Numerical Modelling Methods of Biomass Combustion in Packed Beds

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***Abstract*— The cyclic nature of biomass as a fuel, has taken its advantages over fossil fuel Biomass contributes to the largest share of the renewable energy supply of present world. For effective utilization of energy stored in biomass by combustion a good understanding of the mechanisms involved in the combustion process should be obtained. Study of the mechanisms can be done through experiments or using Computational Fluid Dynamics (CFD) method. The numerical simulation approaches related to packed bed combustion modeling retrieved from research papers, books and other publications is presented in this work. This will provide a basis for understanding the complexities in biomass combustion modeling in packed beds.**

Keywords—biomass; Computational Fluid Dynamics; combustion; numerical modeling; packed beds

I. Introduction

Rapid depletion of fossil fuel and the increasing pressure on the environment by fossil fuel has created an important place for the alternative energy sources within the present context of energy. Therefore the cyclic nature of biomass as a fuel, has taken its advantages over fossil fuel. Biomass contributes to the largest share of the renewable energy supply of present world.

Total primary energy supply has been increased from 6106 Mtoe in 1973 up to 13371 Mtoe in 2012. The share of renewable energy sources in the primary energy supply is 13.5 %. The bio-fuel contributes to 10 % of the world total primary energy supply[1].

Combustion is the main conversion technology to use biomass for energy. It is considered to be the most economical and simplest method of conversion technology and is being used around 90 % in the world[2]. The high moisture content, high volatile content, ash formation characteristics and high oxidation reactivity of the biomass adds complexity to the prediction of biomass combustion processes specially in industrial applications.

II. Fixed Bed Combustion Of Biomass

Fixed bed combustion technology is commonly used in industrial applications due to its simplicity and degree of controllability. When the fuel rests on the bed combustion agent is injected through the distributor plate at the bottom. The fuel is subjected to the major steps of drying, pyrolysis, gasification and combustion during its stay on the bed. There is no sharp separation of the occurrence of these processes in the bed. The biomass particle may undergo simultaneous drying and pyrolysis or pyrolysis and char combustion. The combustion agent changes its composition and the temperature when it percolates through the fuel bed. Therefore drying , pyrolysis, gasification and char combustion are distributed irregularly on the bed. The volatiles released from the reactions will not be fully utilized during its stay in the furnace and unburned char may be discharged without being used. In addition the burnouts make holes in the bed and exposes the bed to higher atmosphere temperatures. This will damage the grate. Channels form in the fuel bed where the pressure drop is low and if the fuel is dry it makes local combustion zones[3].

Fixed bed arrangements can be classified into three categories according to the flow direction of flue gas and fuel.

The biomass combustion occurs through the major steps of drying, pyrolysis, gasification and combustion.

A. Counter Current Flow

Counter current flow arrangement is shown in *Fig 1*.Counter current flow is suitable for fuels with low heating values. Hot flue gases passes over the fresh fuel entering the combustion chamber allowing the moisture in the fuel to be vaporised. Counter current flow fuel beds produces colder gases with more tar content than the co current flow.

B. Co Current Flow

Co current flow is suitable for fuels with low moisture content or systems where preheated primary air is used. The residence time of the unburned gases increases in this system and NOx emission is reduced due to enhanced contact of flue gas with the charcoal bed. Higher fly ash entrainment can be occurred.

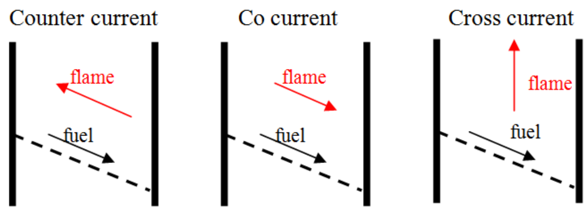

Fig. 1. Classification of grate combustion technologies

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C. Cross Flow

Cross flow combustion is applied in combustion systems with vertical secondary combustion chambers. In this type of furnaces a mixture of counter current flow and co current flow occurs. Cross flow furnaces are used with coarse particle sizes. The fuel is transported by a moving grate. In different parts of the bed air supply can be changed.

III. Computational Fluid Dynamics Modelling for Fixed bed Combustion

Computational fluid dynamics is a tool used to analyse and design fluid flows which involves mass transfer, heat transfer, chemical reactions, phase changes and other associated phenomena. thermo chemical conversions are represented by Partial Differential Equations(PDE) and it utilizes power of computers to convert these PDEs to algebraic form and solve them.

CFD provides the benefit of obtaining accurate results with less financial involvement than experimental procedures. In addition it reduces the time involvement and advantageous for the situations where it is difficult to conduct full scale tests.

CFD modeling approach consists of the following elements

- Pre –processor

In pre processor the geometry of the study has to be defined. In this pre processor stage grid generation, selection of physical & chemical phenomena, defining fluid properties, specification of appropriate boundary conditions are done Solver

Solver is used to convert the PDEs describing the system to algebraic form. There are number of methods used for this purpose.

-Finite element method

- Finite difference method

- Spectral methods

- Finite volume method

Finite volume method is the most commonly used method due to its easiness in understanding, programming and versatility. It involves the formulation of control volumes to convert the PDEs to algebraic form. The governing equations describing the system are integrated over all the control volumes and then converted to algebraic form using discretisation methods. Solution for these algebraic equations is obtained by iterative calculations[4].

- Post – processor

Post processor is used for visualization of data.

Numerous CFD packages were used by different researchers for the simulations. Fluent was used in[3]–[7].The commercial code CFX was used for the work presented in[8], [9]. FLIC and Fluent combination was used by Yang et al. to model the effect of channeling in fixed bed combustion[10]

The CFD modeling can be split into two categories i.e. the conversion of biomass in the fuel bed and the modeling of mixing, combustion, pollution formation, deposit in the free board[11].

The most popular method of modeling fixed bed combustion of biomass involves simulating the bed with a different model and simulating the free board with CFD. The two models are coupled with the mass and heat transfer at the interface. In this approach bed model provides the inlet conditions to the free board and the freeboard simulation returns the heat flux released from the flame and the furnace walls onto the fuel bed.

The other approach considers the fuel bed as a part of the CFD simulation domain. In this method precise size distribution of the biomass particles fed into the furnace is of high importance for the final results of the CFD simulations[11].

There are three modeling approaches which was used by the previous researchers to model the fuel bed.

Approach 1- FLUENTs porous media model is used to simulate the fuel bed on the grate. The results of this simulation are used as the inlet conditions to model the freeboard area.

Approach 2 - Freeboard modeling is carried out by taking inlet conditions from experience or measurements. When the combustion rate is prescribed as a function of the position of the grate the inlet conditions can be calculated by overall heat and mass balances for fuel components and primary air.

Approach 3 - Separate models are formulated to study the biomass conversion of the fuel bed. The ignition front and the combustion front of the fuel bed are tracked and the temperature, species concentrations and the velocity at the bed top is solved which is used as the inlet conditions for freeboard modeling.

Combustion of packed bed includes models for mass, momentum, energy and species conservation, models for thermo chemical reactions, models for turbulence and radiation heat transfer.

The following are the basic governing equations applied for fluid flow system.

Equation for conservation of mass

$$\partial\rho/\partial t+\nabla.(\rho u)=S_p \tag{1}$$

Equation for conservation of momentum

$$\partial\rho u/\partial t+\nabla.(\rho uu)=-\nabla p+\nabla.(\mu\nabla u)+S_u \tag{2}$$

Equation for conservation of energy

$$\partial\rho H/\partial t+\nabla.(\rho uH)=+\nabla.(\lambda\nabla T)+S_H \tag{3}$$

Equation for conservation of species

$$\partial\rho Y_i/\partial t+\nabla.(\rho uY_i)=+\nabla.(D\nabla(\rho Y_i))+S_Y+R_f \tag{4}$$

In the above equations D is diffusion coefficient(m^2/s),u is velocity(ms^{-1}), ρ is density(kg/m3), R_f is net rate of production of species, Sp mass source term(kg/m^{3}s), S_u momentum source term(kg/m^{2}s^2), S_H energy source term(W/m^3),S_Y is the species source term which includes gaseous reactions, drying, pyrolysis and heterogeneous reactions, t time(s) Y mass fraction, λ thermal conductivity (W/mK),μ viscosity (Pas).

IV. Thermochemical Reaction Models

A. Drying

Constant temperature drying model

Constant temperature drying model- Drying starts when a predefined temperature(Normally 100 ^oC) is reached and it is assumed that the entire drying process takes place through heat transfer. When the moisture in the wood reached the predefined temperature ,all the heat given to the moisture is absorbed until the drying ceases. The implementation of this method is valid under two conditions. One is the drying front is assumed to be infinitely thin and the particle is divided into moist and dry sections or the governing equation must contain a conditional statement. This will not hold for the cases where the biomass particles are thermally thick. The second method is not computationally efficient as it includes additional complications into the governing equations.

Kinetic model

Kinetic model treats drying as a thermally activated process and uses first order Arrhenius rate equation to describe it. The activation energy and pre exponential factor is chosen in a way that the evaporation rate increases rapidly when the evaporation temperature increases. It offers the advantage of describing the drying as another reaction in particle models and results in smooth intra particle gradients. The disadvantages in this method are that drying takes place before reaching the evaporation temperature and the kinetic parameters in the literature shows wide variation.

Equilibrium Model

In this model it is assumed that the bound and free water is in equilibrium with local gas phase. Partial pressure of water is defined by the local saturation pressure. This method results in depression in pressure ahead of the drying front and requires simultaneous solutions for algebraic and differential equations.

B. Pyrolysis

Pyrolisis is the process of conversion of biomass into char, gases and other liquid products in the absence of oxygen. Products of pyrolysis are largely defined by the temperature, heating rate, residence time and the properties of biomass[12]. Pyrolysis of large biomass particles is a complex process. The models used to describe the pyrolysis process is categorized either as network models or empirical models. Global one step model, competitive reaction models, and pseudo component models come under empirical models. Many of these models were first developed for reaction of coal and extended for reactions of biomass.

Three major network models can be found in literature. The first one is the Functional Group, Depolymerization, Vaporization and Cross linking(FG-DVC) model. This has two models, one for functional groups which have similar chemical reactivities and other model explains Depolymerization, Vaporization and Cross linking.

chemical percolation devolatalisation (CPD) depends on the structure of the biomass. The data on the fraction of carbon atoms with different types of bonds obtained by solid-state nuclear magnetic resonance (NMR) spectroscopy data is used as input for this second type of model.

The third approach is FLASHCHAIN approach. This uses the biomass structure simplified into linear chain. The input parameters are obtained by ultimate analysis, NMR data and extract yield.

C. Heterogeneous Reactions

Char particles reacts with the gases of O_2, H_2O,H_2 and CO_2 on the surface of the particle. Some authors have neglected the reactions of char with H_2O,H_2 and CO_2 considering slow reaction rates of these reactions compared with the char oxidation under the experimental conditions of their research[13].

The reaction rate of the char is determined by three processes. The transfer of reactant gas from the bulk gas flow to the particle surface, diffusion of the reactant gas to the pores of the particle and the rate at which the reaction occurs. Therefore three zones of reactions which are governed by the above mentioned processes were identified for char combustion of biomass.

Zone I - The reaction rate is kinetically controlled. Since the diffusion rate of the oxidation agent is so fast the concentration of oxidation agent at the reaction surface is almost equal to the concentration of the oxidation agent at the bulk flow.

Zone II - In this zone combustion rate is determined by the combined effect of surface reaction rate and the diffusion of oxidation agent. Simultaneous occurrence of the reduction of particle diameter and particle density can be observed in this combustion zone.

Zone III - In this zone reaction is determined by the diffusion of oxidation agent through the particle boundary layer. The surface reaction rate is much fast therefore the penetration of oxidation agent to the particle is very low.

Char reactions models are classified into one step or two step models where one step models are further classified into global kinetic models or intrinsic kinetic models. Global kinetic models are widely used by the researchers for mathematical modeling of biomass combustion as it reduces the burden of finding unknown parameters associated with the complex nature of various biomass chars used in other models. The detailed classification on heterogeneous reactions can be found in Smoot and Smith[14].

V. Turbulence Modelling

Modeling turbulence is important in combustion applications as it increases the mass, energy and momentum transfer. Reynolds averaged Navier -Stokes equation(RANS) model, Large Eddy Simulation models(LES) and Direct Numerical Simulation(DNS) are used for turbulence modeling.

RANS approach uses the time averaged Navier -Stokes equations to model the turbulence effects of flow in combustion applications.

LES uses spatial filtering to separate large eddies and small eddies. LES model helps to differentiate between the characteristics of small eddies and large eddies.

For an incompressible turbulent flow instantaneous continuity equation and Navier Stokes equation can form a closed set of four equations with four unknowns which is used in DNS modeling to form transient solution with sufficiently fine spatial mesh and sufficiently small time steps.

VI. Radiation Modelling

The radiation models were classified mainly into four categories by Viskanta 2008 as shown below[15].

- directional averaging approximations
- differential approximations (moment, modified moment, spherical harmonics, etc.);
- energy balance (zone, Monte Carlo, finite volume, finite element, boundary element, etc.) methods
- hybrid (discrete transfer, zone-Monte Carlo, ray tracing, etc.) methods.

Finite Volume Method(FVM) and Discrete Ordinate Method(DOM) from the category of energy balance method are suitable for the application of CFD in combustion systems. The Discrete Transfer Method(DTM) which is categorized under hybrid methods is proven to be suitable for CFD applications.

A. Discrete Ordinate Method

Two types of Radiation Transfer Equations(RTE) are used in DOM. The first one is the classical approach which approximates the RTE to first order ordinary differential equation. The second approach is named as even parity formulation which is a second order partial differential equation.

B. First Order Differential Approximations Model-P_1 Model

This is a differential approximation method. P_n approximation is taken from obtaining moments of RTE. This results in n^2 number of equations. P_1 approximation is widely applicable due to its simplicity and sufficient accuracy. This method is based on expansion of radiation intensity into orthogonal series of spherical harmonics. This transfers RTE into set of simultaneous partial differential equations(PDEs).

C. Discrete Transfer Method

DTM method is a hybridization of flux methods and Monte Carlo Method. This method divides the geometry into isothermal control volumes and surfaces which have constant radiation properties. The RTE is integrated analytically and iteratively solved along an arbitrary path.

The solution of the RTE gives the local intensity of any ray in the selected direction. This method is flexible in handling complex geometries and the accuracy can be manipulated by changing the number of rays without affecting much for the computer storage capacity. The disadvantage of this method is that handling the anisotropic scattering problems.

D. Finite Volume Method

The radiance in each discrete direction is assumed to be constant as in DOM . RTE is solved for discrete angles which covers solid angle of 4π steradians. The RTE is discretisised using unstructured meshes.

VII. Mathematical Modelling Of Solid Fuel Combustion In Packed Beds

Numerous modeling techniques were used by different researchers to model the solid fuel combustion in packed beds. They can be broadly classified according to the following categories[10].

- Continuous -medium models
- Neighbouring layers models
- Well-stirred reactor models
- 1d+1d model

A. Continuous -Medium Models

A one dimensional transient approach was used in [16] to study the effect of air supply rate, particle size and calorific value. It was identified that the when the particle size is getting larger the bed deviates from the continuous assumption. It was identified that the air supply rate affect the bed combustion pattern. At low air flow rates the reaction rate is determined by the oxygen concentration and when the air flow rate is increased combustion is reaction limited. When the air flow rate is increased further the flame will extinct.

B. Neighouring Layers Models

In this approach fuel bed was divided into four layers of fuel, drying, pyrolysis and ash. This approach was used by Adams [17] to model an overfeed bed. He used two models; a fixed bed model and a fluidized bed model to predict the behavior of entrained particles. He used the fixed bed model to predictions to determine the off gas temperature, composition and velocity. Since the fuel bed is overfeed he assumed that the drying occurs at the top horizontal layer with other steps of pyrolysis, gasification and char combustion takes place at the subsequent layers. He coupled the fixed bed model with fluidized bed model since the models developed based on the bulk flow velocity calculated based on the simplification of complete combustion which is valid for cases where the air is fed below the fuel feeders[17].

Another research was done in order to use the modeling approach for control purposes in a horizontally moving grate. It is assumed that the combustion behavior inside the chamber is co-current . The bed was separated into layers of moist fuel , dry fuel, char and ash. Thermal decomposition was assumed to be occurred in the first emergence of dry fuel and the complete burning out of char. The model was guaranteed to be accurate in steady state as it is based in mass balances[18].

C. Well-Stirred Reactor Models

The bed was simulated by a cascade of well stirred reactors. This modeling approach was used for 1D modeling of fixed bed by Mätzing et al.[19] assuming that the fuel bed is a porous medium consists of spherical particles. Cylindrical shape fuel bed was assumed to have monolayers of spherical particles arranged in closest packing. Each monolayer is single reaction unit with single composition and temperature. Therefore it does not have axial or radial gradients of composition and temperature. Energy exchange between the layers occurred by conduction, convection and radiation. The mass transfer occurs only by gas phase transport.

A serial cascade of continuous stirred reactors assumption was used by Beckmann and Scholz to model the combustion in stoker systems. The steady state and transient state were described through batch process model, continuous stoker process model and a model for gasification[20]

D. 1d+1d Model

In this approach transient and one dimensional single particle model which uses spherical coordinates was implemented in one dimensional transient fuel bed model. This approach considers the gradients both inside the particle and in the fuel bed. In this approach the packed bed is divided into two subsystems that is the gas phase inside the bed and the gas phase inside the particles. The packed bed is described by 1-D Cartesian coordinates and the particles are described by 1-D spherical coordinate system[21].

Another research was conducted using 1d+1d model in which the conservation equations for mass momentum, energy and species applied for both gas and solid phases. One dimensional particle model was applied to describe the conversion of solid phase which was assumed to be occurred inside the thermally thick particle[22].

Bruch et al [23]used one dimensional transient model to describe the thermal conversion of single particle and a continuum approach only for the gas phase. The global conversion of packed bed is represented by the contributions of single particles. Each particle is in relation with the gas phase by heat and mass transfer[23].

VIII. DISCUSSION

Numerous models were developed by different researchers to understand the combustion process of biomass in packed beds. The efforts being taken to incorporate the effects of complex processes of chemical reactions , turbulence mass transfer and heat transfer, fuel bed packing into these models.

Due to the computer resource requirement, time involvement and scarcity of appropriate data many researchers preferred simplified descriptions of the process involved. Many researchers used constant temperature drying models due to its simplicity with some additional parameters fixed into the basic model. This is to take account of the fraction of energy utilized for drying during particle heating up process[7], [13].

For the heterogeneous reaction kinetics many researchers used the global kinetic models due to their simplicity. Although the char reacts with CO_2, H_2 and H_2O many researchers assumed that reaction occurs only with oxygen[13], [18].

Zero dimension, one dimension, two dimension and three dimension models following steady state conditions or transient conditions are presented in numerous work.

One dimensional unsteady state modeling approach was used by Yang et al.[10] to model the channeling in fixed bed with novel approach of experimenting with an instrument for measuring the parameters while it is passed through the bed with the fuel.

One dimensional transient model was used to describe the thermo chemical conversion of single wood particle in a packed bed consists of finite number of wood particles. Heat and mass transfer relations coupled the interaction between the particle and the flow in the voids of the packed bed. Researchers obtained good match with experimental results and the results of the model for single particle model[24].

In [25] the researchers used a dynamic model of a static bed combustion which was expanded for steady state combustion of a travelling grate.

A two dimensional model was developed by Thunmann and Hermansson to model the char conversion in fixed bed [26]. The bed constitutes of continuous non isothermal porous char bed. The gas flow through the char bed is represented by multi component gas flow through a porous medium. Their purpose was to reduce the high temperatures and reducing conditions along the grate surfaces to minimize the deterioration of grate material.

An unsteady three dimensional models were developed for the combustion of wood in fixed bed biomass boilers by Collazo et al.[13] which applies for both freeboard and fuel bed.

A transient three dimensional model for packed bed combustion of thermally thick particles was presented in[27]. As in[13] one of the objectives of the researchers to develop a fully coupled model which includes both the freeboard and the packed bed.

A three dimensional transient model was developed to study the effect of non uniformities in the bed which is useful in optimizing the grate design in[12]. In this research initially developed two dimensional model was extended to three dimension without altering all the features.

IX. CONCLUSIONS

Packed bed combustion of biomass in an important conversion technological route to convert biomass into energy. Numerical simulation of biomass combustion using CFD has been proved to be an effective tool for predicting the performance of packed bed combustion. This paper presented the importance of biomass as an energy source, the technology behind packed bed combustion systems, basics of CFD approach for packed bed combustion and the efforts made by various researchers in the implementation of CFD for packed bed combustion of biomass. To be more industrially applicable further studies have to be done which couples the complexities of the biomass combustion with the industrial experiences.

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