CFD Modeling and Validation of Oxy-Fired and Air-Fired Entrained Flow Gasifiers

PRAVIN NAKOD

ANSYS Inc. Rajiv Gandhi Infotech Park PUNE 411 057 India, email: pravin.nakod@ansys.com

ABSTRACT

Environmental drivers like carbon capture and other emission controls are creating a great opportunity for growth and adoption of clean coal technologies. Gasification is one of the more established and matured clean coal technologies and numerical simulations are playing crucial role in its development. Different models and approaches have been proposed and discussed in the literature.

In the present work, a step by step approach is proposed to evaluate the fractions of different species as a result of volatile break-up during gasification. The volatile component of a given solid fuel like coal or biomass consists of Carbon, Hydrogen, Oxygen, Nitrogen and Sulfur. Mass of these elements in the evaluated species is balanced with their individual masses in the original solid fuel composition. CFD simulations for ConocoPhillips' EGas technology based gasifier and Mitsubishi Heavy Industries (MHI) research scale two stage air blown gasifierare performed including volatile break-up evaluated using current approach in ANSYS FLUENT 14.5. The reaction rates are computed using the Finite rate/Eddy dissipation reaction model. The Discrete Ordinates radiation model with Weighted Sum of Gray Gas Model (WSGGM) for gas absorption coefficient along with particle radiation interaction is employed in these simulations. The predicted syngas composition and exit temperature are compared with the experimental results. The simulation predictions are within 10% of accuracy compared to the experimental measurements

Introduction

Coal remains the key fuel for the electricity generation in spite of its major contribution to the greenhouse effect and other emissions. Around 41% of the electricity generated in the world utilizes coal as the fuel [1]. Collection of Clean Coal Technologies (CCTs) like chemical washing, gasification, oxy-fuel combustion, carbon capture sequestration, etc. are explored to mitigate the environmental impact of energy generation from coal. Gasification, one of the more established and matured clean coal technologies, is integrated with combined steam and gas turbine cycles for power generation, referred to as Integrated Gasification Combined Cycle (IGCC). Numerical studies like Computational Fluid Dynamics (CFD) simulations are playing an important role in the designing and commissioning of

gasifiers. CFD simulations are becoming popular to provide an insight into thermal and chemical conversion of the coal as it travels through the gasifier and effect of hydrodynamics on these processes. They also help to understand the effect of operating parameters like pressure, temperature, flow rates, mixing, coal quality, etc. on syngas composition. Over the years, many such studies are published in the literature [2-12]. Wen and Chaung [2] simulated an entrained flow pilot plant gasifier and compared temperature and species concentration profiles with the experimental data. Based on their study of effect of operating parameters, they also suggested the optimum operating conditions for efficient operation of the gasifier. Syamlal and Bissett [3] developed a detailed devolatilizationand tar cracking model and predicted the syngas composition and temperature in moving bed gasifier close to respective experimental data. They extended their study for fluidized bed gasifier in their work presented in 2003 [4]. Shi et al. [5] using Euler-Granular multiphase modeling simulated large scale transport gasifier for predicting accurate syngas composition. Radmanesh et al. [6] studied the effect of operating conditions on the performance of bubbling fluidized bed reactor for biomass (beech wood) gasification by conducting several experiments and CFD simulations. Recently, We et al. [7] studied the effect of turbulent mixing and controlling mechanism in an entrained flow coal gasifier. Silaen and Wang [8] investigated the gasification process inside a 2000 Tons per Day (TPD), two stage gasifier under various operating conditions. Kumar and Ghoniem [9-10] investigated the sensitivity of turbulence models and particle turbulent dispersion for entrained flow gasification. Qian et al. [11] studied the effect of reaction kinetic parameters on the syngas composition for an entrained flow coal gasifier. Xu and Qiao [12] examined the influence of different parameters related to physical and chemical processes on the overall gasification performance in a well-stirred reactor.

One of the most important sub-models in performing numerical simulations for gasification is the evaluation of species concentration during devolatilization process. Several approaches determining concentration of species as a result of devolatilization are available in the literature. One of the earliest approaches suggested by Loison and Chauvin [13] is in the form of empirical correlations as a function of dry ash free (DAF) volatile fraction. Because of its empirical nature, this model may not conserve the elements (C, H, N, O, S, etc.) in the volatile while converting them into species concentration for different types of coal. Another approach presented by Syamlal and Bissett [3] expected to provide accurate species evaluation during devolatilization for variety of coal types. Ma and Zintney [14] recently developed another approach and validated it for oxygen blown entrained flow gasifiers.

In the present work, an approach for evaluation of species as a result of devolatilization, referred as volatile break-up, is developed using step by step conversion of the elements in volatile into the species

concentrations. This approach conserves the mass of each of the elements as well as overall heat content in the solid fuel during this conversion. Therefore, it is suitable for any type of coal, biomass or other solid fuels. The approach along with other sub-models is applied in CFD simulation of two entrained flow gasifiers, 2550 TPDConocoPhillips' EGas technology based oxygen blown gasifier and 200 TPD Mitsubishi Heavy Industries (MHI) research scale two stage air blown gasifier. ANSYS FLUENT 14.5 [15] solver is used in these simulations. Syngas compositions and temperature results predicted by the simulations are compared with respective experimental data and agreement within 10% is achieved.

Volatile Break-Up Approach

Volatile break up approach developed in this work assumes that the volatile from the solid fuel consists of Carbon (C), Hydrogen (H), Oxygen (O), Nitrogen (N) and Sulfur (S). Other constituents (like Chlorine) exist invery small amount and therefore are neglected in this approach. Volatile matters from solid fuel are initially converted to a pseudo gas phase species, referred to as *volatile* using a devolatilization model. A gas phase volatile break-up reaction, R1is added to convert this gaseous volatile to several other gas phase species. Species *TAR* is another pseudo gas phase species added to account for left over carbon from the volatiles, if any. Step by step approach outlined in Figure 1 is developed to evaluate the mass fractions of resultant species. Stoichiometric coefficients *a*, *b*, *c*, *d*, *e*, f, *g* and *h* for the resultant species are calculated form the obtained mass fractions and molecular weights of these species. Using current approach, a SCHEME script is written to automatically calculate stoichiometric coefficients of volatile break-up reaction and set up the gasification simulation in ANSYS FLUENT. This script in the form of add-on module is referred to as “Gasification calculator”.

$$Volatile \rightarrow a\,CO + b\,H_2S + c\,CH_4 + d\,H_2O + e\,H_2 + f\,N_2 + g\,O_2 + h\,TAR \qquad \textbf{(R1)}$$

Heating value of species, *Volatile*s obtained by first converting as-received heating value of coal to its lower heating value and then subtracting the lower heating value of fixed carbon (Char) from it. Latent heat of water vapor formed from moisture content and hydrogen is considered appropriately while converting as-received heating value of coal to its lower heating value.

Numerical Methedology

In this work, a three dimensional CFD solver ANSYS FLUENT 14.5 is used to solve a set of governing equations for the gas phase and the solid phase. Reynolds Averaged Navier-Stokes (RANS)

based mass, momentum, turbulence, energy and species conservation equations are solved in Eulerian reference frame for the transport of gas phase. Solid-particles/droplets are tracked using Lagrangian reference frame referred to as Discrete Phase Model (DPM). As both of the gasifiers considered are entrained flow gasifiers operating with low particle concentration, particle-particle interactions are not considered in this work. Details on the set of transport equations and terms included in these transport equations are available in reference [16].

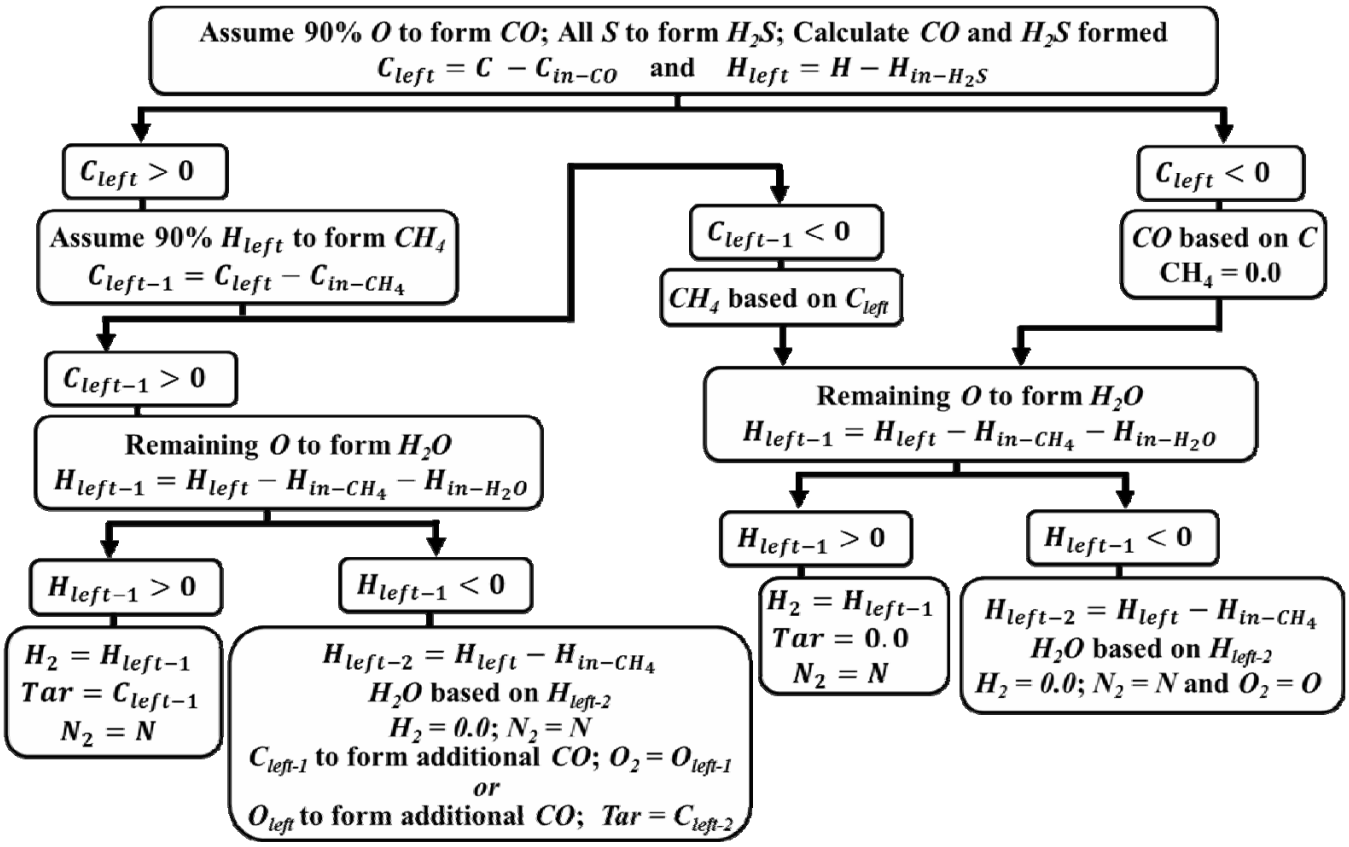


Figure 1: Volatile Break-Up Algorithm

Models

ANSYS FLUENT 14.5 offers variety of models for modeling turbulence, reactions in turbulent flows, radiation including particle-radiation interaction, etc. In this section, details on different models and sub-models employed in this work are discussed.

Turbulence Model: 2 equations standard k-epsilon model is employed to model turbulence. Turbulence dispersion of particles is modeled using Discrete Random Walk Model.

Radiation Model: Discrete Ordinates (DO) radiation model including particle-radiation interaction is used in this work. Weighted Sum of Gray Gas Model (WSGGM) is used for the calculation of gas absorption coefficient.

Droplet Evaporation Model: Moisture release from coal and evaporation of water content in the coal-water slurry are modeled using Convection/Diffusion Controlled Model adopted from Sazhin [17] and Miller et al. [18].

Devolatilization Model: Devolatilization rate is obtained from two competing rate expressions of the form proposed by Kobayashi et al. [19].

Reaction Models: Gas phase mixture has ten species. Nine gas phase reactions listed in Table 1 are modeled using Finite rate/Eddy dissipation model which considers the reaction rate as the minimum of Arrhenius reaction rate and Eddy dissipation (turbulent mixing) reaction rate. Four particle surface heterogeneous gasification reactions listed in Table 2 are modeled using a Multiple Surface Reaction Model in ANSYS FLUENT 14.5, which calculates Kinetic-Diffusion controlled reaction rate based on work suggested by Smith [23].

Table 1: Gas Phase Reactions

S N	Reaction	A	Ea (J/kmol)	N1	N2	N3	Reference
R1	Vol → a CO + b H_2S + c CH_4 + d H_2O + e H_2 + f N_2 + g O_2 + h Tar	2.119e+11	2.027e+08	1.5	-	-	Westbrook and Dryer, Methane comb [20]
R2	CO oxidation reaction: CO + 0.5 O_2 → CO_2	2.239e+12	1.7e+08	1	0.25	0.5 (H_2O)	Westbrook and Dryer [20]
R3	Forward water-gas shift reaction (FWGS): CO + H_2O → CO_2 + H_2	2.35e+10	2.88e+08	0.5	1	-	Bustamante et al. [21] (At high pressure)
R4	Reverse water-gas shift reaction (RWGS): CO_2 + H_2 → CO + H_2O	1.785e+12	3.260e+08	1	0.5	-	Equilibrium with FWGS
R5	Hydrogen oxidation: H_2 + 0.5 O_2 → H_2O	9.87e+08	3.1e+07	1	1	-	ANSYS FLUENT 14.5 [16]
R6	Reverse of hydrogen oxidation: H_2O → H_2 + 0.5 O_2	2.06e+11	2.728e+08	1	-	-	Equilibrium with Hydrogen oxidation
R7	Methane oxidation: CH_4 + 1.5 O_2 → CO + H_2O	5.012e+11	2e+08	0.7	0.8	-	Westbrook and Dryer [20]
R8	Steam methane reforming: CH_4 + H_2O → CO + 3 H_2	5.922e+08	2.09e+08	0.5	1	-	Hou and Hughes [22]
R9	Tar oxidation reaction: Tar + O_2 → CO	1e+15	1e+08	1	0.5	-	Estimated

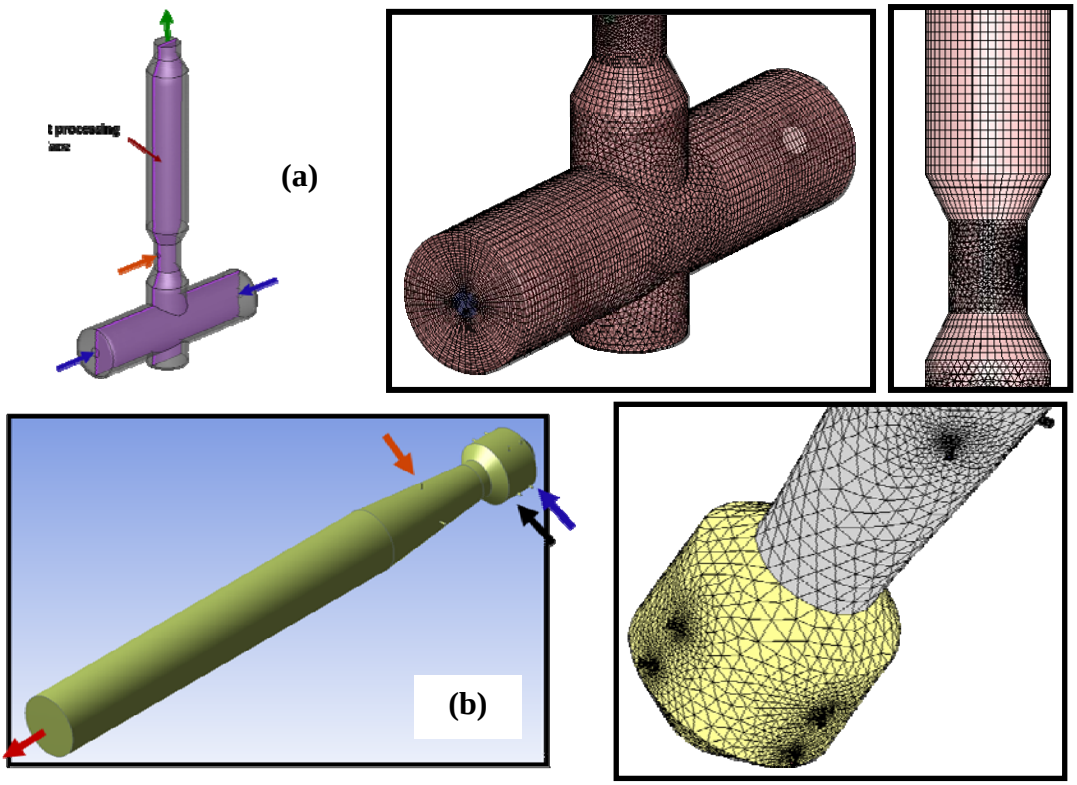
Description Of The Test Cases

Two test cases used in this work for validating the current approach for volatile break-up are 2550 TPDConocoPhillips' EGas technology based oxygen blown gasifier and 200 TPD Mitsubishi Heavy Industries (MHI) research scale two stage air blown gasifier. Figure 2 shows geometries and meshes used in performing three dimensional CFD simulations. Details on the geometrical dimensions can be found in

references [14] and [24-26] respectively for 2550 TPD and 200 TPD gasifiers. Coal properties and operating conditions for both of these gasifiers are listed in Table 3. Boundary conditions for 2550TPD gasifiers are mentioned in Table 4 [27] and those for a 200TPD gasifier are listed in Table 5 [24-26]. Flow rates mentioned in Table5 are combined for 4 burners at a given location. Combination of tetrahedral and hexahedral mesh with about 275000cells issued for 2550 TPD gasifier whereas 200 TPD gasifier is resolver with tetrahedral mesh of about 121000 cellsin this study.

Table 2: Heterogeneous Particle Surface Reactions

S N	Reaction	A	Ea (J/kmol)	N1	Reference
R10	Char combustion: C<S> – 0.5 O_2 → CO	300	1.3e+08	0.65 (O_2)	Wu et al. [7]
R11	CO_2 gasification: C<S> – CO_2 → 2 CO	2224	2.2e+08	0.6 (CO_2)	
R12	H_2O gasification: C<S> – H_2O → CO + H_2	42.5	1.42e+08	0.4 (H_2O)	
R13	H_2 gasification: C<S> – 2 H_2 → CH_4	1.62	1.5e+08	1 (H_2)	



(a) 2550 TPD Gasifier; (b) 200 TPD Gasifier Figure 2: Geometry and Mesh

Table 3: Coal Properties and Operating Conditions

Gasifier		2550 TPD	200TPD
Proximate Analysis	Volatile	30.84%	46.80%
	Fixed Carbon	42.85%	35.80%
	Moisture	15.28%	5.30%
	Ash	11.23%	12.10%
Ultimate Analysis (DAF)	Carbon	79.22%	78.25%
	Hydrogen	5.55%	6.50%
	Oxygen	9.70%	13.90%
	Nitrogen	1.65%	1.13%
	Sulfur	3.38%	0.22%
As received HHV (J/kg)		2.476e+7	2.704e+7
Operating Pressure (MPa)		2.84	2.70

Table 4: Boundary Conditions for 2550 TPD Gasifier

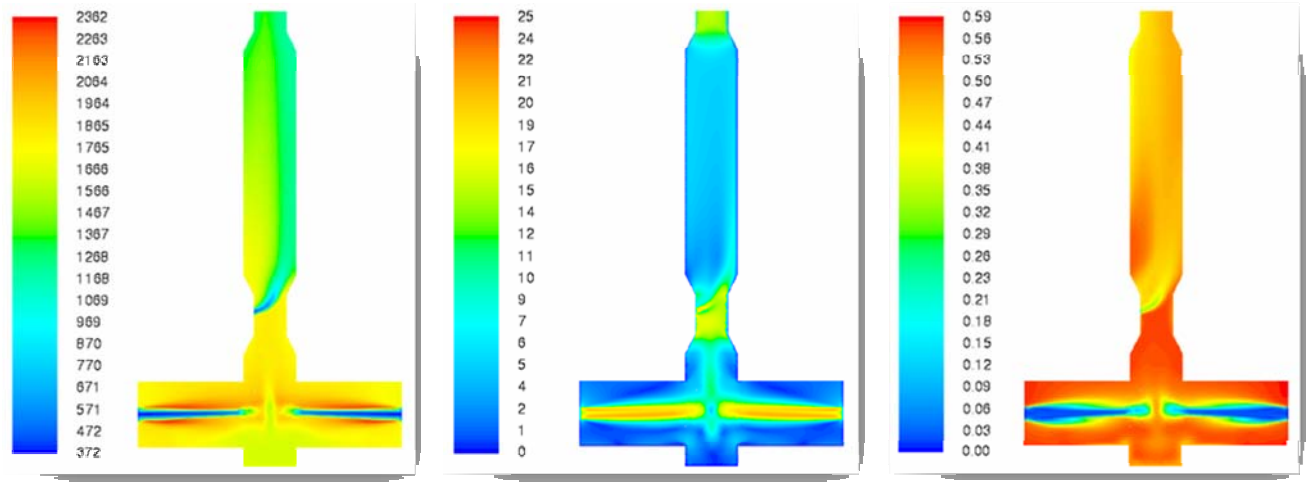
Boundary condition	Magnitude
First stage inlet flow rate (kg/s)	2 x 10.6
Inlet temperature (K)	390
Oxygen mass fraction (rest is Nitrogen)	0.944
First stage coal feed rate (kg/s)	2 x 10.84
First stage water feed rate (kg/s)	2 x 5.583
Second stage coal feed rate (kg/s)	6.11
Second stage water feed rate (kg/s)	3.15

Table 5: Boundary Conditions for 200 TPD Gasifier

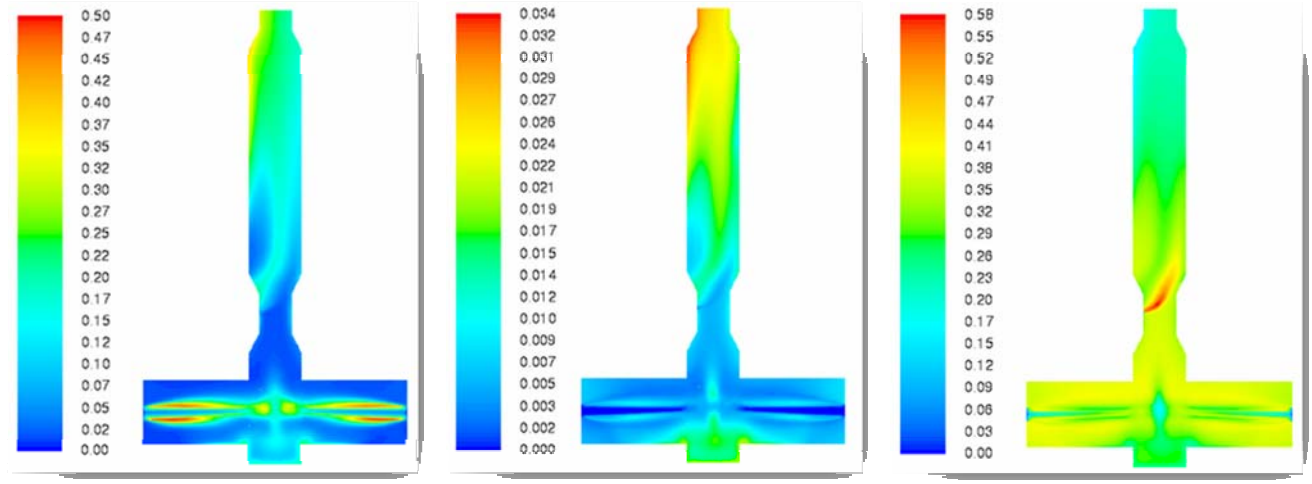
Boundary condition	Magnitude
Combustion burners air flow rate (kg/s)	4.708
Combustion burners coal flow rate (kg/s)	0.472
Char burners air flow rate (kg/s)	4.708
Char burners coal flow rate (kg/s)	1.112
Reducer burners air flow rate (kg/s)	1.832
Reducer burners coal flow rate (kg/s)	1.832
All burners inlet temperature (K)	521

Results And Discussions

Contours of various quantities of interest obtained from 3D simulations for 2550 TPD and 200 TPD gasifiers are shown in Figure 3 and 4, respectively. It is observed from the results that most of the heat release occurs in the primary stage combustion region. Peak temperature and higher CO_2 concentrations are predicted in the vicinity of primary stage inlet regions. Peak temperatures of about 2350K and 2150K are observed in 2550 TPD and 200 TPD gasifiers, respectively. Predicted peak temperature of 2362K for 2550 TPD gasifier, is within 5% of that presented in earlier published numerical study [28]. Gasification reactions dominate the region away from the main flame and thus, cause increase in carbon-monoxide concentration and reduction in temperature in second stage of the gasifiers.



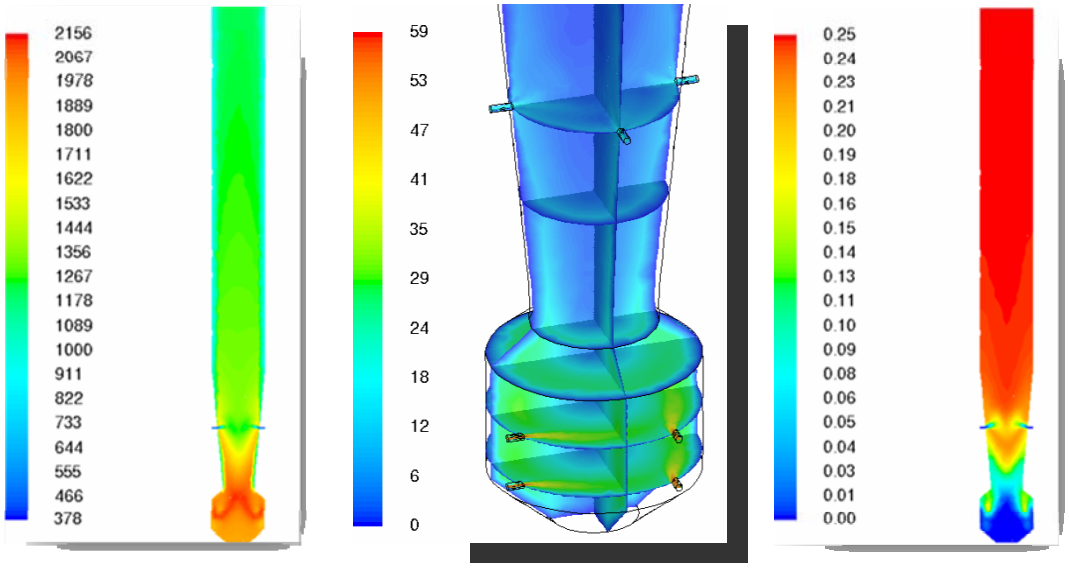
(a) Temperature **(b) Velocity** **(c) CO Mass Fraction**



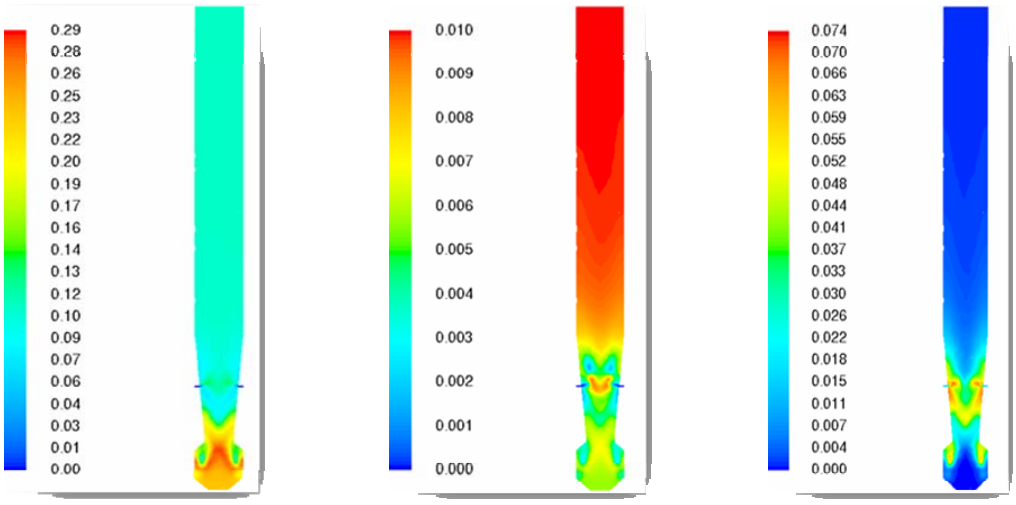
(a) CO_2 Mass Fraction **(b) H_2 Mass Fraction** **(c) H_2O Mass Fraction**

Figure 3: Contours of Variables for 2550 TPD Gasifier

Comparison of axial temperature profile for 200 TPD gasifier predicted by the numerical simulation with that of measured data reported in reference [25] is shown in Figure 5. Reasonable agreement between predicted temperature profile and measured data is observed. The differences in the predicted results for the data points close to the bottom of the gasifier can be attributed to the assumptions made on some of the geometrical details which are not available in reference [24]. It is already reported in reference [24] that the gasifier performance is very sensitive to the variation in geometrical dimensions in this region. Predicted average syngas temperature of 1272K is within 3% of the measured average value of 1311K for 2550 TPD gasifier.



(a) Temperature **(b) Velocity** **(c) CO Mass Fraction**



(a) CO_2 Mass Fraction **(b) H_2 Mass Fraction** **(c) H_2O Mass Fraction**

Figure 4: Contours of Variables for 200 TPD Gasifier

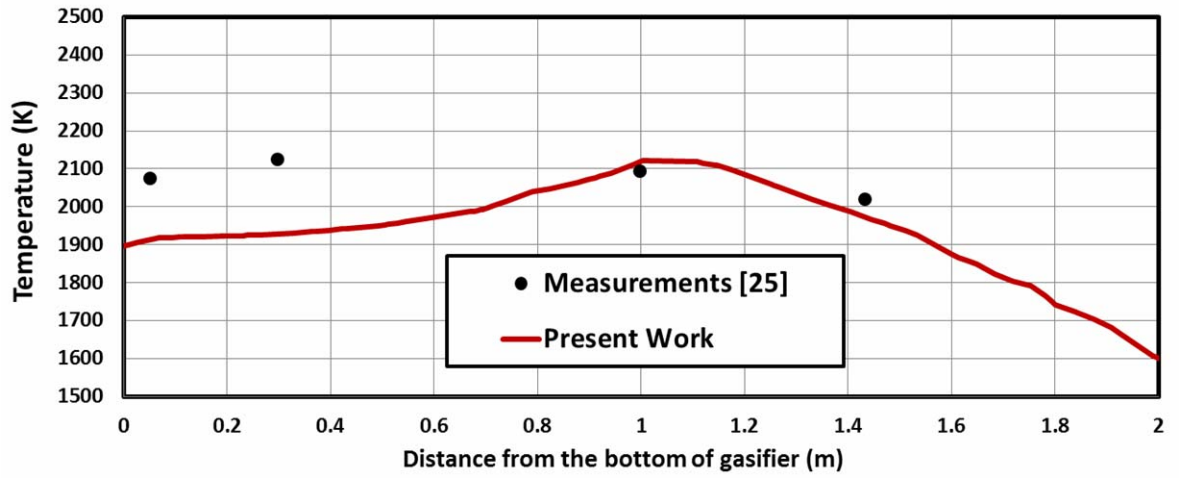
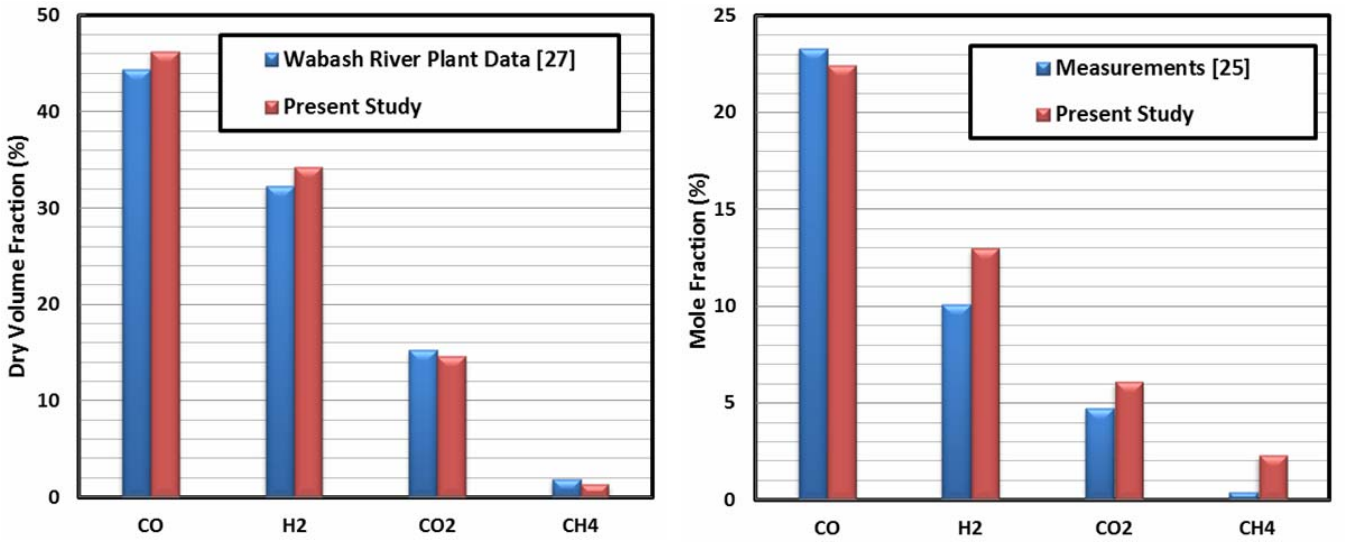


Figure 5: Comparison of Axial Temperature for 200 TPD Gasifier



(a) 2550 TPD gasifier **(b) 200 TPD gasifier**

Figure 6: Comparison of Syngas Composition

Comparison of syngas composition predicted by numerical simulations with actual measured composition is shown in Figure 6. It is observed that the predicted syngas composition for both the gasifiers compares well with measured composition. There are some differences in the predicted mole fractions of hydrogen and methane in 200 TPD gasifier compared to measured data. These differences are almost of the same order as reported in reference [25].

CONCLUSIONS

An approach of calculating species composition as a result of volatile break-up required for performing CFD simulations on gasification is proposed in this work. Conservations of mass of elements in the volatile matter and overall heat content of the solid fuel are ensured in this approach. 3D CFD simulations for two entrained flow gasifiers, 2550 TPD ConocoPhillips' EGas technology based oxygen blown gasifier and 200 TPD Mitsubishi Heavy Industries (MHI) research scale air blown gasifier, are performed to validate the proposed approach. The syngas composition and temperature predicted from the CFD study are compared with respective measured data. Very good agreement between simulation results and measured data is achieved for both the gasifiers. In present work, as both of the validation cases include low particles concentrations, future work is suggested to perform a validation study for fluidized bed or transport type gasifiers using proposed approach for volatile break-up.

REFERENCES

1. World Energy Outlook 2012, Executive Summary, <http://www.iea.org/publications/freepublications/publication/English.pdf>.
2. C Y Wen and T Z Chaung," Entrainment Coal Gasification Modeling", Ind. Eng. Chem. Process Des. Dev., 1979, 18 (4), pp. 684-695.
3. M Syamlal and L A Bissett, "METC Gasifier Advanced Simulation (MGAS) Model", Technical note, DOE/METC-92/4108, NITS/DE92001111, National Technical Information Services, Springfield, 1992.
4. T J O'brien, M Syamlal and C Guenther, "Computational Fluid Dynamics Simulations of Chemically Reactive Fluidized Bed Processes", Third International Conference on CFD in the Minerals and Process Industries, CSIRO, Melbourne, Australia, 2003.
5. S Shi, C Guenther, S Orsino, "Numerical Study of Coal Gasification Using Eulerian-Eulerian Multiphase Model", POWER2007-22144, ASME Power conference, 2007, pp. 497-505.
6. R Radmanesh, J Chaouki and C Guy, "Biomass Gasification in a Bubbling Fluidized Bed Reactor: Experiments and modeling", AIChE Journal, 2006, 52 (12), pp. 4258-4272.
7. Y Wu, P J Smith, J Zhang, J N Thornock and G Yue, "Effects of Turbulent Mixing and Controlling Mechanisms in an Entrained Flow Coal Gasifier", Energy Fuels, 2010, 24 (2), pp. 1170-1175.
8. A Silaen and T Wang, "Investigation of the Coal Gasification Process under Various Operating Conditions Inside a Two-Stage Entrained Flow Gasifier", J. Thermal Sci. Eng. Appl. 2012, 4(2).

9. M Kumar and A F Ghoniem, “Multiphysics Simulations of Entrained Flow Gasification. Part I: Validating the Nonreacting Flow Solver and the Particle Turbulent Dispersion Model”, Energy Fuels, 2012, 26 (1), pp. 451-463.
10. M Kumar and A F Ghoniem, “Multiphysics Simulations of Entrained Flow Gasification. Part II: Constructing and Validating the Overall Model”, Energy Fuels, 2012, 26 (1), pp. 464-479.
11. F Qian, X Kong, H Cheng, W Du, and W Zhong, “Development of a Kinetic Model for Industrial Entrained Flow Coal Gasifiers”, Ind. Eng. Chem. Res., 2013, 52 (5), pp. 1819-1828.
12. J Xu and L Qiao, “Mathematical Modeling of Coal Gasification Processes in a Well-Stirred Reactor: Effects of Devolatilization and Moisture Content”, Energy Fuels, 2012, 26 (9), pp. 5759-5768.
13. R. Loison, R. Chauvin, “Pyrolise rapide du carbon”, Chimie et Industrie 91 (1964) 269.
14. J Ma and S E Zitney, “Computational Fluid Dynamic Modeling of Entrained-Flow Gasifiers with Improved Physical and Chemical Sub models”, Energy Fuels, 2012, 26 (12), pp. 7195-7219.
15. ANSYS, Inc, <http://www.ansys.com>.
16. ANSYS FLUENT 14.5 Theory Guide Help Document <http://www.ansys.com>.
17. S S Sazhin, "Advanced Models of Fuel Droplet Heating and Evaporation", Progress in Energy and Combustion Science, 2006, 32, pp. 162–214.
18. R S Miller, K Harstad and J Bellan, "Evaluation of Equilibrium and Non-Equilibrium Evaporation Models for Many Droplet Gas-Liquid Flow Simulations", International Journal of Multiphase Flow, 1998, 24 (6), pp. 1025-1055.
19. H Kobayashi, J B Howard and A F Sarofim, "Coal Devolatilization at High Temperatures", Symposium (International) on Combustion, 1977, 16 (1), pp. 411-425.
20. C K Westbrook and F L Dryer, “Simplified Reaction Mechanism for the Oxidation of Hydrocarbon Fuels in Flames”, Combustion Science and Technology, 1981, 27, pp. 31-43.
21. F. Bustamante, R M Enick, R P Killmeyer, B H Howard, K S Rothenberger, A V Cugini, B D Morreale, M V Ciocco, “Uncatalyzed and Wall-Catalyzed Forward Water-Gas Shift Reaction Kinetics”, AIChE Journal,2005, 51 (5), pp. 1440-1454.
22. K Hou and R Hughes, “The Kinetics of Methane Steam Reforming over a Ni/α-Al_2O Catalyst”, Chemical Engineering Journal, 2001, 82, pp. 311-328.
23. I W Smith. "The Combustion Rates of Coal Chars: A Review", Symposium (International) on Combustion, 1982, 19, pp. 1045–1065.
24. C Chen, T Miyoshi, H Kamiya, M Horio, T Kojima, “On the Scaling-Up of a Two-Stage Air Blown Entrained Flow Coal Gasifier”, The Canadian Journal of Chemical Engineering, 1999, 77 (4), pp. 745-750.

25. C Chen, M Horio, T Kojima, "Numerical Simulation of Entrained Flow Coal Gasifiers. Part I: Modeling of Coal Gasification in an Entrained Flow Gasifier", Chemical Engineering Science, 2000, 55, pp. 3861-3874.
26. C Chen, M Horio, T Kojima, "Numerical Simulation of Entrained Flow Coal Gasifiers. Part II: Effects of Operating Conditions on Gasifier Performance", Chemical Engineering Science, 2000, 55, pp. 3875-3883.
27. U.S. Department of Energy, Technical Report, "Wabash River Coal Gasification Repowering Project: A DOE Assessment", DOE/NETL-2002/1164, 2002.
28. S Shi, S Zitney, M Shahnam, M Syamlal and W A Rogers, "Modeling Coal Gasification with CFD and the Discrete Phase Method", ICCHMT'05 – 273, 4th International Conference on Computational Heat and Mass Transfer, 2005.