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Flow Simulation & Thermal Analysis Of Pyrolysis Of Wood Particle In Vertical Column

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Abstract

This paper outlines the flow simulation of thermal plasma pyrolysis of wood particle in vertical column and mathematical model has been applied to analyze the pyrolysis reaction of wood at high temperatures (1000-2000K) in thermal torch based plasma pyrolyser. Computational domain consists of a ceramic pyrolyser and two thermal plasma torches placed in ceramic wall. CFD commercial code FLUENT, along with the subroutines developed, and is used to model the flow of high temperature air and its interaction with wood at high temperature. Computation is done at different power supply to torches and mass flow rate of air (plasma gas) through torches. Interaction of wood with high temperature air in absence of oxygen is analyzed. Spatial distribution of variables such as temperature, velocity is presented. We have discussed how wood particle behaves in high temperature field using particle tracking method. Plots of particle mass fraction, particle temperature, particle velocity magnitude with respect to time are obtained.

1. Introduction

Waste management is an important issue in both developed and developing countries nowadays. Today's society uses, and quickly discards, a large volume of an increasingly diverse range of polymeric materials. Organic wastes, such as used rubber and plastic are among the waste materials that represent problematic wastes on one hand and valuable potential as secondary raw materials on the other hand [1]. Most of the organic residue and agricultural waste consists of wood. Many researchers have presented mathematical models on pyrolysis of plastics [10-11] and pyrolysis of medical waste [12-13]. In this paper we tried to build a mathematical model to study pyrolysis of wood.

Thermal plasma technology has been under active development for a long time. The technology is now well established in metallurgical processing, materials synthesis etc. The extremely high temperatures generated by plasma torches have spurred development of their application to waste processing, as they are capable of significantly decreasing the waste volume to a non-leachable residue. By far the most important application of thermal plasma waste treatment is focused on the destruction of hazardous wastes rather than recycling because of economic issues. Nevertheless, in recent years, the interest in energy and resource recovery from waste has grown significantly, and substantial research studies on the use of plasmas in organic

Pyrolysis is the thermochemical process that converts biomass into liquid (bio-oil or bio crude), charcoal and noncondensable gases, acetic acid, acetone and methanol by heating the biomass in the absence of air. The basic phenomena that take place during pyrolysis are: (1) heat transfer from a heat source, leading to an increase in temperature inside the fuel; (2) initiation of pyrolysis reactions due to this increased temperature, leading to the release of volatiles and the formation of char; (3) outflow of volatiles, resulting in heat transfer between the hot volatiles and cooler unpyrolysed fuel;(4) condensation of some of the volatiles in the cooler parts of the fuel to produce tar; and (5) autocatalytic secondary pyrolysis reactions due to these interactions. [2]

In our study, we have focused on computing and analyzing the high temperature air-wood interaction and the flow of plasma gas (air). For our study, we have chosen alumina ceramic as a pyrolyser wall material. Two torches are placed in pyrolyser wall. The aim of this study is three fold, thermal and flow simulation, understanding the thermal interaction between the air and the wood and understanding the effect of decomposition on the plasma gas flow. We have adopted an approach in which we model the following: the pyrolyser, the plasma flow field, the energy transfer between the plasma gas and wood particle. Calculations are carried out using the commercial software FLUENT version 12.0, with user defined function subroutine added to incorporate the effects specific to thermal plasmas. The mathematical formulation of the two-dimensional model is presented in sections 2. Section 3 gives details of the system, computational domain and the boundary conditions. Section 4 presents results and discussion.

Section 5 product of combustion gases for different boundary condition.

2. Mathematical Model

In this section, we present the mathematical model for the system. System consists of two thermal plasma torches placed in wall. System is modeled as a three dimensional model. As the plasma can be approximated to a fluid, the Navier-Stokes equations are used to describe the plasma flow field. Apart from the Navier-Stokes equations, various equations governing chemical reaction and particle tracking have also been added.

2.1 Assumptions

We have carried out our simulations under the following assumptions:

- The flow is assumed to in steady state.
- Properties of the plasma gas depend on the local temperature.
- Distribution of temperature inside the system walls is not considered.
- Formation of soot and particulate effects are neglected.
- Formation of intermediate species is not considered.
- The reaction occurring is assumed to be mixing limited.

2.2 Governing equations

Plasma gas and its temperature and velocity distribution in the flow field are major components of the computational domain. Governing equations for these two domains are presented in subsection 1. Equations governing the fluid (plasma gas)-solid (wood particle) interaction are presented in subsection 2. As the temperature of the plasma domain are very high, radiation heat transfer plays an important role. Subsection 3 present the details of the method we have used to account for radiation heat transfer. Velocity analysis in subsection 4.

2.2.1. Conservation equations for plasma gas:

The conservation equations for various quantities such as energy, mass, momentum, turbulent kinetic energy and its dissipation rate etc. can be written in the generalized form suggested by Patankar [3]:

The dissipation function ϕ in equation 5 can be given as-

$$\Phi = \mu\left\{2\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2\right] + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)^2\right\} + \lambda(\mathrm{div}\,\mathbf{u})^2$$

Table 1

Conservation equations in the generalized form [4]

Conservation Quantity	**Conservation Equation**
Mass	$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \boldsymbol{u}) = 0$ (2)
X momentum	$\frac{\partial(\rho u)}{\partial t} + \mathrm{div}(\rho u \boldsymbol{u}) = -\frac{\partial p}{\partial x} + \mathrm{div}(\mu\ \mathrm{grad}\ u) + S_{Mx}$ (3)
Y momentum	$\frac{\partial(\rho v)}{\partial t} + \mathrm{div}(\rho v \boldsymbol{u}) = -\frac{\partial p}{\partial y} + \mathrm{div}(\mu\ \mathrm{grad}\ v) + S_{My}$ (4)
Z momentum	$\frac{\partial(\rho w)}{\partial t} + \mathrm{div}(\rho w \boldsymbol{u}) = -\frac{\partial p}{\partial z} + \mathrm{div}(\mu\ \mathrm{grad}\ w) + S_{Mz}$
Energy	$\frac{\partial(\rho i)}{\partial t} + \mathrm{div}(\rho i \boldsymbol{u}) - p\ \mathrm{div}\ \mathbf{u} + \mathrm{div}(k\ \mathrm{grad}\ T) + \Phi + S_i$ (5)

Where λ is second viscosity to relate volumetric deformations.[4]

$$\vec{\nabla}\cdot(\rho\upsilon\vec{\phi}) = \vec{\nabla}\cdot(\Gamma_{\phi}\ \vec{\nabla}_{\phi}) + S_{\phi}. \tag{1}$$

where, ϕ represents the scalar quantity for which the conservation equation is to be solved, ρ is the fluid mass density, V the velocity vector, Γ ϕ the diffusion coefficient for the scalar, Sϕ the source term. ϕ is replaced by T, the temperature, u, v, w the Cartesian components of the velocity or V while solving for energy and momentum conservation equations respectively. The various quantities for which the conservation equations are solved for a three dimensional system are presented in table 1. In equations (2)–(5), u, μ, κ, CP, ϕ are, respectively, the velocity vector, the viscosity, the thermal conductivity, and specific heat of the gas and dissipation function due to viscous stresses. The thermodynamic and transport properties depend on the local temperature. P represents the pressure.

2.2.2. Reaction modeling: The conservation equation for each species (reactants and products) mass fraction Yi takes the form as: [3]

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla\cdot(\rho\vec{v}Y_i) = -\nabla\cdot\vec{J}_i + R_i + S_i \tag{7}$$

Where *Ri* is the net rate of production of species *i* by chemical reaction and *Si* is the rate of creation by addition from the dispersed phase plus any user-defined sources. *Ji* is diffusion flux of species i.

The reaction rate is calculated by using The Eddy Dissipation Model [5] available in Fluent as the net rate of reaction is controlled by turbulent mixing. The net rate of production of species *i* due to reaction *r*, *Ri,r*, is given by the smaller (i.e. limiting value) of the two expressions below Y_R

$$R_{i,r} = v'_{i,r} M_{w,i} A \rho \frac{\varepsilon}{k} \min_R \left(\frac{Y_R}{v'_{R,r} M_{w,R}} \right)$$

$$R_{i,r} = v'_{i,r} M_{w,i} A B \rho \frac{\varepsilon}{k} \frac{\sum pYp}{\sum_j^N v''_{j,r} M_{w,j}} \tag{8}$$

Where- [5]
Y_P is the mass fraction of any product species, P
Y_R is the mass fraction of a particular reactant, R
A is an empirical constant equal to 4.0
B is an empirical constant equal to 0.5
k/ε is eddy mixing time scale.

2.2.3. Radiation Heat transfer: The pyrolyser walls are here considered as surfaces from which radiation occurs. To find out intensity of radiation from those surfaces, a pre-defined mathematical model i.e. Discrete Transfer Radiation Model (DTRM) from Fluent is used. [5]

In this section, we present the mathematical model for the system. System consists of two thermal plasma torches placed in wall. System is modeled as a three dimensional model. As the plasma can be approximated to a fluid, the Navier-Stokes equations are used to describe the plasma flow field. Apart from the Navier-Stokes equations, various equations governing chemical reaction and particle tracking have also been added.

2.2.4. Velocity Analysis: For 8 kW power supply and 0.001042 kg/s (50 lpm) mass flow rate, velocity calculated.
For torch, power supply=8 kW
For torch, mass flow rate=0.001042 kg/s
Temperature generated=6286 K
Initial temperature=300 K
Torch inlet hydraulic diameter=0.009 m
Operating atmospheric pressure=101325 Pa
Universal gas constant=290 J/kgK
From ideal gas equation, [15]

$$PV = mRT$$

$$\frac{V}{m} = \frac{RT}{P}$$

Where, V = volume and V/m= specific volume= $1/\rho$

$$\frac{1}{\rho} = \frac{RT}{P}$$

$$\rho = \frac{P}{RT}$$

$$\rho = \frac{101325}{(290 * 6286)}$$

$$\rho = 0.05558 \text{ kg/m}^3$$

From continuity equation we know that

$$m = \rho AV$$

$$0.001042 = 0.05558*0.009*0.009*V$$

$$V = 231.44 \text{ m/s}$$

Which is approximately equal to V = 237 m/s velocity coming from analysis shown in figure 3.

3. System Description

The system considered for simulation is in the design process and is to be installed. Schematic of cross section of the pyrolyser is shown in the figure 1.

The pyrolyser schematic shown in figure 1 is L shaped. The vertical height of longer column is 2246mm and horizontal shorter base has 1146mm length. The cross section of pyrolyser is a square of 396mm x 396mm. The ceramic wall is of thickness 73mm which is throughout the same.

The two torch inlets and outlet of residual gases are of 9mm x 9mm each and 47mm x 47mm square cross sections respectively. There is a provision made for feeding of wood particles at the top of pyrolyser.

This inlet is assumed to be of cone type [5] having 7mm cone radius and cone angle 45^0.

The thermal torches are provided with different power supply and mass flow rate of plasma gas i.e. air. The wood particles are supplied at different rates in two streams as shown in Table [4].

The outer wall of the system is exposed to air. So, the heat transfer coefficient at the wall boundary is calculated as 5.2 W/m2K. The properties of plasma gas are varying and dependent on the local temperature.Proper subroutines are developed to calculate the material properties of plasma gas. All the important boundary conditions are shown in table 2.

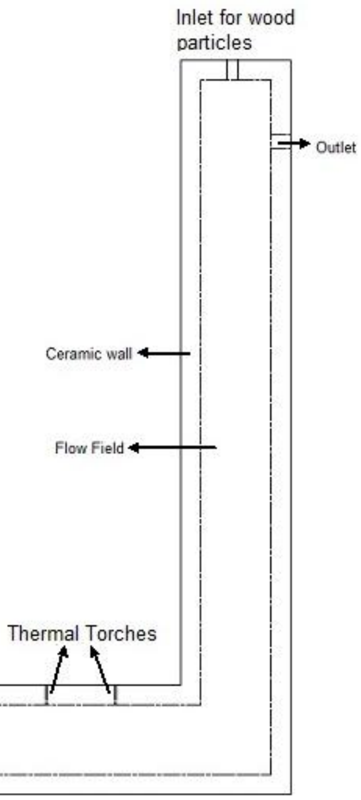

Figure 1: Schematic of Pyrolyser

The computation domain was meshed using hexahedral elements. The mesh consists of 245988 cells, 755340 faces, 263706 nodes.

The various properties of wood like density, specific heat, thermal conductivity, activation energy for pyrolysis etc are taken from prvious research papers[8-9]

3.1 Reaction mechanism:

The basic phenomena that take place during pyrolysis are: heat transfer from a heat source leading to an increase in temperature inside the fuel; initiation of pyrolysis reactions due to this increased temperature leading to the release of volatiles and the formation of char; flow of volatiles towards the ambient resulting in heat transfer between hot volatiles and cooler unpyrolysed fuel; condensation of some of the volatiles in the cooler parts of the fuel to produce tar; and auto-catalytic secondary pyrolysis reactions due to these interactions. Although the oxidation of char and the combustion of volatiles are two major processes in combustion, they may be excluded from the stage of pyrolysis. [6] In our study we have concentrated only on volatilization of

H_2O from wood particles and secondary pyrolysis reaction of devolatilized wood which results is formation of residual gases. The overall process of pyrolysis of wood is believed to proceed as follows: At around 160^0C the removal of all moisture (dehydration) is complete. Over the temperature range 200^0C to 280^0C, all the hemicellulose decomposes, yielding predominantly volatile products such as carbon dioxide, carbon monoxide and condensable vapors.

Table 2

Boundary Conditions

Boundary			Description
Ceramic wall	-	h=5.2 w/m^{2}K	wall
Torch inlets	Flow rate=0.00125kg/s	T=5780K	Mass flow inlet
	Flow rate=0.001042kg/s	T=6286K	
	Flow rate=0.00125kg/s	T=4165K	
	Flow rate=0.001042kg/s	T=4872K	
Outlet	Gauge pressure= -2000 Pascal	T=300K	Pressure outlet
Inlet for wood	Flow rate= 3.6 & 7.2kg/hr	T=300K	Injection

From 280^0C to 500^0C the decomposition of cellulose picks up and reaches a peak around 320^0C. The products are again predominantly volatiles. The decomposition rate of lignin increases rapidly at temperatures beyond 320^0C. This is accompanied by a comparatively rapid increase in the carbon content of the residual solid material. [6]

Table 3

Pyrolysis products, composition of the light gases (% vol.) for beech and pine wood [7]

	Beech wood	Pine wood
CO$_2$	38.2	37.6
Ethylene	0.4	0.6
Ethane	0.8	1
Propylene	0.2	0.3
Propane	0.1	0.2
Hydrogen	9.3	8.8
Methane	15.4	15.5
CO	35.5	36.1

Typical pyrolysis products obtained after complete pyrolysis of wood are shown in table 3.

As the proportion of ethylene, ethane, propylene, propane are very small in comparison with proportion of methane, so they are neglected while modeling in Fluent. Only four product gases (CO, CO$_2$, Methane and Hydrogen) are considered as final pyrolysis products during simulation.

4. Results

Simulations have done different mass flow rate of torch, power supply of torch, particle size and particle feed rate. From Table 4 we have considered 0.001042kg/s flow rate of plasma gas (air) and at 8kW power supply to each torch which produce about 6286K temperature and particle size 0.002m and particle feed rate 0.002kg/s. We have presented and discussed the profiles of temperature and velocity, profile of tracking of wood particles with respect to time, profile of rate of reaction, profiles of mass fraction of wood and pyrolysis products.

Figure 2 shows the temperature distribution of plasma gas in the flow field. As it is seen that, the temperature of plasma gas is maximum at the torch inlets.(6286K)

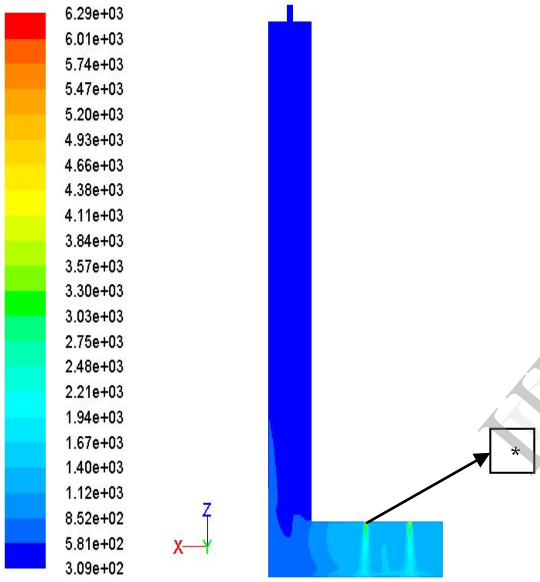

Figure 2: Temperarute Distribution in Pyrolyser (K)

As air flows further the system, its temperature goes on reducing uniformly. But we can see the region (shown in fig.2 by asterisk) where temperature drop occurs abruptly. This is the region where pyrolysis of wood takes place. When wood particles are coming down, their temperature goes on increasing and at that position they are provided with enough heat to start pyrolysis. As pyrolysis reaction is endothermic, so we observe temperature drop at that position.

Figure 3 shows the velocity distribution of air in the flow field. The highlighted portion shows the velocity vectors near the torch inlet region. Due to high mass flow rate the velocity at torch inlets is about 237m/s. Air enters at such a high speed in the pyrolyser. Due to two high velocity streams there is formation of eddies which promotes better heat transfer & better temperature distribution.

Figure 4 describes the tracking of wood particles. As said earlier the wood particles are introduced to the system from inlet at the top in two streams. This figure shows particle traces at various positions in the pyrolyser at various time periods ranging from its introduction to the system (0 second) to its existence (0.85 seconds).

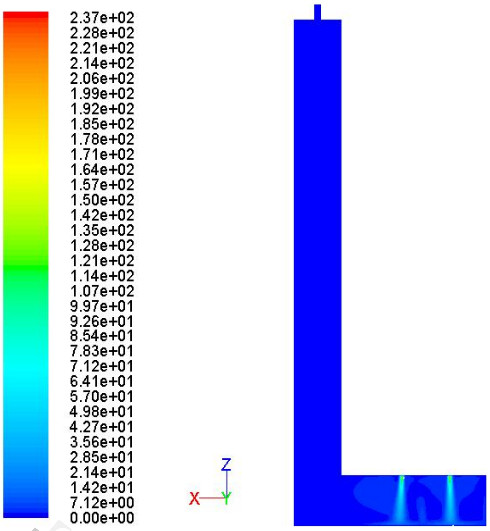

Figure 3: Velocity Distribution (m/s)

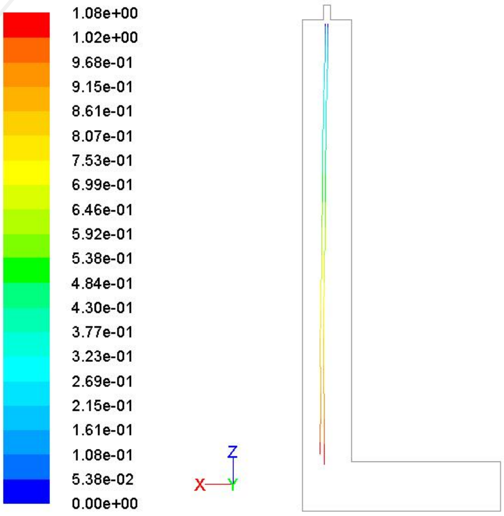

Figure 4: Particle traces colored by particle residence time in system (s)

So we can trace the position of particles with respect to time. As per the simulations carried out by us, the particles are completely pyrolysed within 1.2 second.(1.07s) This is due to very small size of particles considered during simulation and very high temperature field. The temperature where the pyrolysis reaction is carried out is described in later figure.

Figure 5 shows the plot of particle mass (kg) against time(s). This figure traces the mass of wood particles starting from their entrance in the system till their existence in the system. At the inlet the total mass of wood particles is 4.50 x e-7 kg and after 1.07s, the complete pyrolysis takes place and mass of wood particles reduces to zero.

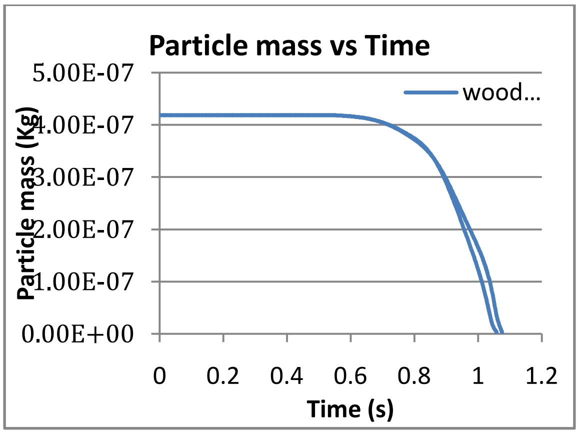

Figure 5: Particle mass (kg) vs. Time(s)

The mass of particles remains the same i.e. wood remains un-reacted up to 0.6 seconds. After then its temperature reaches a value where reaction starts and it is decomposed completely into final products. Hence its mass drastically falls to zero after 0.6 seconds.

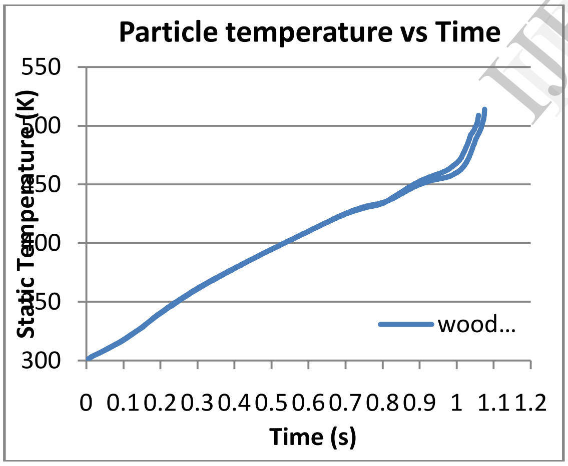

Figure 6: Particle temperature (K) vs. Time(s)

Figure 6 shows the plot of particle temperature against time. As particle descends down the pyrolyser its surrounding temperature goes on increasing. So, it shows the increase in the particle temperature as it descends down the pyrolyser. The particles are entered into the system at ambient temperature (300K). When the temperature of the particle reaches 400K, (at 0.5 second) the pyrolysis reaction starts. Once the reaction is started, particles are started to consume up. It results in increase in surface to volume ratio which in turn promotes the rate of pyrolysis. So there is abrupt increase in the temperature of wood particles. The wood is completely decomposed at about 510K.

Figure 7 shows the plot of particle velocity against time. As particle moves down the pyrolyser its velocity goes on increasing.

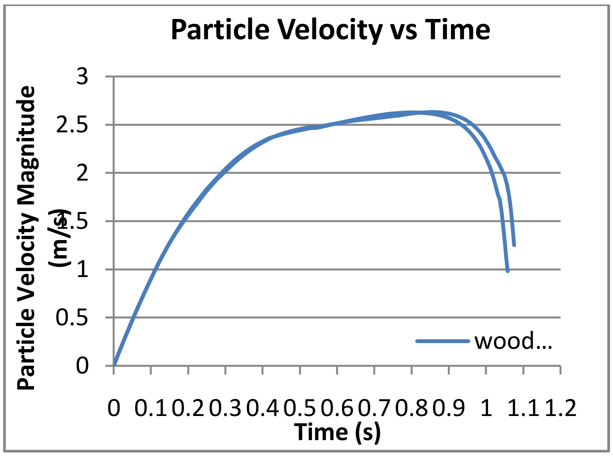

Figure 7: Particle Velocity (m/s) vs. Time(s)

This increase in velocity is not linear as the particles' motion is opposed by the upcoming air draught from torch inlets. Up to 0.6 second i.e. before initiation of pyrolysis the graph shows linear characteristics, but once the reaction is started particles start to eaten up. So they lose their mass, strongly opposed by flowing air, so slope of the plot slightly reduces. The maximum velocity reached by the particle is 2.7m/s.

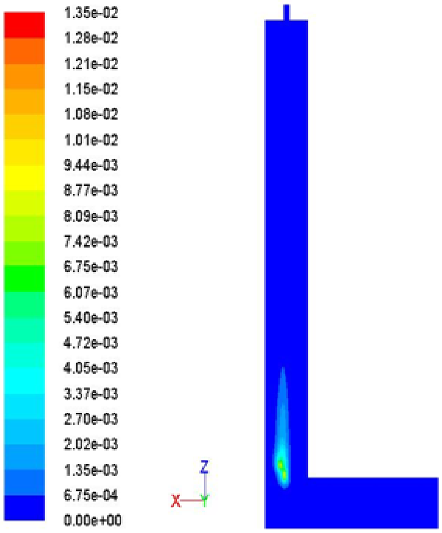

Figure 8: Contours of Rate of reaction (kgmol/m^3-s)

Figure 8 shows the contours of rate of reaction (kgmol/m3-s) of pyrolysis in the flow field. Rate of reaction is the conversion of the number of moles of reactants into products in unit time. As the temperature of wood particles goes on increasing the rate of reaction also goes on increasing reaching the maximum value of 1.35 x e-2 kgmol/m3-s where the wood is completely consumed.

Figure 9 shows the contours of mass fraction of wood after volatilization of water vapour from it. As wood particle moves down the pyrolyser its temperature goes on increasing and hence water vapour in the wood particles starts vaporizing and wood becomes volatilized. The volatilized wood particles are then pyrolysed into products.

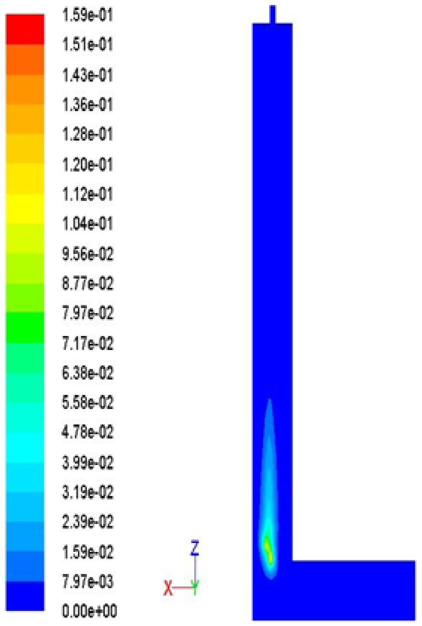

Figure 9: Contours of mass fraction of wood (after volatilization)

5. Product Characteristics

Typical distribution of thermal plasma pyrolysis gases obtained in different power, mass flow rates, particle size and feed rate are given in Table 4. Major combustible products gases are H_2, CO, CH_4 and CO_2, were produced during the pyrolysis processes. The concentration of each product can vary according to particle size and feed rate. For different particle size and feed rate check for volatilization wood up to reaches to the bottom of L shape. Mass fraction of wood after volatilization (wvol).The combustion heat value of the product is in range of 4-9 MJ/Nm3, so it can be used directly as a fuel in various energy applications such as direct firing in boilers, gas turbine or gas engine. The product gas may be utilized in syngas applications. It is known that synthesis gas having different H2/CO molar ratio is suitable for different applications. [1]

6. Conclusion

The result presented in the paper analyzed for pyrolysis of the wood particle completed in vertical column of L-shape for different power supply, mass flow rate, particle size and feed rate. The flow of plasma gas (air) and pyrolysis of wood is simulated and analyzed in thermal torch based plasma pyrolyser used for carrying out pyrolysis of various wastes. Computational domain includes the fluid region throughout the pyrolyser chamber. The complex pyrolysis process is presented in the way which is easier to understand. Heat transfer models are considered while modeling which affect the temperature distribution in the chamber. This paper might help people working on wood pyrolysis for their experimental analysis as well as modeling. The results presented in the paper by considering a single value for physical properties of wood like its

Table 4

Product distribution from thermal plasma pyrolysis for different boundary conditions

Power (kW)	**Mass flow Rate (lpm)**	**Particle Size (mm)**	**Feed Rate (kg/hr)**	**Mass Fraction of wood volatilization (%)**	**Gas product distribution (mass fraction %)**				**Pyrolysis of Particle Completed vertical column**
					H_2	**CO**	**CH_4**	**CO_2**	
8	60	3.0	7.2	19.50	2.17	30.20	4.32	11.80	Yes
8	60	3.5	7.2	17.20	2.35	32.60	4.67	12.80	No
8	60	4.0	3.6	15.10	1.96	27.20	3.90	10.70	Yes
8	50	3.0	7.2	13.50	2.35	32.60	4.67	12.80	Yes
8	50	3.3	7.2	14.00	2.67	37.10	5.31	14.60	No
8	50	2.0	7.2	15.90	2.36	32.80	4.70	12.90	Yes
8	50	4.0	3.6	12.10	2.19	30.50	4.36	12.00	Yes
6	60	3.0	7.2	39.90	3.44	35.90	6.85	18.60	No

6	60	2.0	7.2	15.30	2.22	30.80	4.41	12.10	No
6	60	1.0	7.2	16.40	2.13	29.60	4.23	11.60	Yes
6	60	2.0	3.6	12.70	2.06	28.50	4.08	11.20	Yes
6	50	3.0	7.2	54.70	3.45	37.80	6.87	11.90	No
6	50	2.0	3.6	11.80	2.16	30.10	4.30	11.80	Yes
6	50	1.0	3.6	34.40	3.53	36.50	7.00	19.10	No

density, specific heat, thermal conductivity. These properties are different for different types of wood. So, the experimental results will depend on the type of wood used & size of wood particles. This paper gives the clear understanding of pyrolysis and differentiates it from combustion reaction which is exothermic but pyrolyser being endothermic reaction.

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