero}) \end{aligned} \quad (4.1)$$

Then discretized with respect to y;

$$\left( \frac{\partial Y_{g,i}}{\partial t} \right)_{n+1} = K_1 Y_{g,i,(n+1)} + K_2 \quad (4.2)$$

Where ;

$$\left(\frac{\partial Y_{g,i}}{\partial t}\right)_{n+1} = \frac{Y_{g,i}(n+1) - Y_{g,i}(n)}{\Delta y} \quad (4.3)$$

$$\frac{\partial^2 Y_{g,i}}{\partial y^2} = \frac{Y_{g,i}(n+1) - 2Y_{g,i}(n) + Y_{g,i}(n-1)}{\Delta y^2}; \quad (4.4)$$

When (n-1)<sup>th</sup> and n<sup>th</sup> point is known, n+1 point can be calculated.

After discretized second order differential equation becomes first order differential equation with time;

$$K1 = \left(\frac{1}{\varepsilon_b \rho_g}\right) \left(\frac{\varepsilon_b D_{g,i}}{\Delta y^2} - \frac{\varepsilon_b \rho_g U_g}{\Delta y}\right) \quad (4.5)$$

$$K2 = \left(\frac{1}{\varepsilon_b \rho_g}\right) \left(\left(\frac{-2\varepsilon_b D_{g,i}}{\Delta y^2} + \frac{\varepsilon_b \rho_g U_g}{\Delta y}\right) Y_{g,i}(n) + \left(\frac{\varepsilon_b D_{g,i}}{\Delta y^2}\right) Y_{g,i}(n-1) + \sum_j r_{i,homo} + \sum_i r_{i,hetero}\right) \quad (4.6)$$

Gas phase Energy balance;

Since a uniform high temperature gas flow is introduced throughout the process, it can be assumed that in the furnace gas temperature is equal.

Solid phase Energy balance;

Similarly, Solid phase energy equation is also discretized.

$$\frac{\partial T_s}{\partial t} = \left(\frac{1}{(1 - \varepsilon_b) \rho_s C_s}\right) \left((1 - \varepsilon_b) k_s \frac{\partial}{\partial y} \left(\frac{\partial T_s}{\partial y}\right) - (1 - \varepsilon_b) \rho_s C_s U_s \frac{\partial T_s}{\partial y} - hA(T_s - T_g) - \sum_i \Delta H_i r_{i,hetero} - Q_{walls}\right) \quad (4.7)$$

Here, bed shrinkage is considered to be zero;  $U_s=0$

$$\left(\frac{\partial T_s}{\partial t}\right)_{n+1} = P_1 T_{s,(n+1)} + P_2 T_{g,(n+1)} + P_3 \quad (4.8)$$

$$P_1 = \left(\frac{1}{(1-\varepsilon_b)\rho_s c_s}\right) \left(\frac{(1-\varepsilon_b)k_s}{\Delta y^2} - hA\right) \quad (4.9)$$

$$P_2 = \left(\frac{1}{(1-\varepsilon_b)\rho_s c_s}\right) (hA) \quad (4.10)$$

$$P_3 = \left(\frac{1}{(1-\varepsilon_b)\rho_s c_s}\right) \left( \left(\frac{-2(1-\varepsilon_b)k_s}{\Delta y^2}\right) T_s(n) + \left(\frac{(1-\varepsilon_b)k_s}{\Delta y^2}\right) T_s(n-1) + \sum_i r_{i,homo} + Q_{walls} \right) \quad (4.11)$$

#### 4.2.1 Initial Conditions

$T_s = 300$  K

Volatile fraction in biomass (Dry basis) = 81%

Free carbon fraction (Dry basis) = 14%

Ash fraction (Dry basis) = 5%

Initial Moisture content (wet basis) = 10%

Initial Mass in the packed bed reactor = 3.5 kg

Initial Gas Concentration

Oxygen – 23%

Nitrogen – 76.4%

H<sub>2</sub>O – 0.06%

#### **4.2.2 Other parameters**

$T_G = 800 \text{ K}$  (uniform within the bed)

$U_g = 9 \text{ m/s}$

$D_p = 20 \text{ mm}$

Bed height = 25 cm

Mean bed porosity = 0.5

Mean biomass density =  $500 \text{ kg/m}^3$



## 5. Results and Discussion

The mathematical model based on aforementioned assumptions was solved using MATLAB solver. To solve differential equation discretized form is used with ode45 solver. The procedure used here is method of line with two different for loops.

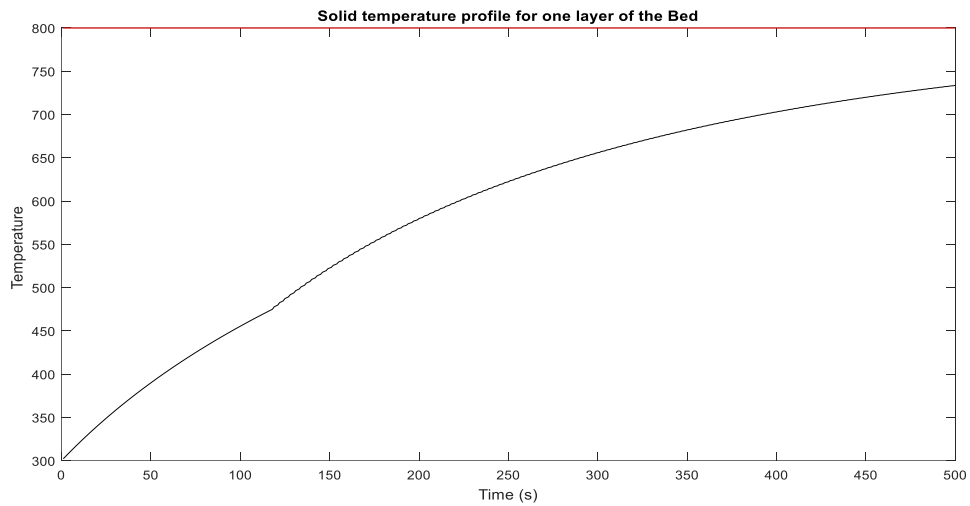


Figure 5-1: Solid Temperature Profile for one layer of the Bed

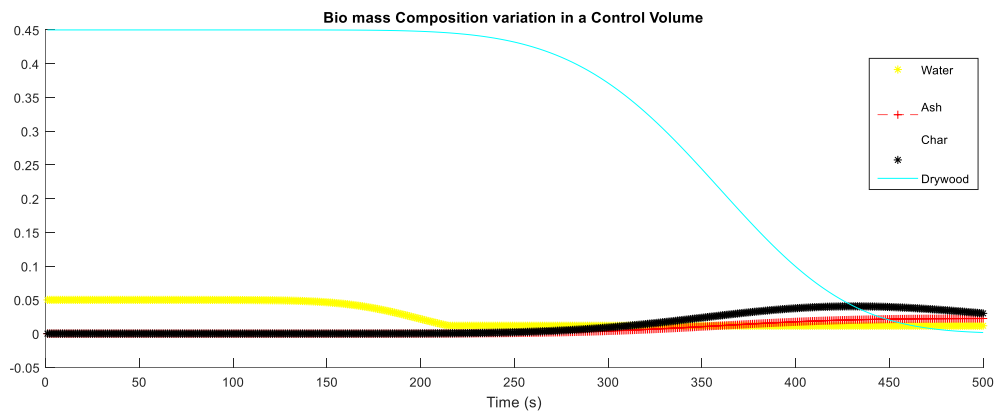


Figure 5-2: Solid Fuel composition variation in Control volume

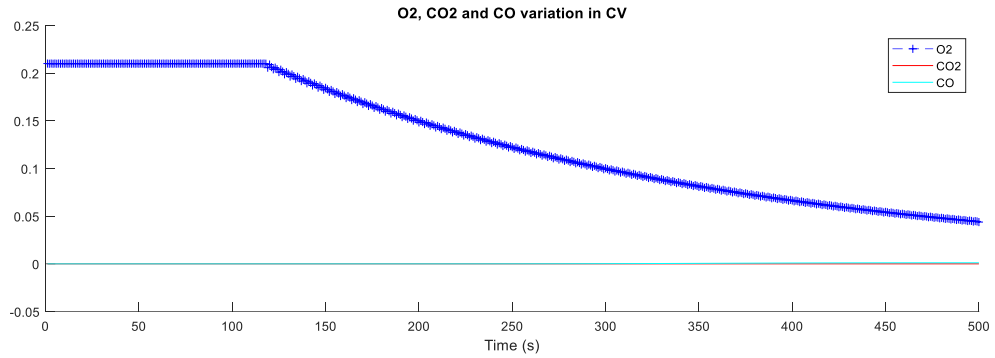


Figure 5-3: O<sub>2</sub>, CO<sub>2</sub> and CO variation in the Control Volume

In accordance with above graphs, packed bed combustion can be conducted with a high temperature gas flow and heterogeneous and homogeneous reactions are initiated after solid temperature increased above 450 K.

Then the mathematical model was solved for the entire biomass bed by considering simple layer lumped model. The results for the solid temperature variation, CO<sub>2</sub> and CO generation are presented in the figure 5-4,5,6 respectively. (For the MATLAB code please refer the appendix)

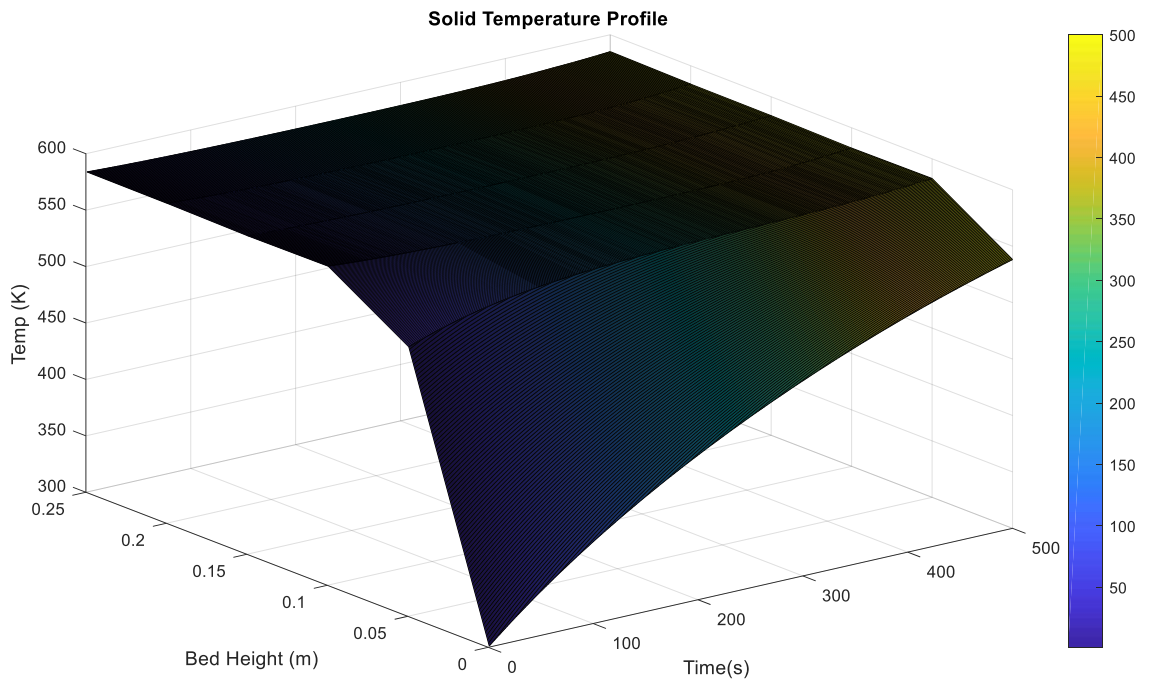


Figure 5-4 : Solid Temperature profile

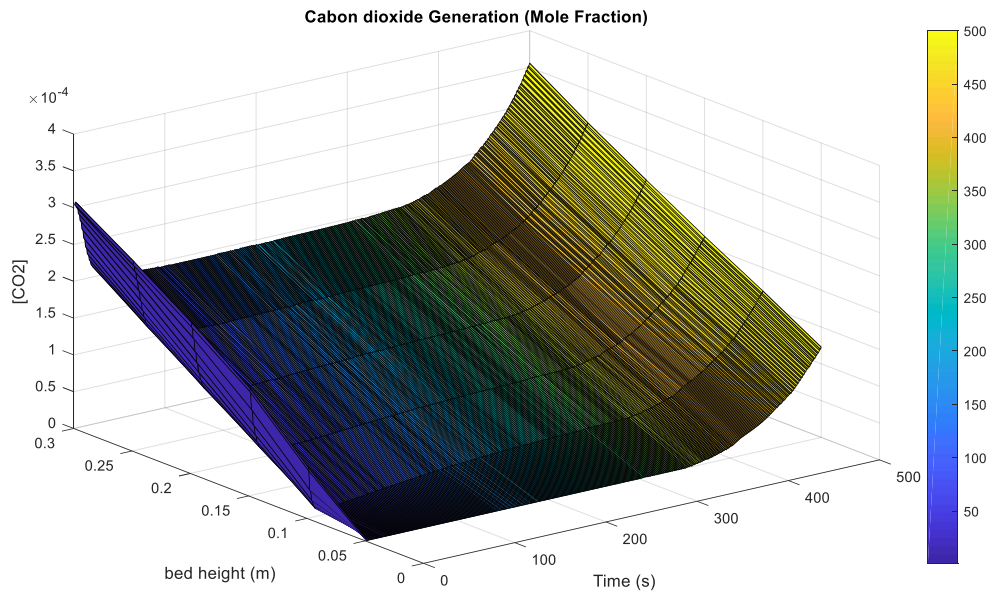


Figure 5-5: CO<sub>2</sub> Generation

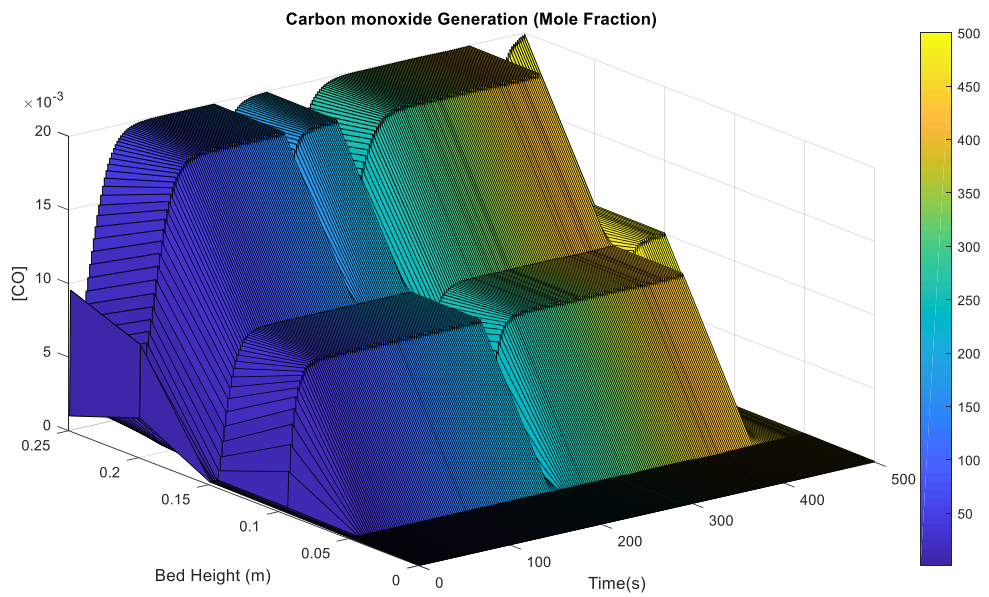


Figure 5-6: CO Generation

## 5.1 Validating Results

When the dimensions used for the simulation are from the lab scale biomass combustion unit located at the Department of chemical and process engineering, University of Moratuwa; comparison figures are 5-7 and 5-8. Although the dimensions was used for the simulation, radiation heat is not included in the simulation for the simplicity of the model. Therefore validation using the measurements from that system would not very well fitted. In future the simulation should be developed by incorporating packed bed radiation to get the exact validation results.

In the figure (5-7) the bed temperature in the simulation is constant at the end of the combustion because of the constant hot air inlet. In the experiment temperature is decreasing with the radiation heat loss.

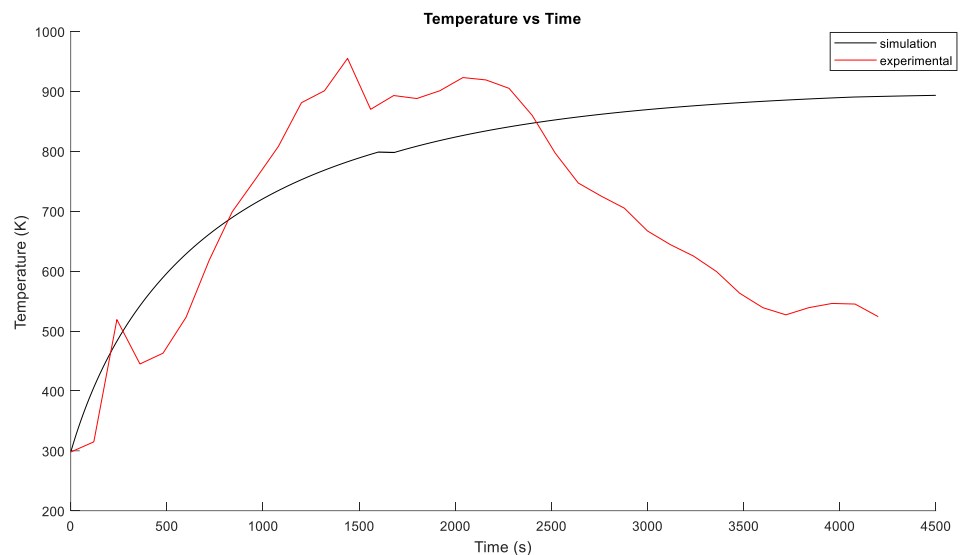


Figure 5-7: Temperature Variation of biomass bed

In the figure (5-8) a sudden mass loss can be seen in the model simulation between the time 500 -1300 s. But in the experiment it is a gradual loss. It can be assumed that it is because of the heat loss due to thermal radiation. In the simulation unique hot air inlet and no radiation heat loss is assumed, rapid pyrolysis and char combustion can be resulted rapid mass loss in the simulation.

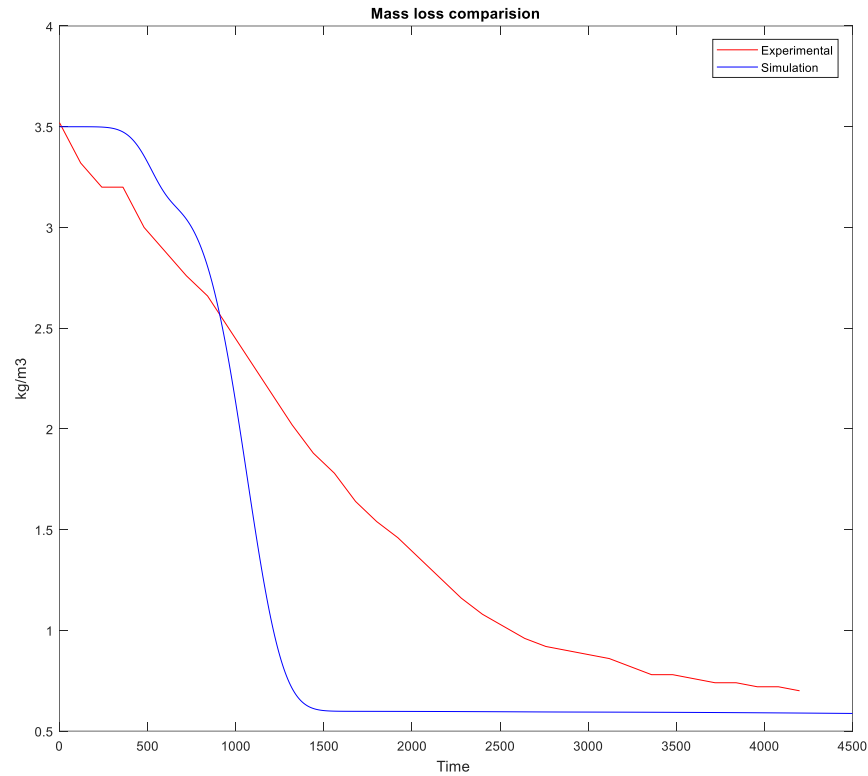


Figure 5-8: Mass Loss Comparison

## 5.2 Representation of moving grate

Industrial furnaces are usually equipped with moving grates to feed the system and remove ash with better burnout of solid biomass. In accordance with the results we can predict the moving packed bed combustion system. And we can find an efficient length of the bed by using walking column approach method. When we consider 1-D model in a particular time step it can be assumed to be equal to the one particular stage of a moving bed. (Figure 5-9) Therefore from this transient analysis of fixed bed combustion system can be related with a corresponding position on the moving grate with a simple relationship.

$$x = (M^0 \times t \times CV) \tag{5.1}$$

Where  $M^0 = \text{mass feed rate to the grate [kg/m}^2\text{s]}$

CV=Volume of Control Volume

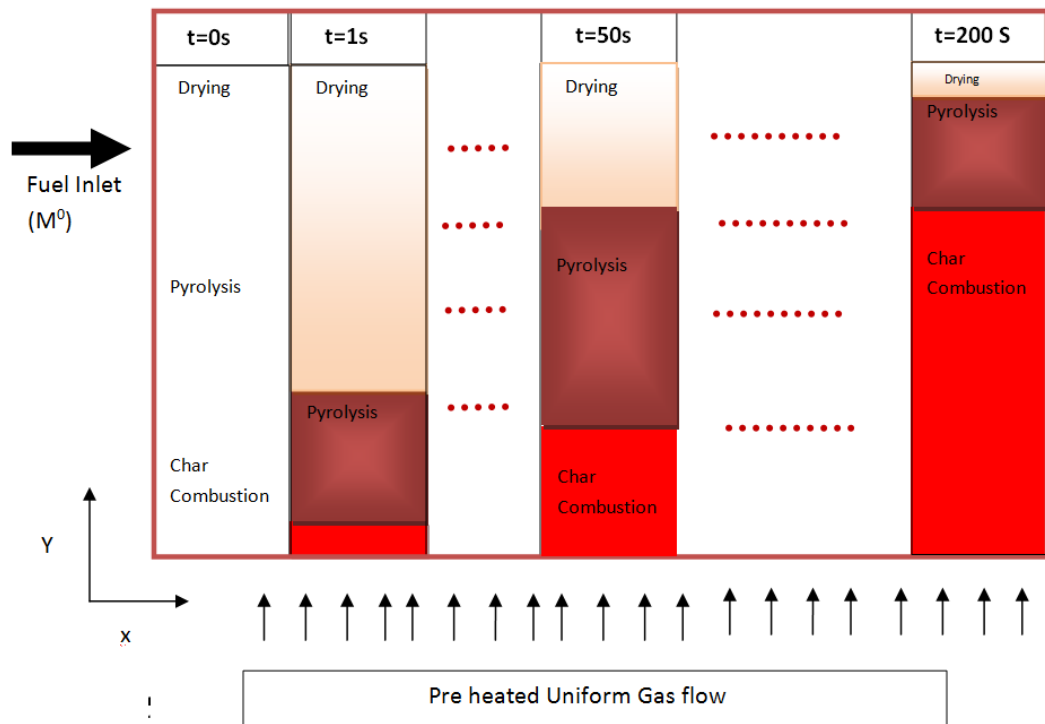


Figure 5-9 Walking Column approach

In accordance with the simulated results from the layer lumped model for the fixed bed solid temperature profile for different time steps can be presented as the Figure 5.10.

Simulation time taken to convert the biomass into ash = 1500 s

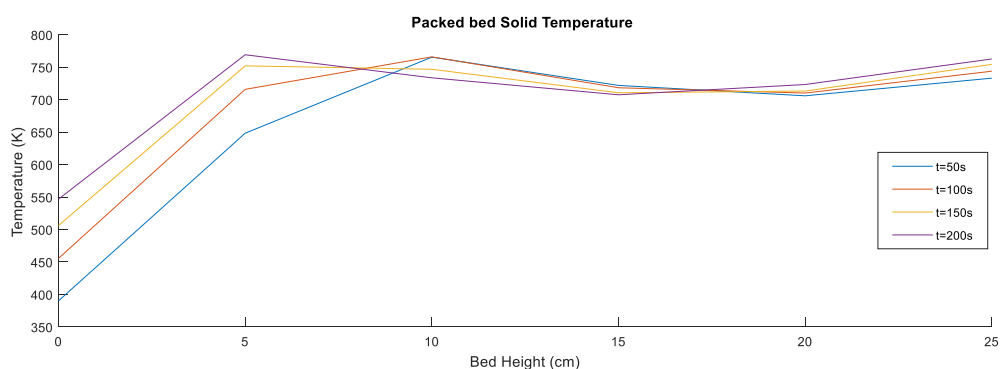


Figure 5-10 Packed bed Solid temperature at time 50,100,150 & 200s

This temperature profile can be validated with the results taken from the research work conducted to simulate 2-D woodchip combustion in a hot air generation system by Rajika and Narayana [19]

## 6. Conclusion

A mathematical model for fixed bed biomass combustion was developed with a layer lumped model approach and simulated using MATLAB solver. Conservation laws were considered to study the heat and mass transfer and the homogeneous and heterogeneous reactions in the gas and the solid phase of the biomass bed. The equations were discretized with respect to the y direction of the bed to convert the equations into ordinary differential equations.

From the results industrial moving bed process was deduced with the walking column approach method. It can be applied to calculate the efficient length of the moving grate furnace.

Finally, simple layer lumped model can be used to analyze packed bed combustion system instead of complex CFD modeling approach with finite difference method. And MATLAB can be used to solve one dimensional two phase heterogeneous transient fixed bed biomass combustion processes with lower simulation time hence with a lower computational cost.

### 6.1 Future works

MATLAB can be used in variety of complex combustion simulation works by considering all the varying parameters which are considered as constant in this present study. Specially shrinkage can be included for developing the transient packed bed model. Instead of uniform high temperature gas flow radiation heat can be incorporated and develop the existing MATLAB code accordingly. And variation of solid density and bed porosity with the thermal decomposition of biomass can be taken into account when developing the model.

Since MATLAB is user friendly mathematical tool, development based on this may applicable in wide variety of industries with low computational cost.

For the smooth simulation it can be used lower spatial step and time step as well.

## 7. References

- [1] S. Ladanai and J. Vinterbäck, “Global Potential of Sustainable Biomass for Energy.”
- [2] IEA, “IEA Energy Technology Essentials - Biomass for Power Generation and CHP,” *High Temp.*, pp. 1–4, 2007.
- [3] R. Mehrabian, A. Shiehnejadhesar, R. Scharler, and I. Obernberger, “Multi-physics Modeling of Packed Bed Biomass Combustion,” *Fuel*, vol. 122, pp. 164–178, 2014.
- [4] N. Duffy, “Investigation of Biomass Combustion in Grate Furnaces using CFD,” *02.03.01\_CombustionBiomass*, no. December, 2012.
- [5] H. Khodaei, Y. M. Al-Abdeli, F. Guzzomi, and G. H. Yeoh, “An overview of processes and considerations in the modelling of fixed-bed biomass combustion,” *Energy*, vol. 88, pp. 946–972, 2015.
- [6] S. Ranasinghe, “Promoting Sustainable Biomass Energy Production and Modern Bio-Energy Technologies.”
- [7] R. P. Van Der Lans, L. T. Pedersen, A. Jensen, P. Glarborg, and K. Dam-Johansen, “Modelling and experiments of straw combustion in a grate furnace,” *Biomass and Bioenergy*, vol. 19, no. 3, pp. 199–208, 2000.
- [8] D. Vortmeyer and R. J. Schaefer, “Equivalence of one- and two-phase models for heat transfer processes in packed beds: one dimensional theory,” *Chem. Eng. Sci.*, vol. 29, no. 2, pp. 485–491, 1974.
- [9] J. S. Ryan and W. L. H. Hallett, “Packed bed combustion of char particles: Experiments and an ash model,” *Chem. Eng. Sci.*, vol. 57, no. 18, pp. 3873–3882, 2002.
- [10] H. Zhou, A. D. Jensen, P. Glarborg, P. A. Jensen, and A. Kavaliauskas, “Numerical modeling of straw combustion in a fixed bed,” *Fuel*, vol. 84, no. 4, pp. 389–403, 2005.
- [11] W. Yang, C. Ryu, and S. Choi, “Unsteady one-dimensional model for a bed combustion of solid fuels,” *Proc. Inst. Mech. Eng. Part A J. Power Energy*, vol. 218, no. 8, pp. 589–598, 2004.
- [12] R. Mehrabian Bardar, “CFD Simulation of the Thermal Conversion of Solid Biomass in Packed Bed Furnaces by Ramin Mehrabian Bardar,” no. November, 2013.
- [13] L. Shan *et al.*, “Studies on combustion behaviours of single biomass particles using



- a visualization method,” *Biomass and Bioenergy*, vol. 109, no. September 2017, pp. 54–60, 2018.
- [14] J. Porteiro, J. L. Míguez, E. Granada, and J. C. Moran, “Mathematical modelling of the combustion of a single wood particle,” *Fuel Process. Technol.*, vol. 87, no. 2, pp. 169–175, 2006.
- [15] S. Kumar and S. Dasappa, “Modeling and analysis of single particle conversion of biomass in a packed bed gasification system,” vol. 112, pp. 1382–1395, 2017.
- [16] J. Cooper and W. L. H. Hallett, “A numerical model for packed-bed combustion of char particles,” *Chem. Eng. Sci.*, vol. 55, no. 20, pp. 4451–4460, 2000.
- [17] D. Shin and S. Choi, “The combustion of simulated waste particles in a fixed bed,” *Combust. Flame*, vol. 121, no. 1–2, pp. 167–180, 2000.
- [18] H. Ström, S. Sasic, and H. Thunman, “Challenges and opportunities in the Eulerian approach to numerical simulations of fixed-bed combustion of biomass,” *Procedia Eng.*, vol. 102, pp. 1573–1582, 2015.
- [19] J. K. A. T. Rajika and M. Narayana, “Modelling and simulation of wood chip combustion in a hot air generator system,” *Springerplus*, vol. 5, no. 1, 2016.
- [20] M. A. Gómez, J. Porteiro, D. Patiño, and J. L. Míguez, “CFD modelling of thermal conversion and packed bed compaction in biomass combustion,” *Fuel*, vol. 117, pp. 716–732, 2014.
- [21] A. Srivivasan, “One-Dimensional Pseudo-Homogeneous Packed Bed Reactor Modeling Including No-Co Kinetics,” p. 206, 2011.
- [22] K. Kwiatkowskia and P. Zukb, “Biomass gasification solver based on OpenFOAM,” *Comput. Phys. Commun.*, no. November, pp. 1–29, 2013.
- [23] T. Jurena, *Numerical modelling of grate combustion Ph.D. Thesis*. 2012.
- [24] N. Fernando and M. Narayana, *A comprehensive two dimensional Computational Fluid Dynamics model for an updraft biomass gasifier*, vol. 99. Elsevier Ltd, 2016.
- [25] N. Wakao and S. Kaguei, “Heat and mass transfer in packed beds,” vol. 1, p. 18, 1983.
- [26] F. Grinnell, *Second Edition*. 2018.

## 8. Appendix

### A ) MATLAB Code for Modelling Packed bed Combustion

```
function fi=finalpackedbedmodel
clc;
clear all;

% -----
epsilonb0=0.5; % Bed porosity
MT=3.5; % biomass weight in the packedbed [kg]
MH2O0=0.10*MT; % Moisture mass (Dry basis)
Mdrywood0=0.90*MT; % Initial drywood mass
Mchar0=0; % Initial Char
Mash0=0; % Initial ash
Mvol=0; % Initial Volatile
rho_S=200; % Initial Solid density
rho_g=1.225; % Gas density
hvap=2257.92*10^3; % Water evaporation enthalpy (J/kg)

% Initial concentration of gas
Y_O20=0.23; % Initial O2 molar fraction
Y_N20=0.764; % Initial Nitrogen molar fraction
Y_CH40=0; % Initial Methane molar fraction
Y_H20=0; % Initial Hydrogen molar fraction
Y_CO20=0; % Initial Carbon dioxide molar fraction
YCO20=0; % Initial Carbon dioxide molar fraction
Y_CO0=0; % Initial Carbon monoxide molar fraction
Y_H2Og0=0.006; % Initial Water vapour fraction
YH2Og=0.006; % Initial Water vapour fraction
HCOg=-10.1*10^6; % enthalpy of CO gas [J/kg]
HH2g=-1.42919*10^8; % enthalpy of H2 gas
HCH4g=-1.7473*10^7; % enthalpy of CH4 gas
HH2Og=13435; % H2O(liquid/gas)enthalpy of formation [J/kg]
HCs_CO2=14.38*10^6; % Char to carbon dioxide fomation enthalpy (J/kg)
HCs_H2O=10.95*10^6; % Char to water vapour fomation enthalpy (J/kg)
r_out=0.075; % Reactor outer Radius [m]

% Calculating TS & TG values
Ug0=9; % Initial Gas velocity
%-----
dp=0.02; % Particle Diameter
dy=0.05; % Height of the CV
%-----
TS0=298; % initial Solid Temprature
TG0=800; % Initial gas temperature

% Define Intial Values-----
TS=TS0;
T_S=298;
TG=TG0;
T_G=800;
Ug=Ug0;
MH2O=MH2O0;
Mdrywood=Mdrywood0;
Mchar=Mchar0;
Mash=Mash0;
epsilonb=epsilonb0;
Y_O2=Y_O20;
```

```

YO2=0.23;
Y_CH4=Y_CH40;
YCH4=0;
Y_H2=Y_H20;
YH2=0;
Y_CO=Y_CO0;
YCO=0;
Y_CO2=Y_CO20;
YCO2=YCO20;
Y_H2Og=Y_H2Og0;
epsilon=0.7;

%---Init array for storing values for plotting

tSize =4500; %--Length of 't'
nSize = 6;%--y=0.05: 0.3( bed height=0.3 and dy=0.05)

IData = zeros(nSize,tSize);
tsData = zeros(nSize,tSize);
tgData= zeros(nSize,tSize);
UgData = zeros(nSize,tSize);
MH2OData = zeros(nSize,tSize);
MdrywoodData = zeros(nSize,tSize);
McharData = zeros(nSize,tSize);
MashData = zeros(nSize,tSize);
MTData = zeros(nSize,tSize);
Y_O2Data = zeros(nSize,tSize);
Y_CH4Data = zeros(nSize,tSize);
Y_H2Data = zeros(nSize,tSize);
Y_CO2Data = zeros(nSize,tSize);
Y_COData = zeros(nSize,tSize);
Y_H2OgData = zeros(nSize,tSize);
%-----

% For loop to calculate all temperature values along the y direction

for n=1:nSize
    % For loop to calculate all temperature values along at the y=0.05m
    for I=1:tSize

        if(n~=1)
            TS = tsData(n-1,I);
            TG= tgData(n-1,I);
            MH2O = MH2OData(n-1,I);
            Mdrywood = MdrywoodData(n-1,I);
            Mchar = McharData(n-1,I);
            Mash = MashData(n-1,I);
            MT = MTData(n-1,I);
            Y_O2 = Y_O2Data(n-1,I);
            Y_CH4 = Y_CH4Data(n-1,I);
            Y_H2 = Y_H2Data(n-1,I);
            Y_CO2= Y_CO2Data(n-1,I);
            Y_CO = Y_COData(n-1,I);
            Y_H2Og=Y_H2OgData(n-1,I);
            Ug=UgData(n-1,I);
        end

        Ap=6*epsilonb/dp; % Specific surface area

% Drying equation-----

```

```

if MH2O>0
Rdry=5.6*10^6*exp(-10584/TS0)*(1-epsilonb)*MH2O; % kg/m3 s]
else
Rdry=0;
end

% Pyrolysis equation-----
if Mdrywood>0 && (TS0>=473.15) && (TS0<=1173.15)
Rpyr=1*10^8*exp(-15083/TS0)*(1-epsilonb)*Mdrywood % [kg/m3 s]
else
Rpyr=0
end

if MH2O <Rdry
MH2O=MH2O
else
MH2O=MH2O-Rdry % [kg/m3]
end

if Mdrywood <Rpyr
Mdrywood= Mdrywood;
else
Mdrywood=Mdrywood-Rpyr; % [kg]
end

%-----
%Char reaction -----
if (Y_O2>0) && (Mchar>0)
Kchar=33*exp(-4700/TS);
alpha=(2+Kchar)/(2+2*Kchar);
KC1=8620*exp(-15900/TS);
KD1=r_out/(2.53*10^-7*TS^0.75);
Rchar1=(Ap*Y_O2/(alpha*32))/((1/KC1)+(1/KD1)) % [kg/m3 s]
else
Rchar1=0;
alpha=0;
end
deltaHc=(2*(1-alpha))*9.8*10^6+(2*alpha-1)*33.1*10^6; %
[combustion reaction enthalpy (J/kg)]

Mchar=Mchar+0.14*Rpyr-Rchar1;
Mash=Mash+0.05*(Rpyr); % [kg/m3]
Mvol=Mvol+(Rpyr)*0.81; % [kg/m3]

MT=Mash+Mchar+Mdrywood+MH2O;

%-----

Ug=Ug0+((0.81*Rpyr*0.1*dy)/(rho_g*epsilonb)); % [m/s]
%-----
% Parameters required to calculate convective heat transfer

cp_g=990+0.122*TG-5680*10^3*(TG)^-2; % Heat capacity of gas [
J/kg K]
cp_s=420+2.09*TS+6.85*10^4*(TS)^-2; % Heat capacity of solid
phase [J/kg k]

meu=(1.98*10^-5)*(TG/300)^(2/3);

```

```

k_g=4.8*(10^-4)*TG^0.717; % thermal conductivity [ W/m K]
Re=rho_g*Ug*dp/1.523; % Renolds Number
Pr=(cp_g*meu)/k_g; % Prandtl Number
Nu=2+0.1*(Pr^(1/3))*(Re)^0.6; % Nusselts Number
k_S=0.8*k_g+0.5*Re*Pr*k_g; % thermal conductivity [W/m k]

%-----
% Homogeneous reaction rates

%CO combustion rate
if Y_CO>0 && Y_H2Og>0
    if(Y_CO/28) >(Y_O2/(0.5*32))
        rt_CO=(4*rho_g*epsilon/k_g)*(Y_O2/(0.5*32)); % [kg/m3 s]
    else
        rt_CO=(4*rho_g*epsilon/k_g)*(Y_CO/28);
    end
else
    rt_CO=0;
end

if Y_CO>0 && Y_H2Og>0
    rCO=3.25*10^7*exp(-
15098/TG)*(Y_CO/28)*(Y_H2Og/18)^0.5*((Y_O2/(0.5*32))^0.5); % [kg/m3
s]
else
    rCO=0;
end

RCO=min(rt_CO,rCO);
%-----
%H2 combustin rate
if Y_H2>0 && Y_O2>0
    if (Y_H2/2) >(Y_O2/(0.5*32))
        rt_H2=(4*rho_g*epsilon/k_g)*(Y_O2/(0.5*32));
    else
        rt_H2=(4*rho_g*epsilon/k_g)*(Y_H2/2);
    end
else
    rt_H2=0;
end

if Y_H2>0 && Y_O2>0
    rH2=5.18*(TG^1.5)*exp(-3420/TG)*(Y_O2/(0.5*32))*(Y_H2/2)^1.5;
else
    rH2=0;
end

RH2=min(rt_H2,rH2);
%-----
% Metane cmbustion rate
if Y_CH4>0 && Y_O2>0
    if (Y_CH4/16) >(Y_O2/(2*32))
        rt_CH4=(4*rho_g*epsilon/k_g)*(Y_O2/(2*32));
    else
        rt_CH4=(4*rho_g*epsilon/k_g)*(Y_CH4/16);
    end
else
    rt_CH4=0;
end

```

```

end

if Y_CH4>0 && Y_O2>0
rCH4=1.6*10^10*exp(-24157/TG)*((Y_CH4/16)^0.7)*(Y_O2/(2*32))^0.8;
else
rCH4=0;
end

RCH4=min(rt_CH4,rCH4)

%-----
%Species balance in gas phase;

sigmaCO2_Air=0.5*(3.617+3.996);
sigmaCO_Air=0.5*(3.617+3.590);
sigmaCH4_Air=0.5*(3.617+3.780);
sigmaH2_Air=0.5*(3.617+2.915);
sigmaO2_Air=0.5*(3.617+3.433);
sigmaH2O_Air=0.5*(3.617+3.176);
EpsilonCO2=(113*97)^1/2;
EpsilonCO=(110*97)^1/2;
EpsilonH2=(38*97)^1/2;
EpsilonO2=(99.8*97)^1/2;
EpsilonCH4=(154*97)^1/2;
EpsilonH2O=(123*97)^1/2;

% YCO2 balance
if (Y_CO2>=0)

DCO2Air=0.0018583*sqrt(TG^3*((1/28.97)+(1/44.01)))*(1/(sigmaCO2_Air^2)
*(44.54*EpsilonCO2^(-4.909)+1.911*EpsilonCO2^(-1.575))^0.1); % [m2/s]

K1=(-
epsilonb*rho_g*Ug/dy+DCO2Air*epsilonb/dy^2)*(1/(epsilonb*rho_g));
K2=((epsilonb*rho_g*Ug/dy-
2*DCO2Air*epsilonb/dy^2)*Y_CO2+YCO2*(epsilonb*DCO2Air/dy^2)+RCO+(Rchar
1*(2*alpha-1))+0.443*(Rpyr))*(1/(epsilonb*rho_g));

dYCO2dt=K1*Y_CO2+K2;

tspan=[0:1:3];
[t,Y_CO2]=ode45(@ (t,Y_CO2) K1*Y_CO2+K2,tspan,Y_CO20);

B0=[Y_CO2];

YCO2=B0(1,1);
Y_CO2=B0(2,1);
else
YCO2=0;
Y_CO2=0;
end
if (Y_CO2<0)
Y_CO2=0;
else
Y_CO2= Y_CO2;
end
Y_CO20=Y_CO2;

% YCO balance

```

```

if (Y_CO>=0)

DCOAir=0.0018583*sqrt(TG^3*((1/28.97)+(1/28)))*(1/(sigmaCO_Air^2))*(44.
54*EpsilonCO^(-4.909)+1.911*EpsilonCO^-1.575)^0.1);

K3=(-epsilonb*rho_g*(2*Ug-
Ug0)/dy+DCOAir*epsilonb/dy^2)*(1/(epsilonb*rho_g));
K4=((epsilonb*rho_g*Ug0/dy-
2*DCOAir*epsilonb/dy^2)*Y_CO+YCO*(epsilonb*DCOAir/dy^2)+(RCH4-
RCO+Rcharl*2*(1-alpha)+0.28*Rpyr))*(1/(epsilonb*rho_g));

dYCOdt=K3*Y_CO+K4;

tspan=[0:1:3];
[t,Y_CO]=ode45(@ (t,Y_CO) K3*Y_CO+K4,tspan,Y_CO0);

B1=[Y_CO];
YCO=B1(1,1);
Y_CO=B1(2,1);
else
YCO=0;
Y_CO=0;
end
Y_CO0=Y_CO;

% YH2 balance
if (Y_H2>=0)

DH2Air=0.0018583*sqrt(TG^3*((1/28.97)+(1/2)))*(1/((sigmaH2_Air^2))*(44.
54*(EpsilonH2)^(-4.909)+1.911*EpsilonH2^-1.575)^0.1));

K5=(-epsilonb*rho_g*(2*Ug-
Ug0)/dy+DH2Air*epsilonb/dy^2)*(1/(epsilonb*rho_g));
K6=((epsilonb*rho_g*Ug0/dy-
2*DH2Air*epsilonb/dy^2)*Y_H2+YH2*(epsilonb*DH2Air/dy^2)+(-
RH2+0.03*Rpyr))*(1/(epsilonb*rho_g));

dYH2dt=K5*Y_H2+K6;

tspan=[0:1:3];
[t,Y_H2]=ode45(@ (t,Y_H2) K5*Y_H2+K6,tspan,Y_H20);

B2=[Y_H2];

YH2=B2(1,1);
Y_H2=B2(2,1);
else
YH2=0;
Y_H2=0;
end
Y_H20=Y_H2;

% YCH4 balance
if (YCH4>=0)

DCH4Air=0.0018583*sqrt(TG^3*((1/28.97)+(1/16)))*(1/((sigmaCH4_Air^2))*(
44.54*(EpsilonCH4)^(-4.909)+1.911*(EpsilonCH4^-1.575)^0.1));

```

```

    K7=(-epsilon*b*rho_g*(2*Ug-
Ug0)/dy+DCH4Air*epsilon/b/dy^2)*(1/(epsilon*b*rho_g));
    K8=((epsilon*b*rho_g*Ug0/dy-
2*DCH4Air*epsilon/b/dy^2)*Y_CH4+YCH4*(epsilon*b*DCH4Air/dy^2)+(-
RCH4+0.056*Rpyr))*(1/(epsilon*b*rho_g));
    dYCH4dt=K7*Y_CH4+K8;

    tspan=[0:1:3];
    [t,Y_CH4]=ode45(@(t,Y_CH4) dYCH4dt,tspan,Y_CH40);

    B3=[Y_CH4];
    YCH4=B3(1,1);
    Y_CH4=B3(2,1);
    else
    YCH4=0;
    Y_CH4=0;
    end
    Y_CH40=Y_CH4;

    % YO2 balance
    if (Y_O2>0)

DO2Air=0.0018583*sqrt(TG^3*((1/28.97)+(1/32)))*(1/((sigmaO2_Air^2)*(44
.54*EpsilonO2^(-4.909)+1.911*EpsilonO2^(-1.575)^0.1)));

    K9=(-epsilon*b*rho_g*(2*Ug-
Ug0)/dy+DO2Air*epsilon/b/dy^2)*(1/(epsilon*b*rho_g));
    K10=((epsilon*b*rho_g*Ug0/dy-
2*DO2Air*epsilon/b/dy^2)*Y_O2+YO2*(epsilon*b*DO2Air/dy^2)-
0.5*RCO+(Rchar1*(-alpha))-1.5*RCH4-0.5*RH2)*(1/(epsilon*b*rho_g));

    dYO2dt=K9*Y_O2+K10;

    tspan=[0:1:3];
    [t,Y_O2]=ode45(@(t,Y_O2) K9*Y_O2+K10,tspan,Y_O20);

    B4=[Y_O2];

    YO2=B4(1,1);
    Y_O2=B4(2,1);
    else
    YO2=0.23;
    Y_O2=0.23;
    end
    Y_O20=Y_O2;

    % YH2O balance
    if (Y_H2Og>0)

DH2OAir=0.0018583*sqrt(TG^3*((1/28.97)+(1/18)))*(1/((sigmaH2O_Air^2)*(
44.54*EpsilonH2O^(-4.909)+1.911*EpsilonH2O^(-1.575)^0.1)));

    K11=(-epsilon*b*rho_g*(2*Ug-
Ug0)/dy+DH2OAir*epsilon/b/dy^2)*(1/(epsilon*b*rho_g));
    K12=((epsilon*b*rho_g*Ug0/dy-
2*DH2OAir*epsilon/b/dy^2)*Y_H2Og+YH2Og*(epsilon*b*DH2OAir/dy^2)+(Rdry/18
)+RH2)*(1/(epsilon*b*rho_g));

    dYH2Odt=K11*Y_H2Og+K12;

```



```

tspan=[0:1:3];
[t,Y_H2Og]=ode45(@ (t,Y_H2Og) K11*Y_H2Og+K12,tspan,Y_H2Og0);

B5=[Y_H2Og];

YH2Og=B5(1,1);
Y_H2Og=B5(2,1);
else
    YH2Og=0.0006;
    Y_H2Og=0.0006;
end
Y_H2Og0=Y_H2Og;

US=0; %Considering No shrinkage

% % % % % % %-----
%energy balance;

S_solid=(Rchar1*deltaHc)-(Rdry*hvap)-(170.2*10^3*0.81*Rpyr);

hconvec=k_g*epsilonb*Nu/dp;

S_gas=(RCO*HCOg+RCH4*HCH4g+RH2*HH2g)-Rchar1/12*HCs_H2O;

P1=((k_S*(1-epsilonb)/dy^2)-hconvec*Ap-(rho_S*(1-
epsilonb)*US*cp_s/dy))/((1-epsilonb)*rho_S*cp_s);
P2=hconvec*Ap/((1-epsilonb)*rho_S*cp_s);
P3=(1/((1-epsilonb)*rho_S*cp_s))*((-2*(1-
epsilonb)*k_S/dy^2)+(rho_S*(1-epsilonb)*cp_s*US/dy))*TS+T_S*((1-
epsilonb)*k_S/dy^2)+S_solid);

L1=(hconvec*Ap+0.81*Rpyr*cp_g)/(epsilonb*rho_g*cp_g); %
L2=((k_g*epsilonb/dy^2)-(hconvec*Ap)-
(0.81*Rpyr*cp_g))/(epsilonb*rho_g*cp_g)-Ug/dy;
L3=(1/(epsilonb*rho_g*cp_g))*((-
2*k_g*epsilonb/dy^2+(epsilonb*rho_g*Ug*cp_g/dy))*TG+(epsilonb*k_g/dy^2
)*T_G+S_gas);

F=@(t,y)[P1*y(1)+P2*y(2)+P3; L1*y(1)+L2*y(2)+L3];
tspan=[0:1:3];
y0=[TS0,TG0];
[t,Y]=ode45(F,tspan,y0);

A=[Y];
T_S=A(1,1);
T_G=750;
TS=A(2,1)
TG=800;
TS0=TS;
TG0=800;
%---Adding values to array for plotting.
    tsData(n,I)=TS;
    tgData(n,I)=TG;
    IData(n,I)= I;
    UgData(n,I)= Ug;
    MH2OData(n,I)= MH2O;
    MdrywoodData(n,I) =Mdrywood;

```

```

McharData(n,I) = Mchar;
MashData(n,I) = Mash;
MTData(n,I) = MT;
Y_O2Data(n,I) = Y_O2;
Y_CH4Data(n,I) = Y_CH4;
Y_H2Data(n,I) = Y_H2;
Y_CO2Data(n,I) = Y_CO2;
Y_COData(n,I) = Y_CO;
UgData(n,I)=Ug;

end
end

%Plotting the graphs -----

figure('Name','TS')
hold on
plot(tsData(:,50)) % plot solid temperature profile at t=50s
plot(tsData(:,100)) %plot solid temperature profile at t=100s
plot(tsData(:,150)) %plot solid temperature profile at t=150s
plot(tsData(:,200)) %plot solid temperature profile at t=200s
hold off

figure('Name','TS') %plot the solid temperature values
surf(tsData,IData);
figure('Name','Y_CO') % Plot CO generation
surf(Y_COData,IData)
figure('Name','Y_CO2') % Plot CO2 generation
surf(Y_CO2Data,IData);

```