MODELLING OF COAL SLAG FLOW AND LAYER THICKNESS IN A HIGH TEMPERATURE ENTRAINED FLOW GASIFIER

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ABSTRACT

A 2-D model for the slag flow simulation in an entrained flow gasifier has been developed. In addition to mass, momentum and energy conservation equations, volume of fluid (VOF) equation was solved to track the liquid-gas interface. Liquid phase consists of melted coal ash particles which deposits on the wall and move downward. The gasification reaction is not considered here but it is postulated to have a mass flow through the interface towards the mass of the liquid phase. The reactor walls are usually kept cold so a temperature gradient and then a solid layer form within the slag layer. The solidification and its effect on the slag layer thickness are also considered here. Results show that, depending on the ash composition which determines the fluid's rheological properties, the solid phase constitutes a large part of the slag layer.

Key words: *coal, gasification, slag flow, simulation*

INTRODUCTION

Coal gasification offers one of the cleanest and most reliable ways to convert coal into gas and other valuable products. It can also be applied to convert low-or negative-value feed stocks or wastes such as petroleum coke to high value products. Various types of gasifires are utilized for gasification process in which carbon reacts with oxygen and steam to produce a mixture of gaseous products, mostly carbon monoxide and hydrogen called syngas. The product can be used either as a source of energy or as a raw material for the synthesis of chemicals, liquid fuels or other gaseous fuels (Collot, 2002). This process has several advantages over direct burning of coal; it has higher efficiency, and a much lower release of pollutant and harmful gases (e.g. SOX and NOX) into the atmosphere. This technology significantly reduces the environmental impact of using coal in accordance with regulations on reduction of greenhouse gas emissions (Higman and Vander Burgt, 2003). As a consequence of this, the Integrated Gasification Combined-Cycle (IGCC) power plants which combine the advantages of relatively cheap fuel with the efficiency and environmental performance of gas turbines, have been recognized as an excellent replacement for coal-fired ones.

In addition to gas production, gasification reaction leads to the formation of ash as coal particles burn. The coal ash comprises primarily of SiO2, Al2O3, alkali and alkaline earth components along with some heavy metals such as iron and nickel. It contains trace amount of titanium and vanadium oxides considered as trace elements but sometimes they play an important role in coal properties.

The effect of mineral matter in coal during combustion has been widely studied. On the other hand, there are also a lot of works on gasification reactions, especially at low temperatures, reviews by Johnson (1979) and Kristiansen (1996) being among them. The impact of minerals on the gasification reactions however, have recently become important and works such as those of Dyk et. al. (2009), Hurst et. al. (1999), Wenjia et. al. (2009) and Wanjia et. al. (2010) have addressed this. For high temperature gasification– which has a higher conversion- there are only few studies on the behaviour and effects of the slag.

In an entrained-flow coal gasifier operating at high temperature, molten coal ash particles from the gas phase move to the reactor wall and accumulate on the refractory under the action of centrifugal forces. After a while, a film of slag is formed which flows down along the sides of the reactor. The slag properties adversely affects the proper operation of the reactor as it can plug the tap hole at the bottom; so it is very important to predict the slag thickness on the reactor wall as a function of time.

The behaviour of slag depends on a number of factors including its composition and operating condition. Due to the cold wall, a temperature gradient will be be formed in the slag layer, changing the physical properties within the reactor. The temperature is lower near the reactor wall, therefore a solid slag layer may be formed influencing the reactor efficiency. The aim of this work is to investigate the flow pattern of slag in the gasification reactor by predicting the slag thickness as well as its temperature profile. This will help in identifying the optimum operating conditions and feedstock composition required to attain reliable and stable performance.

SLAG PROPERTIES

A smooth operation of an entrained flow gasifier depends heavily on the steady removal of slag from the reactor. Various types of coal have different ash contents with different mineral composition, therefore it is necessary to investigate the slag behaviour by measuring the characteristics of feedstock as far as the rheological properties are concerned.

The viscosity and temperature of critical viscosity (TCV) are the two main characteristics to assess the slag flow behaviour (Lowe et al., 2008). The slag viscosity is the most important factor as it governs the flow behaviour of the slag. The thickness of the slag layer particularly at the discharging section depends on the viscosity since a smooth and continuous removal of the slag requires a lower viscosity. Although the viscosity can be reduced by increasing the temperature, that on the other hand would require additional combustion by injecting more oxygen and resulting into the reduction of the process efficiency. Alternatively, slag viscosity can be decreased by using a fluxing agent such as limestone. Blending different feed stocks also have been reported to have a positive effect on the slag viscosity reduction.

The other important parameter is the temperature of critical viscosity. At this temperature the slag flow behaviour starts to deviate from Newtonian flow. This point is characterized by a rapid increase in viscosity of the melt for small temperature variation. This phenomenon has been related to the onset of crystallization and then formation of some kinds of solid in the melt. This event would affect the slag viscosity remarkably (Lowe et al., 2008). Blending and also adding a fluxing agent can change the temperature of critical viscosity although it may also increase the operating costs.

From above, it is therefore apparent that the prediction of viscosity and the temperature of critical viscosity is required. TCV is dependent on the composition while the viscosity depends on both composition and temperature. The network theory is applied to explain the dependency of viscosity on chemical composition. In this method each component is categorized according to their effect on the silica network. Some oxides act as either network formers or acids (increasing the viscosity) and modifiers or base (decreasing the slag viscosity). According to this theory, the temperature of critical viscosity (TCV) is given by

$$T_{CV} = 1385.44 + 74.1\,(A/B)$$

where A/B is the acid to base ratio defined as

$$A/B = \frac{SiO_2 + Al_2O_3 + Tio_2}{Fe_2O_3 + CaO + MgO + Na_2O + K_2O}$$

A lot of equations have been proposed for viscosity predictions but one of the simplest, used by Seggiani (1998) is based on an Arrhenious-type equation as shown below:

$$\log\eta = 4.468S^2 + \frac{1.265\times 10^4}{T} - 7.4$$

where η is the viscosity in poise, T is the temperature in K and S is the silica ratio defined as:

$$S = \frac{SiO_2}{SiO_2 + Fe_2O_3 + CaO + MgO}$$

The density and heat transfer properties are assumed to be constant in this study. The coal composition and properties based on the Seggiani (1998) and used here are shown in Table 1. In this table the ash characteristics after 50% limestone addition are presented as well. Mixing limestone with coal particles has caused a reduction in the viscosity and the temperature of critical viscosity.

Table 1: Coal ash and Coal+limestone ash composition

Component	Coal ash	Coal+limestone ash
	wt%	wt%
Fe_2O_3	5.36	4.9
SiO_2	53.37	48.78
Al_2O_3	27.88	25.49
CaO	6.94	14.93
MgO	1.3	1.19
Na_2O	0.33	0.3
K_2O	2.18	1.99
TiO_2	0.65	0.6
P_2O_5	0.1	0.1
SO_3	1.89	1.72
Acid/base ratio	5.08	3.21
Silica ratio	0.797	0.699
T_{CV} (K)	1762	1623
Viscosity (poise)	$2.59.\ 10^{-5}$ exp(29095/T)	$5.59\ .10^{-6}$ exp(29095/T)
Density (kgm^{-3})	2490	2535
Specific heat Cp ($kJ\ kg^{-1}\ K$)	1.69	1.67
Thermal conductivity ($Wm^{-1}\ K^{-1}$)	1.89	1.9
Emissivity	0.83	0.83

MODEL FORMULATION

The motion of the slag layer in entrained flow gasifiers is a multiphase flow with heat and mass transfer. The slag as shown in Fig. 1 consists of two layers, liquid and solid. Due to temperature difference between the inside and outside of the reactor and also continuous heat flux into the slag layer, a temperature gradient through the slag layers and reactor walls will be developed and as a result, the liquid slag somewhere may become cold enough (i.e. below melting point temperature) and makes a deposition of solid layer on the wall. It is usually assumed that the transition temperature of solidification is the temperature of critical viscosity. The solid layer can sometimes be the larger part of the slag layer.

As the gasification reaction proceeds, continuous input of molten ash particles as well as the heat flux from the gas phase into the liquid phase occur. Different models have been used for slag flow simulation. Goldman, 1981, proposed a technique for simulation of slag flow in which he included conservation equations solved by some simplifying assumptions. Seggiani, 1998, developed a single phase model in which the mass, energy and momentum conservation equations are written for a few number of control volumes. The domain of solution had been divided to fifteen cells in which the thickness and temperature profiles are calculated by solving conservation equations simultaneously. Recently Liu and Hao, 2007, used VOF model which is a technique to track interface and model the slag flow in a coal gasification reactor. They have used some assumptions to simplify the solution. For example, they assume that the viscosity is constant and not changing with the temperature variation. A commercial computational software, Fluent was utilized to solve the equations. Their results however are very qualitative and do not show the effect of operating temperature or feed composition on the slag thickness.

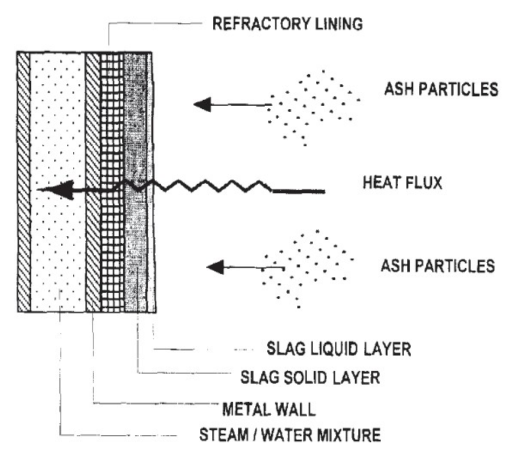

Fig. 1: Slag deposition (Seggiani, 1998)

To model the slag flow in a gasifier, an energy equation along with a momentum and mass transfer equations using a two-phase flow method should be coupled to represent the phase boundary. In Fluent, it is possible to set up such a model by coupling the VOF (volume of fluid) two-phase flow application mode with the other equations. As the slag layer thickness is small compared to the gasifier diameter, a 2-D model is developed. However, this simulation is implemented based on the assumption that the slag is a Newtonian fluid at the temperature above the temperature of critical viscosity and the flow at the temperature below that point is negligible, i.e. it is considered as the solid phase. Fig. 2 gives heat and mass flux details.

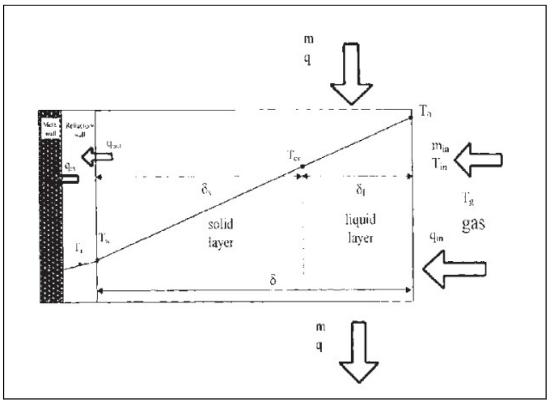

Fig. 2: Heat and mass flux inside the layers (modified from Seggiani, 1997)

Governing Equations

In order to describe the behaviour of the slag inside the reactor, the mass, energy and momentum conservation equations are written. The momentum balance for this situation is:

$$\rho\frac{\partial u}{\partial t}-\nabla\cdot\left[\eta\left(\nabla u+(\nabla u)^{T}\right)-\frac{2\eta}{3}(\nabla.u)I\right]+\rho u.\nabla u+\nabla P=\rho g$$

Where u is the fluid velocity, P denotes pressure, η viscosity, ρ density. In addition to momentum balance equation, the conservation of mass is expressed as:

$$\frac{\partial\rho}{\partial t}+\nabla.(\rho u)=0$$

VOF model is used to determine the gas-liquid interface. By solving the following equation for the volume fraction of one (or more) of the phases, the interface can be tracked. For the q_{th} phase, this equation has the following form:

$$\frac{1}{\rho_q}\left[\frac{\partial}{\partial t}(\alpha_q\rho_q)+\nabla.\left(\alpha_q\rho_q\overrightarrow{u_q}\right)=S_{\alpha q}\right]$$

where $S_{\alpha q}$ on the right-hand side denotes the source term which is zero by default but due to mass input from gas to liquid phase in this model, a user-defined mass source should be specified.

The energy transfer is described by the following equation for the temperature:

$$\rho C_P\frac{\partial T}{\partial t}+\nabla\cdot(-k\nabla T)=-m_{in}H_{in}-\rho C_P u\cdot\nabla T$$

where Cp denotes heat capacity, k thermal conductivity, and T temperature. The first term on the right-hand side of the equation is a source term that accounts for heat flux from the gas phase; H denotes heat transfer flux flows into the slag layer, while m is the interfacial mass flux.

In this two-phase system, the material properties such as density and viscosity are calculated by the following relations:

$$\rho=\rho_g+(\rho_l-\rho_g)\alpha_l$$

$$M=M_g+(M_l-M_g)\alpha_l$$

The subscripts “g” and “l” denote the gas and liquid phases, respectively. M is a physical property parameter which can be density, viscosity, heat transfer coefficient or heat capacity.

Model Geometry and computational methods

In an entrained flow gasifier, the reactants including coal particles, steam and oxygen are injected concurrently from the top. The gasification reaction takes place inside the chamber and gives syngas and fly/molten ash. The ash particles at high temperature form a falling film of slag on the wall and syngas leaves the reactor from the bottom. In the present model, the slag flow, heat and mass transfer and solidification are considered. A 2-D model is developed to describe that system shown in Fig. 3. Quad mesh is used for mesh generation. The number of mesh is 30000 and Fluent was used to solve the equations in implicit mode. The discretization of equations is implemented by second order upwind method; Pressure is treated by PRESTO!. PISO is used to couple the pressure and velocity. Presto! is a scheme in Fluent used for more accurate interpolation of face pressure values from all cell pressures. PISO (Pressure-Implicit Split-Operator) is a sub-scheme in Fluent as well and recommended for unsteady simulation as it usually allows faster convergence of each step through the use of higher under-relaxation factors than are permissible with other schemes.

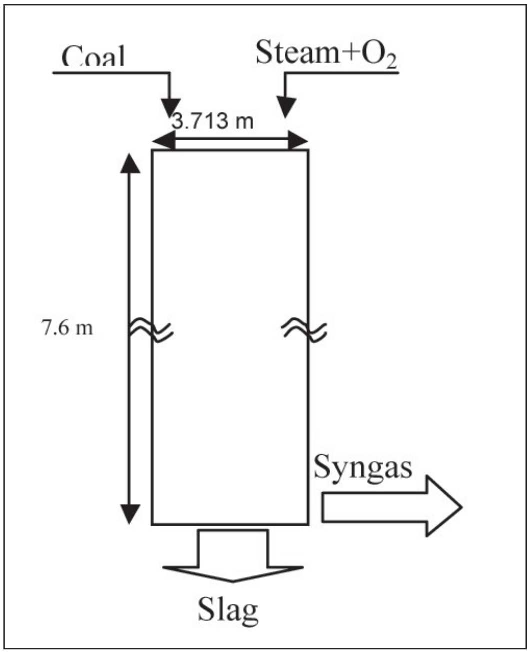

Fig. 3: The geometry of the gasifier

All the conservation equations were solved using unsteady state multiphase mode in Fluent. It was assumed that the reaction takes place in the gas phase and the hot melted ash particles are transferred through the interface and deposited on the wall. The mass and heat flux passing the interface are taken from Seggian's model. As these values should be defined per cell volume through the user-defined-functions, the fluxes have been converted to the equivalent units in Table 2. These values are considered as the source term of mass and energy while the conservation equations are solved.

Table 2: The mass and heat flux from gas to slag phase

Seggiani's section	Seggiani		This model	
	m_{in} (kg/s)	q_{in} (kW)	m_{in} (kg/m^3.s)	q_{in} (kW/m^3)
1	0.129	116	0.73	192.223
2	0.145	130	0.73	192.223
3	0.164	147	0.73	192.223
4	0.516	536	1	786.5
5	0.516	536	1	786.5
6	0.516	536	1	786.5
7	0.516	536	1	786.5
8	0.516	649	1	786.5
9	0.516	649	1	786.5
10	0.516	649	1	786.5
11	0.516	649	1	786.5
12	0.232	251	1	786.5
13	0.158	171	0.63	217.901
14	0.093	101	0.63	217.901
15	0.066	71	0.63	217.901

SIMULATION RESULTS

As initially indicated, the aim of this paper is to predict the thickness of the slag layer as the gasification reaction proceeds. Fig. 4 shows the interface between the two phases of slag and gas obtained by solving VOF equation coupled with the other conservation equations in Fluent.

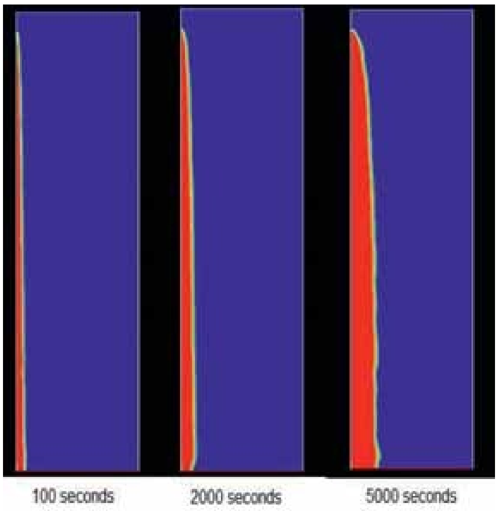

Fig. 4: Growth of over time

As illustrated, the slag layer is growing over time so that it reaches to steady-state condition. The temperature distribution is also important as the viscosity and subsequently the solidification depends on the temperature. The heat flows outward due to temperature difference between the chamber inside and the wall. The temperature distribution is presented in Fig. 5. As the temperature decreases near the wall and falls below the critical viscosity temperature, solidification starts and the solid layer becomes thicker and thicker. The solidification phenomenon plays an important role in the growth of the slag layer.

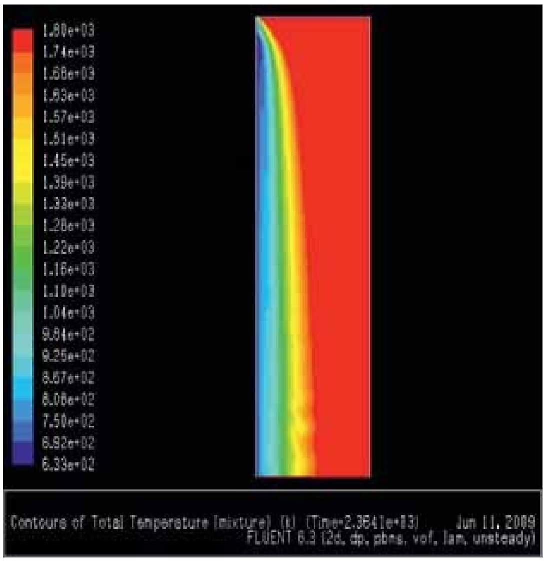

Fig. 5: Temperature distribution inside the gasification chamber

The temperature at the wall is controlled by the ambient temperature or mostly using a coolant such a cooling water. It is also applied to supply a portion of hot steam needed for the unit. Here, it is assumed that the wall temperature is kept constant at 640 K. The temperature increases by passing the solid and liquid parts of the slag layer toward the gas phase. The reaction takes place at a temperature which was assumed to be 1800K. This temperature can be changed by varying the oxygen to steam ratio at the inlet. However, the operating temperature has a remarkable effect on the rate of gasification reaction which influences the slag properties as well. It is also makes a huge decrease in the viscosity of the slag to have a thinner layer on the wall. The temperature profile against the radial length is presented in Fig. 6 for different heights of the reactor. It can be seen that the temperature levels off only after a short distance from the wall, in this case it is only about 15 cm, regardless of the difference in reactor heights. Before leveling off however, at a distance about 10 cm from the wall, the effect of reactor height can be seen with temperatures being higher at the lower part of the reactor as compared to the top one.

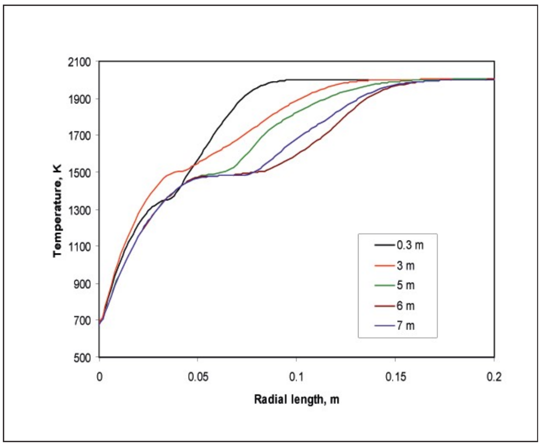

Fig. 6: Radial temperature variation inside the gasification chamber at different reactor heights; gas temperature is assumed to be 2000K.

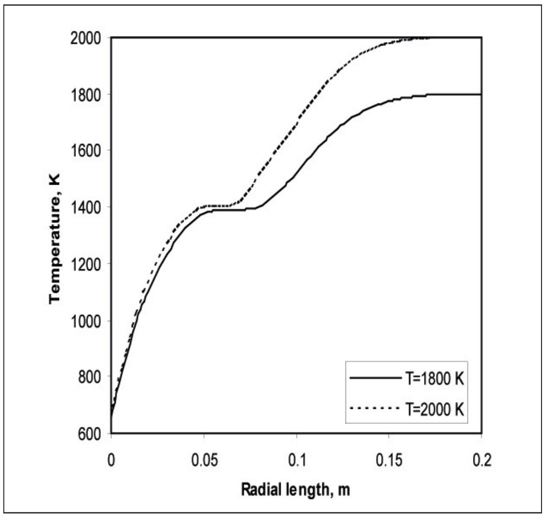

Fig. 7: The effect of operation (gasification reaction) temperature on the temperature distribution inside the chamber.

Fig. 7 shows the effect of the temperature of gas phase on the temperature distribution in the slag layer. The slag layer becomes thinner by adding more oxygen to reactor. The reaction efficiency will be decreased because more coal particles burn in oxygen instead of reacting with steam to produce syngas, but as shown in Fig. 8 the slag deposition on the wall will be also decreased as a consequence. The viscosity decreases with increasing temperature thus as long as the gasifier operates far enough above the temperature of critical viscosity a thinner slag layer deposits on the wall. Fig. 8 furthermore shows that the time needed to reach the steady state condition decreases by working at higher temperatures

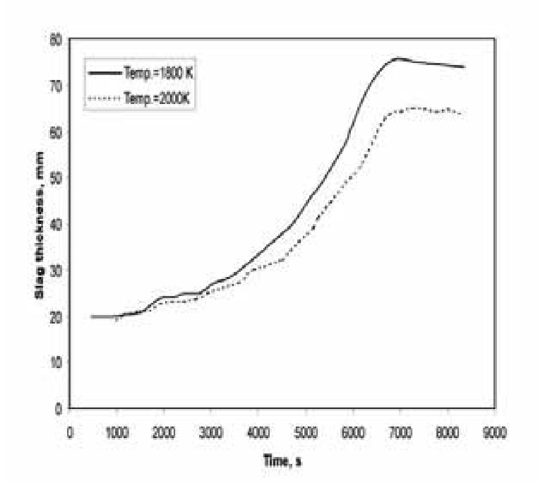

Fig. 8: Slag layer thickness as a function of time.

The effect of fluxing agent addition on the thickness of the slag along the gasification chamber is presented in Fig. 9. As the slag flows down the reactor the thickness will increase until it reaches the maximum at the outlet. This point is very crucial because if the layer thickness continues to grow, it may cause a plugging in the taping system.

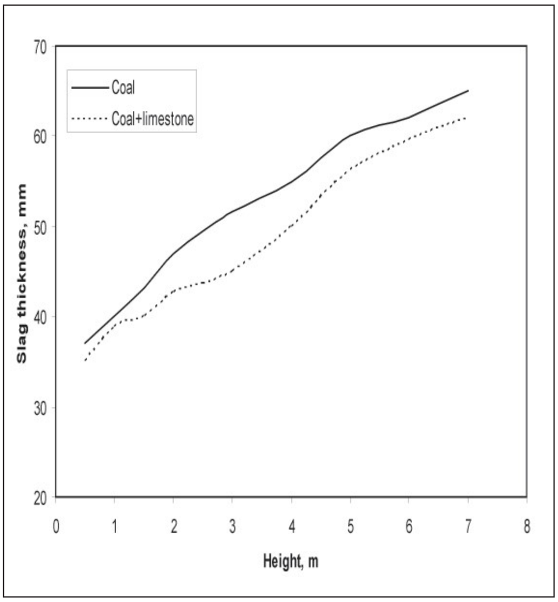

Fig. 9: The slag thickness versus height from top to bottom of the reactor

As illustrated in Fig. 9, adding limestone to the feed made a considerable reduction in the slag thickness. Fluxing agents such limestone change the ash properties; the temperature of critical viscosity and the viscosity itself will be reduced by increasing calcium oxide content therefore larger amount of liquid slag can leave the chamber. The slag thickness growth over time is obtained by doing a simulation for two different types of feedstock, i.e. coal and a mixture of coal and limestone as Seggiani used with the properties in Table 1. Another feed having a lower viscosity was also evaluated to investigate the effect of viscosity reduction by coal blending on the slag thickness. The comparison of the three types of feedstock as far as their effect on slag layer thickness is concerned is shown in Fig. 10 and shows thickness decrease by up to 15%.

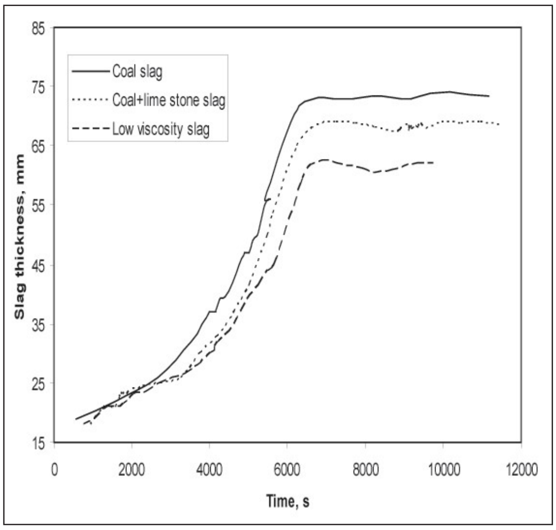

Fig. 10: Slag layer thickness as a function of time for three different feed stocks

The effect of composition on temperature distribution inside the gasification chamber is shown in Fig. 11. As it can be seen, the thicker layer also has a wider range of temperature distribution.

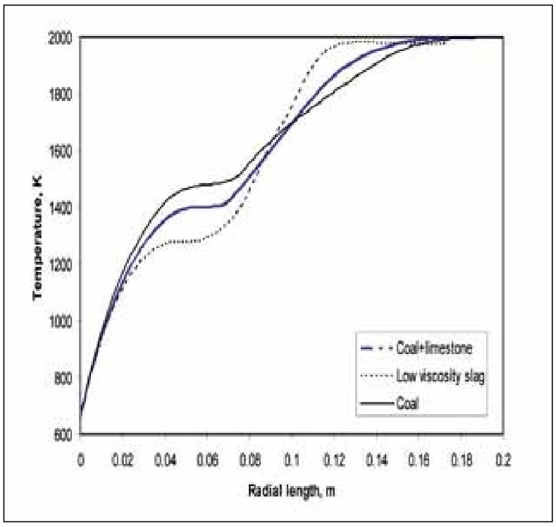

Fig. 11: Effect of composition on temperature distribution inside the gasification chamber

CONCLUSION

The motion of slag layer in entrained flow gasifiers is a multiphase flow with heat and mass transfer. In this study the slag flow was modelled using Fluent to solve all the conservation equations and to track the interface between the gas phase and the liquid phase. Results show that the slag layer thickness is about 5-10 cm for an entrained-flow gasifier, with the larger part of the layer consisting of a solid phase. Increasing the operating temperature will reduce the slag thickness. This however requires extra oxygen be injected to reach such a high temperature which in turn reduces the reaction efficiency. The better solution is to add fluxing agent like limestone to change the composition. The fluxing agent makes a reduction in viscosity and consequently the slag layer thickness by 15%. Generally, the simulation has shown ability to predict the required parameters required for slag layer thickness control and can be a useful tool in avoiding tap hole blockages in entrained flow gasifiers.

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