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CFD OPTIMIZATION OF A BIOMASS 
BRIQUETTE DOMESTIC COMBUSTOR

by

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Abstract

This work aims to develop a Computational Fluid Dynamics (CFD) model of a domestic biomass briquette combustor as a means of providing a platform to enhance combustion performance in such combustion systems. In addition to the numerical modelling which forms the core of the project, experimental tests were conducted as a means of evaluating model accuracy. The combustor used in the experiment has a cylindrical combustion chamber of length 25cm and a diameter of 11cm.

A variety of fuels were used in the experimental tests conducted. However, the fuel chosen for use for purposes of model validation is a peanut shell-cow dung mixture briquette formed under a 5 ton load. The proximate analysis reveals the constituent moisture, medium volatile and combustible matter and ash contents to be 3.44%, 64.99% and 31.57% respectively. On the other hand, the calorific value is determined to be 17.1 MJ/kg.

Due to resource constraints, only devolatilisation is modelled. This decision is precipitated by the determination made by the proximate analysis showing the volatiles to be the most abundant constituent of the fuel. The computational domain of the model represents the combustion chamber which is separated into two regions—namely, freeboard and fuel bed. The freeboard consists only of the gas phase while the fuel-bed consist of multiple phases in interaction, that is, the solid fuel and gas phases. The multiphase nature of the model is captured by an Eulerian-Eulerian model where the fuel region is considered a packed bed with the solid fuel represented by a granular phase.

The combustion modelled is based on the homogeneous reactions taking place in the freeboard which transfer heat to the solid fuel to initiate and sustain mass transfer of reactants to the freeboard. The exchange of heat between the gas and solid phases is carried out through radiation and convection. However, the inability of the commercial CFD package in use (Ansys Fluent 17.0) to calculate multiphase heat transfer necessitates the introduction of User Defined Functions (UDFs) to capture the radiation and convection contributions to the source term of the solid fuel energy equation.

The rate of volatile species mass transfer, on the other hand, is determined by an iterative process. The constant species volatile fractions for the volatile fuel component of a woody biomass obtained from literature are used as the upper limit mass transfer rates for the respective species. The lower limit is based on the estimated average mass loss rate determined from the experimental mass decay curve. The proportions of the species were kept the same for each iteration. The values of mass transfer rates of each iteration were determined by dividing the species mass transfer rates of the upper limit with the n\textsuperscript{th} integer iteration number. Comparisons carried out at 60 seconds of combustion between each iteration and the experimental temperatures at the exit as well as within the freeboard (4cm from the exit) along the central axis showed improved predictions with each iteration. As a consequence of resource constraints, the most important being time, only ten iterations could be carried out with each case run for 5 minutes.

The temperatures measured at the exit as well as the freeboard (4cm from the exit) show the freeboard temperatures to be greater than the exit temperatures. The reverse situation is the case for the model predicted temperatures in this region. This relational agreement between the model and experiment is observed only within 3cm of the exit. Also, as modelled, the mass transfer rates specified are consistently higher than those predicted. This shows the specified rates to be upper limits. The predicted rates are also observed to be dependent on the specified values and independent of the species being transferred. Furthermore, the reaction rates for each of the homogeneous reactions are revealed to be heavily dictated by the large-eddy mixing time scale in the longitudinal
direction while influenced by wall effects in the radial direction. Turbulence is modelled by the standard k-epsilon model. In the longitudinal direction, the reaction rates are generally seen to decrease further away from the freeboard/fuel-bed interface situated at a longitudinal position/height of 0.1 meters. This is associated with an increase in the large-eddy mixing time scale in the same direction which is seen to correspond with a progressive decrease in the turbulence kinetic energy (TKE). On the other hand, the radial reaction rate distribution for most heights is seen to be influenced by both turbulence as well as the no wall reactions defined. This is evidenced by the sharp drop in the reaction rates very near the wall.
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\( A_i \) Pre-exponential factor \((s^{-1})\)
\( A_v \) Area-volume ratio \((m^{-1})\)
\( C_p \) Constant pressure specific heat \((J.\, kg^{-1}K^{-1})\)
\( E_i \) Activation energy \((J.\, mol^{-1})\)
\( h \) Convection coefficient \((w.m^{-2}K^{-1})\)
\( I \) Irradiation intensity \((wm^{-1}sr)\)
\( J_i \) Diffusive flux of species
\( K \) Char reaction constants \((m.\, s^{-1})\)
\( M_i \) Molecular weight \((kg.\, mol^{-1})\)
\( n \) Refractive index
\( Nu \) Nusselt number
\( Pr \) Prandtl number
\( Re \) Reynolds number
\( \rho \) Density \((kg.\, m^{-3})\)
\( Sc \) Schmidt number
\( Sh \) Sherwood number
\( S_i \) Source term
\( T \) Temperature \((K/\circ C)\)
\( Y_i \) Mass fraction
\( \varepsilon \) Solid fraction
\( \dot{\omega}'\prime\prime \) Generation or consumption rates of wood components \((kgm^{-3}s^{-1})\)
\( \sigma \) Stefan-Boltzman coefficient \((Wm^{-2}K^{-4})\)
\( \sigma_{scat} \) Scattering coefficient \((m^{-1})\)
CHAPTER 1: INTRODUCTION

1.1 Background

A significant proportion of the South African population living in rural areas rely on biomass in the form of round wood for domestic cooking and space heating [1]. In 2007, it was estimated that 20.5% of all South African households rely on wood for cooking [1]. However for most of Africa, the proportion could be as high as 80%. This significant reliance on wood as a source of energy has adverse effects on the environment including deforestation, land degradation and desertification [1]. Beyond the South African context, countries such as Nigeria and Mali also face the same threat to their forests as a consequence of reliance on round wood for domestic cooking and heating [2].

The pressure on forests resulting from the demand for fuel wood can be alleviated by the adoption of an alternative but renewable biomass energy source such as biomass briquettes also known as densified biomass briquette fuel [3]. Biomass briquettes are solid fuels made from the densification of loose, low bulk density biomass residues obtained from forest residues, agricultural and industrial wastes [3] [4] [5]. Common agricultural wastes used for briquetting include rice and maize husks, coffee residues, peanut stalks and shells while industrial wastes are dominated by saw dust. Elephant grass, that is widely available on the African Savanah, is also a potentially unexploited source of biomass briquetting residues. In spite of the numerous advantages provided by biomass briquettes, among which is environmental sustainability, a study conducted by Mwampamba et al [3] shows that the adoption of this fuel type as a substitute for round wood has been limited in Sub-Saharan Africa. This is partly attributable to the relatively poor combustion properties of biomass briquettes in comparison to wood fuel [3]. Mwampamba et al [3] also suggest the redesign of stoves in order to enhance the combustion efficiency of biomass briquettes.

1.2 Problem statement

The above discussion shows that the widespread adoption of biomass briquettes as a fuel for domestic cooking would be beneficial with regard to forest sustainability. It can also be observed that the relative inefficient combustion properties of biomass briquettes are a prohibitive factor to its widespread adoption. Also, the literature survey that has so far been conducted has failed to yield a study that addresses the enhancement of the combustion efficiency of biomass briquettes in a domestic cooking combustor. As such a study of the combustion characteristics of a domestic biomass briquette combustor will constitute the main focus of the proposed research.
1.3 Aims and Objectives of the Research

The proposed research is aimed at developing a complete Computational Fluid Dynamics (CFD) model of a biomass briquette combustor for domestic cooking applications. This is meant to provide a detailed understanding of the energy conversion processes undergone by the fuel-combustor system during combustion. This is necessitated by the numerous mechanisms and parameters involved in the combustion of solid biomass fuels which make certain aspects of the combustion process prohibitively difficult to measure experimentally without disrupting the progress of the process. CFD provides means by which numerous field variables of a combustion system can be evaluated. Therefore, this work should provide a platform where the quantitative as well as qualitative behaviour of the combustion system under consideration is understood. This allows for improvements in both energy conversion and extraction.

The objectives of the research are based on the understanding that two separate phases-namely, solid and gas-are involved in an interaction that precipitates the combustion process under consideration. Therefore, the specific objectives of this work are as follows: (1) modelling the behaviour of the gas phase, (2) modelling the behaviour of the solid phase, (3) modelling the interaction of the solid and gas phases, (4) setting up and conducting the relevant combustion experimental tests, (5) comparing empirically observed behaviour with model behaviour to determine the effectiveness of the chosen modelling approach.

1.4 Hypothesis

A representative CFD model capturing the behaviour of a domestic biomass briquette combustor can be developed.

1.5 Scope of Work

The proposed investigation will involve both a CFD simulation and experimentation. Firstly, the CFD model will be developed based mainly on the understanding provided by the relevant literature. Secondly, experiments will be conducted to determine the relevant macroscopic parameter values of the combustion process together with the values of the parameters which will serve as inputs for the model. Finally, validation of the model is carried out wherein a comparison of the model and experimentally obtained data is conducted together with model refinements aimed at achieving the closest agreement between the model and experiment.
Chapter 1 – Introduction

This chapter highlights the context of the research by presenting the research background, problem statement, aims, objectives, hypothesis as well as the scope. The background provides broader context of the backdrop against which the research is done, while the problem statement identifies the specific problem to be addressed within this background. The aim speaks to the desired outcome of the research achieved through the steps enumerated by the objectives. The hypothesis, on the other hand, provides the research question to be answered, whereas the scopes considers the confines within which the research will be conducted.

Chapter 2 - Literature review

This chapter will be split into three sections each considering a facet of the topic deemed necessary to facilitate the understanding required to effectively model the combustion system. The first section considers combustion theory in general. The second section considers in particular the factors involved in the combustion of solid biomass fuels. Finally, the third section will examine the literature specifically concerning the CFD modelling of solid biomass combustion systems.

Chapter 3 - Experimental design and testing

This chapter serves as a description of the experimental work to be done. This will include a description of the means by which the nature and amount of the flow, the temperature profile, as well as other relevant parameters will be measured and captured.

Chapter 4 – Experimental results

The experimental results presented in this chapter serve two significant purposes. Firstly, they provide pertinent input variable values for the model. Secondly, they provide a means by which the model physics can be validated.

Chapter 5 – CFD model

This chapter will describe in detail the various aspects of the model considered in the development of the model for the desired combustion system. This description will entail details of the geometry as well as those of the various aspects of the model physics.

Chapter 6 – CFD results

This chapter presents results obtained from the CFD model. The model results reveal the behaviour of the model under the influence of various parameters. These results are to be presented in a manner that is sufficiently clear so as to elucidate the underlying drivers of the behaviour observed.
Chapter 7-Conclusions and recommendations

This chapter will summarise the main findings of the study including the set of parameter values at which optimization is obtained. Additionally, recommendations for further work may be made in this chapter.
Chapter 2: Literature review

2.1 Background

This chapter presents literature relevant to the current study. The topics discussed herein will be presented in three separate sections namely, combustion theory, combustion of solid biomass and, finally, computational fluid dynamics modelling of solid biomass combustion systems. The first section will consist of four subsections to be chronologically presented as chemical thermodynamics, chemical kinetics, explosive reactions and finally flame phenomena. The second section will consist of subsections sequentially entitled carbon neutrality of biomass, biomass briquetting, the combustion of biomass fuels and heat and mass transfer.

The final section will sequentially consider the solid phase, gas phase, energy exchange between the phases as well as mass exchange between the phases. In the solid phase section two subsections are discussed, namely, bed mass and energy conservation and bed thermo-chemical conversion. The latter subsection is further divided into three subsections chronologically entitled moisture evaporation, volatile release and combustion, char oxidation and gasification. On the other hand, the gas phase is divided into subsections sequentially entitled gas flow, homogeneous reactions and combustion models.

2.2 Introduction

Combustion requires the presence of a fuel and an oxidant and is a consequence of a rapid sequence of reactions through which the fuel is oxidised by the oxidant [6]. This results in the evolution of heat and/or light from the combustion system [6]. Fuel may come in three forms namely solid, liquid and gaseous. Common examples are respectively coal, petrol and synthesis gas (syngas) while the oxidant for most combustion systems is oxygen. The aspects of our lives in which combustion finds everyday use are vast and varied and may in certain instances be influenced by socio-economic factors. An example of this being access to electricity, a resource which is still being largely produced by combustion. Associated with combustion systems are pollutant emissions whose severity depends on both the nature of the fuel as well as the nature of the combustion system. This chapter will consider the literature available on combustion theories, the combustion of solid biomass as well as the modelling of solid biomass combustion systems.
2.3 Combustion theory

2.3.1 Chemical thermodynamics

Associated with every chemical reaction is either an absorption or evolution of energy consistent with the first law of thermodynamics i.e. conservation of energy. One of the most important thermodynamic facts to know about a chemical reaction is its heat of reaction \( \Delta H \). This refers to the net change in energy or heat content of the reacting system at a particular temperature where the reactants and products are at a standard state \([6]\)[7][8]. This standard state is usually defined by the state of the particular substances at atmospheric pressure for any temperature \([1]\). If the heat of reaction of a particular chemical system is known for a particular temperature \( T_0 \), then it can be determined for another temperature \( T_1 \) as a consequence of the first law of thermodynamics \([1]\). This is shown by the equation (1) \([6]\):

\[
\left\{ \sum_{j \text{ reactant}} n_j \left( (H_{T_1}^r - H_0^r) - (H_{T_0}^r - H_0^r) \right) \right\} + \Delta H_{T_1} \\
= \Delta H_{T_0} + \left\{ \sum_{i \text{ products}} n_i \left( (H_{T_1}^e - H_0^e) - (H_{T_0}^e - H_0^e) \right) \right\} \\
\]

(1)

where \( H_{T_1}^r, \Delta H_{T_1}, H_0^r, n_j \) and \( n_i \) are respectively the standard enthalpy for the \( i \)th temperature, heat of reaction at the \( i \)th temperature, standard reference enthalpy, number of moles of the \( j \)th reactant and the number of moles of the \( i \)th product.

An alternative and more convenient approach to calculating the heat of reaction is through the use of a quantity known as the heat of formation, \( \Delta H_f^r \). This is the enthalpy of a substance in its standard state referred to its elements in their standard states at the same temperature \([8]\). From this quantity the heat of reaction is obtained as shown in equation (2) \([8]\):

\[
\Delta H_{T_0} = \sum_{i \text{ prod}} n_i (\Delta H_{f,i}^r) - \sum_{j \text{ react}} n_j (\Delta H_{f,j}^r) \\
\]

(2)

In the instance that all the heat evolved from the reaction is used to heat up the products, the product temperature would be referred to as the adiabatic flame temperature \([6]\). If the \( n_i \) of the reaction are known, the adiabatic flame temperature can be determined \([6]\). However, in the case of combustion processes that reach temperatures greater than 1250K, dissociation of the products of combustion is observed and as such the equilibrium concentrations of the products cannot be easily obtained from stoichiometry \([6]\). It then becomes necessary to consider additional equations to solve
for the equilibrium concentrations of each product (including those resulting from dissociation) and the flame temperature. These additional equations come in the form of the combined first and second laws of thermodynamics for a reversible process for a control mass as well as the enthalpy and Gibbs’ free energy equations [9].

From these equations emerge the conditions that must be met for a chemical system to be considered to be at equilibrium. The first condition is that the sum of the chemical potential, also known as the partial molal free energy, for all chemical species of a chemical system must be zero [7] [9]. Secondly, for a constant temperature and pressure system the rate change in free energy is zero [7]. This reveals the sole temperature dependency of the constant pressure equilibrium constant and as such the temperature dependency of the concentration based equilibrium constant [6]. These equations show that an increase in temperature leads to an increase in the equilibrium constant.

If one applies the definition of the adiabatic flame temperature to equation (2) and considers the enthalpy of formation of elements to be at reference state, then it can be observed that many moles of product will form for every one mole of fuel consumed as is represented in the following inequality [6]:

$$\sum_{i, prod} n_i (\Delta H_f^i) \gg \sum_{j, react} (\Delta H_f^j)$$  \hspace{1cm} (3)

This indicates that flame temperature is determined only by the reacting atoms and the atomic ratios of the atoms involved as opposed to specific reactants [6]. The reacting atoms determine the products formed [6]. Therefore, for any C-H-O system, the products will be the same that is CO$_2$, H$_2$O and their dissociated products [6]. The importance of the knowledge of the molar amounts of each of the products in the temperature equation should be noted. The endothermic nature of the dissociation reactions of the products may lead to the reduction of the flame temperature which may not be apparent if dissociation is not considered [6]. As earlier stated, an increase in temperature beyond a certain threshold yields the dissociation of certain products [6]. Additionally, there are certain temperature ranges and pressures within which specific dissociation reactions can be expected [1]. For example, if $T > 2200 K$ at $P = 1 \text{ atm}$ or $T > 2500 K$ at $P = 20 \text{ atm}$ then the following dissociation reactions for CO$_2$ and H$_2$O can be expected [6]:

$$\text{CO}_2 \leftrightarrow \text{CO} + \frac{1}{2} \text{O}_2, \hspace{1cm} Q_p = -67.6 \text{ kcal}$$  \hspace{1cm} (4)

$$\text{H}_2\text{O} \leftrightarrow \text{H}_2 + \frac{1}{2} \text{O}_2, \hspace{1cm} Q_p = -57.8 \text{ kcal}$$  \hspace{1cm} (5)
\[ H_2O \leftrightarrow \frac{1}{2}H_2 + OH, \quad Q_p = -67.9 \text{ kcal} \] (6)

\( Q_p \) refers to the heat of reaction at constant pressure from the perspective of the flame, meaning that the above dissociation reactions are endothermic [6]. In the instance of over-oxidisation, if \( T > 2400 K \) at \( P = 1 \text{ atm} \) or if \( T > 2800 K \) at \( P = 20 \text{ atm} \), then the dissociation of \( O_2 \) and \( H_2 \) have to be considered and proceed as follows [1]:

\[ H_2 \leftrightarrow 2H, \quad Q_p = -104.2 \text{ kcal} \] (7)

\[ O_2 \leftrightarrow 2O, \quad Q_p = -119.1 \text{ kcal} \] (8)

In air combustion systems as opposed to pure oxygen combustion systems, nitrogen is fairly non-reactive below 1800K. Above this temperature value, nitrogen begins to participate in reactions [6]. The above discussion should make it apparent that the level of complexity involved in determining the flame temperature is dependent on the number of products for the given combustion system.

The temperature of a flame is known to vary with the ratio between the oxidizer and the fuel. This ratio is usually given by a quantity referred to as the equivalence ratio \( \Phi \) [7]. This quantity is defined as the ratio of the actual fuel-oxidant ratio to the stoichiometric fuel-oxidant ratio. For fuel rich systems, there is more than the stoichiometric amount of fuel hence \( \Phi > 1 \). For over-oxidised or fuel lean systems \( \Phi < 1 \). In the case of the stoichiometric fuel-oxidant ratio \( \Phi = 1 \). The temperature of a flame is found to be at its maximum at the stoichiometric equivalence ratio. In the over-oxidized case, the excess air lowers the flame temperature as it is heated to the flame temperature while on the other hand the fuel rich system lacks sufficient oxidant to achieve complete oxidation of the fuel and maximum energy release [8].

2.3.2 Chemical kinetics

Flames propagate in chemical mixtures that have the capability to react sufficiently fast to be termed explosive [6]. It is therefore of great importance to the study of combustion to understand the aspects of a chemical system that have a bearing on the rate of reaction. The rate of reaction can be described as the rate at which a given reactant disappears or alternatively as the rate at which a particular product forms [6]. This is usually considered in terms of concentration. Equation (9) gives a condensed form of the stoichiometric relation of a one-step reaction [6]:
\[
\sum_{j=1}^{n} v_j' M_j = \sum_{j=1}^{n} v_j'' M_j \quad (9)
\]

where \(v_j'\) refers to the stoichiometric coefficient of the reactants, \(v_j''\) is the stoichiometric coefficient of the products, \(M\) is an arbitrary specification of all chemical species and \(n\) is the number of all chemical species involved. According to the law of mass action which is based on experimentation, the rate of reaction, \(RR\), is proportional to the product of the reactants’ concentrations each raised to its stoichiometric coefficient. The generic formula for the rate of change of the concentration of a species \(M_i\) is given by equation (10) [1]:

\[
\frac{d(M_i)}{dt} = [v_i'' - v_i']k \prod_{j=1}^{m}(M_j)^{v_j'} \quad (10)
\]

where \(k\) refers to the specific reaction rate coefficient. The description for a second order reaction rate is given by the Arrhenius rate expression [6]. This is based on the postulate by Arrhenius that in order for a reaction to occur from a bimolecular collision the reacting molecules would have to possess a specific minimum amount of energy referred to as activation energy. A bimolecular collision for reactants that did not possess this minimum energy would not result in a reaction [6]. In this case the specific reaction rate coefficient is given by the following expression [6]:

\[
k = p\sigma^2 \left[\frac{8\pi k_B T}{\mu}\right]^{1/2} \exp\left(-\frac{E}{RT}\right) \quad (11)
\]

where \(\sigma\) refers to the hard sphere collision diameter, \(k_B\) the Boltzmann constant, \(\mu\) is the reduced mass of the two reacting species, \(p\) is the steric factor, \(E\) is the activation energy, \(R\) is the universal gas constant and \(T\) refers to temperature. From equation 11, the temperature dependency of the Arrhenius specific reaction rate coefficient is evident.

The transition state theory is the most suitable for capturing the nature of the temperature dependence of the specific reaction rate coefficient in the case of low activation energy free radical reactions where the reactants are assumed to be in equilibrium with the activated complex that has a mode of vibration that leads to the decomposition of the activated complex to form products [6].

In combustion processes, reactions tend to be more complex than one-step reactions. The more general type of reaction is a simultaneous interdependent reaction that is, a reaction which moves both forward and backwards. In this case the rate of formation of the product is found as the sum of
the forward and backward reaction rates that relate to that particular product [6]. The equilibrium of such a reaction yields a relationship between the forward and backward reaction rate coefficients as well as the equilibrium constant based on concentration. This relationship makes the forward reaction rate coefficient the only independent rate coefficient for such a reaction [6].

Also associated with combustion are chain reactions. These are reactions which are initiated by an elementary reaction which forms free radicals from one of the reactants [6]. This is followed by a series of successive steps called chain propagating steps that continue based on the formation of high activity radicals that propagate the formation of the product [7]. This type of reaction is terminated by another elementary reaction that either yields the recombination of two radicals, the formation of a molecular species or a low activity radical that cannot propagate the chain [7]. A special variant of the chain propagating step found responsible for non-thermal explosive reactions is the chain branching step. This is characterised by the formation of two radicals from the consumption of one radical. It is precisely this multiplication effect that is responsible for the explosive nature of branching reactions [6] [7].

2.3.3 Explosive reactions

As stated above, flames will propagate only in a mixture that reacts sufficiently fast to be deemed explosive. A distinction is made between two different types of explosions, namely chain branching explosions and thermal explosions [6] [7]. A thermal explosion takes place when insufficient heat is removed from an exothermic chemical system which causes a temperature increase which consequently results in an exponential increase in the reaction rate as described by the Arrhenius expression for the specific reaction rate coefficient. On the other hand, the chain branching explosion runs away because of the very nature of chain branching reactions; that is, a multiplication factor greater than unity [6] [7]. It should be noted that albeit chain branching reactions result in two radicals for each radical consumed, the multiplication factor is usually greater than one but less than two. This is attributable to competing reactions such as recombination that result in a decrease of the expected number of radicals available for reaction [7]. The critical multiplication factor that deems a particular chain branching reaction system as explosive is determined by considering the following generic chain branching reaction:

\[
M \overset{k_1}{\rightarrow} R \quad (\text{initiation step}) \quad (12a)
\]

\[
R + M \overset{k_2}{\rightarrow} \alpha R + M' \quad (\text{overall chain branching step}) \quad (12b)
\]
\[ R + M \xrightarrow{k_3} P + R \quad (\text{propagating step forming product}) \quad (12c) \]

\[ R + M \xrightarrow{k_4} P' \quad (\text{gas} - \text{phase terminating step forming product}) \quad (12d) \]

\[ R \xrightarrow{k_5} P'' \quad (\text{surface destruction} - \text{termination step}) \quad (12e) \]

where \( \alpha \) is the multiplication factor, \( M \) and \( M' \) are reactant molecules, \( R \) is representative of all radicals that are chain carriers and \( P, P' \) and \( P'' \) represent products formed in the reaction system and the last three reactions collectively represent termination reactions [7].

Considering the rate of formation of the main product \( (P) \) in the third reaction and the application of the steady-state assumption for the determination of the expression for the concentration of radicals in the system provides the following expression for the critical multiplication factor [7]:

\[ \alpha_{\text{crit}} = 1 + \frac{k_4(M) + k_5}{k_2(M)} \quad (13) \]

The parentheses in equation (13) designate the volumetric concentration of the chemical species of interest. Generally \( (M) \) is considered to be proportional to the total pressure of the system [7].

Combustion systems in which chain branching is prevalent exhibit a dependence on both temperature and pressure with regard to the explosiveness of fuel-oxidizer mixtures. This dependence defines, for each mixture, sets of temperatures and pressures within which reactions are either explosive or not [7]. The set of temperatures and pressures which constitute the boundaries that separate the sets of temperatures and pressures of fast and slow reactions are referred to as explosive limits [6]. It should be noted that these limits can only be evaluated for a single mixture ratio at a time; that is, explosion limits are unique to a particular mixture ratio. Explosion limits can be understood qualitatively by considering the effect of both temperature and pressure on the relative rates of competing reactions namely, chain-breaking and chain-branching reactions [6] [7]. However, the specific mechanisms involved in the transition from the exhibition of an explosive character to a non-explosive character and vice versa require the evaluation of the specific combustion system [7].
2.3.4 Flame phenomena

Combustion can be categorised into two major groups namely; premixed and non-premixed (or diffusion) combustion [6]. The premixed combustion phenomenon, as suggested by the name, pertains to the combustion of fuel-oxidizer systems that have been premixed. These fuel-oxidiser mixtures are usually non-reactive at room temperature and pressure [6]. The introduction of an ignition source would result in a substantial temperature increase or cause a substantial concentration of radicals. This would result in the propagation of an explosive region through the mixture provided that the mixture is within flammability limits [6]. Given the conditions under which the explosive region or combustion wave propagates the mixture, the speed of the combustion wave may be lower or higher than the speed of sound of the unburned gases [6]. The combustion wave that propagates the gaseous mixture at a subsonic speed is referred to as a flame or deflagration whereas that which traverses the mixture at supersonic speed is referred to as a detonation. The burned and unburned gases in a premixed system are separated by the combustion wave [6].

The second category of combustion phenomena (diffusion flames) is more relevant to this research as premixed combustion is exclusive to gaseous mixtures. In the literature so far reviewed, the condensed phase diffusion flame is considered using the analysis of the single liquid droplet in gaseous oxidizer environment [6, 7]. The analysis can, however, be extended to explaining the combustion of other condensed phases such as solid fuels [7]. In the case of the liquid fuel droplet in an oxidizing atmosphere, the fuel is evaporated at the droplet surface and diffuses to the flame front while the oxygen is also diffused from the surrounding environment to the flame front [6].

Most of the theoretical models used to describe this combustion process consider a double-film model. This model supposes that there is a film that separates the droplet surface and the flame front and another that separates the flame front and the surrounding oxidizing atmosphere [6] [7]. In most theoretical developments the liquid surface is assumed to be at the normal boiling point of the fuel. However, surveys of the temperature fields in burning liquids indicate that the temperatures of the liquid fuel surfaces are in fact a few degrees below boiling point [6]. In the film separating the fuel surface and the flame front, heat is conducted from the flame front to the fuel surface to vaporize the fuel. Many analyses assume that in this very film the fuel is heated to the flame temperature and only reacts when it reaches the flame front [7]. In the film between the flame front and the surrounding atmosphere, oxygen is diffused to the flame front while combustion products and heat are transported away from the flame into the surrounding [6] [7].
The combustion of a liquid fuel droplet generally involves the evaluation of the following three parameters: mass burning rate (evaporation), the flame position above the fuel surface and the flame temperature [7]. The mass burning rate enables the evaluation of the evaporation coefficient which is an experimentally measurable quantity [6] [7]. The evaporation coefficient is defined as follows [6]:

$$d^2 = d_0^2 - \beta t$$  \hspace{1cm} (14)

where \(d_0\) is the original drop diameter and \(d\) is the droplet diameter after time \(t\). It should be noted that the term evaporation coefficient arises from mass and heat transfer experiments without combustions that is, evaporation experiments [6].

The combustion of condensed fuels also allows for the measurement of the mass consumption rate which is also known as the rate of regression of the condensed fuel [6] [7]. Since the combustion of condensed phase fuels requires the gasification of the surface, an energy input is required. Hence the heat flux at the surface determines the regression rate of the fuel [6] [7]. This is expressed as follows [7]:

$$q_s = \dot{r} \rho_f Q$$  \hspace{1cm} (15)

where \(q_s\) is the heat flux to the surface of the fuel, \(\dot{r}\) is the regression rate, \(\rho_f\) is the density of the fuel and \(Q\) is the sum of the two terms representing the heat of vaporization and the energy required to raise the temperature of the fuel from its original value to that of vaporization.

If no radiation is assumed then the heat flux at the surface can be represented through the Fourier heat transfer equation as follows [6]:

$$q_s = -\lambda \left( \frac{\partial T}{\partial y} \right)_s$$  \hspace{1cm} (16)

where \(y\) is the distance below the droplet surface. The validity of the expression relating heat flux to regression rate is maintained even in the presence of convective effects [6] [7]. In this case the heat flux at the surface of the fuel is expressed as follows [7]:

$$q_s = \bar{h}_c (T_\infty - T_s)$$  \hspace{1cm} (17)
2.4 Combustion of solid biomass

2.4.1 Carbon neutrality of biomass

The widely accepted consensus is that biomass derived fuels do not contribute to the increase in greenhouse gases. This is attributed to the CO\(_2\) neutrality of the energy conversion of such fuels for which the renewability of biomass is responsible [10]. Biomass refers to vegetable mass or phytomass produced by the effect of solar energy on photosynthesis, that is, polymers of carbon (C), hydrogen (H) and oxygen (O) that are responsible for making cell walls and other plant parts [11]. In addition to the above mentioned constituents of biomass, small concentrations of phosphorus, nitrogen and potassium can be found together with trace amounts of other elements responsible for cellular function [11].

The action of photosynthesis in the formation of biomass can be illustrated by the following chemical equation [11]:

\[
CO_2 + H_2O + \text{sunlight} \rightarrow CH_2O + O_2
\]  

(18)

The carbon dioxide is obtained by the atmosphere through leaves while water is provided by a plant’s vascular system and roots. The sunlight on photosynthetic centres dissociates water molecules into oxygen, protons and electrons [11]. The oxygen is released into the atmosphere through the leaves while the protons react with the carbon dioxide to form the photosynthate \(CH_2O\) which is the basic building block for sugars, starches and cellulose [11].

Cellulose is the most commonly produced natural polymer followed by lignin which is formed from phenyl propane units [11]. Lignocellulosic material resources are the most commonly used biomass energy resources as they constitute over half of the above ground biomass produced by photosynthesis [11]. These refer to trees, most woody plants and stalks and straws of cereal crops whose fibres are formed from cellulose, hemicellulose and lignin (polymers of oxygen, carbon and hydrogen) which serve different functions in the formation of plant cell walls. Energy can be derived from biomass by means of combustion in oxygen or through metabolic processes. The following chemical equation describes the evolution of energy from biomass for both cases [2]:

\[
CH_2O + O_2 \rightarrow CO_2 + H_2O + \text{heat}
\]  

(19)

It can be seen from the two chemical equations immediately above that the formation of biomasses and the processes through which energy is derived from them form a solar powered closed loop between plant matter and the atmosphere [11]. It is this closed loop that is attributed to the carbon
dioxide neutral character of biomass energy conversion [11]. In addition, carbon neutrality of biomass energy conversion does not extend to the mitigation of carbon emissions in the form of \( \text{CO}_2 \) or \( \text{CH}_4 \) during biomass decomposition [12]. Fossil fuels, on the other hand do not participate in the above discussed closed loop and as such increase the net amount of carbon dioxide in the atmosphere [11].

2.4.2 Biomass briquetting

The need to mitigate both net carbon emissions of fossil fuels for climate change reasons as well as deforestation that takes place in developing countries, which are dependent on fuel wood as a source of energy, has stimulated interest in biomass residues as a renewable energy source. These are obtained from activities in agriculture and industry [13]. However, raw biomass residue has a number of disadvantages as energy feed stock. These include (i) relatively low calorific values, (ii) variability of quality and calorific value, (iii) difficulty in controlling the rate of burning, (iv) rapid burning which necessitates frequent refuelling, (v) large volume or area required for storage and (vi) problematic with regards to transportation and distribution [14]. Most of the above mentioned disadvantages can be attributed to the low bulk density of raw biomass residue [14]. Therefore, densification of such energy feed stocks is required for its improvement on several fronts [13] [14]. These include increased energy density, reduced cost of transportation and improved handling and combustion characteristics [15].

These densified biomass fuels come in one of three forms: pellets, briquettes and agglomerated spheres [13]. Pellets and briquettes are both typically cylindrical in form differing solely in their individual range of dimensions [16]. In order to ensure the quality of these fuels, numerous standards exist in order to regulate such quality measures as length, diameter, density, water content, ash content and higher heating value (HHV) [16]. Agglomerated spheres, on the other hand, are characterised by a diameter less than 50 mm [13]. These densified forms are obtained by aggregating biomass particles through the application of pressure and/or a binding agent to the loose raw biomass [13]. Two classes of briquetting machines can be found: piston presses and screw presses [13]. In the former, compaction is achieved through strokes of hydraulic cylinders while the latter achieves compaction through the extrusion of the biomass by a screw extruder into a tapered die [13]. The piston press is usually inefficient with regard to energy consumption while the screw press produces better quality products [13].
In an experimental study conducted by Chin and Siddiqui [17], compaction pressure, dwell time, moisture and binder content were investigated on the quality of briquettes for several biomasses. The biomasses tested included sawdust, rice husks, peanut shells, coconut fibres and palm fibres. The parameters of interest in determining quality were relaxation behaviour, shear strength, combustion rate and durability.

The compaction pressure was varied between 0.5 and 7 MPa. The relaxation length for each type of biomass was observed to decrease with an increase in the pressure. The density calculated after a relaxed state was obtained for each biomass and showed an increase in pressure corresponding to an increase in density. The shear strength of the briquettes for each of the biomass types increases in correspondence to an increase in pressure.

The combustion rate was determined by mounting the combustor with the briquette on a mass balance and measuring the mass loss after ignition of the fuel. The tests showed a decrease in the rate of combustion for an increase in pressure which could be as follows [17]:

$$\dot{m} = ap^n$$

(20)

where $a$ and $n$ refer to constants associated with individual biomass types while $p$ is the pressure. The values of $n$ were found to be negative. The effect of dwell times was tested at a constant compaction pressure of 4 MPa while dwell times were varied up to 60s. An increase in the dwell time led to a decrease in the relaxed lengths of the briquettes of each of the biomasses until optimal relaxation was achieved. Additionally, an increase in the dwell time also led to a slight increase in the shear strength of the briquettes which was initially exponential before becoming asymptotic at dwell times between 60 and 70 seconds. Also, a power law relationship was observed between the combustion rate and the dwell time which may be expressed as follows:

$$\dot{m} = at^{-b}$$

(21)

where $a$ and $b$ are empirical constants and $t$ is the dwell time in seconds.

2.4.3 Combustion of solid biomass fuels

The most recent technologies used for the direct combustion of solid biomass include fluidised beds (FB) and grates. Grates were the first systems to be used for combustion processes [16]. Currently, this combustion system is used in the combustion of biomass, municipal solid waste and in some small coal furnaces [16]. This type of combustion system releases an average of $4\, MW/m^2$. 


of energy per grate area which results in an abundance of volatiles and a reduced amount of ash for biomass fuels [16]. Grate systems are composed of four components: the fuel supply, the grate, the primary and secondary air intakes [16]. The grate is situated at the bottom of the combustion chamber and serves the dual function of longitudinally distributing the fuel as well as primary air which enters the combustion chamber from the bottom through the grate [16]. Grates can be found in one of two categories: stationary or mechanical. The mechanical grate is either reciprocal (with upwards and downwards movement of its bars), balanced, vibrating or mobile [16]. The primary air serves to facilitate the proper distribution of air throughout the combustion bed while secondary air- air above the combustion bed- promotes mixing with the exhaust gases from the combustion bed [16].

On the other hand, fluidised bed combustion equipment consists of two distinct regions namely the bed and the freeboard (also known as the free space above the bed) [16]. The former refers to a region where the concentration of solids is high while the latter refers to a region where the concentration of solids is significantly lower. Therefore, a fluidised bed is a volume of particles (bed) which are varied in nature, mainly biomass ash and sand, which are supported by a gas distribution plate [16]. The function of a fluidised bed is characterised by the particle (bed elements) moving vigorously [16]. This is achieved only when the upward velocity of the air is increased beyond the minimum fluidisation velocity “the critical” air velocity beyond which the particles are no longer stationary [16]. The fluidised bed combustion process requires that the combustion chamber be preheated with gas to temperatures within the range of $400 - 500^\circ C$ before the start of the process [16]. The preheating temperature is determined by the type of the biomass to be combusted [16]. The bed temperature is further increased to $800 - 900^\circ C$ through the introduction of solid biomass fuels [16].

The combustion of solid biomass is characterised by a sequence of steps which take place either sequentially or in parallel [16]. These steps include heating and drying, pyrolysis (also known as devolatilisation) and char burnout [18]. The thermal conversion of biomass begins with the drying process [18]. Due to heating up, moisture is released from the fuel particle [18]. Subsequently pyrolysis converts dry biomass into volatiles and char [18]. Finally, char burns out and leaves another layer which only contains ash [18]. Drying, pyrolysis and char burn out fronts proceed from the surface of the fuel particle towards its centre [18].
The fuel particle entering the combustion chamber heats to the temperature close to that within the combustion chamber [16]. It is due to this heating that the water on the surface and pores of the fuel particle, which exists in the form of humidity, evaporates at a fixed boiling temperature [16, 18]. The drying process acts as a heat sink meaning that any additional energy beyond that required for evaporation is further consumed for the same purpose [18]. If the moisture content of a biomass fuel particle is too high, combustion cannot take place steadily and as a consequence pre-drying of the fuel may be required before combustion [16].

Biomass pyrolysis (also known as devolatilisation in the absence of oxygen) refers to the thermal decomposition of the three pseudo-components of biomass-cellulose, hemicellulose and lignin [16, 18]. Hemicellulose is easily decomposed and its pyrolysis takes place at a temperature range of 493-588K [19]. The pyrolysis of cellulose, on the other hand, takes place at a temperature range of 588-673K, while that of lignin proceeds over a much wider temperature range of 423-1176K [19]. The composition and amount of the resultant volatiles are determined by the heating rate of the particle, the final temperature, fuel composition (important for the C/H ratio), the particle size and pressure [16]. The main gaseous components are \( H_2O, CO, H_2, CO_2, CH_4 \) and tars [16, 19].

At temperatures below 773K, pyrolysis yields primary volatiles while tars form from depolymerisation reactions [19]. The pyrolytic water produced at these temperatures results from dehydration reactions [19]. In this case the main gaseous products that form are \( CO_2 \) and \( CO \) [19]. At temperatures above 773K primary volatiles undergo secondary pyrolysis processes during which tars are converted into various gases, in particular \( CO \), light hydrocarbons, \( H_2 \) and \( CO_2 \) [19]. At high heating rates biomass decomposes rapidly yielding gases, vapours and carbon enriched char [19].

The transient 3-dimensional model of packed bed biomass combustion by Mehrabian et al. [18], which considers the combustion from the intra-particle perspective as well as bed shrinkage, uses the hypothesis of the pseudo-components of biomass being pyrolysed independently. The Arrhenius rate equation is used to describe the decomposition of each pseudo-component [18]. This is given in equation (22) [18]:

\[
k = A \exp \left( -\frac{E}{RT} \right)
\]  

(22)

where \( A \) is the pre-exponential factor, \( E \) is the activation energy and \( R \) is the universal gas constant. The overall rate of mass loss for a fuel particle is therefore described by the equation [18]:

\[
\]
\[- \frac{dm}{dt} = \sum_{i=1}^{3} c_i \frac{d\alpha_i}{dt} \tag{23}\]

where \(i\) is representative of each pseudo-component, \(c_i = m_{0,i} - m_{f,i}\) and represents the mass loss of the \(ith\) pseudo-component as a fraction of the overall mass loss \(m_0 - m_f\) and as such acts a means of measuring the individual contribution of each pseudo-component to the overall mass loss [18]. The conversion of each pseudo-component \(\alpha_i\) can be expressed as follows [18]:

\[\alpha_i = \frac{m_{0,i} - m_i}{m_{0,i} - m_{f,i}} \tag{24}\]

Since the pseudo-components are assumed by Mehrabian et. al. [18] to decompose individually, the decomposition rate of each pseudo-component is described in equation (25) [18].

\[\frac{d\alpha_i}{dt} = A_i \exp \left( \frac{-E_i}{RT} \right) (1 - \alpha_i) \tag{25}\]

A process called fragmentation also takes place in parallel with devolatilisation and occurs as a consequence of thermal shock, drying and the release of volatile matter [18]. This process is important as it is involved in the oxidation process of the fuel [18].

Combustion involves the oxidation of the volatiles released during the pyrolysis process [16]. It also involves the oxidation of \(CO\) gas species which results from the oxidation of carbonized materials [16]. In the intra-particle model by Mehrabian et. al. [18] the char conversion reactions are assumed to occur at the interface between the char and the ash layers. The conversion reactions of char involve oxidation with \(O_2\) and gasification with \(CO_2\), \(H_2O\) and \(H_2\) as shown by the following chemical equations [18].

\[\Omega C + O_2 \rightarrow 2(\Omega - 1)CO + (2 - \Omega)CO_2 \tag{26a}\]
\[C + CO_2 \rightarrow 2CO \tag{26b}\]
\[C + H_2O \rightarrow CO + H_2 \tag{26c}\]
\[C + 2H_2 \rightarrow CH_4 \tag{26d}\]

Char conversion rate is influenced by both the kinetic rate at the reaction surface as well as the mass transfer to or from the reaction surface [18]. Assuming a global reaction rate of first order with respect to the concentration of the oxidising or gasifying agent leads to the following description for the char conversion rate [18]:
where \( i \) corresponds to the 4 heterogeneous reactions above (equation 26a-d), \( \Omega_i \) represents the stoichiometric ratio of the moles of carbon for each mole oxidising or gasifying agent for the particular reaction. \( M_c, S, k_i, \delta_{ash}, X_{\infty,i} \) respectively represent the molecular weight of carbon, the surface area of the char burnout front, the kinetic rate constant of the heterogeneous reaction \( i \), the thickness of the ash layer and the molar concentration of the oxidising/gasifying agent for the \( ith \) reaction in the bulk flow. The mass transfer coefficient of the reactants in the boundary layer \( h_m \) is obtained through the Sherwood number whereas the effective diffusivity of the ash layer is dependent on the ash porosity and the molecular diffusivity of the penetrating gaseous component [18].

2.4.4 Heat and mass transfer

In a transient 3-D model developed by Mehrabian et. al. [18], in which the two zones constituting a solid biomass combustion system, namely, fuel bed and free-board-were studied, the fuel particle was assumed to be thermally thick. In an attempt to reduce the complexity of the model, only the radial temperature gradients were considered. In order to apply this one dimensional model to a finite cylindrical fuel particle size, the Thunman discretisation approach was implemented. This approach is based on the assumptions that the particle boundary conditions are homogeneous and that every point in the fuel particle at the same distance from the surface of the particle has the same temperature and conversion state.

The convective heat transfer rate inside the fuel bed of the Mehrabian et. al. [18] model was determined through a semi-empirical approach in which the Nusselt number is a function of the mean Reynolds number as follows.

\[
Nu_{l\text{am}} = 0.664Pr^{1/3}(Re/\varnothing)^{1/2}
\]

\[
Nu_{t\text{ur}} = \frac{0.037Pr(Re/\varnothing)^{0.8}}{1 + 2.443 \left( Pr^{2/3} - 1 \right) (Re/\varnothing)^{-0.1}}
\]

\[
Nu_p = 2 + (Nu_{l\text{am}}^2 + Nu_{t\text{ur}}^2)^{1/2}
\]

The \( 2 \) in equation (30) above is the asymptotic value as \( Re \to 0 \). It should also be noted that variables \( Pr, Re, \varnothing, Nu_{l\text{am}} \) and \( Nu_{t\text{ur}} \) respectively represent Prandtl number, Reynolds number, bed porosity, laminar and turbulent Nusselt numbers.
\( Nu_p \) is then used to determine the mean Nusselt number in the manner given in equation (31):

\[
Nu = f(\theta)Nu_p
\]  

(31)

where \( f(\theta) \) is an empirically determined factor which is a function of the bed-porosity \( \theta \) [18]. The relationship is given as:

\[
f(\theta) = 1 + 1.5(1 - \theta)
\]  

(32)

In the Mehrabian et al. [18] model, the radiation heat transfer is considered from the perspective that each fuel particle in the packed bed emits radiation which is absorbed by surrounding fuel particles. The influence of the surrounding fuel particles on radiative heat transfer is considered by changing the boundary conditions on the surface of the fuel particle:

\[
q_{rad,i} = \sum_{j=1}^{NP} \epsilon \sigma F_{ij}(T_j^4 - T_i^4)
\]  

(33)

where \( q_{rad,i} \) refers to radiation heat flux of the surrounding fuel particles to the \( i^{th} \) particle of interest, \( \epsilon \) is the emissivity of the particle, \( \sigma \) is the Stefan-Boltzmann constant, \( F_{ij} \) is the view factor between particle \( i \) and \( j \), \( NP \) refers to the number of particles while \( T \) refers to the surface temperature of the respective fuel particles.

The application of equation (33) in a simulation, however, is difficult as it requires the summation of the radiative heat exchanges between the surrounding fuel particles and the particle of interest [18]. The difficulty in this stems from the need to determine individual view factors for each particle with which the fuel particle of interest exchanges heat through radiation [18]. In order to circumvent this limitation, an appropriate control volume \( \vartheta \) (see Figure 1) is defined around the particle of interest and the assumption is made that the target particle exchanges its radiation with this control volume [18]. The exchange is then described as:

\[
q_{rad,i} = \epsilon \sigma F_{i\vartheta}(T_{\vartheta,i}^4 - T_i^4)
\]  

(34)

Given that the particle of interest is completely enclosed by the control volume and as a consequence exchanges all its radiation with it and vice versa, then \( F_{i\vartheta} = 1 \) [18, 20]. The parameter \( T_{\vartheta,i} \) refers to the average temperature of the particles and gas phase enclosed within the control volume \( \vartheta \) and is described as:
where $\varnothing$, $T_{g,\varnothing}$, $NP_{\varnothing}$, respectively refer to bed porosity, gas temperature in the control volume and the number of particles inside the control volume.

If, on the other hand, the particle of interest is close to the wall of the combustor placing some of the surrounding particles adjacent to the wall gives the following average temperature $T_{\varnothing,i}$ description within the relevant control volume which factors in the influence of the wall radiation [18]:

$$T_{\varnothing,i} = (1 - \zeta) \left[ \varnothing T_{g,\varnothing} + (1 - \varnothing) \frac{1}{NP_{\varnothing}} \sum_{j=1,j\neq i}^{NP_{\varnothing}} T_j \right] + \zeta \frac{1}{NP_{\varnothing}} \sum_{j=1}^{NP_{\varnothing}} T_{wall}$$  \hspace{1cm} (36)

where $NP_{\varnothing}$ refers to the number of particle within the control volume adjacent the wall while $T_{wall}$ refers to the combustor wall temperature.

In the case of particles located at the top of the fuel bed, the average temperature description in the relevant control volume is given by equation (37):

$$T_{\varnothing,i} = 0.5 \left( \frac{q_{rad}}{\sigma} \right)^{1/4} + 0.5 \left[ \varnothing T_{g,\varnothing} + (1 - \varnothing) \frac{1}{NP_{\varnothing}} \sum_{j=1,j\neq i}^{NP_{\varnothing}} T_j \right]$$  \hspace{1cm} (37)

where $q_{rad}$ refers to the radiation from the freeboard [18].
In the work done by Collazo et al. [21] a three-dimensional transient CFD model for the simulation of a fixed bed combustion system is presented. The two zones of the combustion system namely, fuel bed and freeboard are solved simultaneously as a result of the strong coupling provided by the embedded formulations of the bed model. The solid phase is modelled through the use of C++ user defined functions (UDFs) which are simultaneously solved with the gaseous phase. In this model the fuel bed was modelled as a porous zone where five scalar variables were defined, namely solid fraction, moisture density, wood density, char density and temperature. In this model, convective heat and mass transfer between solids and gases are given by experimental correlations of Wakao and Kaguei for the Nusselt and Sherwood numbers as given in the following equations [21]:

\[ Nu = 2 + 1.1 Re^{0.6} Pr^{1/3} \]  
\[ Sh = 2 + 1.1 Re^{0.6} Sc^{1/3} \]

where \( Sh \) and \( Sc \) respectively refer to the Sherwood and Schmidt number. The definition of these parameters is used in the determination of the convective heat transfer coefficient as well as the mass transfer coefficient in the following manner [21]:
where $h_t$, $k$, $h_d$, $D$ and $d_{eq}$ respectively refer to convective heat transfer coefficient, thermal conductivity, convective mass transfer coefficient, diffusivity and equivalent diameter.

Radiation is responsible for a significant amount of heat transferred between the solid and gas phases [21]. The homogeneous reactions taking place in the freeboard emit a radiation flux which heats the solid phase in the fuel bed thus facilitating the thermo-chemical processes which take place in the fuel bed [21]. However, the absorption of the radiation flux is not constant and depends on the depth of the particle in the bed [21]. This model used a method that estimated the heat distribution due to radiation in a manner that follows an exponential decay [21]. This is expressed in equation 42:

$$Q_{rad}(z) = \alpha \sigma (\varepsilon_g T_{fl}^4 - \varepsilon_s T_s^4)e^{-\alpha(z_0-z)}$$

where $\alpha$, $\varepsilon_g$, $\varepsilon_s$, $T_{fl}$, $T_s$ and $z$ respectively refer to decay coefficient, emissivity of gas, emissivity of solid, temperature of flame, temperature of solid and bed depth.

2.5 CFD modelling of solid biomass combustion systems

2.5.1 Introduction

As already mentioned in section 2.4.4, a fixed bed grate biomass combustor consists of two sections, namely, fuel bed and freeboard. The behaviour of these individual regions as well as their interactions with each other are revealed by literature to be integral to the function of biomass energy conversion systems and as such are of interest. This section will explore the available literature as regards the Computational fluid dynamics (CFD) modelling of fixed bed grate biomass combustors.

The approach to be taken in presenting this section will first consider the modelling of the solid phase of these combustors. According to a review by Khodaei et al. [22], the spatial treatment of the solid phase found in the available literature separates bed models into three categories namely the single porous fuel particle [23, 24, 25, 26], continuous porous medium [27, 28, 29, 30] and particle resolved modelling [31, 32, 33, 34].

The single porous fuel model places a great emphasis on capturing the details of intra-particle heat and mass transfer. This positions the model well for the study of both thermally thick and thin
fuels. The continuous porous medium model, on the other hand, considers the bed as a continuous porous medium. This model does not consider the intra-particle behaviour of the solid fuel thereby making it suitable only for the study of thermally thin fuel particles. Finally, the particle resolved modelling approach can be understood as a combination of the two formerly discussed models. This model considers the combined transient individual particle and fuel bed model. Also, the entire bed shrinkage is captured by this model. The combined intra-particle and fuel bed analysis approach of this model leads to better accuracy in the modelling of the individual sub-processes.

This will be followed by a discussion of the various aspects of gas phase modelling found in the surveyed literature. This will be succeeded by a consideration of the models used to capture the behaviour of both mass and energy exchange that takes place between the two regions.

The majority of the literature explored conducted the modelling of these systems through the use of various versions of ANSYS Fluent, the same package - barring specific versions - to be used in this study. A commonality found in all of them was the ineptitude of the packages to resolve the fuel bed. This is circumvented by the introduction of User Defined Functions (UDFs) coded in either C or C++ to enhance the capabilities of the package.

2.5.2 Solid Phase

The models used to capture the behaviour of the solid phase found in the fuel bed (a gas and solid region) will be presented in this sub-section. The chronology of the presentation is as follows: bed mass and energy conservation, bed thermochemical conversion, moisture evaporation process, volatile release and combustion and char oxidation and gasification.

2.5.2.1 Bed mass and energy conservation

Mehrabian et. al [35] presents a one dimensional thermally thick particle model. In this case the fuel particle is represented by a layer model wherein the various stages of the fuel conversion are represented by concentric layers. This model identifies 4 layers, namely, wet fuel, dry wood, char and ash. The reaction fronts for each of the sub-processes (drying, pyrolysis and char burnout) are represented by the boundaries of the respective layers.

The chronology of the layers, as mentioned above, represents the order in which they succeed each other from the centre going out. The procession of each sub-process, chronologically moving from the inner layer outwards, is characterised by a shrinkage of the relevant layer to the centre. This process is accompanied by a mass and energy transfer from the layer of interest into the neighbouring layer as described by equation 43 and 44, respectively.
\[ \frac{\partial}{\partial t} \sum_{c} m_{c,L_i} = \sum_{c=\text{in}} m_{c,B_{i-1}} - \sum_{c=\text{out}} m_{c,B_{i}} \tag{43} \]

\[ \frac{\partial}{\partial t} \sum_{c} m_{c,L_i} H_{c,L_i} = \sum_{c=\text{in}} m_{c,B_{i-1}} H_{c,B_{i-1}} - \sum_{c=\text{out}} m_{c,B_{i}} H_{c,B_{i}} + k_{L_i} \Delta x_{0,L_i} (T_{B_{i-1}} - T_{L_i}) \]

\[ - k_{L_i} \Delta x_{1,L_i} (T_{L_i} - T_{B_i}) \tag{44} \]

where the summations with the subscripts \( c, c = \text{in} \) and \( c = \text{out} \) respectively represent the summation over all components (solid and gas) of the layer, summation over all components entering the layer from the previous boundary and the summation over all components exiting the layer to the next boundary. \( m_{c,L_i} \) and \( H_{c,L_i} \) are, respectively, the mass and specific enthalpy of every component present in layer \( L_i \). \( m_{c,B_{i}} \) and \( H_{c,B_{i}} \) are the mass flow rate and specific enthalpy of each component at the boundary \( B_{i} \). \( K_{L_i} \) is thermal conductivity of the layer \( L_i \). \( \Delta x_{0,L_i} \) is the ratio of the area of the boundary \( B_{i-1} \) to half of the layer \( L_i \) thickness. \( \Delta x_{1,L_i} \) is the ratio of the boundary \( B_{i} \) to half the thickness of layer \( L_i \). Also, \( T_{L_i} \) and \( T_{B_i} \), respectively represent the temperature at the centre of the layer \( L_i \) and the boundary \( B_i \).

The model is used to simulate a single cylindrical particle. This is validated by experiments carried out in a single particle reactor. Although the model manages to closely predict the intraparticle behaviour of the thermally thick particles, the computational resources that would be needed to extend this model to the scale of the bed would be prohibitive given the particle tracking that would be required [36].

On the other hand, Kaer [37] uses a Lagrangian (or walking column) model to represent a slow moving grate combustor in which straw is the fuel. The fuel region is represented by a number of 3-Dimensional volumes, each of which is divided into horizontal slabs. At the centre of each of these slabs exists a node wherein the cell parameter values are stored, both gas and solid. In contrast to the above case, the fuel used is thermally thin.

The velocity of the moving grate is assumed to be constant and as such a relationship is found between the residence time of the fuel and its position on the grate. Therefore, for each new time step, which corresponds to a particular position, the fuel temperature and composition of the previous control volume are transferred to the new control volume as initial conditions.
The transport of mass of the bed is assumed to only be taking place in the direction of the movement of the grate. Also, the short residence time of the fuel in any one computational cell in the x-direction, the direction of grate movement, is short and as such conduction heat transfer is unable to reach steady state in this direction. As a result the, the energy transfer in the fuel is governed by a one dimensional time dependent conduction equation along the length of the fuel. Equation 45 and 46 respectively describe the fuel’s mass and energy conservation [37].

\[
\frac{\partial (\rho_{bed})}{\partial t} + \frac{\partial (\rho_{bed} U_{bed})}{\partial x} = S_{mass,drying} + S_{mass,devol} + S_{mass,char}
\] (45)

where \( \rho_{bed} \) is the bed density and \( S_i \) are source terms which account for the mass loss due to the conversion of the bed.

\[
\frac{\partial (\rho_{bed} C_{p,bed} T_{bed})}{\partial t} = \frac{\partial}{\partial y} (k_{bed} \frac{\partial T_{bed}}{\partial y}) + S_{heat,exchange} + S_{heat,drying} + S_{heat,char}
\] (46)

where \( C_{p,bed}, T_{bed} \) and \( k_{bed} \) are, respectively, the bed specific heat, bed temperature and the thermal conductivity of the bed. Also, \( S_{heat,t} \) accounts for the heat release as a result of conversion processes as well as heat exchanges with the gas phase.

2.5.2.2 Bed thermo-chemical conversion

2.4.2.2.1 Moisture evaporation (drying process)

The model presented by Collazo et.al [21] above presents the drying process as a thermally controlled process. The drying process is assumed to take place at a constant atmospheric saturation temperature of \( 373.15K \). At this temperature all the heat received is dedicated to the drying process until all the moisture has evaporated while the temperature is kept constant. The rate of moisture loss is described by equation 47.

\[
\omega'' = \begin{cases} 
\frac{a \cdot \rho C_p}{\Delta H_m} \frac{\partial T}{\partial t} & \text{if } T \geq T_{evap} \cup \rho_m > 0 \\
0 & \text{rest of the cases}
\end{cases}
\] (47)

where \( a, \rho, C_p, \Delta H_m \) and \( T \) respectively are heat distribution during drying, density, specific heat, heat of reaction of moisture and solid temperature.

2.5.2.2.2 Volatile release and combustion

Gomez et.al [38] presents a three dimensional transient model of solid biomass combustion. The particles in the packed bed are assumed to be thermally thin. The Eulerain multi-phase model is employed wherein the fuel bed is defined as a porous region to which a shrinkage model is also applied. The model is developed using ANSYS Fluent which, as already mentioned, is unable to
capture the thermal conversion of the bed. Therefore, this model resolves the thermally driven time evolution of the bed and its interaction with the freeboard through the use of UDFs.

To capture the conversion of the solid component of the fuel bed the following variables are defined: solid temperature, solid fraction, moisture density, dry biomass density and char density. The mass loss during the thermal decomposition of the solid fuel is modelled by an assumed change only in density during both drying and devolatilization, and a combined change in volume and density during char consumption. The devolatilization is characterised by three competing rates of the formation of the three products of the process, namely, gas(1), tar(2) and char(3). This is reflected in the Arrhenius equation; that is, equation 48 [38].

\[
\dot{\omega}_{\text{wood}}'''' = \rho_{\text{wood}} \sum_{i=1}^{3} A_i \exp \left(-\frac{E_i}{RT_s} \right)
\]

(48)

where \( \rho_{\text{wood}} \) and \( \dot{\omega}_{\text{wood}}'''' \) respectively represent the density of the dry wood and the devolatilization rate. \( A_i \) and \( E_i \) are respectively the \( i \)th pre-exponential factor and activation energy. \( R \) and \( T_s \) are the ideal gas constant and the solid temperature, respectively. On the other hand, equation 49 captures the time rate of change of the density of the dry fuel during the process.

\[
\frac{\partial (\varepsilon \rho_{\text{wood}})}{\partial t} = -\dot{\omega}_{\text{wood}}'''' \varepsilon
\]

(49)

where \( \varepsilon \) represents the solid fraction; that is, the solid volume fraction in the fuel bed.

2.5.2.2.3 Char oxidation and gasification

A one dimensional thermally thick particle model similar to the one presented by Mehrabian et.al [35] is given by Thunman et.al [39]. The reactions taking place at the char reaction front are the oxidation and gasification reactions as expressed by equations 26(a) through 26(d). The rate of char consumption presented by the model is given by equation 50.

\[
R_{b,3}'' = \frac{\tau_{b,3}}{\tau_{b,4}} \left( R_{b,1}'' + R_{b,II}'' + R_{b,III}'' + R_{IV}'' \right)
\]

(50)

where \( R_{b,3}'' \), \( \tau_{b,3} \) and \( \tau_{b,4} \) are, respectively, the char consumption rate at the char consumption front (the boundary separating the char and ash layers), the surface area of the of the char consumption front and the surface area of the fuel particle external boundary. Additionally, equation 51 gives \( R_{b,i}'' \).

\[
R_{b,i}'' = (1 - \alpha) \Omega C_i \left( (\eta \beta_{r,i})^{-1} + (\beta_d)^{-1} \right)^{-1}
\]

(51)

where \( i \) represents the \( i \)th char conversion reaction and \( \alpha \) the fraction of oxygen consumed by volatiles. \( \eta \), \( \beta_{r,i} \), \( \beta_d \) (equation 52) and \( C_i \) are, respectively, the efficiency factor, the rate of reactant
diffusion from the bulk onto the surface, the reaction rate at the reactive surface and the molar concentration of the \(i\)th reactant. \(\Omega\) (equation 53) is the char oxidation parameter.

\[
\beta_d = \frac{Sh. D_c}{d} \tag{52}
\]

\[
\Omega = \frac{2(1 + 4.3 \exp[-3390/T])}{2 + 4.3 \exp[-3390/T]} \tag{53}
\]

where \(Sh, D_c, d\) and \(T\) refer respectively to the Sherwood number, diffusivity, equivalent diameter and solid temperature.

Additionally, the model developed by Gomez et.al [38] keeps track of the time evolution of char density. This is determined as the difference between the char generation and consumption rates as expressed by equation 54. The heterogeneous reactions considered by this model are those represented in equations (26a) through (26c).

\[
\frac{\partial (\varepsilon \rho_c)}{\partial t} = (\omega''_{G,\text{char}} - \omega''_{C,\text{char}}) \varepsilon \tag{54}
\]

where \(\varepsilon\) and \(\rho_c\) are solid fraction and char density respectively. \(\omega''_{G,\text{char}}\) (equation 55) and \(\omega''_{C,\text{char}}\) (equation 56) are char generation and consumption rates respectively.

\[
\omega''_{G,\text{char}} = \rho_{\text{wood}} A_3 \exp\left(-\frac{E_3}{RT_s}\right) \tag{55}
\]

where \(\rho_{\text{wood}}, A_3, E_3, R\) and \(T_s\) are, respectively, dry wood density, char generation pre-exponential factor, char generation activation energy, ideal gas constant and solid temperature.

\[
\omega''_{C,\text{char}} = K_{\text{glob}}^{\text{ox}} A_v [O_2] M_c + K_{\text{glob}}^{g,1} A_v [CO_2] M_c + K_{\text{glob}}^{g,2} A_v [H_2O] M_c \tag{56}
\]

\(K_{\text{glob}}^{\text{ox}}\) (equation 57), \(K_{\text{glob}}^{g,1}\) (equation 58) and \(K_{\text{glob}}^{g,2}\) (equation 59) are known as global char constants and control the heterogeneous reactions thermally and through the diffusion of oxygen, carbon dioxide and water. \(A_v\) and \(M_c\) are area-volume ratio and molecular weight of carbon, respectively. \([O_2], [CO_2]\) and \([H_2O]\) refer, respectively, to the molar concentrations of oxygen carbon dioxide and water.

\[
K_{\text{glob}}^{\text{ox}} = \frac{1}{K_0^{\text{ox}} + 1} \tag{57}
\]

\[
K_{\text{glob}}^{g,1} = \frac{1}{K_0^{g,1} + 1} \tag{58}
\]

\[
K_{\text{glob}}^{g,2} = \frac{1}{K_0^{g,2} + 1} \tag{59}
\]
where \( K^i \) (equations 60, 61 and 62) and \( K'_m \) (captured by equation 52) are respectively the reaction surface reaction rate and the reactant diffusion rates for the heterogeneous reactions.

\[
K^{ox} = 1.715 . T_s . \exp \left( - \frac{9000}{T_s} \right) \tag{60}
\]

\[
K^{g,1} = 3.42 . T_s . \exp \left( - \frac{1.56 \times 10^4}{T_s} \right) \tag{61}
\]

\[
K^{g,2} = 5.7114 . T_s . \exp \left( - \frac{1.56 \times 10^4}{T_s} \right) \tag{62}
\]

2.5.3 Gas Phase

2.5.3.1 Gas flow

Collazo et al. [40] presents a three dimensional transient model of a 18\( kW \) biomass pellet boiler. The gas phase flow is modelled as turbulent to account for high flow speeds of the gases in certain areas of the domain. The effect of turbulence is captured through the realizable \( k - \varepsilon \) model with enhanced wall treatment.

The model represents the fuel bed as a porous region. The impedance of the flow by the solid phase is accounted for by a momentum source (equation 63). This momentum source is determined from three parameters i.e. permeability, inertial losses and porosity. The permeability (equation 64) and inertial losses (equation 65) are estimated from the Ergun equation [40]. The determination of the parameters requires sphericity as well as equivalent diameter values as expressed by equations 66 and 67 respectively.

\[
S_p = - \left( \frac{\mu}{\alpha_p} v_i + C_2 \frac{\rho g}{\sqrt{\varepsilon}} |v| v_i \right) \tag{63}
\]

\[
\alpha = \frac{\psi^2 d_{eq}^2}{150} \frac{\varepsilon^3}{(1 - \varepsilon)^2} \tag{64}
\]

\[
C_2 = \frac{3.5}{\psi d_{eq}} \frac{(1 - \varepsilon)}{\varepsilon^3} \tag{65}
\]
\[ \psi = \frac{\pi^{1/3}(6V_p)^{2/3}}{A_p} \]  

(66)

\[ d_{eq} = D_{cil} \left( \frac{3L_{cil}}{2D_{cil}} \right)^{1/3} \]  

(67)

where \( \mu, v, \rho_g \) and \( i \) respectively refer to the dynamic viscosity, gas velocity, gas density and the \( ith \) coordinate. \( \varepsilon, V_p \) and \( A_p \) are void fraction, particle volume and particle surface respectively. Finally, \( D_{cil} \) and \( L_{cil} \) are, respectively, diameter and length of a cylindrical particle.

2.5.3.2 Homogeneous reactions

Collazo et al. [21] presents the constituent gases of the gas component of pyrolysis products as \( C_6H_6, CH_4, H_2, CO \) and \( CO_2 \). The production of these gases is sustained by the radiation derived from the oxidation of the gases during the homogeneous reactions given by equations 68a through 68e.

\[ C_6H_6 + \frac{9}{2}O_2 \rightarrow 6CO + 3H_2O \]  

(68a)

\[ CH_4 + \frac{3}{2}O_2 \rightarrow CO + 2H_2O \]  

(68b)

\[ H_2 + \frac{1}{2}O_2 \rightarrow H_2O \]  

(68c)

\[ CO + \frac{1}{2}O_2 \rightarrow CO_2 \]  

(68d)

\[ CO_2 + H_2 \rightarrow H_2O + CO \]  

(68e)

The kinetic rates of the homogeneous reactions represented in equations 68a through 68e are given by equations 69a through 69e.

\[ r_{C_6H_6} = 1.3496 \times 10^9 \exp \left( - \frac{1.256 \times 10^8}{RT} \right) [C_6H_6]^{-0.1}[O_2]^{1.85} \]  

(69a)
\[ r_{CH_4} = 5.012 \times 10^{11} \exp \left( -\frac{2 \times 10^8}{RT} \right) [CH_4]^{0.7} [O_2]^{0.8} \] \hspace{1cm} (69b)

\[ r_{H_2} = 9.87 \times 10^8 \exp \left( -\frac{3.1 \times 10^7}{RT} \right) [H_2][O_2] \] \hspace{1cm} (69c)

\[ r_{CO} = 2.239 \times 10^{12} \exp \left( -\frac{1.702 \times 10^8}{RT} \right) [CO][O_2]^{0.25} [H_2O]^{0.5} \] \hspace{1cm} (69d)

\[ r_{CO_2} = 5.0 \times 10^8 \exp \left( -\frac{1.702 \times 10^8}{RT} \right) [CO_2] \] \hspace{1cm} (69e)

where \( R \) and \( T \) respectively refer to the ideal gas constant and the temperature. The corner brackets represent the molar concentrations of the respective gases enclosed.

2.5.3.3 Combustion models

Shiehnejadhesar et.al [41] develops a gas phase combustion model which distinguishes between laminar and turbulence dominated regions of the flow field in order to calculate the respective reaction rates. The disparate nature of the flow field with regard to flow regimes can be found just above the fuel bed of small scale biomass grate furnaces (less than 500kWth). In these cases, the gas phase mixing and reaction rates are heavily dependent on the laminar and low turbulence zones.

The model emphasizes the difference between finite-rate kinetics (FRK) and eddy break-up (EDU) models with particular emphasis being placed on the eddy dissipation concept model. These kinetic models serve as a means of accounting for net rate of species creation in the species transport model. The species transport equation of a multi-component system is given by equation 70.

\[ \frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i \] \hspace{1cm} (70)

where \( \rho, Y_i, \vec{v}, \vec{J}_i \) and \( R_i \) respectively refer to the mixture density, the mass fraction of the \( ith \) species, velocity vector, diffusion flux of species \( i \) as a result of concentration gradients and the net rate of production of the \( ith \) species by chemical reactions.
The FRK determines the rate of species production term through the Arrhenius rate approach while ignoring the effects of turbulent fluctuations. The net reaction source of the $ith$ chemical species is obtained as the sum of the Arrhenius reaction sources over the $N_R$ number of reactions in which the species participates as expressed in equation 71.

$$\left( R_i \right)_{FRK} = M_{w,i} \sum_{r=1}^{N_R} \overline{R_{i,r}}$$  \hspace{1cm} (71)

where $M_{w,i}$ is the molecular weight of the $ith$ species, $\overline{R_{i,r}}$ (equation 72) is the molar rate of creation/destruction of species $i$ during reaction $r$.

$$\overline{R_{i,r}} = \left( v_{i,r}'' - v_{i,r}' \right) \left[ k_{r,f} \prod_{j=1}^{N} \left[ C_{j,r} \right]^{\eta_{j,r}} - k_{r,b} \prod_{j=1}^{N} \left[ C_{j,r} \right]^{v_{j,r}''} \right]$$  \hspace{1cm} (72)

where $N$ is the number of chemical species in the system, $v_{i,r}'$ and $v_{i,r}''$ are respectively the stoichiometric coefficients of reactant $i$ and product $i$ in reaction $r$, $k_{r,f}$ is the forward reaction rate constant for reaction $r$, $k_{r,b}$ is the backward reaction rate constant for reaction $r$, $\eta_{j,r}$ is the rate exponent for reactant species $j$ in reaction $r$ and $C_{j,r}$ is the molar concentration of species $j$ in reaction $r$.

On the other hand, the EBU models are based on the assumptions of infinitely fast chemistry as well as turbulence mixing as the reaction rate limiting/controlling factor. The EBU models are the most popular Reynolds Averaged Navier-Stokes (RANS) based combustion models. A popularity derived from the low computational costs incurred in running RANS simulations.

The eddy dissipation concept (EDC) model is based on the eddy energy cascade. This refers to the particular characteristic of turbulent flow wherein large scale eddies progressively break up into smaller scale eddies. This process is accompanied by a transfer of mechanical energy until the finest scale eddies are achieved where viscous effects become dominant [42]. The central supposition to the EDC model is that reactions take place at the level of the fine structures where mixing takes place at a micro scale [41].

The EDC model separates the fluid into two volume fractions: the fine structure volume fraction ($\gamma^* = \gamma^3$) and the volume fraction of the inert surroundings ($\gamma_0 = (1 - \gamma^3)$). The length fraction of the fine structures is modelled as:

$$\gamma = C_{\gamma} \left( \frac{v_e}{k^2} \right)^{0.25}$$  \hspace{1cm} (73)
Where

\[ C_\gamma = \left( \frac{3C_{D2}}{4C_{D1}} \right)^{0.25} = 2.1377 \text{ with } C_{D2} = 0.134 \text{ and } C_{D1}^2 = 0.5 \quad (74) \]

The EDC time scale (equation 75), on the other hand, is for the mass transfer from the fine structures to the surroundings as well as the residence time in the fine structures.

\[ \tau_{EDC} = C_\tau \left( \frac{\nu}{\varepsilon} \right)^{0.25} \quad (75) \]

where

\[ C_\tau = \left( \frac{C_{D2}}{3} \right)^{1/2} = 0.4082 \quad (76) \]

\( \nu, \varepsilon \) and \( k \) respectively refer to kinematic viscosity, turbulent dissipation rate and turbulent kinetic energy.

Given turbulent Reynolds number as \( Re_t = k^2/\nu \varepsilon \), the length fraction as well as the EDC time scale can be rewritten as shown in equations 77 and 78 respectively.

\[ \gamma = C_\gamma (Re_t)^{-1/4} \quad (77) \]

\[ \tau_{EDC} = C_\tau Re_t^{-1/2} \frac{k}{\varepsilon} \quad (78) \]

There are two approaches taken to determining the mean reaction rate that determines the source value. The first is \( \gamma^2/\tau \) while the second is \( \gamma^2/\tau \) which is used most recently. This latter approach is based on the assumption that mass transfer within the fine structures is contained and does not take place with surrounding flow. Based on this assumption the species mass conservation source term is as given in equation 79.

\[ (R_i)_{EDC} = \rho \frac{\gamma^2 \chi}{\tau_{EDC}} (Y_i^* - Y_i^0) \quad (79) \]

\( \chi \) represents the probability of reaction supporting conditions in the fine structures. \( Y_i^* \) and \( Y_i^0 \) are the mass fractions of the \( i^{th} \) species inside and outside the fine structures respectively.

Equation 80 shows the relationship between the mass averaged state and the surrounding species mass fraction.
This translates to the following representation of the surrounding species mass fraction (equation 81):

$$Y_i^0 = \frac{\bar{Y}_i - \gamma^3 \chi Y_i^*}{(1 - \gamma^3 \chi)}$$  \hspace{1cm} (81)

This leads to an alternative expression for the mean chemical reaction rate as expressed in equation 82.

$$ (R_i)_{EDC} = \frac{\rho \gamma^2}{\tau_{EDC}(1 - \gamma^3)} (Y_i^* - \bar{Y}_i) $$  \hspace{1cm} (82)

### 2.5.4 Energy exchange between the phases

The model presented by Gomez et. al. [43] is that of a steady state heat transfer model in a packed bed through CFD. The model develops this as a general model illustrated and validated through a solar collector. One of the major assumptions of the model is thermal non-equilibrium between the gas and solid phases. The packed bed is modelled as a porous medium and the mass as well as the energy transport of the solid component is modelled through the aid of UDFs. In particular, two UDSs (User Defined Scalars) are considered namely, volume fraction of the solid (solid fraction) as well as energy/temperature.

Heat transfer takes place through conduction, convection and radiation. In the case of the gas phase the commercial code used, ANSYS Fluent, is able to represent the gas phase energy equation as presented in equation 83. On the other hand, the solid energy equation is externally defined as a UDS as expressed in equation 84.

$$ \frac{\partial}{\partial t} (\rho_g e_g(T_g)) + \nabla \cdot \tilde{v}_g (\rho_g e_g(T_g) + P) = \nabla \cdot (k_{g,eff} \nabla T_g) + S_g $$  \hspace{1cm} (83)

$$ \frac{\partial}{\partial t} (\rho_s e_s(T_s)) + \nabla \cdot \tilde{v}_s (\rho_s e_s(T_s)) = \nabla \cdot (k_{s,eff} \nabla T_s) + S_s $$  \hspace{1cm} (84)

where the subscripts $s$ and $g$ respectively refer to solid and gas. $e$, $\rho$, $T$ and $\tilde{v}_i$ represent the volume fraction, density temperature and the velocity vector of the $i$th phase respectively. $k_{i,eff}$ and $S_i$ are, respectively, the effective diffusive coefficient of the $i$th phase and the energy source of the $i$th phase.

The effective diffusivities are determined by both geometric and thermal conductivities of the respective phases. The gas phase effective diffusivity coefficient is given as the porosity scaled thermal conductivity of the phase by equation 85. However, the heat transfer that takes place in the
solid phase is dependent on the packing for it is at the points of contact where solid heat transfer takes place. In this case equation 86 describes the energy transfer through the particle.

\[ k_{g,eff} = \gamma \cdot k_g \]  
\[ \dot{Q}_c = \frac{k_{s,eff} \cdot 4R^2 \Delta T_s}{2\lambda_e R} = G \cdot \Delta T_s \]  
\[ G = \frac{G_S G_C}{G_S + G_C} \]  
\[ G_S = \frac{1}{2} k_s \lambda_s \pi R \]  
\[ G_C = k_s \lambda_c \cdot \frac{\delta}{f_r} \]

where \( \gamma, k_g, k_s, R, G, G_S, G_C, \lambda_e, \lambda_s, \lambda_c, \Delta \) and \( f_r \) are respectively bed porosity, gas thermal conductivity, solid thermal conductivity, particle radius, thermal conductance through unit cell, thermal conductance through particle, thermal conductance through point of contact, dimensionless geometrical correction factor for cell conductance, dimensionless geometrical correction factor for particle conductance, dimensionless geometrical correction factor for contact conductance, average contact area between spheres and the average height of the short-range particle roughness.

The source terms, on the other hand, represent both convective and radiation heat transfer. These are also the means by which energy is transferred between the two phases. In the case of convection, the magnitude of energy transferred from the one phase equals that transferred to the other phase. This is captured in equation 90 as:

\[ S_{g,conve} = -S_{s,conve} = h_c A (T_s - T_g) \]  

where \( h_c \) and \( A \) respectively represent convective coefficient and the area of interaction of the phases. The convection coefficient is determined using the Nusselt number obtained through the correlation in equation 38.

This model [43] considers, in modelling the radiation source, the high participative nature of the porous medium as a consequence of the high absorptivity and emissive coefficients introduced by the presence of solid particles. It is determined by the authors of [30] that the DO (Discrete ordinate) model is best suited to resolve the RTE (radiative transfer equation). Equation 91 presents the RTE. The standard DO model offered by commercial CFD codes is only equipped to resolve the gas phase. In the model presented by [30] external functions are introduced by means of UDFs to enhance the limited DO model to enable it to incorporate the solid phase as given in the evolved
equation 92. The DO model solves the RTE for each of a finite number of solid angles characterised by an associated fixed direction vector \( \vec{s} \) in the Cartesian coordinate system.

\[
\nabla I(\vec{r}, \vec{s}) + (\alpha + \sigma^{scat}) I(\vec{r}, \vec{s}) = \frac{\alpha n^2 T^4}{\pi} + \frac{\sigma^{scat}}{4\pi} \int_0^{4\pi} I(\vec{r}, \vec{s}) \Phi(\vec{s}, \vec{s}')d\Omega
\]

\( I, \alpha, \sigma^{scat}, n \) and \( \sigma \) respectively refer to the radiation intensity, absorption coefficient, scattering coefficient, refractive index and the Boltzmann constant. The first term on the left hand side of equation 91 is the change of the intensity in the position \( \vec{r} \) along the fixed direction \( \vec{s} \). The second term on the left represents the loss in intensity from the absorption and scattering of the radiation. The first term on the right represents an increase in the intensity due to emission of the gas. Finally, the second term on the right is the scattering contribution in all directions.

\[
\nabla I(\vec{r}, \vec{s}) + (\alpha_s + \alpha_g + \sigma^{scat}_g + \sigma^{scat}_s) I(\vec{r}, \vec{s})
\]

\[
= \frac{\alpha_s n_s^2 T_s^4}{\pi} + \frac{\alpha_g n_g^2 T_g^4}{\pi} + \frac{\sigma^{scat}_s + \sigma^{scat}_g}{4\pi} \int_0^{4\pi} I(\vec{r}, \vec{s}') \Phi(\vec{s}, \vec{s}')d\Omega
\]

The solid and gas phase radiation sources derived from equation 92 are respectively given in equations 93 and 94. These equations represent the difference of the radiation absorbed and emitted by the phases under consideration in the particular direction \( \vec{s} \). Equations 95 and 96 are the solid and gas radiation sources in all directions.

\[
S_{s}^{rad}(\vec{r}, \vec{s}) = \alpha_s I(\vec{r}, \vec{s}) - \frac{\alpha_s n_s^2 T_s^4}{\pi}
\]

\[
S_{g}^{rad}(\vec{r}, \vec{s}) = \alpha_g I(\vec{r}, \vec{s}) - \frac{\alpha_g n_g^2 T_g^4}{\pi}
\]

\[
S_s^{rad} = \int_0^{4\pi} S_{s}^{rad}(\vec{r}, \vec{s})dw
\]

\[
S_g^{rad} = \int_0^{4\pi} S_{g}^{rad}(\vec{r}, \vec{s})dw
\]

2.5.5 Mass exchange between the phases

According to [38], the exchange of mass between the gas and solid phase takes place during solid fuel drying, devolatilization and heterogeneous reactions. The mass balance in the model as pertains to the exchange of mass between the phases is captured by density changes in the solid phase and corresponding species sources for the individual gaseous species \( H_2O, CH_4, C_6H_6, CO, CO_2 \) and
The composition of the ascending gases is estimated using a method based on the C, H, O balance as well as the energy balance. The water vapour species source produced by the drying process is presented in equation 97 whereas equation 98 presents the \textit{ith} volatile gas species source. Finally, equations 99 through 103 represent the contribution of the heterogeneous reactions to the gaseous species source terms.

\begin{align*}
S_{H_2O,\text{moist}} &= \dot{\omega}_{\text{moist}}'' \cdot \varepsilon \\
S_{i,\text{vol}} &= \gamma_i (\dot{\omega}_{\text{wood}}'' - \dot{\omega}_{\text{G, char}}'') \cdot \varepsilon \\
S_{CO,\text{char}} &= \left( (2\varphi - 1)K_{\text{glob}}^{o_x}A_v[O_2]M_{CO_2} - K_{\text{glob}}^{g,1}A_v[CO_2]M_{CO_2} \right) \cdot \varepsilon \\
S_{CO,\text{char}} &= \left( (2(1 - \varphi)K_{\text{glob}}^{o_x}A_v[O_2]M_{CO} + 2K_{\text{glob}}^{g,1}A_v[CO_2]M_{CO} + K_{\text{glob}}^{g,2}A_v[H_2O]M_{CO} \right) \cdot \varepsilon \\
S_{H_2O,\text{char}} &= -K_{\text{glob}}^{g,2}A_v[H_2O]M_{H_2O} \cdot \varepsilon \\
S_{H_2\text{char}} &= K_{\text{glob}}^{g,2}A_v[H_2O]M_{H_2} \cdot \varepsilon \\
S_{O_2,\text{char}} &= -\varphi \cdot K_{\text{glob}}^{o_x}A_v[O_2]M_{O_2} \cdot \varepsilon
\end{align*}

where $S_j$, $\gamma_i$, $M$, $\varepsilon$, $\omega$, $A_v$, $K$ and $\varphi$ are respectively the gaseous species source of the \textit{jth} species, the mass fraction of the \textit{ith} volatile, molecular weight, solid fraction, reaction rate, area-volume ratio, char reaction constants (equations 57 through 59) and the char oxidation parameter (equation 53).

2.6 Conclusion

The literature showed that the combustion chamber of interest consisted of the solid and gas phases in interaction. The fuel-bed, which is the area of the combustion chamber occupied predominantly by the solid fuel, can be modelled by one of three approaches: the single porous particle, the continuous porous medium and the particle resolved models. The single porous particle fuel bed model places the greatest emphasis on intra-particle heat and mass transfer. On the other
hand, the continuous porous medium model considers the bed as a continuous porous medium which does not take into account intra-particle behaviour. Finally, the particle resolved model can be seen as a combination of the two above mentioned models.

During the combustion process the solid fuel goes through three sub-processes: drying, devolatilization and char consumption. Drying is revealed by the literature as the thermally driven removal of the solid fuel’s moisture content. This process behaves as a heat sink which takes place at a constant saturation temperature. Devolatilization is characterised by the formation of three products from the dry biomass. These are gas, tar and char. The tar undergoes secondary cracking processes which breakdown the tar into smaller hydrocarbons. The gas together with the broken down tar are consumed by homogeneous reactions modelled in the freeboard region of the combustion chamber. The consumption of the solid char, however, takes place through the gasification and oxidation of the carbon (the only constituent of char) in heterogeneous reactions. The rate of char consumption is dependent on the diffusion of oxygen, carbon monoxide and water vapour towards and away from the char surface. The energy that evolves from the heterogeneous and homogeneous reactions is exchanged between the gas and solid phases through convection and radiation. The modelling of this through ANSYS Fluent takes place through the introduction of UDFs which enable this commercial CFD package to capture the heat transfer between the phases when thermal equilibrium is not assumed.
Chapter 3: Experimental Design and Testing

3.1 Introduction

This chapter aims to give a description of the individual experimental apparatus used in obtaining the results from the experiments conducted as well as an overview of the entire experimental setup. The chapter will first describe the aims of the experimental tests conducted. This will be followed by a detailed description of the experimental materials used. Subsequently, a detailed description of the experimental equipment is given. This is followed by a description of the experimental procedure to elucidate the manner in which the equipment will be used in order to conduct the combustion test. The experimental matrix is described next. Finally, a conclusion of the chapter is given.

3.2 The aim of the experiments

The experiments conducted herein are only aimed at validating the results obtained from the CFD model. This includes the experimental determination of model input parameters as well as output data for purposes validating the combustion model. In addition to the combustion test itself, experimental tests are carried out to characterise the fuel in order to help in accurately representing it in the model.

3.3 Materials used in the experiments

3.3.1 Fuel (geometric and body properties)

The experiments conducted used briquettes made with two separate sets of feed stock (namely, cow dung (80% mass) and yellow thatching grass (20% mass) (Figure 3) and cow dung (80% mass) and peanut shells wherein the cow dung serves as the binding agent for the two instances) prepared under various pressure conditions. In all the test cases, two briquettes prepared in the same way would be tested at a time. Table 1 presents both geometric as well as body properties of the briquettes tested. This table further presents the minimum and maximum mass fraction estimates occupied by the fuel in the fuel bed.
### Table 1: Geometric and body properties of the test fuels

<table>
<thead>
<tr>
<th>Mass of briquettes(g)</th>
<th>Briquette dimensions(cm)</th>
<th>Volume of the briquettes (m³)</th>
<th>Volume fraction occupied by 2 briquettes</th>
<th>Density of the briquettes(kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Peanut shells</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(5 Tons)</td>
<td>175</td>
<td>Diameter=9.5</td>
<td>Min=0.36</td>
<td>352.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Thickness=3.5</td>
<td>Max=0.42</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.000496</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Peanut shells</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(10 tons)</td>
<td>221</td>
<td>Diameter=9.5</td>
<td>Min=0.46</td>
<td>346.4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Thickness=4.5</td>
<td>Max=0.54</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.000638</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Yellow thatching</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>grass(5 Tons)</td>
<td>123.5</td>
<td>Diameter=9.5</td>
<td>Min=0.46</td>
<td>193.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Thickness=4.5</td>
<td>Max=0.54</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.000638</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Yellow thatching</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>grass(10 Tons)</td>
<td>128.5</td>
<td>Diameter=9.5</td>
<td>Min=0.36</td>
<td>259</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Thickness=3.5</td>
<td>Max=0.42</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.000496</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Yellow thatching</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>grass(15 Tons)</td>
<td>146</td>
<td>Diameter=9</td>
<td>Min=0.41</td>
<td>254.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Thickness=4.5</td>
<td>Max=0.48</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.000573</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Figure 2: Yellow thatching grass and cow dung briquette**
3.3.2 Thermogravimetry (proximate analysis)

The thermogravimetric analysis of the fuel specimens of interest is conducted according to ASTM E1131 [44]. This is an empirical approach to determining the amounts of highly volatile, medium volatile, combustible material and ash components of the solid fuels under investigation. This is achieved by first exposing the specimen to an inert gas environment while mass loss is observed as a consequence of the specimen being heated at a predetermined rate of temperature change between 10 and 100°C/min. The various constituents of the specimen are determined on the basis that each has a distinctive thermostability range. These are the distinctive temperature ranges within which each of the components is lost during the thermal decomposition of the specimen. The temperature range of the test is between 25 and 1000°C.

The ASTM E1131 [44] standard in use dictates that the apparatus used consists of the following: a thermobalance, temperature controller, data collection device, containers and gas flow device. The thermobalance is comprised of a furnace which provides a means by which the specimen can be uniformly heated in the range of 25 to 1000°C; a temperature sensor which indicates the specimen and furnace temperatures; an electrobalance which allows for the continuous measurement of the specimen mass with a minimum value of 30mg and a sensitivity of 1μg. The temperature controller is required to be able to operate the furnace between predetermined temperature limits at a rate of change of temperature between 10 and 100°C. The data collection device is the instrument through which the three minimum signals required for thermogravimetry namely mass, temperature and time are acquired, stored and displayed. The containers are required to be inert to the specimen and to remain dimensionally unchanged when subjected to the range of temperatures of the test. Finally, the gas flow device should be able to switch between the reactive and nonreactive gases.

In the case of a sample which constitutes a mixture or blend such as the briquettes currently under consideration, ASTM E1131 [44] dictates that measurement be taken to obtain a specimen that is representative of the sample for purposes of analysis. In instances involving a solid specimen, then this can be done in one of two ways. Multiple specimen can be extracted from different areas of the sample and either combined for a single test or run separately where the final determination is the average of the multiple tests. This work employs the former approach where specimen is obtained from four areas of each sample tested.

The standard in use, ASTM E1131 [44], gives tools for carrying out the proximate analysis for five different sets of materials from the thermally driven mass decay data obtained from
thermogravimetric tests. These five sets of materials include coal, elastomers, thermoplastics, lubricants and thermosets. Based on the similarity of application of coal and biomass briquettes, the analysis approach employed for coal is used to approximate the components of the biomass briquettes under consideration.

According to this standard, the mass percent of the initial mass of coal which constitutes highly volatile matter is obtained at 110°C. On the other hand, the medium volatile matter component is determined as the mass percent of the coal lost between 110 and 900°C. The amount of combustible matter is obtained as the mass percent lost in the presence of a reactive gas between 900 and 1000°C. The remaining substance at this point is the ash component. However, the temperature range used in this work is between the ambient temperature and 900°C. As a result, the amounts of highly volatile and medium volatile matter are individually determined while the amount of combustible material and ash present in the relevant fuel specimen is given as a single combined value.

3.4 Experimental Equipment

3.4.1 Stove/combustor

The combustor is a hollow cylinder where the hollow represents the combustion chamber. The inner diameter of the cylinder is 11cm whereas the outer diameter is 23.5cm. In between these diameters resides a refractory and insulating material in the form of a ceramic material. The depth of the combustion chamber is 25cm which is where the grate is situated. Immediately below the grate, the primary air inlet is found on the periphery of the outer diameter of the combustor. It is itself a short hollow cylinder with an inner diameter of 6cm.

3.4.2 Scale (mass balance)

The combustor mentioned above is placed on an electronic scale. This electronic scale is used to capture the mass loss of the stove-fuel system in time thereby enabling the determination of the mass loss rate. This scale is directly connected to a computer which logs the time changing mass of the combustor-fuel system through the aid of a custom interfacing program without the intervention of a data logging module. The sensitivity of the scale is 0.5 grams whereas the upper limit of the mass that can be measured is 30kg. The data is logged at a frequency of a reading per second.

3.4.3 Thermocouples

The temperatures of the ambient air, inlet air, exhaust gas outlet as well as the freeboard are captured by a total of 4 thermocouples each placed immediately above mentioned points where the temperature values are of interest. The first two thermocouples are K-type thermocouples whereas the latter two are N-type industrial thermocouples with plug in capability. The thermocouples used to
record the exhaust gas outlet and freeboard temperatures are inserted at the gas outlet at the top end of the combustor. The depth of the freeboard thermocouple into the combustion chamber lies at 4cm from the top of the combustion chamber. Both the flue gas thermocouple as well as the freeboard thermocouple are fixed in their desired position with the aid of the four-legged stand. Data logging modules are used to record the temperature measured by each of the thermocouples. This is done at a frequency of a reading per second.

3.4.4 Flow meter

The flow velocity of the inlet air is captured by a hot wire anemometer. This device consists of a telescopic probe and a cable which relays measurements to a display that allows for the display of both the measured velocity and temperature of the flow. The resolution of the flow velocity and temperature are, respectively, 0.1 m/s and 0.1°C. Given that a dedicated thermocouple had been positioned to capture the primary air inlet temperature, only the velocity values measured by the hot wire anemometer was considered for use. Table 2 gives the range of primary air velocities for the tests conducted for the briquettes considered in Table 1.

<table>
<thead>
<tr>
<th>Table 2: Primary air velocity ranges</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peanut shells (5 tons)</td>
</tr>
<tr>
<td>Velocity ranges (m/s)</td>
</tr>
</tbody>
</table>

3.4.5 Calorimetry

The calorific values of the briquettes tested are thought to be of interest in fully describing the characteristics of the solid fuels. To this end a Cal2k bomb calorimeter was used. Such an instrument consists of the following components: a combustion chamber, crucible, crucible holder, vessel, firing cotton and firing wire. The function of the bomb calorimeter is complemented by a filling station, oxygen cylinder, a high precision mass scale as well as a data logger in the form of a computer.

In conducting the bomb calorimeter tests, the following procedure is observed: firstly, the mass of the fuel of interest is weighed using the high precision scale. The maximum allowable mass of the fuel is 0.5g. This mass of fuel is subsequently placed into the crucible held by a crucible holder. In this configuration, the firing cotton, which is attached to the firing wire is placed inside the crucible together with the fuel to act as an ignition aid. The fuel-crucible-holder system is placed inside the vessel which is tightly closed and pressurized by the oxygen tank at the filling station. The required
vessel pressure is 3000kPa and as such the vessel is removed from the filling station when this pressure is reached.

The vessel is then placed inside the open combustion chamber. From this point onwards instructions are followed from the display on the combustion chamber. The first instruction displayed on the combustion chamber display requires the insertion of the fuel mass obtained from the scale into the combustion chamber system through the keyboard of the computer used to log the progress of the test. This is followed by the instruction to close the combustion chamber. This is immediately followed by an initializing process which is in turn succeeded by the combustion of the fuel which is observed through the computer monitor by means of a vessel temperature-time curve generated/logged by Cal2k-eco. The combustion chamber display gives the measured calorific value of the fuel at the end of the process. Table 2 presents the calorific values of both yellow thatching grass as well as peanut shell briquettes made under 5, 10 and 15 tons of load.

Table 3: Calorific values (CV) of yellow thatching grass and peanut shell briquettes for 5, 10 and 15 tons of production load

<table>
<thead>
<tr>
<th></th>
<th>CV (MJ/Kg) - 15 ton</th>
<th>Mass (g)</th>
<th>CV (MJ/Kg) - 10 ton</th>
<th>Mass (g)</th>
<th>CV (MJ/Kg) - 5 ton</th>
<th>Mass (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>yellow thatching grass</strong></td>
<td>14.35</td>
<td>0.489</td>
<td>15.79</td>
<td>0.488</td>
<td>15.57</td>
<td>0.487</td>
</tr>
<tr>
<td><strong>Peanut shells</strong></td>
<td>16.08</td>
<td>0.496</td>
<td>16.85</td>
<td>0.489</td>
<td>17.1</td>
<td>0.496</td>
</tr>
</tbody>
</table>

3.5 Experimental procedure

The experiments were carried out in a configuration that placed the stove on the electronic scale (Figure 2). The purpose of this was to capture the rate of mass loss of the combustor-fuel system. Thermocouples were placed at the inlet of the primary air as well as at some point in the room in order to capture the ambient temperature (Figure 2).

Two more thermocouples are required. One was used to capture the temperature at a point in the freeboard whereas another was placed at the flue gas outlet to capture the temperature of the flue gases (Figure 2). This is to give an indication of what temperatures can be deemed reasonable inside of the system being simulated. These two thermocouples were inserted into the combustion chamber through the flue gas outlet at the top end of the cylindrical combustor.

A more accurate temperature representation along the longitudinal direction of the combustion chamber (in both the fuel bed and freeboard) could be obtained with more thermocouples placed at different points along the length of the combustion chamber. However, the combustor used for these experiments does not allow for this as these thermocouples can only be inserted from the top. This
means that an addition of thermocouples may start to significantly affect the flow area of the flue gases in addition to the difficulty in accurately determining the depth at which the thermocouples would be placed. This would not be so if the combustor was such that the thermocouples could be inserted into the combustion chamber radially (from the side).

The primary air intake into the combustion chamber occurs through a cylindrical inlet on the lower periphery of the cylindrical combustor. The experiment keeps the flow as a natural up-draught. A hot wire anemometer is utilised to capture the speed of the primary air as it enters the combustion chamber. The flow speed was sampled at the centre of the inlet at various times in order to determine the range of maximum flow speeds and subsequently approximate the mass flow rate for each test case.

The experiment is carried out inside an enclosed space and as such ventilation is provided through a conical chimney as shown in Figure 2. The chimney is held up by a four-legged stand with a meshed top. In addition, this stand provides support for 3 of the 4 thermocouples used in the setup.

The ignition process, as observed in the preliminary tests, required the aid of ignition agents. In this case the chosen ignition agents consist of a measured amount of loose biomass in the form of twigs as well as off-the-shelf “firelighters”. The preliminary tests further revealed that solid briquettes with no holes which fill a significant proportion of the circular cross-section of the test stove leaving little room for air flow either smoulder or completely fail to combust.

The combustion test proceeded by first placing the twigs and firelighters on the grate which were then ignited. This was followed by throwing into the combustion chamber two briquettes each of which would be broken up into smaller pieces in order to allow for more air flow. An additional piece of firelighter would be dropped onto the top of the briquettes in order to ensure successful ignition. Once the ignition process is deemed successful, which is determined by the presence of flame, the combustor-fuel system is placed on the scale where the three thermocouples measuring the outlet, inlet and freeboard temperatures as well as the hot wire anemometer are put in place. Subsequently, recording of data from the various instruments commences. The ignition approach employed in this work, however, does not account for the fuel mass loss that takes place during the ignition process but assumes it to be negligible. This assumption is based on the mass comparison before and immediately after ignition.

Given the nature of the process followed in igniting the fuel, it is difficult to measure the depth of both the fuel bed and the freeboard for each case at the beginning of the combustion process. In an attempt to estimate these values a measurement of the depth of the freeboard was taken before ignition
for two cases. The depth of the freeboard was estimated to be between 12.5 cm and 15 cm. It is this value that is used to estimate the depths of the respective regions in the CFD model.

Figure 3: An overview of the experimental setup

3.6 Experimental matrix

The measured output parameters of interest for the purposes of validation are the freeboard flame temperature, outlet temperature at the top of the combustion chamber and the mass loss rate of the combustor-fuel system. These outputs will be validated given the primary air velocity and temperature as well as fuel properties as input parameters. Given that the end goal of the study is to represent as accurately as possible the combustion behaviour of a biomass briquette combustor such as the one used in these experiments, the test conditions are kept the same as they would be in the case of normal domestic use. This means that the test parameters (i.e. primary air velocity, primary air temperature as well as the ambient temperature) are not controlled but instead observed. Therefore, repeatability of the results of these experiments cannot be tested.

3.7 Concluding Remarks

The work done in this chapter is aimed at giving a description of the individual experimental apparatus used in obtaining the results from the experiments conducted as well as an overview of the entire experimental setup. The results obtained herein constitute the means by which the model to be developed is validated. The briquettes used in the experimental tests are formed from a peanut-shell/cow-dung mixture as well as a yellow-thatching-grass/cow-dung mixture. These briquette
mixtures were compacted by 5 ton, 10 ton and 15 ton loads. The proximate analysis is carried out by means of a TGA guided by the ASTM E1131 Standard. The temperatures measured are those of the ambient air, inlet air, exhaust gas outlet and freeboard. The inlet (primary) air velocity is captured by a hot wire anemometer. A bomb calorimeter test is conducted to determine the calorific values of the solid fuel while the mass loss of the combustor-fuel system is captured by an electronic scale.
Chapter 4-Experimental Results

4.1 Introduction

This chapter presents the experimental data obtained with the objective of providing a means by which the basic physics of the CFD model discussed in the next chapter can be both setup and validated. As discussed in Chapter 3, the briquettes under consideration are the peanut shell (formed under 5 and 10 ton loads) and yellow thatching grass (compacted at loads of 5, 10 and 15 ton) briquettes all using cow dung as the binding agent. The validation of the CFD model for each of the samples is done through the measurement of macroscopic aspects of the combustion process, namely, temperature and mass loss. On the other hand, determinations that were made to aid in setting-up the model include the proximate analysis of the fuel samples.

This chapter is divided into three sections. First, the temperature profiles measured during the combustion of the above mentioned solid fuel samples. Second, the mass loss profiles of the fuel-combustor systems obtained during the combustion of the same fuels. Finally, the thermogravimetric data of the fuels. This gives an indication of the amount of moisture, volatile matter, combustible matter and ash contained within the fuel.

4.2 Temperature

The temperature profiles presented for all the fuel samples tested are measured at the same places. The temperature values deemed to be of interest are as follows: the ambient temperature, air inlet temperature, flue gas outlet temperature and the freeboard temperature. Figures 4, 5, 6 and 7 respectively represent the temperature profiles of peanut shells (5 tons), yellow thatching grass (5 tons), peanut shells (10 tons) and yellow thatching grass (10 tons).

The temperature plots in Figures 4, 5, 6 and 7 all behave in a manner similar to each other. In all cases, the flue gas temperatures are lower than the freeboard temperatures throughout the duration of the respective tests. Furthermore, the temperature profiles measured in the freeboard and flue gas outlets move in tandem with each other for all the samples presented.

It turns out from mere inspection of the temperature plots, however, that in cases where the fuel samples are prepared under similar conditions with respect to pressure, the yellow thatching grass produces comparatively higher measured temperatures in the freeboard and the flue gas outlet. Additionally, the briquettes produced under higher pressure conditions show higher peak temperatures. However, given the difference in the ambient conditions under which the tests under consideration were conducted it is more meaningful to consider the temperature difference achieved for the individual tests as opposed to the peak temperatures. Table 4 indicates the peak temperatures.
achieved in each of the tests together with the maximum and minimum temperature differences achieved. These are determined with respect to the minimum and maximum air inlet temperatures, respectively.

An observation of all the temperature plots reveals both the ambient and inlet temperatures not to be clearly distinguishable in all the cases under consideration. Table 5 gives the maximum and minimum temperature values of these quantities as a means to more clearly distinguish them.

Figure 4: Peanut shells (5 tons) temperature profile

Figure 5: Yellow thatching grass (5 tons) temperature profiles
Figure 6: Peanut shells (10 tons) temperature profiles

Figure 7: Yellow thatching grass (10 tons) temperature profiles
Table 4: Flue gas peak temperatures, minimum and maximum differences between the flue gas exit temperature and air inlet temperatures

<table>
<thead>
<tr>
<th></th>
<th>Peak temperatures(℃)</th>
<th>Minimum temperature difference(℃)</th>
<th>Maximum temperature difference(℃)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peanut shells (5 tons)</td>
<td>347.03</td>
<td>322.79</td>
<td>326.72</td>
</tr>
<tr>
<td>Peanut shell (10 tons)</td>
<td>430.75</td>
<td>409.52</td>
<td>412.99</td>
</tr>
<tr>
<td>Yellow thatching grass (5 tons)</td>
<td>435.56</td>
<td>415.45</td>
<td>418.64</td>
</tr>
<tr>
<td>Yellow thatching grass (10 tons)</td>
<td>548.5</td>
<td>527.95</td>
<td>530.52</td>
</tr>
</tbody>
</table>

Table 5: Minimum and maximum inlet and ambient temperatures

<table>
<thead>
<tr>
<th></th>
<th>Minimum inlet temperature(℃)</th>
<th>Maximum inlet temperature(℃)</th>
<th>Minimum ambient temperature(℃)</th>
<th>Maximum ambient temperature(℃)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peanut shells (5 tons)</td>
<td>20.31</td>
<td>24.24</td>
<td>19.25</td>
<td>20.03</td>
</tr>
<tr>
<td>Peanut shells (10 tons)</td>
<td>17.76</td>
<td>21.23</td>
<td>18.04</td>
<td>19.42</td>
</tr>
<tr>
<td>Yellow thatching grass (5 tons)</td>
<td>16.92</td>
<td>20.11</td>
<td>16.63</td>
<td>17.47</td>
</tr>
<tr>
<td>Yellow thatching grass (10 tons)</td>
<td>17.98</td>
<td>20.54</td>
<td>17.46</td>
<td>17.82</td>
</tr>
</tbody>
</table>

4.3 Mass decay

Figures 8, 9, 10 and 11 respectively show the mass decay of the combustor-fuel system during the combustion processes for peanut shells (5 tons), yellow thatching grass (5 tons), peanut shells (10 tons) and yellow thatching grass (10 tons). The importance of this particular section is to estimate, as
best as possible, the mass loss rate of each of the combustor-fuel systems tested. This is done through the determination of the initial and final masses in each case together with the time taken to move from one extreme to another in order to determine a path independent average mass loss rate as presented in table 6.

![Figure 8: Mass decay curve for combustor-peanut shell (5 tons) briquette system](image1)

![Figure 9: Mass decay curve of the combustor-yellow thatching grass (5 tons) briquette system](image2)
Figure 10: Mass decay curve for the combustor-peanut shell (10 tons) briquette system

Figure 11: Mass loss curve of the combustor-yellow thatching grass (10 tons) briquette system
Table 6: Average mass loss rates for the tests conducted at 1500s

<table>
<thead>
<tr>
<th>Description</th>
<th>Initial mass (g)</th>
<th>Final mass (g)</th>
<th>Mass change (g)</th>
<th>Duration (s)</th>
<th>Average mass loss rate (g/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peanut shells (5 tons)</td>
<td>7591</td>
<td>7454</td>
<td>137</td>
<td>1499.38</td>
<td>0.091</td>
</tr>
<tr>
<td>Peanut shells (10 tons)</td>
<td>7663</td>
<td>7566</td>
<td>97</td>
<td>1499.88</td>
<td>0.065</td>
</tr>
<tr>
<td>Yellow thatching grass (5 tons)</td>
<td>7548.5</td>
<td>7440</td>
<td>108.5</td>
<td>1499.38</td>
<td>0.072</td>
</tr>
<tr>
<td>Yellow thatching grass (10 tons)</td>
<td>7550</td>
<td>7436</td>
<td>114</td>
<td>1499.88</td>
<td>0.076</td>
</tr>
</tbody>
</table>

4.3 Thermogravimetric Analysis (TGA)

Thermogravimetric analysis was carried out in order to determine the highly volatile (moisture), medium volatile, combustible matter and ash proportions of the respective groups of briquettes under consideration, namely, yellow-thatching-grass/cow-dung and peanut-shells/cow-dung. This guides the manner in which the solid fuel in the CFD model is represented. As a consequence of a lack of sufficient samples to spread around for the various tests, only the briquettes produced by 10 tons were analysed in this regard.

According to ASTM E1131 [44], a determination of all the above mentioned constituents requires the test to be run up to 1000°C. However, given that this work is to model only the homogeneous reactions taking place, the range of the temperatures applied in the decomposition processes was limited to 900°C. This is the temperature at which the standard dictates the volatile component to be determined for a material most comparable to those under examination in this work—that is, coal. More specifically, the highly volatile component is determined between the ambient temperature and 110°C whereas the medium volatile component resides between 110°C and 900°C.
The use of the mentioned temperature limit means that both the combustible matter and ash proportions cannot be individually determined and as such are estimated together.

Figures 12 and 13 display the temperature driven mass decay of peanut shell and yellow thatching grass briquettes respectively. The temperatures measured during the TGA tests are recorded discretely. As a consequence the upper limit temperature value of 110°C outlined in the standard for determining highly volatile matter measured during the test is not precisely obtained but instead estimated. This is achieved by employing the closest temperature to 110°C to estimate the amount of highly volatile matter as given in Table 7. Furthermore, it is observable from the temperature driven mass decay plots that 900°C is not exactly obtained as the upper temperature limit of the tests albeit the aim. The upper limit temperatures are presented in Table 7 while Table 8 presents the proximate analysis.

Figure 12: TGA temperature driven mass decay curve for peanut shell briquette
Figure 13: TGA temperature driven mass decay curve for yellow thatching grass briquette specimen

Table 7: Actual upper limit temperatures used to determine the highly and medium volatile matter proportions

<table>
<thead>
<tr>
<th></th>
<th>Highly volatile matter temperature (°C)</th>
<th>Medium volatile matter upper limit temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peanut shell briquette specimen</td>
<td>109.9892</td>
<td>890.068</td>
</tr>
<tr>
<td>Yellow thatching grass briquette specimen</td>
<td>110.0017</td>
<td>889.8303</td>
</tr>
</tbody>
</table>

Table 8: Proximate analysis for peanut shell and yellow thatching grass specimen

<table>
<thead>
<tr>
<th></th>
<th>Peanut shell</th>
<th>Yellow thatching grass</th>
</tr>
</thead>
<tbody>
<tr>
<td>Moisture (%)</td>
<td>3.44</td>
<td>4.46</td>
</tr>
<tr>
<td>Medium volatiles (%)</td>
<td>64.99</td>
<td>60.63</td>
</tr>
<tr>
<td>Combustible matter and ash (%)</td>
<td>31.57</td>
<td>34.91</td>
</tr>
</tbody>
</table>

4.4 Concluding remarks

The temperature results obtained above are measured at the primary air inlet, in the room (ambient air), in the freeboard and the exhaust gas outlet. The temperatures at the first two locations where the temperatures are measured are fairly indistinguishable in magnitude and remain largely constant throughout the tests for all the fuels. The latter two locations, on the other hand, present
significant variations in temperatures observed for each individual location but similar in behaviour for the two locations. In both locations, the temperature begins by increasing in magnitude until a peak point is reached. Beyond this point the temperature starts to steadily decrease. The freeboard temperatures at the point measured (4cm from the exit) are observed to be higher than the exit temperatures for the duration of each test for all the fuels tested.

The measured mass decay plot for all the combustor-fuel systems concerned show a steep decrease in the mass followed by a sustained but significantly diminished mass loss rate. The area exhibiting high mass loss rates is understood to be associated with the loss of mainly volatiles while the sustained diminished mass loss rate is associated with char consumption. Observation reveals the volatile mass loss rate to take place at the same time as the high rate temperature decrease. This region of volatile mass loss is heuristically judged to be up to 1500 seconds for the 5 ton peanut shell briquette chosen for validation. It is within this duration that the average mass loss rate is estimated.

Finally, the TGA obtained proximate analysis is to be used to aid in representing the solid fuel in the model. The peanut shell briquettes are found to consist of 3.44% moisture (mass), 64.99% medium volatiles (mass) and 31.57% of combustible matter and ash (mass). On the other hand, the yellow thatching grass briquettes consist of 4.46% moisture (mass), 60.63% medium volatiles (mass) and 34.91% of combustible matter and ash (mass)
Chapter 5: CFD Model

5.1 Introduction

As earlier mentioned, this project aims to develop a fully representative numerical model of a domestic biomass briquette combustor. This chapter presents a detailed description of the CFD modelling of the combustion process in the biomass briquette combustor of interest to be validated by the peanut shell briquette (5 ton) combustion test case. To this end, the model geometry and mesh, modelling approach and assumptions, governing equations and model settings are chronologically discussed.

The model geometry gives a description of the geometric features of the solution domain. Additionally, the nature of the grid used in the solution as well as the process undertaken to choose the appropriate grid parameters will be considered in the mesh discussion. The modelling approach and assumptions will detail the combination of models used together with some of the restrictions placed on the model as regards each of the regions of the model. The important equations required to elucidate the mathematical formulation of the model are presented under governing equations. Finally, model parameter values for various parameters will be considered, especially ones that have been modified.

5.2 Material description

5.2.1 Material properties

The materials used in the model are presented in Table 9. This presents various properties of the materials used in the model both at a species and phase level.

Table 9: Material properties for phases 1 and 2

<table>
<thead>
<tr>
<th>Components</th>
<th>Phase 1</th>
<th>Phase 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene vapour ($C_6H_6$)</td>
<td></td>
<td>Wood</td>
</tr>
<tr>
<td>Carbon dioxide ($CO_2$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Carbon monoxide ($CO$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hydrogen ($H_2$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Methane ($CH_4$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nitrogen ($N_2$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water vapour ($H_2O$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Density (kg/m$^3$)</td>
<td>Incompressible ideal gas</td>
<td>700</td>
</tr>
</tbody>
</table>
### 5.2.2 Fuel representation

This work represents the solid fuel as a combination of segmented fuel components, namely moisture, dry wood, char and ash. The moisture component is not defined separately but instead defined within the larger wood component which excludes char and ash. This minimizes the number of phases and as such makes the model less computationally expensive. Each of these components is defined as a granular phase. All four fuel constituent components are kept stationary in the fuel bed. Based on the volume of the fuel used in the experimental program together with the volume of the combustion chamber designated as the fuel bed, the volume fraction occupied by the fuel is determined. In addition, the results obtained from the thermogravimetric analysis (TGA) of the fuel gives a measurement of the proportions of each of the fuel components (refer to Table 8).

### 5.3 Geometry and Mesh

The geometry in use is a 3 dimensional representation of the combustion chamber. This is cylindrical in form and separated into two regions, namely, the freeboard and the fuel-bed as shown in Figure 14. The freeboard constitutes the top cylinder. This represents the area in which the homogeneous reactions take place. On the other hand, the gas phase interaction with the granular phase, solid fuel representation is localised in the bottom cylinder defined as the fuel-bed. The top and bottom boundaries of the composite structure under consideration are respectively defined as pressure-outlet and velocity-inlet boundaries while the peripheral boundaries of the fuel-bed and freeboard are both defined as wall boundaries. This cylindrical combustion chamber representation...
has a uniform cross-section of diameter 11 cm. Additionally, the lengths of the fuel-bed and freeboard are respectively 10 and 15 cm.

The solution domain is meshed using hexahedral cells in both its regions as shown in Figure 14. Given the cylindrical form of both regions and consequently the entire solution domain a structured (hexahedral) mesh is typically indicated. The boundary layer mesh is captured by prism cells stratified into five layers. The size of this prism layer is determined through a smoothing function which takes into consideration the prescribed and imposed smoothness (cell growth rate) of 20%.

![Figure 14: The front/upright (a) and top (b) views of the meshed combustion chamber solution domain](image)

A mesh sensitivity study is carried out to determine the mesh size at which further reduction of the cell size no longer offers significant increases in accuracy given the associated computational cost. In this case, four cell sizes are tested each one being half the size of the immediately larger value; 10 mm, 5 mm, 2.5 mm and 1.25 mm. Table 10 gives the details of both mesh size as well as mesh quality measures. As the mesh size is varied the exit flame temperature is monitored; that is, the flame temperature at the outlet boundary. Given the transient nature of the model, comparisons are carried out at 5 seconds of run time as presented in Figure 15.
Table 10: Measures of the size and quality of the various meshes used to conduct the sensitivity study

<table>
<thead>
<tr>
<th>Cell size</th>
<th>10.00mm</th>
<th>5.00mm</th>
<th>2.50mm</th>
<th>1.25mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of nodes</td>
<td>10322</td>
<td>60282</td>
<td>364914</td>
<td>2015671</td>
</tr>
<tr>
<td>Number of cells</td>
<td>9550</td>
<td>57550</td>
<td>355250</td>
<td>1981188</td>
</tr>
<tr>
<td>Minimum aspect ratio</td>
<td>1.5344</td>
<td>1.203</td>
<td>1.0382</td>
<td>1.02</td>
</tr>
<tr>
<td>Maximum aspect ratio</td>
<td>7.6721</td>
<td>7.6248</td>
<td>7.8238</td>
<td>7.7169</td>
</tr>
<tr>
<td>Average aspect ratio</td>
<td>3.7944</td>
<td>3.0123</td>
<td>2.4498</td>
<td>1.9553</td>
</tr>
<tr>
<td>Standard deviation (aspect ratio)</td>
<td>1.9685</td>
<td>1.8743</td>
<td>1.7031</td>
<td>1.5476</td>
</tr>
<tr>
<td>Minimum skewness</td>
<td>0.042763</td>
<td>0.015768</td>
<td>0.0081755</td>
<td>0.0028369</td>
</tr>
<tr>
<td>Maximum skewness</td>
<td>0.53654</td>
<td>0.47723</td>
<td>0.45851</td>
<td>0.5366</td>
</tr>
<tr>
<td>Average skewness</td>
<td>0.11438</td>
<td>0.084567</td>
<td>0.059403</td>
<td>0.061498</td>
</tr>
<tr>
<td>Standard deviation (skewness)</td>
<td>0.089086</td>
<td>0.079233</td>
<td>0.064824</td>
<td>0.075849</td>
</tr>
</tbody>
</table>
The mesh sensitivity study conducted in the plot of Figure 15 indicates that cell sizes 10 and 5mm show a 46% difference in the temperatures predicted at 5 seconds of flow time. On the other hand, the percentage difference between cell sizes 5 and 2.5mm is 4.7% at the same flow time. While the smaller percentage difference indicates insignificant mesh sensitivity between the corresponding cell sizes, both the predicted temperatures significantly deviate from the experimentally obtained values. The 10mm mesh, however, is observed to be significantly sensitive to the reduction of the cell size but predicts temperatures closest to the experimentally obtained values in the shortest period of all the meshes tested. Given the time sensitivity of the project as well as the observed competitive accuracy of the 10mm cell size, it is chosen as the mesh to be used throughout.

5.4 Modelling Approach and Assumptions

5.4.1 Assumptions

As already severally mentioned, the solution domain consists of two regions namely the freeboard and the fuel bed. The freeboard is the region in which homogeneous reactions take place whereas the fuel bed represents the region where heterogeneous reactions take place. The modelling approach taken considers the processes occurring in each of the regions as well as the interaction of the regions by means of mass and energy transfer. The following is a list of assumptions made about the two regions and their interaction:
• The homogeneous reactions taking place in the freeboard are modelled by volumetric reactions in the species transport model
• The flow regime in both regions is assumed to be turbulent
• A multiphase modelling approach is pursued to account for the various phases present in the system under consideration
• The fuel bed is assumed to remain stationary (no translation in any direction)
• No shrinkage of the fuel bed is assumed
• The fuel under consideration is assumed to be thermally thick
• Combustion of volatiles only takes place in the freeboard
• The individual gases as well as the gas mixture are modelled as an incompressible ideal gas
• The exchange of energy between the gas and solid phases takes place through convection and radiation.
• Solid-solid heat transfer in the fuel bed, on the other hand, takes place through conduction and radiation
• The fuel in the fuel bed is defined to be composed of char, dry wood, water and ash separately
• The drying of the fuel occurs at a particular temperature of the water component of the fuel
• The gases generated during drying and devolatilization enter the gas phase instantaneously at the respective trigger conditions

5.4.2 Gas phase Conservation Equations

Five partial differential equations (PDEs) are responsible for the description of a single phase fluid flow in three dimensions namely mass conservation (equation 104), x-momentum (equation 105), y-momentum (equation 106), z-momentum (equation 107) and energy (equation 108) equations [45]. The energy equation can be given in any one of its three variants wherein either the internal energy, enthalpy or temperature is of interest [45].

\[
\frac{\partial \rho}{\partial t} + \nabla (\rho \vec{u}) = 0 \tag{104}
\]

\[
\frac{\partial (\rho u)}{\partial t} + \nabla (\rho u \vec{u}) = -\frac{\partial p}{\partial x} + \nabla (\mu \nabla u) + S_{Mx} \tag{105}
\]

\[
\frac{\partial (\rho v)}{\partial t} + \nabla (\rho v \vec{u}) = -\frac{\partial p}{\partial y} + \nabla (\mu \nabla v) + S_{My} \tag{106}
\]

\[
\frac{\partial (\rho w)}{\partial t} + \nabla (\rho w \vec{u}) = -\frac{\partial p}{\partial z} + \nabla (\mu \nabla w) + S_{Mz} \tag{107}
\]
\[ \frac{\partial (\rho i)}{\partial t} + \text{div}(\rho \vec{u} i) = -p \text{div} \vec{u} + \text{div}(k \text{grad} T) + \varphi + S_i \]  
(108)

In addition to conservation equations 104 through 108 \( \rho, p, i \) and \( T \) are linked by relationships developed under the assumption of thermodynamic equilibrium known as equations of state (equations 109 and 110) if \( \rho \) and \( T \) are used as state variables for \( p \) and [45].

\[ p = p(\rho, T) \]  
(109)

\[ i = i(\rho, T) \]  
(110)

Furthermore, this model makes use of the species transport conservation equation (equation 110a) to predict the local mass fraction of the \( i \)th species in the gas phase [46].

\[ \frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \]  
(110a)

where \( \rho, Y_i, J_i, R_i \) and \( S_i \) are respectively the mixture density, mass fraction of the \( i \)th species, diffusion flux of the \( i \)th species, net rate of production and the rate of creation through addition of the \( i \)th species from the dispersed phase as well as any user defined sources [46]. This equation is a modified form of the equation presented in equation 70. The difference is in the inclusion of the species creation term from the dispersed phase and the user defined species sources, \( S_i \), as seen in equation 110a.

The species diffusive flux term \( J_i \) is representative of the movement of species as a consequence of both concentration and temperature gradients. In a flow field modelled as turbulent as is the case in this work, the species diffusive flux is given by equation 110b [46].

\[ J_i = -\left( \rho D_{m,i} + \frac{\mu_t}{S_{Ci}} \right) \nabla Y_i - D_{T,i} \frac{\nabla T}{T} \]  
(110b)

where \( D_{m,i}, D_{T,i}, \mu_t \) and \( S_{Ci} \) are the mass diffusion coefficient for species \( i \), the thermal diffusion coefficient, the turbulent /eddy viscosity and the turbulent Schmidt number. The first term on the right hand side of equation 110b represents the concentration driven component whereas the second term speaks to the thermal gradient contribution [46].

This work models homogeneous reactions i.e. Equations 68a through 68e in the freeboard. It is due to the creation and consumption of species taking place in these reactions that the net rate of production term \( R_i \), is computed in this work. Ansys Fluent provides three models for the purpose of capturing volumetric reactions in the gas phase, namely finite rate kinetics model, eddy dissipation model and the eddy dissipation concept model [46].
The finite rate kinetics model does not assume turbulence-chemistry interaction and as such computes the species rate of creation using general rate of reaction expressions and not factoring in the effects of turbulent fluctuations [46]. Equation 71 supplemented by equation 72 gives the species net creation rate for this model. On the other hand, the eddy dissipation model assumes the reaction rate to be determined by turbulent mixing of species. This enables the neglect of complicated kinetic rates while assuming that combustion occurs immediately upon mixing [46]. In this case, the minimum or limiting rate of the two presented in equations 110c and 110d is the effective net rate of creation of species \( i \) for reaction [46].

\[
R_{i,r} = v_i'M_{w,i}A\rho\frac{\varepsilon}{k} \min_R \left( \frac{Y_R}{v_{R,r}M_{w,r}} \right) \quad (110c)
\]

\[
R_{i,r} = v_i'M_{w,i}A\rho\frac{\varepsilon}{k} \sum_{P} Y_p \left( \frac{\sum_{j} v_{j,r}M_{w,j}}{\sum_{j} v_{j,r}M_{w,j}} \right) \quad (110d)
\]

where \( Y_p, Y_R, A \) and \( B \) are the mass fraction of any product species \( P \), the mass fraction of a particular reactant, an empirical constant equal to 4.0 and an empirical constant equal to 0.5 respectively [46].

In the case of non-premixed combustion, the eddy dissipation model requires only the presence of turbulence with no ignition source. However, as regards the premixed case, combustion only takes place when the fuel-oxidizer mixture enters the computational domain. Ansys Fluent treats this particular case by making available a Finite-rate/eddy-dissipation model which uses the Finite rate kinetics model to act as a switch as the mixture enters the computation domain as it is likely to be the limiting rate at this stage. Once in the domain, the mixing rate is likely to become slower (that is, the limiting rate) than the finite rate and as such the Eddy dissipation model takes effect [46].

Finally, the eddy dissipation concept (EDC) considers turbulent mixing to be responsible for the net rate of creation in conjunction with detailed chemical mechanisms. These chemical reactions are assumed to be taking place at the scale of small turbulence structures referred to as fine structures [46]. Equations 73 through 82 move from the representation of the length fraction of the fine structures to the development of the expression for the species net rate of creation for the EDC model.

Given the descriptions of the three volumetric reaction models above, it is clear that the EDC is the one that factors in all the drivers of the reaction rate; that is, the effect of turbulence mixing/convection and kinetic rates. Therefore, it is likely to give a more representative behaviour of the model in this work albeit at a larger computational cost. However, Ansys Fluent does not permit the use of the EDC model in conjunction with the chosen multiphase model. Given the assumed turbulent nature of the flow together with the premixed nature of the volatiles as they flow from the fuel-bed into the freeboard, the Finite-rate/Eddy-dissipation model is then indicated.
The species source from the dispersed phase as well as the user defined sources, $S_i$, which appear in equation 110a in this work are only influenced by the user defined species sources that result from the drying and devolatilisation processes. Equation 97 and 117, respectively, represent the drying and devolatilisation sources.

The above discussion hints to the flow field being turbulent. The turbulence model used to capture this aspect of the flow is the standard k-epsilon model which has been observed to work sufficiently well for comparable systems in the surveyed literature [41]. Additionally, the dominant mode of heat transfer in this region is thermal radiation which is modelled by the discrete ordinate (DO) model. The reasoning behind this choice of model is similar to that used for the solid phase below. Additionally, the radiation source in this region is quantified by equation 96.

However, the presence of both gases as well as solids necessitates the introduction of a multiphase approach to the modelling of the system. The modelling of the individual phases, solid and gaseous, in this model is carried out as described next.

### 5.4.3 Solid phase

The presence and thermal response of the solid fuel in the fuel bed impacts both the fluid flow as well as the flame that develops in the freeboard. This makes accurately modelling the behaviour of the solid very important. The fuel bed is modelled as a porous region wherein the solid fuel coexists with the gas phase. This approach to modelling the fuel bed is taken as a means of capturing the pressure drop that is expected to occur in the flow due to the presence of the solid phase in this region. This is represented by the momentum sink that is given by equation 63; that is, the Ergun equation. This equation is completed by the parameters given by equations 64 through 67, respectively, permeability, inertial losses, sphericity and equivalent diameter.

The flow velocity in the porous region can be formulated as either physical or superficial [47]. The relationship between these two velocity formulations is captured by the equation 111.

$$v_{\text{superficial}} = \gamma v_{\text{physical}}$$

(111)

where $\gamma$ is the porosity defined as the ratio of the fluid to the total volume of the relevant region. The superficial velocity outside the porous zone is the same as that inside. This means that such a velocity formulation does not factor in the reduced flow area and the corresponding increased velocities. This velocity formulation is likely to yield inaccurate results in instances where velocity values and gradients are of significance. The physical, or true, velocity yields more accurate results and is consequently the velocity formulation chosen in the porous media representation of the fuel bed.

The solid fuel behaviour in the fuel bed is characterised by thermally driven decomposition of the fuel during the combustion process. The associated sub-processes are the drying,
devolatilization and char combustion processes. Ansys Fluent, the commercial CFD software used in this study, is not equipped to model the three mentioned sub-processes. As a result, UDFs developed in C were introduced to capture the sub-processes of interest.

In this work the solid phase and its behaviour are characterised by five scalar variables. These are (1) solid temperature, (2) solid fraction, (3) moisture density, (4) dry biomass density and (5) char density. However, changes in moisture and dry biomass quantities are represented by a mass transfer model which changes the volume fraction of these fuel constituents while leaving the density values unchanged. On the other hand, the char component of the fuel is included in order to represent the solid fuel as fully as possible, but due to time constraints the changes in the char solid fraction and density are not modelled but their formulations are presented. The relevant equations for the first three solid phase variables are respectively presented in equations 112 through 114. On the other hand, the scalar equations for the last two solid phase variables are respectively presented in equations 49 and 54.

Given the assumption of the stationary fuel bed used in this work, the solid temperature equation given by equation 84 is transformed into the more relevant equation 112.

\[
\frac{\partial (\varepsilon \rho_p C_p T_s)}{\partial t} = \nabla (k_{s,eff} \nabla T_s) + S_s \tag{112}
\]

Where \(\varepsilon, \rho_p, C_p, T_s, k_{s,eff}\) and \(S_s\) respectively represent the solid fraction, fuel particle density, constant pressure specific heat, solid temperature, effective temperature diffusivity and solid energy source term.

\[
\frac{\partial \varepsilon}{\partial t} = -\frac{\dot{\omega}_{c, char}'''}{\rho_p} \varepsilon \tag{113}
\]

Where \(\dot{\omega}_{c, char}'''\) (equation 56) represents the char consumption rate.

\[
\frac{\partial (\varepsilon \rho_m)}{\partial t} = -\dot{\omega}_{moist}'' \varepsilon \tag{114}
\]

where \(\dot{\omega}_{moist}'''\) (equation 47) represents the drying rate.

5.3.3.1 User Defined Functions (UDFs)

As previously mentioned, Ansys Fluent (versions 15 through 17) does not provide the necessary sub-models to enable modelling the thermally driven conversion processes of the solid fuel which has been circumvented by the use of UDFs. These UDFs are a means by which the scalar variables used to define the solid phase (fuel) are incorporated into the model in order to preserve the conservation equations presented in equations 49, 54 and 112 through 114. These five scalar
equations are derived from the generic scalar conservation equation of the form of equation 115 if $\varphi$ is introduced as the general scalar [48].

$$\frac{\partial (\rho \varphi)}{\partial t} + \text{div}(\rho \varphi \vec{u}) = \text{div}(\Gamma \text{grad} \varphi) + S_\varphi$$  \hspace{1cm} (115)

This equation (115) is known as the transport equation for the property $\varphi$ wherein all the necessary transport processes are represented. The first and second terms on the left hand side of equation 115 are, respectively, the rate of change term and the convective term, whereas the first and second terms on the right hand side are, respectively, the diffusive and source terms. $\Gamma$ is the diffusion coefficient.

A comparison of the form of equation 115 with the equation used to define the solid phase energy equation (112) reveals that the energy equation is only comprised of the diffusive and source terms. Given that heat transfer between the solid and gas phase is assumed to be facilitated by both radiation and convection, both these modes of energy transfer will feature as components of the energy source. An additional energy source component for the solid phase is derived from the reactions expected to take place on the surface of the solid fuel during char combustion. Therefore, the solid energy source will assume the form presented in equation 116:

$$S_S = S_\text{react} + S_\text{conv} + S_\text{rad}$$  \hspace{1cm} (116)

where the first, second and third terms represent the reaction, convection and radiation energy sources respectively. The convective energy source component of the solid phase is assumed to be the same in magnitude but opposite in direction to that of the gas phase with which it interacts. This is captured by equation 90. This process is facilitated with the aid of a source UDF [49]. The flow of information in this piece of code is illustrated in the flow diagram presented in Appendix A1.

On the other hand, Ansys Fluent provides five models for capturing radiation behaviour. These are the P-1 radiation model, Rosseland radiation model, Discrete Transfer Radiation Model (DTRM), Surface-to-Surface radiation model (S2S) and the Discrete ordinate model (DO) [46]. The desired radiation model is required to be able to incorporate the participative nature of the solid phase with reasonable computational cost.

The DTRM has two particular disadvantages that disqualify it as a suitable model for use in this case. Firstly, this model does not include the scattering effect of relevant optical media in its calculation of the radiation source. Secondly, it is not compatible with parallel processing, which is necessary to achieve desirable computational times. Similarly, the surface-to-surface model is disqualified based on its ineptitude in modelling participative media.
The P-1, Rosseland and DO radiation models possess no attributes in their formulation which theoretically makes one more apt to capture radiation heat transfer than another [46]. Therefore, based on the proven capabilities of the DO model by the literature surveyed to reasonably capture the radiation energy source component, the same model is given preference to the other two. This source component is introduced into the model by a DOM-Source UDF [49]. The flow chart in Appendix A2 illustrates the logic of the UDF as well as the flow of information within it.

A comparison of the form of equations 49 and 114 to the generic scalar transport equation 115 yields that these equations are only comprised of source terms. In this work, the dry wood component of the fuel is assumed to be that which is consumed during devolatilization. Each volatile that evolves from the fuel dry wood component into the gas phase should be captured by equation 117 which is a modified form of equation 98.

\[ S_{i,\text{vol}} = \gamma_i A_2 \rho_{\text{wood}} \exp \left( \frac{E_2}{RT_s} \right) \]  

(117)

where \( \gamma_i \), \( A_2 \), \( \rho_{\text{wood}} \) and \( E_2 \) are respectively the \( i \)th volatile fraction, pre-exponential for devolatilization, density of the dry wood component and the activation energy for the devolatilization sub-process. The modification comes as a consequence of the approach taken in defining fuel components in this work; that is, as opposed to the dry fuel emerging from competing processes it is defined as a known fixed volume fraction which is then consumed. The moisture component of the fuel is consumed during the drying process and converted into water vapour which is instantaneously propelled into the gas phase. The drying rate should be presented in equation 97 in conjunction with equation 47. The devolatilization and drying processes should both ideally be modelled by mass transfer UDFs [49].

However, due to the temperature dependence of both the devolatization and drying rate formulations, the ignition process employed in this work could not sustain the high temperatures for the length of time required for the combustion process to self-sustain. Given the time limitation of the project, an alternative approach was pursued. This approach gives the mass transfer rates of the various volatile gases including water as constant values. These constants are informed by the volatile mass fractions found in the thermogravimetric data of wood at 850k by Gomez et.al [38]. Validation of the model developed in this work is pursued by varying the mass transfer rates of the volatiles while keeping their proportions the same as presented in Table 11. The proportions are kept the same as a means of complying with equation 117 as closely as possible. An examination of equation 117 reveals that the volatile fraction of a species dictates the proportion of the mass transfer of the species with respect to the global mass transfer rate.
These volatile fractions are assumed to remain constant throughout the consumption of the volatile component of the fuel. The logic and information flow of the devolatilization and drying UDFs are respectively presented in the flow charts of Appendix A3 and Appendix A4 purely for completeness purposes.

An examination of Table 6 gives the estimated mass loss rate. Given that the peanut shell briquettes formed by 5 tons of force are used for purposes of validation, the estimated mass transfer rate of interest up to 1500 seconds is estimated as 0.000091 kg/s. Also, given the length of the cylindrical combustion chamber as 25 centimetres and the diameter as 11 centimetres the volume is determined to be 0.00238 m$^3$. Therefore, the mass loss per unit volume is determined to be 0.0274 kg/m$^3$.s. The volatile mass transfer proportions as seen in the first iteration of Table 11 give the following lower limit mass transfer rates: 0.01528 kg/s-m$^3$ ($H_2O$), 0.01528 kg/s-m$^3$ ($C_6H_6$), 0.00382 kg/s-m$^3$ (CO), 0.003056 kg/s-m$^3$ ($CO_2$), 0.000382 kg/s-m$^3$ ($H_2$) and 0.000382 kg/s-m$^3$ ($CH_4$).

In a manner similar to the drying and devolatilization of solid scalar equations, the char density (equation 54) and solid fraction (equation 113) equations are determined to also only consist of source terms. The char density equation is developed with the aid of the char generation and consumption rates given in equations 55 and 118 respectively where the latter equation is a modified version of equation 56 in order to reflect the assumption made in this work that char consumption only results from char oxidation.

$$\dot{\omega}_{c, char}^{m} = K_{glob}^{ox} A_v [O_2] M_2$$  \hspace{1cm} (118)
where $K_{glob}^{ox}$ represents the global char constants expressed in equation 57 with the aid of equation 60. The solid fraction equation, on the other hand, is dependent on the char consumption rate and as such only becomes relevant during char consumption. Due to time constraints the presence of the char component of the fuel is presented in the model to participate in sensible heat transfer. However, char consumption is not included in the model. Both the solid fraction as well as the char density sources are driven by source UDFs [49]. However, due to limitations in time, heterogeneous reactions are not considered. This is included purely for purposes of completeness.

5.4.4 Multiphase formulation

According to [46], the two currently available methods for modelling multiphase flow are the Euler-Lagrange and Euler-Euler approaches. The former comes in two guises, namely the discrete phase model (DPM) and the discrete element model (DEM). The latter, on the other hand, is represented by three models which are the Volume of fluid (VOF) model, the mixture model and the Eulerian model.

The Lagrangian DPM treats the fluid phase as a continuum and applies Navier-Stokes equations to capture its behaviour. The dispersed phase is solved through the tracking performed for a large number of particles, droplets and bubbles which are able to exchange energy, momentum and mass with the continuous phase. The simplification employed in this model is neglecting particle-particle interaction which is closely approximated by a system in which the volume fraction of the dispersed phase is low. This does not, however, place a restriction on the dispersed phase mass loading. This means that even a high mass loading is acceptable for a low volume fraction, i.e. $m_{\text{particles}} \geq m_{\text{fluid}}$.

The limitation of the DPM as regards modelling particle-particle interaction is circumvented by the DEM. In this case, the high volume fraction particles are treated as moving mass points whose shapes and volumes are represented as abstractions. This model neglects the details of the flow in which the particle is immersed. Newton’s second law is used to capture the motion of the particle as given by equation 119. The collision forces between particles are represented in the last term of equation 119.

$$m \frac{d\vec{v}}{dt} = \vec{F}_{\text{drag}} + \vec{F}_{\text{pressure}} + \vec{F}_{\text{virtual mass}} + \vec{F}_{\text{gravitation}} + \vec{F}_{\text{other}} \quad (119)$$

The Euler-Euler approach generally models different phases as interpenetrating continua [46]. In order to account for the inability for phases to share space, a phasic volume fraction is defined, which is a continuous function of space and time. The sum of all volume fractions is unity.
The VOF model is the only one of the three Euler-Euler sub-models that does not represent the different phases as interpenetrating continua. Instead it models, in a fixed mesh, immiscible fluids wherein the interface between the immiscible fluids is monitored. A single momentum equation is solved for all the phase. Additionally, the volume fraction of each of the fluids is monitored in each computational cell throughout the solution domain.

In contrast, the mixture model does take the interpenetrating continuum approach to multiphase modelling which enables it to model, among other things, the interaction of a dispersed phase with a fluid phase. The mixture model solves the mixture continuity equation (equation 120), the mixture momentum equation (equation 121) and the volume fraction equations for the secondary phases. Algebraic expressions are also provided for capturing relative velocities in instances where phases move at different velocities (equation 122). Additionally, the mixture model also solves the mixture energy equation (equation 123).

$$\frac{\partial}{\partial t} (\rho_m) + \nabla \cdot (\rho_m \bar{v}_m) = 0$$ \hfill (120)

where $\bar{v}_m$ is the average mixture velocity defined in equation 120a and $\alpha_k$ is the volume fraction of phase $k$.

$$\bar{v}_m = \frac{\sum_{k=1}^{n} \alpha_k \rho_k \bar{v}_k}{\rho_m} \hfill (120a)$$

$\rho_m$ being the mixture density defined in equation 120b.

$$\rho_m = \sum_{k=1}^{n} \alpha_k \rho_k \hfill (120b)$$

$$\frac{\partial}{\partial t} (\rho_m \bar{v}_m) + \nabla \cdot (\rho_m \bar{v}_m \bar{v}_m)$$

$$= -\nabla p + \nabla \cdot [\mu_m (\nabla \bar{v}_m + \nabla \bar{v}_m^T)] + \rho_m \bar{g} + \bar{F} + \nabla \cdot \left( \sum_{k=1}^{n} \alpha_k \rho_k \bar{v}_{dr,k} \bar{v}_{dr,k} \right) \hfill (121)$$

Where $n$, $\bar{F}$, $\mu_m$ are, respectively, the number of phases, a body force and the viscosity of the mixture (equation 121a).

$$\mu_m = \sum_{k=1}^{n} \alpha_k \mu_k \hfill (121a)$$
And $\bar{v}_{dr,k}$ is the drift velocity of the secondary phase $k$ (equation 122).

$$\bar{v}_{dr,k} = \bar{v}_k - \bar{v}_m$$  \hspace{1cm} (121b)

The relative velocity is defined as the velocity of the secondary phase $p$ relative to that of the primary phase $q$.

$$\bar{v}_{pq} = \bar{v}_p - \bar{v}_q$$  \hspace{1cm} (122)

$$\frac{\partial}{\partial t} \sum_{k=1}^{n} (\alpha_k \rho_k E_k) + \nabla \cdot \left( \sum_{k=1}^{n} (\alpha_k \bar{v}_k (\rho_k E_k + p)) \right) = \nabla \cdot (k_{eff} \nabla T) + S_E$$  \hspace{1cm} (123)

where

$$E_k = h_k + \frac{p}{\rho_k} + \frac{v_k^2}{2}$$  \hspace{1cm} (123a)

Similar to the mixture model, the Eulerian model also takes the interpenetrating continua approach to multiphase modelling [46]. However, this model solves as many sets of conservation equations as the number of phases, one set for each phase i.e., the continuity equation (equation 124), momentum equation (equation 125) and the energy equation (equation 126) [50, 51]. This model makes no distinction between how it solves fluid-fluid and fluid-solid multiphase flow. The latter is characterised by at least one of the phases being designated as a granular phase [46].

$$\frac{\partial}{\partial t} (\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \bar{v}_q) = \sum_{p=1}^{n} (\dot{m}_{pq} - \dot{m}_{qp}) + S_q$$  \hspace{1cm} (124)

where $\alpha_q$, $\bar{v}_q$, $\dot{m}_{pq}$, $\dot{m}_{qp}$ and $S_q$ are the volume fraction of phase $q$, the velocity of phase $q$, the mass transfer from phase $p$ to phase $q$, the mass transfer from phase $q$ to phase $p$ and the source term, respectively.

$$\frac{\partial}{\partial t} (\alpha_q \rho_q \bar{v}_q) + \nabla \cdot (\alpha_q \rho_q \bar{v}_q \bar{v}_q)$$

$$= -\alpha_q \nabla p + \nabla \cdot \bar{f}_q + \alpha_q \rho_q \bar{g} + \sum_{p=1}^{n} (\bar{R}_{pq} + \dot{m}_{pq} \bar{v}_{pq} - \dot{m}_{qp} \bar{v}_{qp})$$

$$+ (\bar{F}_q + \bar{F}_{lift,q} + \bar{F}_{wl,q} + \bar{F}_{vm,q} + \bar{F}_{td,q})$$  \hspace{1cm} (125)

Where $\bar{f}_q$, $\bar{F}_q$, $\bar{F}_{lift,q}$, $\bar{F}_{wl,q}$, $\bar{F}_{vm,q}$, $\bar{F}_{td,q}$ and $\bar{R}_{pq}$ are respectively the stress-strain tensor for phase $q$ (equation 125a), external body force, lift force, wall lubrication force, virtual mass force, turbulence dispersion force and interaction force between phases.
\[ \tau_q = \alpha_q \mu_q \left( \nabla \bar{v}_q + \nabla \bar{v}_q^T \right) + \alpha_q \left( \lambda_q - \frac{2}{3} \mu_q \right) \nabla \cdot \bar{v}_q \mathbf{l} \tag{125a} \]

where \( \lambda_q \) and \( \mu_q \) respectively represent bulk and shear viscosity.

\[
\frac{\partial}{\partial t} \left( \alpha_q \rho_q h_q \right) + \nabla \cdot \left( \alpha_q \rho_q \bar{u}_q h_q \right) = \alpha_q \frac{dp_q}{dt} + \bar{\tau}_q \cdot \nabla \bar{u}_q - \nabla \cdot \bar{q}_q + S_q + \sum_{p=1}^{n} \left( Q_{pq} + m_{pq} h_{pq} - m_{q} h_{qp} \right) \tag{126} \]

Where \( h_q \) is the specific enthalpy of phase \( q \), \( \bar{q}_q \) is the heat flux, \( S_q \) is the source term that includes source of enthalpy, \( Q_{pq} \) \( (Q_{pq} = -Q_{qp}) \) is the intensity of heat exchange between phase \( p \) and \( q \) and \( h_{pq} \) is the interphase enthalpy.

The DPM is effective only when the solid phase volume fraction is negligible while the VOF model only models immiscible fluids. These characteristics automatically disqualify both models from consideration in this work. Whilst the mixture and Eulerian models are capable of modelling the category of system under consideration, the per-phase approach employed by the Eulerian model makes it more likely to yield greater accuracy albeit at a greater computational cost. However, accuracy is considered a priority in this work and as such the Eulerian model is prioritised between the two. On the other hand, the particle tracking implicit to the Euler-Lagrange approach would make it difficult to adapt the DEM model to more complicated systems [52], which in this case would limit the scale-up potential of this particular modelling approaching that would not be encountered with the Eulerian model. Based on all the above mentioned, the Eulerian model is chosen for use in this work.

5.5 Model settings

This section presents the specific parameters and parameter values used to setup the model. These parameters are separated into the following categories: boundary conditions, which show the manner in which each boundary in the model has been defined (Table 12); discretization methods (Table 13) used to solve each of the governing equations; solution controls (Table 14) which serve as a means of controlling the stability of the solution; and initial conditions (Table 15) which specify initial values for a set of pertinent parameters.
### Table 12: Boundary values for phases 1 and 2

<table>
<thead>
<tr>
<th>Phases</th>
<th>Phase 1</th>
<th>Phase 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundaries</td>
<td>Inlet</td>
<td>Outlet</td>
</tr>
<tr>
<td>Velocity (m/s)</td>
<td>2.4</td>
<td></td>
</tr>
<tr>
<td>Temperature (K)</td>
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<td>293.15</td>
</tr>
<tr>
<td>Species mass fraction</td>
<td>0.79$N_2$</td>
<td>0.79$N_2$</td>
</tr>
<tr>
<td>Volume fraction</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Granular temperature (m$^2$/s$^2$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>momentum</td>
<td>No slip condition</td>
<td>No slip condition</td>
</tr>
</tbody>
</table>

### Table 13: Discretization methods for the various governing equations as well as pressure-velocity coupling

<table>
<thead>
<tr>
<th>Governing equations</th>
<th>Spatial discretization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gradient</td>
<td>Least squares cell based</td>
</tr>
<tr>
<td>Momentum</td>
<td>First order upwind</td>
</tr>
<tr>
<td>Pressure-velocity coupling</td>
<td>Coupled</td>
</tr>
<tr>
<td>Volume fraction</td>
<td>First order upwind</td>
</tr>
<tr>
<td>Turbulent kinetic energy</td>
<td>Second order upwind</td>
</tr>
<tr>
<td>Turbulent dissipation rate</td>
<td>Second order upwind</td>
</tr>
<tr>
<td>Energy</td>
<td>First order upwind</td>
</tr>
<tr>
<td>Discrete ordinates</td>
<td>Second order upwind</td>
</tr>
<tr>
<td>Phase 1-$H_2O$</td>
<td>First order upwind</td>
</tr>
<tr>
<td>Phase 1-$N_2$</td>
<td>First order upwind</td>
</tr>
<tr>
<td>Phase 1-$CH_4$</td>
<td>First order upwind</td>
</tr>
<tr>
<td>Phase 1-$H_2$</td>
<td>First order upwind</td>
</tr>
<tr>
<td>Phase 1-$CO$</td>
<td>First order upwind</td>
</tr>
</tbody>
</table>
Table 14: Solution stability controls for a flow Courant number of 200

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Under relaxation factors</th>
<th>Explicit relaxation factors</th>
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</thead>
<tbody>
<tr>
<td>momentum</td>
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<td>0.5</td>
</tr>
<tr>
<td>Pressure</td>
<td></td>
<td>0.5</td>
</tr>
<tr>
<td>Density</td>
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<td>0.8</td>
</tr>
<tr>
<td>Body forces</td>
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<tr>
<td>Vaporization mass</td>
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</tr>
<tr>
<td>Granular temperature</td>
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<td>0.2</td>
</tr>
<tr>
<td>Turbulent kinetic energy</td>
<td></td>
<td>0.8</td>
</tr>
<tr>
<td>Turbulent dissipation rate</td>
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<td>0.8</td>
</tr>
<tr>
<td>Turbulent viscosity</td>
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<tr>
<td>Energy</td>
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<tr>
<td>Discrete ordinates</td>
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</tr>
<tr>
<td>Phase 1-$H_2O$</td>
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</tr>
<tr>
<td>Phase 1-$N_2$</td>
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<tr>
<td>Phase 1-$CH_4$</td>
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<tr>
<td>Phase 1-$H_2$</td>
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<td>0.8</td>
</tr>
<tr>
<td>Phase 1-$CO$</td>
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<td>0.8</td>
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<tr>
<td>Phase 1-$CO_2$</td>
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<tr>
<td>Phase 1-$C_6H_6$</td>
<td></td>
<td>0.8</td>
</tr>
</tbody>
</table>
Table 15: Initial conditions for phases 1 and 2 in the freeboard and fuel bed regions where $O_2$ is the most abundant reactive species

<table>
<thead>
<tr>
<th>Regions</th>
<th>Freeboard</th>
<th>Fuel-bed</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Phase 1</td>
<td>Phase 2</td>
</tr>
<tr>
<td>X-velocity (m/s)</td>
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<td>0</td>
</tr>
<tr>
<td>Y-velocity (m/s)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Z-velocity (m/s)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>293.15</td>
<td>293.15</td>
</tr>
<tr>
<td>$H_2O$ mass fraction</td>
<td>0</td>
<td>0.01</td>
</tr>
<tr>
<td>$N_2$ mass fraction</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$CH_4$ mass fraction</td>
<td>0</td>
<td>0.01</td>
</tr>
<tr>
<td>$H_2$ mass fraction</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$CO$ mass fraction</td>
<td>0</td>
<td>0.01</td>
</tr>
<tr>
<td>$CO_2$ mass fraction</td>
<td>0</td>
<td>0.01</td>
</tr>
<tr>
<td>$C_6H_6$ mass fraction</td>
<td>0</td>
<td>0.01</td>
</tr>
<tr>
<td>Granular temperature (m^2/s)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Volume fraction</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>
5.6 Conclusion

The model domain is separated into two regions, the freeboard and the fuel bed. The current model is setup so as to only allow homogeneous reactions in the freeboard. The heat generated during these reactions is transferred to the solid phase fuel in the fuel bed through convection and radiation. Both these modes of heat transfer were modelled through the use of UDFs.

By virtue of the presence of both the solid and gaseous phases present in the combustion chamber modelled, a multiphase approach is pursued. This is done through an Eulerian-Eulerian model. The fuel which is modelled as stationary and localised in the fuel-bed is represented by two granular phases which are defined with identical properties except for the volume fraction occupied by each. The one granular phase represents the volatile component (including moisture) of the fuel while the other represents the char and ash component. Given constraints in time, only volatile consumption is modelled through the mass transfer model while the extent of the participation of the char and ash components of the represented fuel is limited to capturing the sensible heat transfer to this fuel component. The mass transfer rates of the volatile species are specified as constant values. However, an iterative approach is pursued in determining the influence of various sets of constant species mass transfer rates guided by a lower limit of mass transfer rates which is informed by the empirically estimated average mass loss rate of the combustor-fuel system.
Chapter 6: Model Results and Discussion

6.1 Introduction

As previously stated, this work aims to develop a CFD model of a domestic biomass briquette combustor which is validated by experiment. The validation of the model is based largely on the temperatures measured at a point in the freeboard of the combustion chamber as well as at the exit. It is against these output quantities that the accuracy of the model is measured. This is done by using experimentally obtained air inlet velocities and temperatures as well as estimated mass loss rates as input variables. The estimated mass loss rates as input variables are of particular prominence in this work as made clear in the discussion in Chapter 5.

This chapter seeks to present a comparison between measured and simulated temperature results at comparable locations in the combustion chamber in order to determine both the quantitative as well as qualitative accuracy of the CFD model in reflecting the experimentally measured behaviour in time. Additionally, the radial temperature distribution along the length of the freeboard is presented. In order to give the temperature distribution context, an examination of the specific parameters suspected to have an impact on these temperatures will be carried out in order to determine and discern relevant relationships. The parameters under consideration include homogeneous reaction rates, 2nd phase temperature distribution, turbulent characteristics (turbulent kinetic energy, turbulent dissipation rate and turbulent intensity), devolatilization rates as well phasic volume fraction distributions of the 2nd phase.

6.2 Model refinement

The outcome of the iterative approach described in Chapter 5 to determine the representative constant mass transfer rates for the volatile species are shown in Figure 16. The temperature distribution show to be predicted by the model at 60 seconds of simulated combustion shows a progressive decrease in exit and freeboard temperatures with every iteration. Every iteration is characterised by a set of constant mass transfer rates which are less than those of the preceding iteration in the manner explained in Chapter 5. Given time constraints, only 10 iterations could be run. At the 10th iteration the exit and freeboard temperatures predicted by the model are 623.81 and 610.09K respectively while the measured are respectively 471.67 and 505.97K. The percentage difference between the experimental and modelled temperature values at the tenth iteration for the exit and freeboard temperatures are respectively 32.3% and 20.6%. Although both these percentage differences still lie outside the 10% range, which is typically deemed sufficient for validation, the trend hints that continued iterations are likely to continue to tend towards the desired error margin for both the freeboard and exit temperatures.
6.3 Model Validation

Due to resource constraints the model under consideration simulates the combustion process under consideration for 300 seconds while the duration of the experimental test spanned 4966 seconds. An additional consequence of the resource constraints encountered was the inability to model all three sub-processes i.e. drying, devolatilization and char consumption involved in the combustion process. An examination of the TGA curve in Figure 12 reveals volatiles to be the largest constituent of the relevant fuel specimen under consideration. As such, the drying and devolatilization processes are chosen for modelling. However, given the manner in which the fuel is modelled in Chapter 5, drying is treated as part of the devolatilisation process.

According to [44], devolatilization is characterised by a greater rate of mass loss than that observed during the consumption of char. Figure 8 reveals that the mass loss rate starts to drop noticeably between 681 and 1189 seconds. This leads to the conclusion that devolatilization is dominant before 681 seconds of combustion.

The contour plot in figure 17, which represents the lengthwise symmetrical cross-section of the combustion chamber modelled, shows the gas phase temperature distribution at 60 seconds. This contour plot shows the gas phase temperature to be increasing along the entire length of the combustion chamber. Additionally, the freeboard, which occupies the region of the combustion chamber situated above the 0.1m position, shows a temperature with two sets of behaviours. One region indicates an increase in temperature towards the wall while another exhibits the opposite trend. This is discussed in more detail in section 6.4. Furthermore, the fuel-bed gas phase temperature
distribution residing below the 0.1m position along the length of the combustion chamber shows that gas phase heat transfer is taking place from the freeboard. This is shown by the increase in temperature given that no homogeneous reactions are modelled in this region. Also, the highest fuel-bed gas phase temperatures observed close to the freeboard/fuel-bed interface (0.1m position) further make the case for heat transfer from the freeboard. On the other hand, the central axis longitudinal gas phase temperature plot (Figure 17, right) shows a temperature increase throughout the length of the combustion chamber except very close to the top where a decrease is observed. This is also discussed in detail in section 6.4 in comparison to the experimentally observed temperature behaviour.

Figure 17: Gas phase temperature contour plot (left) as well as the central longitudinal axis gas phase temperature plot (right) at 60 seconds

The temperature plots of Figure 18 show a progressive decline predicted by the CFD model at the points monitored in the freeboard as well as the exit which both appear to be linear. A comparable behaviour of the experimentally obtained freeboard and exit temperatures is observed in Figure 4 only past the peak temperatures. This looks to be the case within the duration determined to be dominated by devolatilization. Also, the CFD predicted exit temperature is observed to be consistently higher than the numerically predicted freeboard temperature. However, this is inconsistent with the experimentally obtained comparison of these two points in progressing time as
seen in Figure 4 where the behaviour is reversed. The extent of this inconsistency is addressed in section 6.4.

Figure 18: Plot of the CFD values of the exit and freeboard temperatures simulated over 300 seconds

Observing Figures 19 and 20 shows there not to be any discernable qualitative agreement between experimental results and CFD predictions for the freeboard and exit points respectively. However, this is a comparison made over a very short period of time that does not take into consideration the difference in the ignition processes undertaken in the different cases. On the one hand, the ignition process in the experimental case is initially very unsteady and may be responsible for the initial temperature fluctuations observed in Figure 4 for both the freeboard as well as the exit temperatures before the respective peak temperatures are achieved. On the other hand, the difficulties associated with ignition in the experimental case were not encountered in the case of CFD ignition. This may be responsible for the large temperature deviations before flame stability is achieved in the experimental case.

As seen in Figure 4, the freeboard and exit peak temperatures are achieved at 206 and 267 seconds respectively. In the case of the freeboard point temperature, Table 16 shows a progressive decrease in the percentage error between experimental and simulated results from 210 seconds through 300 seconds. On the other hand, in the case of the exit point temperature, this same percentage difference also progressively decreases between 180 seconds and 240 seconds. Although this progressive decrease does not continue past 240 seconds, the percentage error continues to remain low until 300 seconds of combustion is achieved.
Table 16: Percentage difference of the CFD and experimental temperature values for the points monitored in the freeboard and at the exit

<table>
<thead>
<tr>
<th>Time(s)</th>
<th>% error (freeboard)</th>
<th>% error (exit)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>14.41398</td>
<td>24.98171</td>
</tr>
<tr>
<td>60</td>
<td>20.57748</td>
<td>32.25465</td>
</tr>
<tr>
<td>90</td>
<td>25.95131</td>
<td>37.48302</td>
</tr>
<tr>
<td>120</td>
<td>30.78825</td>
<td>42.33168</td>
</tr>
<tr>
<td>150</td>
<td>26.80227</td>
<td>42.44986</td>
</tr>
<tr>
<td>180</td>
<td>12.79368</td>
<td>18.53602</td>
</tr>
<tr>
<td>210</td>
<td>24.35593</td>
<td>5.3176</td>
</tr>
<tr>
<td>240</td>
<td>22.95047</td>
<td>0.247234</td>
</tr>
<tr>
<td>270</td>
<td>17.58546</td>
<td>1.315046</td>
</tr>
<tr>
<td>300</td>
<td>9.464281</td>
<td>3.754101</td>
</tr>
</tbody>
</table>

Figure 19: Experimental and CFD temperatures compared at the monitored freeboard point for the first 5 minutes of combustion
6.4 Freeboard temperature distribution

Figure 21 shows the model to predict a progressive increase in temperatures along the longitudinal direction of the freeboard up to a distance of 0.12 meters above the freeboard/fuel-bed interface. Also observed is the general progressive decrease in the temperature difference along the length of the freeboard over the same distances. This is observed up to the same distance from the interface of 0.12 meters. The radial temperature distribution at 0.15 meters above the interface, however, indicates a reverse of the above mentioned longitudinal temperature progression in specific relation to the point at 0.12 meters above the interface. Additionally, there is an increase in the temperature along the radius observed with the exception of the temperatures at the plane 0.15 above the interface which behaves in a contrary manner. All the above mentioned is observed most distinctly up to 0.03 meters in the radial direction.

On the other hand, the behaviour discussed above sees an inversion at radial distances beyond 0.05 meters, which is very close to the wall. That is, a progressive decrease in temperature is observed in the longitudinal direction in this region. The radial positions between 0.03 and 0.05 meters, however, can be seen as a region of transition where temperature behaviour observed beyond the two limits is seen in some combination. A comparison of the experimental and simulated temperature behaviour as observed in Figures 4 and 21, respectively, show a qualitative agreement within the top 0.03 meters of the freeboard where the exit temperature is less than the temperature inside the freeboard along the central longitudinal axis. This is seen more clearly in Figure 22. Furthermore, the
fact that the qualitative agreement of experiment with the model is localised in the top 0.03 meters of the freeboard explains the failure of qualitative agreement between Figures 4 and 19 as the model monitors the freeboard value at 0.04 meters from the exit which corresponds with the location of the experimentally measured freeboard temperature.

Figure 21: Radial temperature distribution along the length of the freeboard from 0.03m from the interface with the fuel bed to the exit at 60 seconds of combustion

Figure 22: Radial temperature distribution along the top 3cm of the freeboard at 60 seconds of combustion
6.5 Species mass transfer rate

Figures 23 through 28 depict the species mass transfer rates of the gases which are released into the freeboard from the solid fuel. For reasons discussed in Chapter 5, the mass transfer rates are given as constant values. The mass transfer rate radial distribution along the length of the fuel bed shows a similar behaviour for all species under consideration. Firstly, the mass transfer rates progressively decrease along the length of the fuel-bed in the longitudinal direction. Secondly, at each longitudinal height the radial mass transfer rate decreases with an increase in the radial position. This decrease is seen to be most sharp closest to the wall—that is, past the 0.05 meter radial position. Appendixes B1 through B6 show the species mass transfer rates for each of the species over a five minute period of modelling time. The distribution for each of the species is observed to remain the same for the entire simulation duration. However, the magnitude of mass transfer rates for each of the species progressively decreases with time.

Furthermore, the constant mass transfer rates specified for each species are not the same as those predicted by the model. In each case the predicted rates are less than those initially specified which yields the supposition that the specified rates serve as an upper limit. Additionally, in cases where the specified mass transfer rate is the same, the predicted mass transfer rates are also seen to be identical. This suggests that the rates predicted are independent of the specific species for which the rate is calculated.

Figure 23: Radial distribution of the mass transfer rate of $H_2O$ evolution from the solid fuel along the length of the fuel-bed
Figure 24: Radial distribution of the mass transfer rate of $\text{CH}_4$ evolution from the solid fuel volatile component along the length of the fuel-bed.

Figure 25: Radial distribution of the mass transfer rate of $\text{H}_2$ evolution from the solid fuel volatile component along the length of the fuel-bed.
Figure 26: CFD predicted radial distribution of the mass transfer rate of CO evolution from the solid fuel volatile component along the length of the fuel-bed

Figure 27: CFD predicted radial distribution of the mass transfer rate of CO₂ evolution from the solid fuel volatile component along the length of the fuel-bed
6.6 Second phase temperature distribution

An observation of Figure 29 reveals completely contradictory behaviour for the two halves of the fuel-bed in the longitudinal direction. On the one hand, the radial temperature distribution at heights (longitudinal positions) 0.02 and 0.04 meters are such that the temperatures at these height points are consistently greater than those at height positions 0.06 and 0.08 meters up to the radial position of 0.02m. This suggests a progressive decrease in the temperature of the second phase in the longitudinal direction. On the other hand, at radial positions beyond 0.03 meters the behaviour is reversed; that is, the temperatures at heights 0.06 and 0.08 meters remain consistently higher than those at height positions 0.02 and 0.04 meters in a way that shows a progressive increase in the temperature in the longitudinal direction. Additionally, the radial temperature distribution of the two lowest height points are in constant decline while the opposite is seen to be the case for the two top heights.

Given that the initial second phase temperature was 293.15\(K\), the lowest and highest temperature rises achieved by the second phase at 60 seconds of combustion are respectively 148.04 and 168.48\(K\). This indicates that the heat transfer formulation used, as described in Chapter 5, allows for the transfer of heat to the solid fuel as modelled. However, an observation of Figures 23 through 28 as well as Figure 29 show no discernable relationship between the species mass transfer rate for the approach used in modelling the species mass transfer rate in this model and the temperature of the fuel.
6.7 Second phase volume fraction

The predicted radial volume fraction behaviour along the longitudinal direction of the fuel-bed presented in Figure 30 shows a progressive increase along the longitudinal directions. A general increase in the volume fraction is observed in the radial direction at all height points. However, at the height points of 0.02 and 0.04 meters a drastic drop in the volume is observed between radial positions 0.04 and 0.05 meters. This is followed by a sharp recovery very close to the wall. Similarly, at the top two height points i.e. 0.06 and 0.08 meters, a sharp increase is exhibited from within the radial position between 0.04 to 0.05 meters. This continues up to the wall where the highest volume fractions are observed for every height point.

A comparison of the volume fraction distribution shown in figure 30 with the mass transfer rate distribution for the various species considered in figures 23 through 28 reveal an inverse correlation. Where the mass transfer rate is the highest the volume fraction of the fuel is the lowest. This relationship is also observed in areas of the domain where drastic changes occur. This refers to the sharp increases in the volume fraction observed close to the wall accompanied by corresponding sharp drops in the mass transfer rates.

The Arrhenius rate used in the surveyed literature for the determination of mass transfer rates for the various relevant species is seen in equation 117. This equation reveals a direct proportionality between the mass transfer rate and the devolatilisation fraction of the ith species in the volatile fuel component. On the other hand, the inverse correlation predicted by this model is to be expected given...
that the consumption of the fuel should be greatest where the highest mass transfer rate (fuel consumption rate) is found. This, however, does not distinctly suggest influence of the volume fraction on the mass transfer rates. This is expected given the manner in which the mass transfer rate is modelled.

Figure 30: CFD predicted radial distribution of the second phase volume fraction along the height of the fuel-bed at 60 seconds of combustion

6.8 Turbulence behaviour

6.8.1 Turbulent kinetic energy

The turbulent kinetic energy distribution seen in Figure 31 shows the most amount of turbulence to be experienced closest to the fuel-bed/freeboard interface. The turbulence intensity and by extension the turbulent kinetic energy (TKE) progressively decreases further along the longitudinal axis in the freeboard. This can also be observed to be the case for all of the five minutes modelled as shown in Figure 32. Furthermore, the radial TKE distribution at all heights in the freeboard show a progressive decrease towards the wall up to a radial position of 0.05 meters. This decrease in the turbulence towards the wall is likely a result of the no-slip condition imposed at the wall (boundary layer). Beyond the radial position of 0.05 meters a sharp increase is observed at the 0.13m longitudinal position.
Figure 31: CFD predicted radial turbulent kinetic energy along the length of the freeboard at 60 seconds of combustion

Figure 32: Turbulent Kinetic Energy contour plots over 5 minutes

6.8.2 Turbulent dissipation rate

An examination of Figure 33 yields clearer results of the predicted turbulent dissipation rate (TDR) in the radial direction. The TDR observed for all height points in the longitudinal direction remain fairly constant up to the radial position of 0.03 meters. In the region between 0.03 and 0.04 meters in the radial direction a slight dip is observed. Beyond this region, a steep increase is observed up to the wall.
On the other hand, Figure 34 clearly shows the TDR distribution along the length of the freeboard in the longitudinal direction. In the above discussion the TDR is said to be fairly constant at all heights in the radial direction. However, Figure 34 shows a slight but progressive increase of the TDR in the radial direction at each height point. Furthermore, the TDR is observed to decrease progressively along the longitudinal axis.

Figure 33: CFD predicted radial distribution of the turbulent dissipation rate along the length of the freeboard at 60 seconds of combustion

Figure 34: CFD predicted radial turbulent dissipation rate distribution along the length of the freeboard resolved between 0 and 0.35m$^3$/s$^3$ at 60 seconds of combustion
6.8.3 Inverse of the large eddy mixing time scale

The species transport model in use is dependent on the inverse of the large eddy mixing time scale as will be discussed in section 6.9. It is as a consequence of this that an examination of the CFD predicted behaviour of this parameter is deemed pertinent. Figure 35 exhibits the same behaviour in the radial direction as that seen in Figure 33. That is, an insignificant change is observed along the radius at all height positions until close to the wall where a drastic increase occurs. Similarly, Figure 36 shows a more resolved version of Figure 35 so as to better view the behaviour of the inverse of the large-eddy mixing time scale in the longitudinal direction of the freeboard. A progressive decrease in this parameter along the length of the freeboard is predicted in a similar manner as that seen in Figure 34. The slight but progressive increases observed in each height position in the radial direction far from the wall for the TDR in Figure 34 are similar to those observed in Figure 36. This also extends to the behaviour predicted in the longitudinal direction. This is to be expected given the behaviour of both the TKE as well as the TDR in the same regions.

Figure 35: CFD predicted radial distribution of the inverse of the large eddy mixing time scale along the length of the freeboard at 60 seconds of combustion
6.9 Reaction rates

Each of the reaction rates predicted are modelled as the limiting value i.e., the smallest value of equations 110c and 110d. An examination of these equations shows the reaction rate to be dependent on, among other things, the inverse of the large-eddy mixing time scale. Consideration is given to this particular parameter as it is the only variable flow character which can be easily monitored and computed as done above. Additionally, over and above the imposed models for the determination of reaction rates, reactions are modelled where they have been defined.

Looking at Figures 37 through 41 shows a general tendency of all reactions to exhibit a progressive decrease in reaction rates in the radial direction at most height points at radial positions less than 0.05m. Deviation from this pattern is observed in the radial reaction rate distribution of reactions 4 and 5 at the height point 0.013m where an increase is observed instead. However, the reaction rates at this height point all indicate a sharp drop in the reaction rate very close to the wall-at radial positions past 0.05m. This behaviour can also be observed for height point 0.016m for reactions 1, 2 and 4 while all other reaction rates for all other reactions and heights continue to drop fairly steadily. However, an observation of Appendixes C1 through C5 indicate an increase in the in the reaction rates close to wall near the freeboard/fuel-bed interface. Given the behaviour observed in Figures 37 through 41, this behaviour is likely exhibited within 3cm of the freeboard/fuel-bed interface. Additionally, in a manner similar to that observed in the case of species mass transfer, the
distribution of each reaction remains the same over the duration of the simulation while the magnitude of each reaction rate decreases with time.

Furthermore, the longitudinal reaction rate distribution shows a progressive decrease along the length of the freeboard. Exception to this trend is observed in the case of reaction 4 with respect, particularly, to the reaction rates at height point 0.013 meters. At this height point predicted rates are lower than those at height points 0.016 and 0.019 meters at the smallest radial position. The progressive reaction rate growth of the height position 0.013 meters in the radial direction leads to the restoration of the broadly exhibited longitudinal trend close to the radial position of 0.04 meters.

The relationship between the inverse of the large-eddy mixing time scale and the reaction rates predicted by the equation pair of 110c and 110d is one of direct proportionality. Therefore, all other things being equal, an increase in the one parameter should mean a corresponding increase in the other parameter as well. An examination of Figures 35 and 36 in comparison with Figures 37 through 41 show the discernable relationship between the reaction rates predicted with the inverse large-eddy mixing time scale in the longitudinal direction far from the wall (up to the radial position of 0.05 meters). Figure 36 shows a progressive increase in the large-eddy mixing time scales in the longitudinal direction, which is accompanied in general by progressively decreasing reaction rates in the same direction as shown by Figures 37 through 41. However, the general drop in reaction rates observed in the radial direction for most height positions and reactions is inconsistent with the above noted effects of the large-eddy mixing time scale on reaction rates. This is likely caused by the fact that no wall reactions are defined. This is also a likely explanation for the high rate drops experienced near the wall at height positions that generally see high reaction rates.
Figure 37: Radial distribution of the CFD predicted reaction rates of reaction 1 (equation 68a) along the length of the freeboard at 60 seconds of combustion

Figure 38: Radial distribution of the CFD predicted reaction rate of reaction 2 (equation 68b) along the length of the freeboard at 60 seconds of combustion

Figure 39: Radial distribution of the CFD predicted reaction rates of reaction 3 (equation 68c) along the length of the freeboard at 60 seconds of combustion
Figure 40: Radial distribution of the CFD predicted reaction rates of reaction 4 (equation 68d) along the length of the freeboard at 60 seconds of combustion

Figure 41: Radial distribution of the CFD predicted reaction rates of reaction 5 (equation 68e) along the length of the freeboard at 60 seconds of combustion

6.10 Conclusion

As mentioned throughout the document, the work is meant to develop a model that is validated by experiment. The specific parameter compared for validation purposes is the temperature at a point in the freeboard as well at the exit. The temperature behaviour predicted by the model for the 5 minutes modelled predicts freeboard temperatures which are lower than the exit temperatures when the freeboard position under consideration is located 4cm from the exit (Figure 18) but experimental
results predict the reverse outcome. However, the longitudinal temperature distribution predicted along the central axis shows the freeboard temperature to be higher than the exit temperature within 3cm (Figure 22) from the exit. Therefore, qualitative agreement as regards the freeboard and exit temperatures in this area is achieved with experiment, however, quantitative agreement regarding the position of this relationship is not found.

The model fails to replicate the temperature trends of the freeboard as well as the exit at least for the first five minutes modelled as compared to experiment. However, the region past the respective peak temperature points is determined as the volatile consumption period. This region exhibits experimental trends which are comparable to those seen predicted by the model. This is appropriate given that the model only captures the consumption of the volatile component of the fuel.
7.1 General Remarks

This work aims to develop a complete CFD model of a domestic biomass briquette combustor as a means of providing a platform to fully understand and enhance combustion performance in these types of combustor systems. A combustor with a cylindrical combustion chamber of length 25 centimetres and diameter of 11 centimetres was used for this work. Four different biomass briquettes were used in the combustion experimental tests which were conducted. These are: peanut shell-cow dung briquettes formed under a compaction force of 5 tons; peanut shell-cow dung briquettes formed under a force of 10 tons; yellow thatching grass-cow dung briquettes formed under 5 tons and 10 tons compaction forces separately.

The tests conducted on the fuel samples included a proximate analysis done by means of TGA as well as the determination of calorific values by a bomb calorimeter test. The bomb calorimeter tests were conducted for 5 and 10 ton peanut shell briquettes as well as 5 and 10 ton yellow thatching grass briquettes.

The experimental combustion tests, on the other hand, monitored air inlet temperatures, air inlet velocities, exit temperatures, freeboard temperatures 4 centimetres from the exit, ambient temperatures as well as mass decay of the combustor-fuel system in time. The briquettes were broken down into smaller components and so introduced into the combustion chamber. The fuels for each of the tests were estimated to occupy between 10 to 12 centimetres of the lower end of the combustion chamber.

The above discussed was then used as a guide to build a representative CFD model of the combustor. The 5 ton peanut shell briquette combustion case was used for purposes of validating the model. Due to resource constraints, the model focused solely on representing devolatilisation. The decision to model devolatilisation was based on the determination that had been made by the proximate analysis showing volatiles to be the most abundant constituent of the fuel. The model represented by two regions namely, freeboard and fuel-bed. The freeboard consisted only of the gas phase while the freeboard consisted of multiple phases in interaction; that is the solid fuel and gas phases. The multiphase nature of the model was done through an Eulerian-Eulerian model where the fuel region was considered a packed bed with the solid fuel represented by a granular phase.

The combustion modelled is based on the homogeneous reactions taking place in the freeboard which in turn transfer heat to the solid fuel in order to elicit and sustain the evolution of volatiles into the freeboard which form the reactants consumed in the mentioned reactions. The transfer of heat from the gas phase in the freeboard as well as the fuel bed to the solid fuel is modelled through both
radiation and convection. However, the commercial CFD package used, Ansys Fluent 17.0, is only equipped to carry out single phase heat transfer. This necessitated the use of UDFs to calculate the radiation and convection contributions to the solid fuel energy equation source term.

7.2 Literature VS Approach pursued in this work

The literature surveyed suggested that the mass transfer rate of each of the volatile species from the fuel to the freeboard is appropriately determined by an Arrhenius rate. This rate is dependent on the fuel temperature, activation energy of the devolatilisation sub-process as well as the volatile species fraction of each species in the volatile component of the fuel. Mass transfer UDFs were developed to reflect the species transfer rates suggested by the literature. The mass transfer rates calculated by these UDFs were insufficient to sustain the combustion process. An alternative approach was pursued. This approach used constant mass transfer rates for the species transfer rates. The initial mass transfer values used for each species were the volatile species fractions of a comparable fuel obtained from literature. An iterative process was pursued in determining mass transfer rates which gave satisfactory validation wherein the proportions of the species are kept the same in every iteration. This was done by dividing the initial set of species transfer mass transfer rate (i.e. species volatile fraction) with successive integer iteration numbers. The lower limit was determined based on the estimated average mass loss rate. However, given resource constraints, particularly time, only ten iterations could be run, each for five minutes. Comparisons between experimental and simulated temperatures were done at 60 seconds for the exit as well as the freeboard (that is, 4cm from the exit). For both positions the simulated temperatures progressively approached experimentally obtained values with each iteration.

7.3 Conclusions

The above described experimental program together with the modelling approach yields the following conclusions:

- The proximate analysis tests revealed that the peanut shell briquettes were composed of 3.44% moisture, 64.99% medium volatiles and 31.57% combustible matter.
- The yellow thatching grass briquettes consisted of 4.46% moisture, 60.63% medium volatiles and 34.91% combustible matter and ash.
- The calorific values for 5 and 10 ton peanut shell as well as 5 and 10 ton yellow thatching briquettes were respectively determined to be 17.1MJ/kg, 16.85MJ/kg, 15.57MJ/kg and 15.79MJ/kg.
- The experimental temperature variation at the exit as well as the freeboard were much more significant with a temperature difference in excess of 300K and 500K respectively achieved
between the highest and lowest temperatures for the 5 ton peanut shell briquette combustion case.

- The experimentally observed variations in the temperatures of both the inlet as well as ambient air were minimal.
- The freeboard temperatures were consistently measured to be above those of the exit for the tests conducted for all the fuels.
- The temperature behaviour predicted by the model for the 5 minutes modelled predicts freeboard temperatures which are lower than the exit temperatures when the freeboard position under consideration is located 4cm from the exit.
- The longitudinal temperature distribution predicted by the model along the central axis shows the freeboard temperature to be higher than the exit temperature within 3cm from the exit. Therefore, qualitative agreement as regards the freeboard and exit temperatures in this area is achieved with experiment, however, quantitative agreement regarding the position of this relationship is not found.

Therefore, given the aim of the work, a representative model of a biomass briquette combustor has been developed. However, the recommendations made in section 7.4 are believed will further enhance the behaviour of the model.

7.4 Recommendations

The following are recommendations which may aid in addressing some of the shortfalls seen in the development and execution of this model as well as enhancing the accuracy of the model itself:

- Using an experimental combustor that allows for thermocouples to be inserted radially along the entire length of the combustion chamber in order to get an improved view of the temperature distribution generated during experiment to allow for more accurate validation.
- Allow the model to run for at least half the length of the experimental time to see if the model will indeed replicate the experimental temperature trends exhibited in the freeboard as well as at the exit past their respective peak temperatures.
- For the sake of the model achieving wide applicability and adaptability, an approach to making the mass transfer appropriately thermally driven should be pursued. One such approach could include the application of the same approach as that in Appendix 3 applied to the density UDS as opposed to the volume fraction.
- Include the heterogeneous reactions for a more complete model.
• Define reactions at the wall to see the impact it has on the radial distribution of the predicted reaction rates
References


H. Wang, “Numerical simulations of wind driven rain on building facades under various oblique winds based on the Eulerian multiphase model”.
Appendix A: User Defined Functions

Appendix A1: Flow Diagram of Convective Source UDF

Start

Fluent solver passes the mixture level thread pointer, cell index as well as the phase indexes to the UDF

Phase level thread pointers for air and wood are determined

The following variables were accessed from the solver: density (air and wood), air velocity components \((x, y, z)\), effective air viscosity, specific heat capacity (air), air thermal conductivity, temperature (air and wood) and wood surface temperature

Reynolds number calculated
Prandtl number calculated

Nusselt number calculated (eq 38)

Convection coefficient \(\alpha\) calculated (eq 40)

Convective source = 0

Density of wood > 0

Yes

Convective source calculated (equation 90)

No

Density of wood = 0
Fluent solver passes the cell index, pointer to cell thread, solid angle directions, band numbers for non gray DOM, pointer to emission term, pointer to scattering term, pointer to absorption coefficient and pointer to scattering coefficient to the UDF.

**Emission term computed with char absorption coefficient and temperature**

Wood and char component phase level thread pointers are determined

The absorption coefficients as well the temperatures for the wood and char components of the fuel are accessed from the fluent solver and the averages of each computed by the UDF. The refractive index of the fuel as well as the Boltzman constant are manually inputted into the UDF.

**Wood density>0**

**Char_density>0**

Emission term computed with average temperature and absorption coefficient

---

*emission=0
Appendix A3: Devolatilization mass transfer UDF flow chart

Start

The fluent solver passes to the UDF the cell index, mixture level cell thread pointer, index of phase from which mass is transferred, ID of the species from which mass is transferred, index of phase to which mass is transferred, ID of species to which mass is transferred

Phase level thread pointers for the to (benzene, methane, carbon dioxide, hydrogen) and from (dry wood) phases are determined

Activation energies and pre-exponential factors for wood-gas, wood-tar and wood-char reactions are manually inputted as fixed values into the UDF together with the universal gas constant

Mass transfer rate calculated (equation )
Appendix A4: Drying mass transfer UDF flow chart

1. The Fluent solver passes to the UDF the cell index, mixture level cell thread pointer, index of phase from which mass is transferred, ID of species from which mass is transferred, index of phase to which mass is transferred, ID of species to which mass is transferred.

2. Phase level thread pointers for the to (water vapour) and from (liquid water) phases are determined. Also, the Latent heat of water for the Johannesburg altitude (LH) as well as the evaporation temperatures (T_{evap}) are manually entered into the UDF.

3. The UDF accesses from the Fluent solver the physical time step used, moisture density (\rho_{h2o}), moisture heat capacity, moisture temperature (temp_{h2o}) and volume fraction.

4. If Temp_{h2o} > T_{evap} and \rho_{h2o} > 0, then the mass transfer rate is calculated.

5. If Temp_{h2o} \leq T_{evap} or \rho_{h2o} \leq 0, then the mass transfer rate is zero.
Appendix B: Species mass transfer rate contour plots

Appendix B1: H2O mass transfer rates

Figure 42: H2O mass transfer rate contour plots over 5 minutes
Appendix B2: CH4 mass transfer rates

Figure 43: CH4 mass transfer rate contour plots over 5 minutes
Appendix B3: H2 mass transfer rate

Figure 44: H2 mass transfer rate contour plots over 5 minutes
Appendix B4: CO mass transfer rates

Figure 45: CO mass transfer rate contour plots over 5 minutes
Appendix B5: CO2 mass transfer rates

Figure 46: CO2 mass transfer rate contour plots over 5 minutes
Appendix B6: C6H6 mass transfer rates

Figure 47: C6H6 mass transfer rate contour plots over 5 minutes
Appendix C: Reaction rates

Appendix C1: Reaction rate 1

Figure 48: Reaction rate 1 contour plots over 5 minutes
Appendix C2: Reaction rate 2

Figure 49: Reaction rate 2 contour plot over 5 minutes
Appendix C3: Reaction rate 3

Figure 50: Reaction rate 3 contour plot over 5 minutes
Appendix C4: Reaction rate 4

Figure 51: Reaction rate 4 contour plot over 5 minutes
Appendix C5: Reaction rate 5

Figure 52: Reaction rate 5 contour plots over 5 minutes