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Eulerian-Lagrangian CFD modeling of coal gasification

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Abstract

A computational model is applied to investigate thermal flow and gasification of coal in gasifier using commercial CFD (computational fluid dynamics) solver STAR CCM+. The Eulerian-Lagrangian approach is used to model this work. The Eulerian approach is used to model air while theLagrangian approach is used to model coal particle. The objective of this work is to implement devolatilization, char oxidation and homogeneous reaction model in themulti-phase flow. Implementation of model starts with coal moisture evaporation, devolatilization, char oxidation and lastly homogeneous reactions in themulti-phase flow. The results show that moisture evaporation, devolatilization, and char oxidation along with homogeneous reaction model are successfully implemented. Syngas composition of species at outlet mainly consist of CO, CH_4, and H_2. Syngas species composition is validated with experimental results. Hence, coal gasification model has been successfully implemented in thecomputational code of STAR CCM+.

Keywords:*Multiphase flow, Gasification simulation, coal devolatilization, char oxidation, STAR CCM+.*

1. Introduction

Coal is theprimary source of fossil fuel in India. Coal is cheap and readily available in India as compared to other fossil fuel. Hence, it becomes theprimary source of energy in Indian industry. But, coal has its own drawback as it is most polluting fuel. Also, the traditional method used to utilized energy from coal are low efficient and high pollutant prone. Hence, there is must do athing to developed new method to utilized large amount of energy benefits from coal without pollution. For this integrated gasification combined cycle serve our need. As compare to combustion, gasification is amuch cleaner process along with high efficient. As we know, theend product of combustion is only heating source along with polluting product gas. But, in thecase of gasification, syngas gas have heating source ability with productive species such as CO, O_2, methane, etc. Gasification gives heating effect with which we can produce steam and hence electricity. Also, syngas so obtain can chemically process and synthetic fuel can be obtained. This synthetic fuel will be alternative to our conventional fossil fuel. In this century, we have ahighly efficient computer and highly advanced numerical method. The combination of this two can give us anoptimum solution to thermochemical process. Computational fluid dynamics offer aneffective mean of quantifying physical and chemical process in coal thermochemical reactor under various operating condition. The accurate results from simulation help to optimize the system design and operating condition. Also, thedynamic process can be understood clearly within the reactor.
Adam Klimanek (2014) done a research work on anumerical model of coal gasification in circulating fluidized bed. The eulerian-lagrangian approach has been used. To simulate Particle flow in continuous phase has been amodel using discrete dense phase model. Homogeneous and heterogeneous reaction are amodel using eddy dissipation model and finite rate chemistry.G.k.singh (2015), work on pilot scale bubbling fluidized bed gasifier for high ash Indian coal gasification. The eulerian-eulerian approach has been used in this work. The homogenous reaction has been amodel using eddy dissipation model while user defines function has been used for theheterogeneous reaction. Jun Xie (2013), developed athree-dimensional numerical model for coal gasification in fluidized bed gasifier. The Eulerian approach used for continuous phase while Lagrangian used for discrete phase. Jobaidar Khan (2013), investigate the thermal flow and gasification in themild gasifier. The eulerian-eulerian approach is considered. For devolatilization special code has been generated and successfully implemented. Ravi Inder Singh (2013), studied the detailing of combustion and gasification process in afluidized bed. CFD modeling is used to analysis the effect of theoperating parameter.

In this work, numerical analysis is done using commercial CFD solver STAR CCM+. There is no literature available on CFD analysis of coal gasification using STAR CCM+. Also, for present work Eulerian-Lagrangian approach is used to model multiphase flow. The Eulerian approach used to model gaseous phase while Lagrangian approach used solid phase. As mention above Adam klimanek (2014) used Eulerian-lagrangian approach but method used to model chemical kinetics are different. In Adam Klimanek work, user define fuction is used to model chemical kinetics while in this present work Arrhenius equation is used to model chemical kineticsfor both hetereogeneous and homogeneous reaction.

2. Gasification Theory

2.1.Gasification and Combustion

Gasification and combustion these both processes are used to convert solid fuel into productive gases along with heat energy. But, this process occurs at thedifferent environmental condition. Combustion is done in oxygen enriched environment while gasification required alimited amount of oxygen. Combustion is nothing but burning of fuel in boiler, stove, and furnace to generate heat. This heat is then used to produce steam and indirectly electricity through steam turbines. At the end of combustion, we got CO_2 and H_2O as product gas. These product gas can only be used as aheating source. Also, these are polluting gases. Gasification is nothing but the partial combustion of fuel. Gasification is done in alimited oxygen environment. Syngas mainly includes CO, H_2, methane and other species. This syngas has multiple application instead of just using as aheating source. Like it can be used produce methane, methanol, hydrogen and much more. Also, after few chemical process, this syngas can be converted into synthetic fuel which can serve as analternative to fossil fuel.

2.2. Gasification

The thermochemical conversion of fuel in product gas which contains mainly CO, H_2 and methane is called as gasification. For gasification, alimited amount of oxygen, air or air with steam can be used as gasifying agents. Gasification is mainly done through following four stage which is drying, devolatilization, oxidation, and reduction.

2.2.1. Drying

Solid fuel always contains some amount of moisture. For efficient gasification fuel should be completely dry. Hence, in thefirst stage of gasification drying of solid is done. The temperature at this stage is about 100-200°C which helps to remove moisture from fuel and formvapor of it. There will be no further decomposition of fuel as thetemperature is pretty low to decompose fuel.

2.2.2. Devolatilization

Devolatilization is theremoval of volatile matter from solid fuel. Mostly, this process occurs at atemperature ranging from 200-300°C. In thecase of coal as solid fuel, coal consist of char, volatile matter, moisture and ash. In trying process moisture are removed hence, there will be char, volatile matter and ash only. During devolatilization, volatile matter from coal is taken out. As there is theremoval of volatile matter, there will be areduction in weight. Devolatilization is mostly depended upon characteristics and type of coal. This reaction is endothermic hence, to complete this reaction we need to add heat into it.

2.2.3. Char Oxidation

After devolatilization, remaining productsis char and ash where thereactive product is only charred as Ash is sort of inert material. In oxidation stage, O_2, CO_2, and H_2O react with char. This reaction is exothermic which release the heat and supply heat to other endothermic reaction.

2.2.4. Reduction

This stage includes reduction reaction in absence of oxygen. These are anendothermic reaction.
After all stage, product gas that is syngas mostly contain CO, CO_2, CH_4, and H_2.

3. Numerical analysis:

3.1. Geometry and material

Geometry used in this work is shown in figure1. The total height of gasifier is 4m having three opening. Two inlets for agasifying agent and another for coal along with this there will be one outlet for syngas. The diameter for air inlet is 250 mm located at the bottom of gasifier as shown in Figure1. The coal inlet has adiameter of 80mm located at 500mm height and to the left side of thegasifier. An outlet for syngas is given at top of gasifier having 350mm of diameter. The material used is Indonesian coal having adensity of 1200 kg/m^3. The diameter of coal is 10µm. the proximate and ultimate analysis is given in Table 1 and Table 2 respectively.

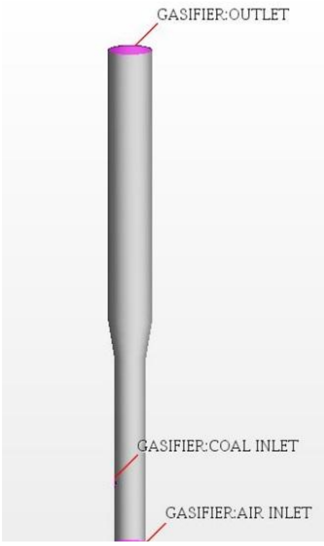

Figure 1: Geometry

Table 1: Proximate analysis of coal

Proximate analysis	
Moisture	15.23%
Ash	3.96%
Volatile matter	40.15%
Fixed carbon	40.66%

Table 2: Ultimate analysis of coal

Ultimate analysis	
Mineral matter	4.67%
Carbon	67.03%
Hydrogen	5.01%
Sulphur	1.12%
Nitrogen	1.16%
Oxygen	21.01%

3.2. Meshing

Mesh is discretized representation of computational domain which is used by physics solver to provide anumerical solution. In this work, we generate mesh with the help of STAR CCM+ meshing tool. Surface remesher, polyhedral meshing, and prism layer mesh have been used in this work. Surface remesherremesh initial surface to provide quality discretized mesh. the surface remesher is used. For volume mesh, we used polyhedral mesher. Polyhedral mesher provide balance solution for complexed mesh generation problem. Polyhedral mesher are relatively easy and efficient to build also, they contain five times lesser cell than tetrahedral mesh for starting surface. Prism layer mesh model is used with core volume mesh to generate orthogonal prismatic cells next to wall or boundaries. This layer of thecell is necessary to improve the accuracy of flow solution. Table 3 shows meshing detail. Figure 2 shows the mesh generated for present work.

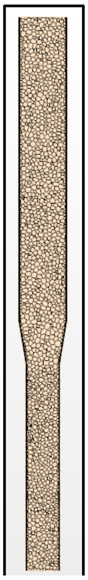

Figure 2: Meshed Geometry

Table 3: Meshing details

Base size	20 mm
Relative minimum size	25% of base size
Relative target size	100% of base size
Prism layer thickness	33.3% of base size
No. of prism layer	5
No. of cells	64461

Mesh sensivity is checked with four different mesh having 50mm, 40mm, 20mm and 20mm with customized fined mesh. To check mesh sensitivity simulation is run for 100s physical time. Detailed of mesh sensitivity is given in table 4.

Table 4: Mesh sensitivity analysis

	Mesh 1	Mesh 2	Mesh 3	Mesh 4
Base size	50mm	40 mm	20 mm	20 mm with customize meshing
Cell count	18426	43543	64461	73786
Mole fraction of CO	0.0901	0.0923	0.1096	0.1038

From mesh sensitivity it is clear that meshing with 20 mm base size with or without customized fined mesh gives almost same reults.Hence, to avoid extra computational time we select mesh of 20mm base size without customized mesh.

3.3. Model description and simulation method:

In this present work, theEulerian and Lagrangian approach has been used, theGasifying agent is taken as continuous phase while coal particle is considered as a discrete phase which models using Lagrangian approach. K-epsilon turbulence used to model turbulent flow. In this method, set of turbulent kinetic energy and turbulent kinetic energy dissipation equation are solved for each phase. Eddy break up model used for modeling of coal gasification reaction while Arrhenius equation has been used for chemical kinetics.

3.4. Governing equation

As in this present work, we are dealing with themultiphase problem. The gasifying agent is considered as continuous phase while coal particle is considered as dispersed phase. Governing equation for each phase is given below,

3.4.1. Governing equation for continuous phase:

(a) Continuity equation:

$$\frac{\partial}{\partial t}(\alpha_c\{\rho_c\}) + \frac{\partial}{\partial x_i}(\alpha_c\{\rho_c u_i\}) = -\frac{1}{V}\sum_k \dot{m}_k$$

(b) Momentum conservation equation:

$$\frac{\partial}{\partial t}(\alpha_c\{\rho_c\}\tilde{u}_i) + \frac{\partial}{\partial x_j}\left(\alpha_c\{\rho_c\tilde{u}_i\tilde{u}_j\}\right) = -\frac{\partial\{p\}}{\partial x_i} + \frac{\partial\{\tau_{ij}\}}{\partial x_i} + \alpha_c\{\rho_c\}g_i - \frac{1}{V}\sum_k v_{k,i}\dot{m}_k - \frac{1}{V}\sum_k \dot{F}_{k,i}$$

(c)Energy equation:

$$\frac{\partial}{\partial t}(\alpha_c\{\rho_c\}\tilde{\imath}_i) + \frac{\partial}{\partial x_i}(\alpha_c\{\rho_c u_i i_c\}) = \frac{\partial}{\partial x_i}\left(k_{eff}\frac{\partial\langle T_C\rangle}{\partial x_i}\right) + \alpha_c\{\emptyset\} - \frac{1}{V}\sum_k v_{k,i}\dot{m}_k - \sum_k \dot{q}_k$$

3.4.2. Governing equation for dispersed phase:

(a)Particle motion:

$$\frac{dv}{dt} = \frac{F_f}{m} + g$$

(b)The trajectory of particle:

$$\frac{dx_p}{dt} = v$$

(c)The temperature of particle:

$$\frac{dT_d}{dt} = \frac{1}{mc_d}(\dot{Q}_d + \dot{m}h_L)$$

3.4.3. Turbulence model:

(a)Equation for turbulent kinetic energy:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho v_j k) = \frac{\partial}{\partial x_j}\left[\mu + \frac{\mu_t}{\sigma_k}\right]\frac{\partial k}{\partial x_j} + G_k + G_b - \rho\varepsilon$$

(b)The equation for Turbulent dissipation rate:

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_i}(\rho v_j \varepsilon) = \frac{\partial}{\partial x_j}\left[\mu + \frac{\mu_t}{\sigma_\epsilon}\right]\frac{\partial\epsilon}{\partial x_j} + G_k + (1 - A_{3\varepsilon})G_b + A_{1\varepsilon}\frac{\varepsilon}{k} - A_{2\varepsilon}\rho\frac{\varepsilon^2}{k}$$

3.4.4. Species Transport equation:

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho u_j Y_k)}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\rho D_k\frac{\partial Y_k}{\partial x_j}\right) + \dot{\omega}_k$$

3.5. Chemical kinetics:

3.5.1. Coal moisture evaporation:

The moisture contains coal particle is assumed to coat the particle moisture evaporation occur rapidly before the mass transfer process takes place. The continuity equation for moisture component in particle p given as

$$\frac{d\alpha_{wp} m_p}{dt} = -r_{wp}$$

3.5.2. Raw coal devolatilization:

Devolatilization is a step where thevolatile matter gets out of coal particle.

$$(Rawcoal) \rightarrow YY_{pn}(volatile\ matter) + \left(1 - YY_{pn}\right)(char)$$

The continuity equation for raw coal component in particle p is given as

$$\frac{d\alpha_{cp}}{dt} = -r_{cp}$$

The net rate of raw coal consumption given as

$$r_{cp} = k_{pn}\alpha_{cp}$$

K_{pn} is reaction rate constant calculate using

$$k_{pn} = A_{pn}exp\left[-\frac{E_{pn}}{R_u T_p}\right]$$

3.5.3. First order char oxidation:

Char remain after devolatilization react with O_2, H_2O, and CO_2 in the following form,

$$(char) + (oxdizer) \rightarrow (product)$$

The continuity equation for char component in particle p.

$$\frac{dm_{hp}}{dt} = -r_{hp}$$

The rate of formation of char from particle p,

$$r_{hp} = r_{vp}\ (1 - YY_{pn})/YY_{pn}$$

The rate of reaction is calculated as follows,

$$k_{pl} = A_{pl}T_p^n exp\left[-\frac{E_{pl}}{R_u T_p}\right]$$

The devolatilization and char oxidation reaction with their properties are given in Table 4 and 5 respectively.

Table 5: Properties of Two step devolatilization

Properties	First step devolatilization	Second step devolatilization
Activation energy (kJ/kmol)	7.36×10^4	2.51×10^5
Pre-exponential factor	3.7×10^5	1.5×10^{13}
YY	0.4	0.8

Char oxidation reaction:

Reaction 1:

$2char + O_2 \rightarrow 2CO$ ……………..… [R1]

Reaction 2:

$char + H_2O \rightarrow CO + H_2$….. [R2]

Reaction 3:

$char + CO_2 \rightarrow 2CO$…………... [R3]

Table 6: Properties of Char Oxidation reaction

Reaction	Activation energy	Pre-exponential factor	Temp exponent
1	9.29×10^7	2.3	1
2	1.47×10^8	1.33	1
3	1.3×10^8	3.149	1

Homogeneous reaction:

Reaction 4:

$volatile + 0.076O_2 \rightarrow 0.583CH_4 + 0.417CO + 0.021N_2$. ………………………………………….. [R4]

Reaction 5:

$CO + 0.5O_2 \rightarrow CO_2$ ………. [R5]

Reaction 6:

$$CO + H_2O \rightarrow CO_2 + H_2 \ldots\ldots \text{[R6]}$$

Reaction 7:

$$H_2 + 0.5O_2 \rightarrow H_2O \ldots\ldots\ldots\ldots \text{[R7]}$$

Reaction 8:

$$CH_4 + H_2O \rightarrow CO + 3H_2 \ldots\ldots \text{[R8]}$$

Table 7: Properties of homogenous reaction

Reaction	Activation energy	Pre-exponential factor	Temp exponent
4	2.027×10^{8}	2.119×10^{11}	1
5	1.7×10^{8}	2.239×10^{12}	1
6	2.88×10^{8}	2.35×10^{10}	1
7	3.1×10^{7}	9.87×10^{8}	1
8	2.09×10^{8}	5.922×10^{8}	1

3.6. Boundary condition:

Geometry and meshing for this work have been generated in STAR CCM+ modeling and mesh. Coal and theair inlet are provided with wall and velocity inlet. Syngas outlet is given as pressure outlet. For aparticle, theinjector has been used. Surface type injector is used in this case and coal inlet surface is taken as input for theinjector. Initial and boundary condition are alist out in Table 7 and Table 8 respectively.

Table 8: Initial condition

Initial condition	
Pressure	0.2bar
Species fraction	$N_2 = 0.79$ $O_2 = 0.21$
Velocity	0.277m/s

Table 9: Boundary condition

Boundary condition	
(1) Air inlet	
Type of boundary	Velocity inlet
Velocity	0.277m/s
Species fraction	O_2 =0.21 N_2 =0.79
Static temperature	850°C
(2) Coal injector	
Type of injector	Surface injector
Mass flow rate	0.0111kg/s
Particle diameter	10µm
Particle temperature	25°C
Species fraction	Rawcoal=0.8081 Ash =0.0396 Moisture=0.1523
velocity	0.001804m/s
(3) Pressure outlet	
Type of boundary	Pressure outlet
Pressure	1 atm
Species fraction	O_2 =0.21 N_2 =0.79
Static temperature	25°C

4. Results and discussion:

Devolatilization and char oxidation of coal particle along with homogenous reaction has been carried out in this work. This reaction releases coal volatile and other species. The mole fraction of CO, CH_4, H_2,N_2,and temperature is analyzed in this work. Results from numerical analysis are validated by experimental results.

4.1. Syngas species distribution:

Char oxidation reaction [R1-3] are heterogeneous reaction occurs between char and anoxidizing agent as O_2, H_2O, and CO_2. After production of gaseous species from theheterogeneousreaction, there will be ahomogenous reaction [R4-8] to from CO, CH_4, and H_2. Figure 3 and 4 shows thecontour of different syngas species. Figure 5 shows, distribution of species along the axis of thegasifier. It is evident that at the bottom of gasifier concentration of CO,H_2 and CH_4 are lower while N_2 is higher. As we move upward along the axis, theconcentration of CO, H_2, and CH_4 shows increasing nature while N_2 shows decreasing one. At thebottom region of thegasifier, there is thepresence of char and H_2O because of devolatilization reaction. Hence, theconcentration of CO, H_2, and CH_4 are lower in thebottom region. As moved upward, char from devolatilization get oxidized and product so formed react homogeneously to give CO, H_2, and CH_4. Because of this reactions, there will be anincrease in theconcentration of CO, H_2, and CH_4 in theupward region of thegasifier.

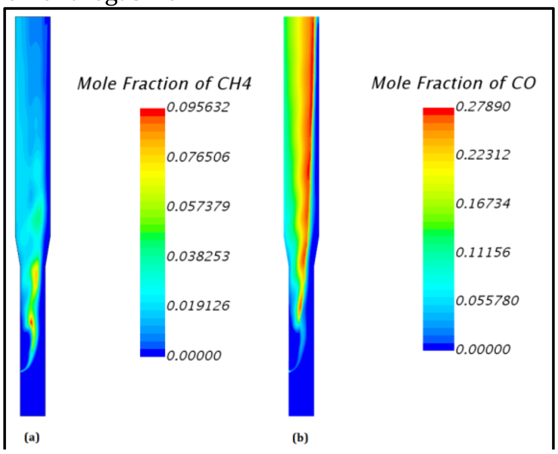

Figure 3: (a) Mole Fraction of CO
(b)Mole Fraction of CH_4

Figure 3(a-b) and 4(c) show thedistribution of CO, H_2, and CH_4. While Figure 5 shows the concentration of these species along the axis of the gasifier. From the bottom of the gasifier, air is coming which have O_2 and N_2 as its constituent. Hence, at a bottom concentration of N_2 is higher and as move upward most of the N_2 combine with another unburnt hydrocarbon to form mineral matter or tar. Because of this N2 concentration shows decreasing behavior along the axis of the gasifier. Figure 4(d) and 5 shows the N_2 distribution in the gasifier.

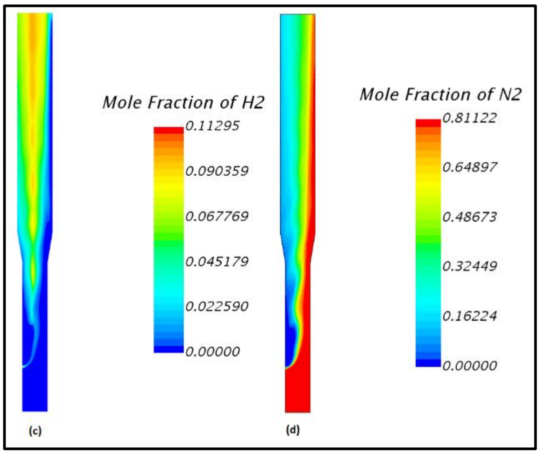

Figure 4: (c) Mole fraction of H_2 (d) Mole fraction of N_2

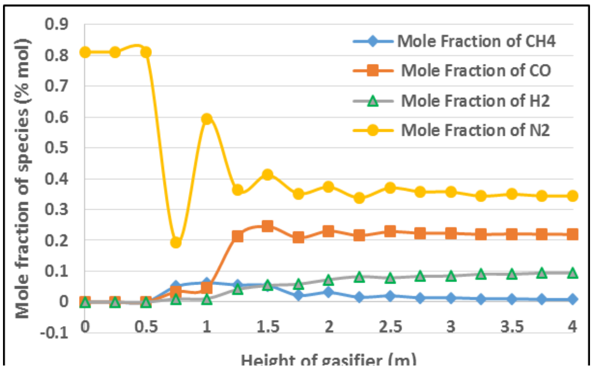

Figure 5: Mole Fraction of species along height

4.2. Progressive generation of CH_4:

Progressive generation of CH_4 is shown in Figure 6(a-b). The initial stage of CH_4 generation is shown in figure 6(a). During theinitialstage, devolatilization occurs which release a large amount of volatile matter. This volatile matter breaks down into CH_4 and CO hence, there will be ahigher concentration of CH_4 during initial stage [R4]. As gasification proceed, formed CH_4get to react with H_2O to form CO and H_2 [R8]. Hence, in thefinalstage, theCH_4 concentration decreases. From figure 6(a-b)we can summarize asCH_4 concentration increased in initial stage while it goes on decreasing in thefinal stage.

4.3. Progressive generation of CO:

Progressive generation of CO is shown in Figure 7(a-b). In gasification, there is thecontinuous formation of CO from heterogeneous [R1-3] and homogeneous reaction [R4, R8].During theinitialstage, there is char oxidation [R1-3] which mostly gives CO hence there is increasing in concentration in this stage. As gasification proceed, thehomogeneous reaction takes place [R4, R8] and CO is generated. Hence, there is acontinuous increase of CO concentration because of heterogeneous [R1-3] and homogeneous [R4, R8] reaction which is shown in Figure 7(a-b).

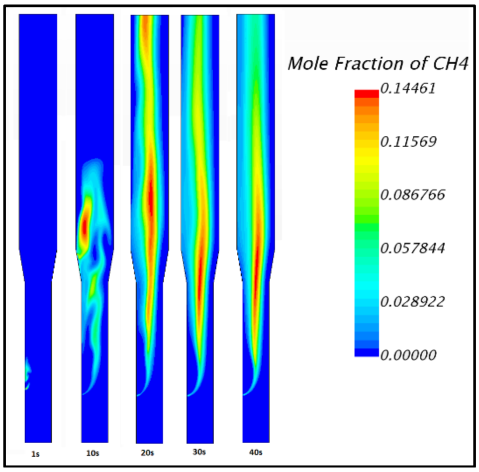

Figure 6(a): Progressive generation of CH_4

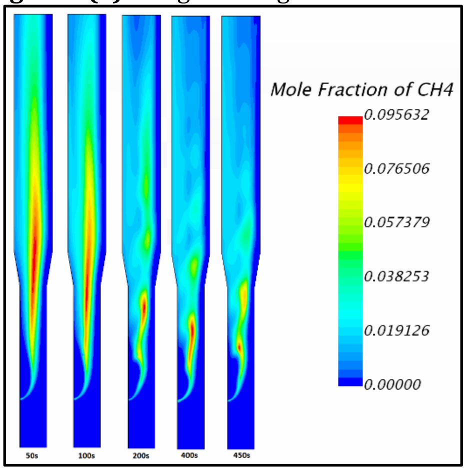

Figure 6(b): Progressive generation of CH_4

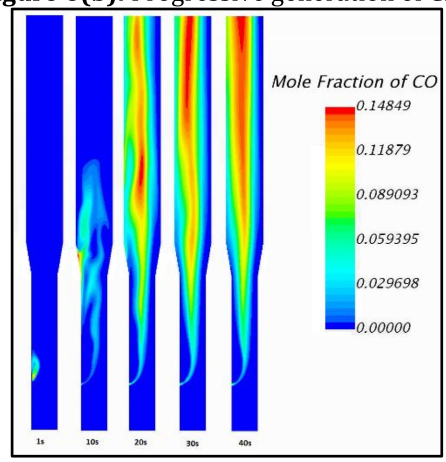

Figure 7(a): Progressive generation of CO

4.4. Progressive generation of H_2:

Progressive generation of H_2 is shown in Figure 8(a-b). Char oxidation [R2] and homogenous reaction [R6, R8] gives out H_2. This will result in higher concentration of H_2 during the initial stage of gasification which is shown in Figure 8(a). As gasification proceed, formed H_2 react with oxygen to give water [R7]. Hence, there will be consumption of H_2 which leads to decrease in concentration of H_2 which is shown in Figure 8(b), Fromthis, we can summarizeas during gasification concentration of H_2 initially increases then decreases.

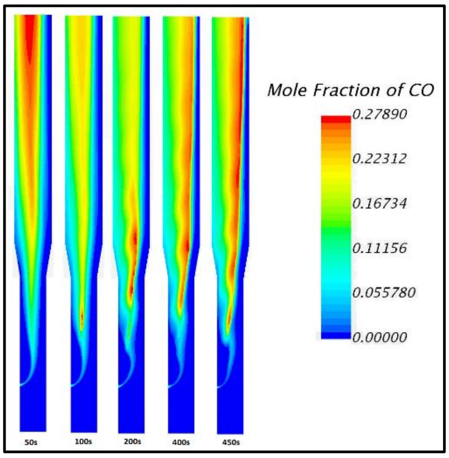

Figure 7(b): progressive generation of CO

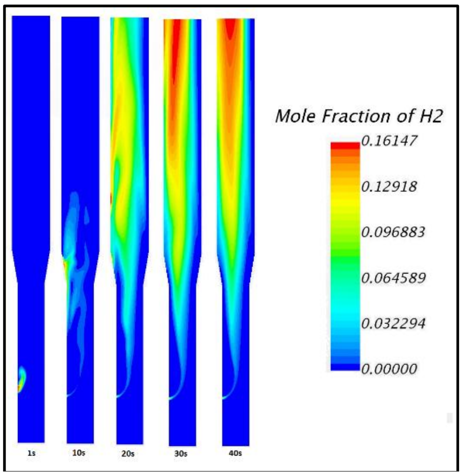

Figure 8(a): Progressive generation of H_2

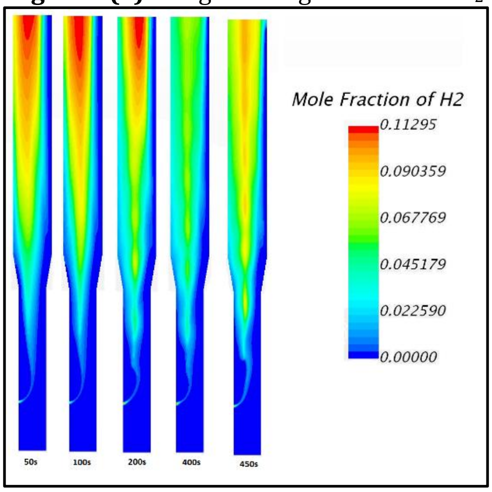

Figure 8(b): Progressive generation of H_2

4.5. Temperature distribution:

The gasifier is initialized with 25°C but as reaction progress, hot air react with coal particle and theexothermic reaction takes place. Because of this reaction, there is acontinuous increase of temperature. After devolatilization, there will be heterogeneous [R1-3] and homogeneous [R4-8] reaction which are endothermic in nature. Hence there will be decreasing in temperature after devolatilization.The temperature distribution along the axis of thegasifier is shown in Figure 9.The contour of temperature profile is shown in Figure 10. Temperature is ahigh in lower region where coal and air come in contact. Because there is a large amount of unreacted coal and oxygen are available which initialized the devolatilization reaction which is highly exothermic. Hence, there is theelevation of temperature in thelower region of thegasifier. As we move upward along axis there will be theoccurrence of endothermic reaction which lowers down the temperature in thegasifier. Figure 9 shows thatbetween the heights of 0.5 to 1.5 m there is increasing temperature. This is a region where theexothermic reaction occurs. While. Above 1.5m height, there is adecrease in temperature because of anendothermic reaction.

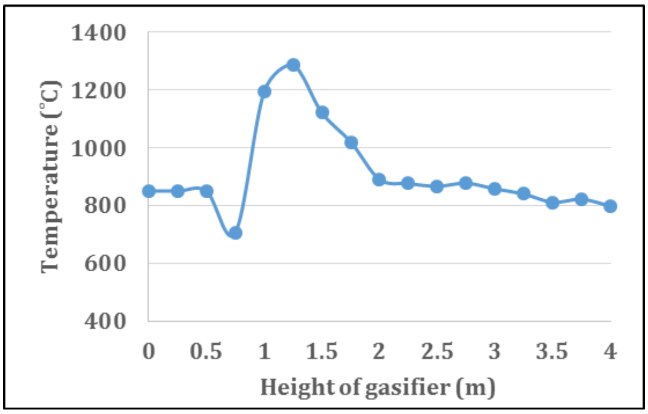

Figure 9: Temperature distribution along height

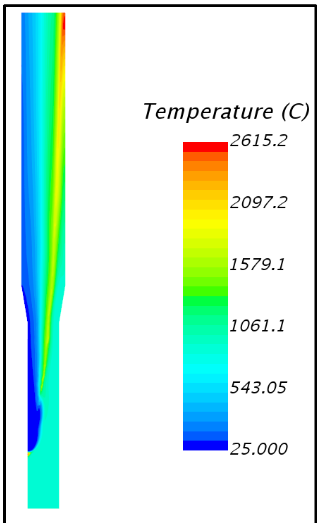

Figure 10: Temperature distribution

5. Experimental validation:

Numerical results obtained from this present work are validated with experimental results of coal gasification in fluidized bed gasifier. Coal used is Indonesian coal as mention in section 3.1. The results from numerical analysis and experiment are shown in Table 9 and Figure11 shows bar chart between experimental and numerical results. Numerical results show good agreement with experimental results.

Table 10: Mole fraction of gaseous species

	Numerical results	Experimental results

Mole Fraction		
CO	0.1904	0.20
CH_4	0.0089	0.01
H_2	0.0764	0.1
N_2	0.3719	0.40
Temperature	937.67°C	950°C

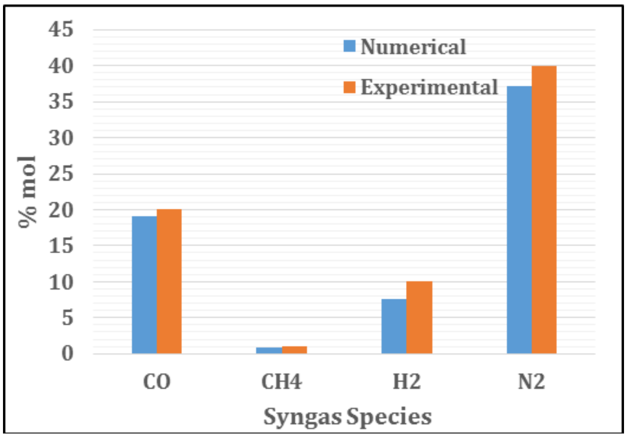

Figure 11: Experimental and numerical results

6. Conclusion:

The results are summarized as follows,

1. Devolatilization, char oxidation of coal particle and thehomogenous reaction has been successfully implemented in thecomputational code of STAR CCM+.
2. The syngas composition i.e. CO, CH_4,and H_2 are validated with experimental results and show good behavior with theexperimental value.
3. As devolatilization is ahighly exothermic reaction. Hence, initially temperature is high but after theendothermicreaction, there is adecrease in temperature.
4. For future scope, effect of coal particle size, mass flow rate of air and mass flow rate of coal on syngas composition has to be investigate

Nomenclature:

Latin letter

m = Mass
v = Velocity
g = Gravity
t = Time
x = Position
c = Specific heat
h = Enthalpy
F = Force
V = Volume
T = Temperature
Q = Heat transfer
E = Energy of activation
A = Pre-exponential factor
R = Universal gas constant
r = Rate of reaction
k = Rate constant
YY = Mass stoichiometric coefficient

Greek letter

α = Volume fraction
ρ = Density
τ = Shear stress

Sub-script

K = Number of particle
c = Continuous phase
d = Dispersed phase
p = Particle
h = Char component
w = Moisture component
C = Raw coal component
n = Devolatilization step

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