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A Review of Sub-models for Computation Fluid Dynamics (CFD) Modelling of Clean Coal Technology

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Abstract: *Environmental drivers like carbon capture and other emission controls are creating a great opportunity for growth and adoption of Clean Coal Technologies (CCTs). Gasification and oxy-fuel combustion are more established and matured technologies out of several clean coal technologies suggested in the literature. Numerical simulations like Computation Fluid Dynamics (CFD) modeling are playing crucial role in their design, development and adoption in the power industry. In the present paper, a review of some of the CFD works carried out by researchers from the academics and industries for gasification and oxy-fuel combustion is presented. The objective of this work is to provide a comprehensive reporton different sub-models required for accurate CFD modeling of gasification and oxy-fuel combustion.*

Keywords: *Clean Coal Technology, Gasification, Oxy-fuel combustion, CFD modeling, Sub-models.*

1. INTRODUCTION

Coal will remain the key fuel for electricity generation in the near future, in spite of its major contribution to the greenhouse effect and other emissions. Out of over 21,000 Terra Watt hours (TWh) of electricity produced from all the sources in the world [1] in 2012, around 41% of the electricity generated in the world utilizes coal as the fuel [2]. The major advantages of using coal for electricity generation are the power from coal is cheap (i.e., less than US$ 0.03 per kWh) and about 40% of the energy from the coal can be converted into electricity. However, coal combustion accounts for the large amount of emissions. Coal combustion adds more carbon dioxide than any other energy source. Further, coal plants emit toxins like mercury, sulfur dioxide, nitrogen oxides, carbon monoxide, hydrocarbons, etc. These toxins cause global warming due to greenhouse effect, acid rain (acid deposition), demise of global clean water reserves, etc. Several techniques are explored to mitigate the environmental impact of energy generation from coal. These techniques/technologies are called Clean Coal Technologies (CCTs). Chemical washing, gasification, oxy-fuel combustion, biomass co-firing, super and ultra-critical pulverized coal combustion boilers, carbon capture sequestration, etc. are some of the clean coal technologies being explored by industrialists, academicians, researchers and technology & equipment suppliers to plan their strategies to mitigate environmental concerns of coal utilization in the 21st century. The main objective of these technologies is to reduce the emission from coal combustion. Efficient and effective design of devices used in clean coal technologies is one of the main challenges for the involved technical communities. Both, experimental and numerical techniques are widely employed to provide insights on several physical and chemical processes involved in these devices which help to optimize the design parameters and overall performance of these devices.

Numerical studies like Computational Fluid Dynamics (CFD) simulations are playing an important role in the designing and commissioning of Clean Coal Technologies. CFD simulations are becoming popular to provide an insight into fluid dynamics, thermal and chemical conversion processes involved in the devices used in clean coal technologies. CFD replicate the hydrodynamics, thermal and chemical processes involved in these devices using several mathematic models and governing equations. These governing equations are solved using numerical tools on high speed computers. Parametric studies of different operating conditions, input parameters and device geometries using CFD are carried out in much less time than that involved in actual field measurements and testing to obtain the best set of operating parameter for effective design of these devices. Therefore, CFD has become an integral part of design and development in many industries. It helps to reduce the overall design cycle time and cost.Appropriate sub-models are required in the CFD modeling to describe the various physical processes (like mixing, turbulence, combustion, radiation, etc.)involved in the device to be analyzed. Accuracy of CFD results significantly depends on the accuracy of these sub-models to mathematically represent the physical processes involved. In this paper, a review of some of the CFD works carried out by researchers from the academics and industries for gasification and oxy-fuel combustion is presented. The objective of this work is to provide a comprehensive report on different sub-models required for accurate CFD modeling of gasification and oxy-fuel combustion.

2. GASIFICATION AND OXY-FUEL COMBUSTION TECHNIQUES

In the late 1980s and early 1990s, the U.S. Department of Energy (DOE) began conducting a joint program with the industry and State agencies to demonstrate clean coal technologies large enough for commercial use. The program, called the Clean Coal Technology & Clean Coal Power Initiative (CCPI), has had a number of successes that have reduced emissions and waste from coal-based electricity generation [3]. The National Energy Technology Laboratory has administered three rounds of CCPI funding and the following projects were selected during each round [4].The main objective of these projects is to capture and sequestrate carbon dioxide instead of releasing it into the atmosphere. These techniques are successfully applied at some of the clean power stations around the world like Wabash River Energy Ltd. Plant, Indiana State, US [5] for full scale electricity generation. Most of these projects use gasification and/or oxy-fuel combustion technologies to reduce the emissions. This section explains the details of the physical and chemical processes involved in the gasification and oxy-fuel combustion techniques.

2.1. Gasification

Gasification is a process of partial oxidation of fuel. Oxygen fraction used is generally half of that used for the combustion process. Any combustible material such as coal, petroleum coke, biomass, heavy oil, natural gas, etc. can be used as a fuel for gasification. The product of gasification is called syngas (which stands for synthetic gas) and it mainly consists of carbon monoxide, hydrogen, methane, carbon dioxide and water vapor. Syngas is then used as a gaseous fuel for combustion. The devices in which gasification takes place are called Gasifiers. Gasifiers are mostly operated with pure oxygen environment to avoid NOx formation. However, some gasifiers operating with air as the oxidizer are also used in the industries.Further, gasifiers are operated under elevated pressures to reduce bulk of the gasifiers. In power plants, gasifiers are integrated with combined steam and gas turbine cycles for power generation, referred to as Integrated Gasification Combined Cycle (IGCC). Syngas combustion produces pure carbon dioxide which is ready to compress and sequestrate. Therefore, gasification is one of the popular clean coal technologies. One of the three types of gasifiers (moving bed; fluidized bed gasifier and entrained flow gasifiers) is used in the industries. Details of the operating conditions in these gasifiers can be found in Ref. [6]. Though, these types of gasifiers differ in the instantaneous volume fraction of the solid fuel existing in them, the operation is similar in terms of physical and chemical processes. Fig.1 shows the chemical changes taking place for the solid fuel while it undergoes the gasification. Any solid fuel consists of four major constituents, i.e., moisture, volatile matter, char and ash in varying proportions. When this particle comes in contact with the hot gas, the heat transfer from the surrounding gas to the solid particle takes place. This causes moisture from the fuel to get converted to water vapor which is released into the surrounding gas. This process is called drying. Once the drying is complete and the particle reached to the

devolatilization temperature, the volatile matter from the fuel gets converted to several gas phase species through the process of pyrolysis. These gas phase species are the main constituents for formation of the syngas. Once all the volatile matter is converted to gaseous species, the char gasification takes place. During char gasification, the gaseous species (like O_2, CO_2, H_2, H_2O, etc.) diffuse to the char surface through the pours of the solid fuel and react on the char surface. These reactions yield other gaseous species like CO, CH_4 and H_2 which diffuse back to the surrounding gas. After completion of the gasification reactions, solid fuel remains only with the residual ash.

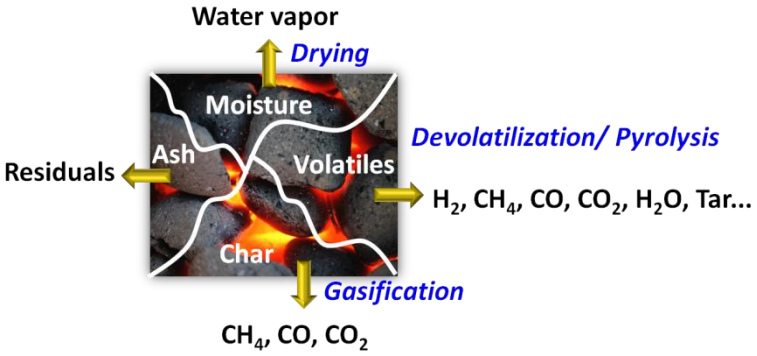

Figure 1. *Solid Fuel Undergoing Gasification*

The main difference between the solid fuel undergoing combustion and gasification is that in combustion volatiles will completely burn to CO_2 and H_2O as sufficient oxygen is available in the surrounding whereas the volatile matter in gasification is partially oxidized to form H_2, CO, CH_4, etc. as the gaseous products. Further, during combustion, char undergoes almost complete combustion whereas in gasification it undergoes several gasification reactions listed earlier.

2.2. Oxy Fuel Combustion

The oxy-fuel combustion cycle for the pulverized coal power plant is shown in Fig.2. In this case, nitrogen is separated out from the air in Air Separation Unit, briefly called ASU and almost pure oxygen is then used for the combustion the fuel in the boiler. The solid coal particles undergo the combustion and release heat in the boiler. On the downstream of the boiler, ash particles are separated out from the flue gas. Flue gas now consists of CO_2 and steam (water vapor) only. Steam can then be condensed and flue gas in the form of CO_2 is ready for the compression and sequestration.

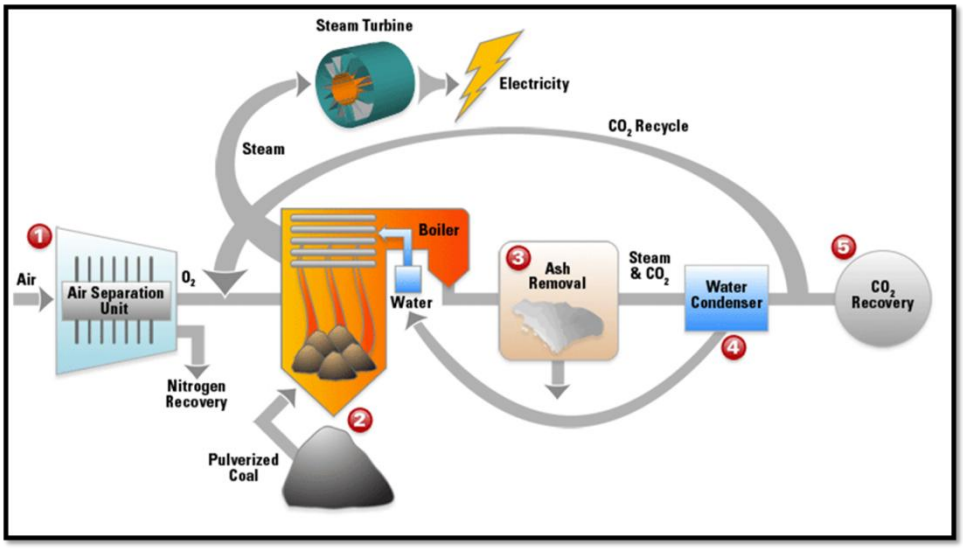

Figure 2. *Oxy Fuel Combustion*

Within the boiler as the combustion takes place in presence of almost pure oxygen, the NOx formation is avoided. However, due to absence of inert gas (like nitrogen), the peak temperature in the boiler can reach to a very high level (3000 to 3500K) compared to that combustion with air

(1800-2200K). The boiler part will fail at such extreme temperature. To avoid failure of boiler components, a stream of fuel gas is recycled into the boiler. This is called recycle stream. Depending on whether this recycle stream consists of only CO_2 or CO_2 and water vapor mixture, the recycle is called dry recycle or wet recycle, respectively.

3. CFD MODELING CONSIDERATIONS

Numerical studies like CFD simulations are playing an important role in the designing and commissioning of gasifiers and oxy fuel combustors. These simulations provide an insight into fluid dynamics, thermal and chemical conversion processes involved in these devices. CFD replicate the hydrodynamics, thermal and chemical processes involved in these devices using several mathematic models and governing equations. As CFD simulations can be completed in much less time compared to that required for actual building and testing the device performance, it has become an integral part of design and development in many industries. Appropriate sub-models are required in the CFD modeling to describe the various physical processes (like mixing, turbulence, combustion, radiation, etc.) involved in the device to be analyzed. Accuracy of CFD results largely depends on the accuracy of these sub-models to mathematically represent the physical process involved. In this section, different sub-models required for CFD analysis of gasification and oxy-fuel combustion are reviewed.

3.1. CFD Modeling of Gasification

Over the years, many CFD studies for gasification modeling are published in the literature [7-17]. Wen and Chaung [7] 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 [8] developed a detailed devolatilization and 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 [9]. Shi et al. [10] using Euler-Granular multiphase modeling simulated large scale transport gasifier for predicting accurate syngas composition. Radmanesh et al. [11] 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. [12] studied the effect of turbulent mixing and controlling mechanism in an entrained flow coal gasifier. Silaen and Wang [13] investigated the gasification process inside a 2000 Tons per Day (TPD), two stage gasifier under various operating conditions. Kumar and Ghoniem [14-15] investigated the sensitivity of turbulence models and particle turbulent dispersion for entrained flow gasification. Qian et al. [16] studied the effect of reaction kinetic parameters on the syngas composition for an entrained flow coal gasifier. Xu and Qiao [17] examined the influence of different parameters related to physical and chemical processes on the overall gasification performance in a well-stirred reactor.

The main objectives of using CFD simulations for gasification are prediction of outlet temperature, species composition for syngas and thereby it heating value, axial and radial temperature profiles, degree of gasification and effect of operating conditions on these parameters. Representation of the physical processes in the CFD is required to predict accurate results. Rate of conversion of mass and energy from solid particles to the gas through moisture release, devolatilization and char combustion/gasification needs to be accounted accurately. Further, the representation and the rate of gaseous homogeneous reactions and heterogeneous char surface reactions are essential for correct syngas temperature and composition prediction. 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 [18] 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 [8] expected to provide accurate species evaluation during devolatilization for variety of coal types. Ma and Zintney [19] recently developed another approach and validated it for oxygen blown entrained flow gasifiers. Most recently, Nakod [20] has presented an approach which uses a 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. Along with other sub-models, this model is used for CFD simulation of two entrained flow gasifiers, 2550 TPD ConocoPhillips' EGas technology based oxygen blown gasifier and 200 TPD Mitsubishi Heavy Industries (MHI) research scale two stage air blown gasifier. The CFD results from these simulations in terms of syngas composition, exit temperature and axial temperature profile are validated against respective available measurement data from the literature. Details of this approach are explained below.

3.1.1. Volatile Break-Up Approach

Volatile component in the coal or any other solid fuel is known in terms of mass fractions of elements like C, H, O, N, S, etc. However, while performing numerical simulations, gas phase species transport equations are solved. Therefore, the known mass fractions of elements in the volatiles need to be converted to mass fractions of species like CO, CH_4, H_2, H_2O, H_2S, N_2 and O_2. System of simultaneous equations can be constructed for the mass balance of each element as given by the equations 1 to 5. In this set of equations, values of m_C, m_H, m_O, m_N and m_S are known and m_{CO}, m_{CH4}, m_{H2S}, m_{H2O}, m_{H2}, m_{O2} and m_{N2} are unknown, where *m* stands for mass. Therefore, seven unknown quantities need to be evaluated from five equations. Solution to these equations can be obtained by making two suitable assumptions. However, physical constrain on the evaluated mass of each species i.e., mass should be positive or zero, may not be accomplished if these equations are solved mathematically.

$$m_C = m_{C_{CO}} + m_{C_{CH_4}} \tag{1}$$

$$m_H = m_{H_{H_2S}} + m_{H_{CH_4}} + m_{H_{H_2O}} + m_{H_{H_2}} \tag{2}$$

$$m_O = m_{O_{CO}} + m_{O_{H_2O}} + m_{O_{O_2}} \tag{3}$$

$$m_N = m_{N_{N_2}} \tag{4}$$

$$m_S = m_{S_{H_2S}} \tag{5}$$

In the approach suggested by Nakod [20], solution to this problem is obtained using step by step method outlined in Fig.3. Species TAR is considered to account for left over carbon, if any. Once the solution to this problem is obtained, 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, R1 is added to convert this gaseous volatile to several other gas phase species. Stoichiometric coefficients *a, b, c, d, e, f, g* and *h* for the resultant species are calculated from the obtained mass fractions using suggested approach outlined in Fig.3 and molecular weights of these species. Heating value of species, Volatile is 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.

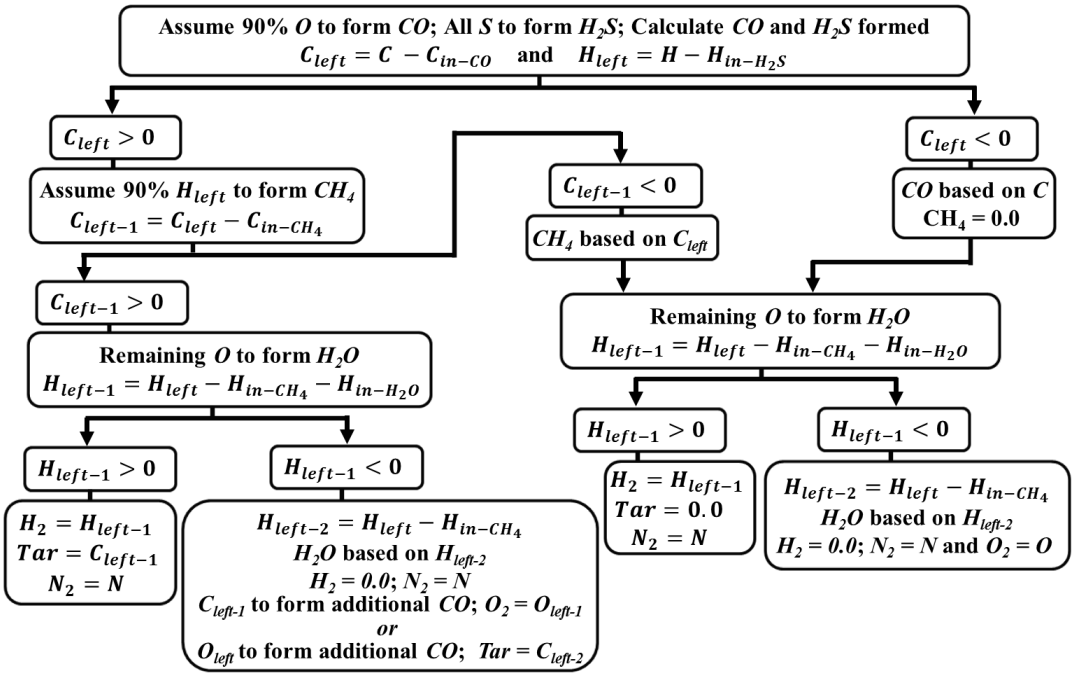

Figure 3. *Volatile Break-Up Approach [20]*

$$Volatile \rightarrow aCO + bH_2S + cCH_4 + dH_2O + eH_2 + fN_2 + gO_2 + hT \quad \text{(R1)}$$

3.1.2. Gasification Reaction Scheme

Important reaction steps taking place in the gasification process are represented in Fig.4. In this case, the first process of drying takes place as soon as the solid fuel is introduced in the gasifier which converts the moisture from the coal (or other solid material) into water vapor. Next step converts the volatile matter into several gas phase species. This can be accomplished using approach presented in section 3.1.1 of this paper. Once the gaseous species are available, the composition tries to achieve chemical equilibrium through several equilibrium reactions like water gas shift reaction, steam methane reactions, hydrogen combustion reaction, etc. This is governed by several parameters prevailing in the gasifier and local conditions such as temperature, pressure, residence time and availability of the reacting species.

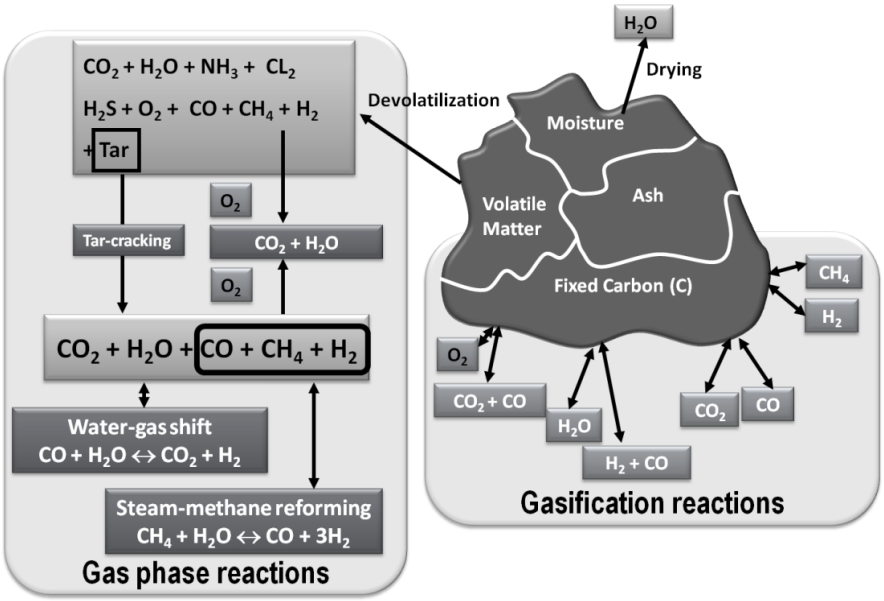

Figure 4. *Gasification Reaction Scheme*

After completion of the devolatilization of the volatile matter, gaseous species diffuse to the char surface and char gasification reactions as shown in the Fig.4 take place. Details of the relative importance of the individual reactions presented in Fig.4 are available in reference [7, 8 and 21].

In CFD simulations, these reactions can be included with the reaction rate parameters as listed in Table 1 and Table 2.

Table 1. *Gas Phase Reactions [7, 8 and 21]*

S N	Reaction	A	Ea (J/kmol)	N1	N2	N3
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	-	-
R2	CO oxidation reaction: CO + 0.5 O_2 →CO_2	2.239e+12	1.7e+08	1	0.25	0.5 (H_2O)
R3	Forward water-gas shift reaction (FWGS): CO + H_2O → CO_2 + H_2	2.35e+10	2.88e+08	0.5	1	-
R4	Reverse water-gas shift reaction (RWGS): CO_2 + H_2 → CO + H_2O	1.785e+12	3.260e+08	1	0.5	-
R5	Hydrogen oxidation: H_2 + 0.5 O_2 → H_2O	9.87e+08	3.1e+07	1	1	-
R6	Reverse of hydrogen oxidation: H_2O →H_2 + 0.5 O_2	2.06e+11	2.728e+08	1	-	-
R7	Methane oxidation: CH_4 + 1.5 O_2 → CO + H_2O	5.012e+11	2e+08	0.7	0.8	-
R8	Steam methane reforming: CH_4 + H_2O → CO + 3 H_2	5.922e+08	2.09e+08	0.5	1	-
R9	Tar oxidation reaction: Tar + O_2 → CO	1e+15	1e+08	1	0.5	-

Table 2. *Heterogeneous Particle Surface Reactions [12]*

S N	Reaction	A	Ea (J/kmol)	N1
R10	Char combustion: C<S> + 0.5 O_2 → CO	300	1.3e+08	0.65 (O_2)
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)

31.3. Other Sub-Models

Other sub-models such as turbulence, turbulence-chemistry interaction in turbulent flows, radiation including particle-radiation interaction, etc. are readily available in Commercial codes like ANSYS Fluent [22]. They can be employed as it is for the gasification simulation.

3.2. CFD Modeling of Oxy-Fuel Combustion

As mentioned earlier in this paper, oxy-fuel combustion, another clean coal technology gaining popularity as a method to reduce the emissions of CO_2 from fossil power plants by flue gas recycling [23]. In this technology, nitrogen is separated out from air in air separation unit before it enters the combustion chamber. Fuel is then burned in either an oxygen-rich (~95% oxygen) environment, as in welding and cutting of metals where higher flame temperature is required, or diluted with recycled flue-gas, as in pulverized coal-fired boilers. The main advantage of separating nitrogen before combustion is to lower the NOx formation. In oxy-fuel combustion the NOx formation takes place only from the available nitrogen content in the fuel such as coal. This fuel NOx, most of the times, is order of magnitude lower than the thermal NOx which is formed from the nitrogen available in the air. In oxy-fuel combustion, if the combustion is carried out with the pure oxygen stream, then the peak temperature in the device would be almost doubled (3000-3500K) compared to that of air-fired case (1800-2200K). If the combustion is carried out for the heat transfer application like boilers, combustion device material will not be able to sustain such a high temperature. Therefore, carbon dioxide (or the mixture of carbon dioxide and water vapor) from the flue gas is re-circulated. This recycling leads to high concentrations of gases

(CO_2, H_2O) participating in radiation which, in turn, can result in significantly different gas emissivity values within the boiler. Fig. 5 compares the level of H_2O/CO_2 ratio in oxy fired and air fired flames. It can be seen that in case of air fired case, the ratio of H_2O/CO_2ratio varies from ~5 in the flame region to 1 away from the flame region. In case of oxy-fired case, the maximum value of H_2O/CO_2ratio is ~0.7 in the flame region and that decreases away from the flame region. Therefore, there is a large difference in the H_2O/CO_2prevailing in oxy-fired case than that existing in air-fired case. This significantly alters the gas emissivity values within the combustor. In this case, the traditionally available radiation properly calculation models which are suitable for air-fired combustion may not apply to oxy-fired combustion.

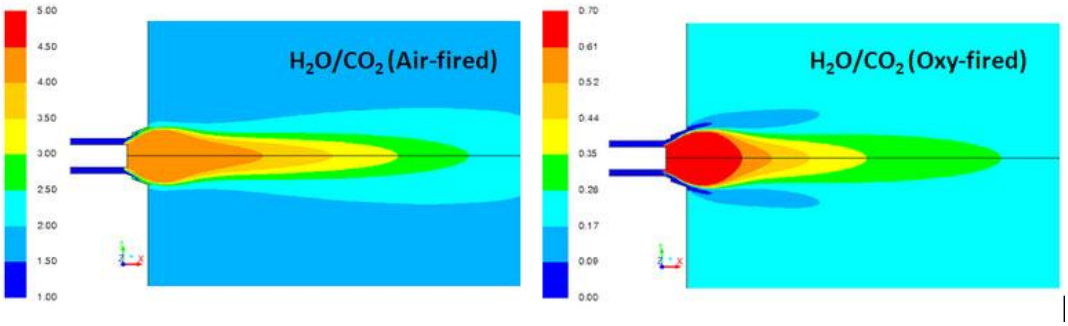

Figure 5. *H_2O/CO_2 Ratio in Air-Fired and Oxy-Fired Combustion*

Current ongoing development efforts in the power-generation industry are either to build a new oxy-fuel combustion facility or retrofit an existing air-fuel combustion plant using current technologies. Multiple oxy-combustion facilities of various scales are being constructed or are in operation around the world today. Developing a better understanding of flame behavior, heat and mass transfer, combustion gas chemistry, char burnout, etc., is a key for successful building or retrofitting of oxy-fuel combustion plants. While retrofitting, it is important to keep heat transfer characteristics in the oxy-fired plant similar to that of the existing air-fired plant. This is accomplished by adjusting oxygen and re-circulated flue-gas levels at the entry of the boiler. Computation fluid dynamics (CFD) analysis can help with faster convergence of the required levels of oxygen and recycled flue-gas. Of the dominant heat transfer modes, radiation heat transfer is altered the most in the oxy-fired scenario, compared to that of the air-fired scenario, due to significantly different radiation properties resulting from high concentrations of participating gases in radiation (CO_2 and H_2O). Therefore, the choice of models to represent radiation properties needs to be made carefully.

3.2.1. Radiation Property calculation Model for Oxy-Fired Combustion

To enable accurate calculations of radiative heat transfer in oxy-combustion scenarios several gas property calculation models have been proposed in recent years [24-26]. The proposed models in [24-26] are all based on the framework of the Weighted Sum-of-Gray-Gases (WSGG) method where the emissivities of gas mixtures are expressed in terms of temperature independent absorption coefficients and temperature-dependent weighting factors. The model absorption coefficients and weighting factors are computed from a fit to total emissivity data of gas mixtures obtained from experimental measurements or narrow band and wide band model calculations. Among the benefits of WSGG models include: ease of implementation within existing CFD frameworks since the absorption coefficients and emissivity weighting factors can be computed locally based on the temperature and specie concentrations and the flexibility to be employed in either gray or non-gray radiative transfer calculations. Highly accurate non-gray calculations can be carried out employing four or five gray gases with a modest increase in computational cost particularly when the radiation calculations are performed once in several fluid iterations. The need for these newer WSGG models [24-26] arose when the older WSGG models (Smith et al. [27] for instance) that were specifically developed for combustion with air as the oxidizer were found to be inaccurate when extended to low H_2O/CO_2 ratios that are encountered during oxy-combustion with dry flue gas recycle. The accuracy of a WSGG model depends on: (1) The accuracies of the experimental measurements or the narrow-band and wide-band model databases employed to generate the total emissivity of gas mixtures and (2) The accuracy to which the emissivity data can be fit to the functional form of a WSGG model to estimate the model

coefficients. Lallemant et al. [28] examined the total emissivities of the combustion gas mixture in a natural gas furnace predicted by different narrow band and wide band models and found significantly variations depending upon the property database being used. Similarly, transmissivity spectra from recently conducted gas cell experiments have concluded that the statistical narrow band models (SNB) RADCAL [29] and EM2C SNB [30] to be accurate within 3% of the measured transmissivities at gas concentrations representative of oxy combustion scenarios [31]. Furthermore, recent benchmark calculations of Chu et al. [32-33] have further reinforced the accuracies of the EM2C SNB model for oxy-combustion scenarios. In their study, line-by-line (LBL) calculations of thermal radiative transfer calculations employing the HITEMP 2010 spectroscopic database were carried out in one-dimensional and two-dimensional media containing mixtures of CO_2 and H_2O representative of air and oxy-flames. The EM2C SNB model predictions that contained estimates of high temperature "hot lines" based on approximate theoretical and empirical formulas were found to agree closely with the LBL calculations. Therefore, the experimental results of Bechera et al. [31] and the LBL calculations of Chu et al. [32-33] suggest the EM2C SNB and the RADCAL SNB to be accurate model databases to generate "benchmark" radiative heat transfer data when LBL calculations are infeasible. However, these SNB models output band averaged transmissivities (path-length dependent properties) that are not readily amenable with the more popular radiation models in CFD codes that employ a differential formulation of the radiative transfer equation (RTE) and require the absorption coefficient as the input property. Therefore, these SNB models are employed to compute total emissivities of gas mixtures and WSGG models are developed from them. For instance, four and five gray gas WSGG models based on the EM2C SNB model database have been developed and formulated and reported by Johansson and co-workers [25]. Similarly, Krishnamoorthy et al. [27, 34 and 35] computed WSGG model coefficients based on total emissivity data from SNB RADCAL [30] and Hottel charts [36]. The performances of these two sets of WSGG models are compared and evaluated in their study of gray and non-gray formulations [35]. The model accuracies and impact on the predicted velocity, temperature and radiative heat fluxes are evaluated by comparisons against experimental data obtained under oxy-firing scenarios. Table 3 summarizes these models along with their model notations employed within their work. The non-gray models are denoted by the number of gray-gases (gg) employed in their formation. It is worth mentioning that the accuracies of the WSGG model may be further improved by directly computing the WSGG model coefficients from high resolution spectroscopic databases. For instance, Denison and Webb [37] developed the Spectral-Line Weighted-Sum-of-Gray-Gases Model (SLW) and Modest and Zhang [38] developed the Full-Spectrum Correlated K (FSCK) models and demonstrated near line-by-line (LBL) accuracies in benchmark problems. However, they are yet to find widespread use in large-scale, fully coupled, CFD simulations of combustion mainly because they require 10-20 gray gases (or equivalently quadrature points) to achieve high fidelities. Therefore, at present, the gray and non-gray models summarized in Table 1 are recommended and can be implemented as User-Defined Models (like User Defined Functions, UDFs) and employed in conjunction with the commercial CFD codes like ANSYS Fluent. Nakod et al [39], using gray and non-gray radiation properly models suggested by Krishnamoorthy et al. [35] predicted the radiation heat transfer in industrial scale coal fired boiler for air fired and oxy fired (both, dry-recycled and wet-recycled) scenarios. The observed agreement between the experimental measurements and simulations is within 100 K in most of the locations and may be deemed as acceptable. An agreement to within 100 K of the experimental measurements is generally the level of modeling accuracies that can be expected in simulations of such large scale furnaces even when accurate particle size distribution and coalkinetic parameters are available [40]. The temperature contours within the full scale boiler during air-firing, dry and wet FGR are shown in Fig. 6. The similarities between the contours obtained from the three firing conditions confirm that the combustion of coal can be completed at these H_2O/CO_2 molar ratios in the dry and wet flue gas recirculation scenarios to achieve a temperature profile within the boiler that is identical to that found in air-fired scenario in order to retrofit the existing air fired boilers/furnaces with oxy fired combustion to achieve cleaner energy objectives. These conclusions are consistent with the observations of Habermehl et al. [41]

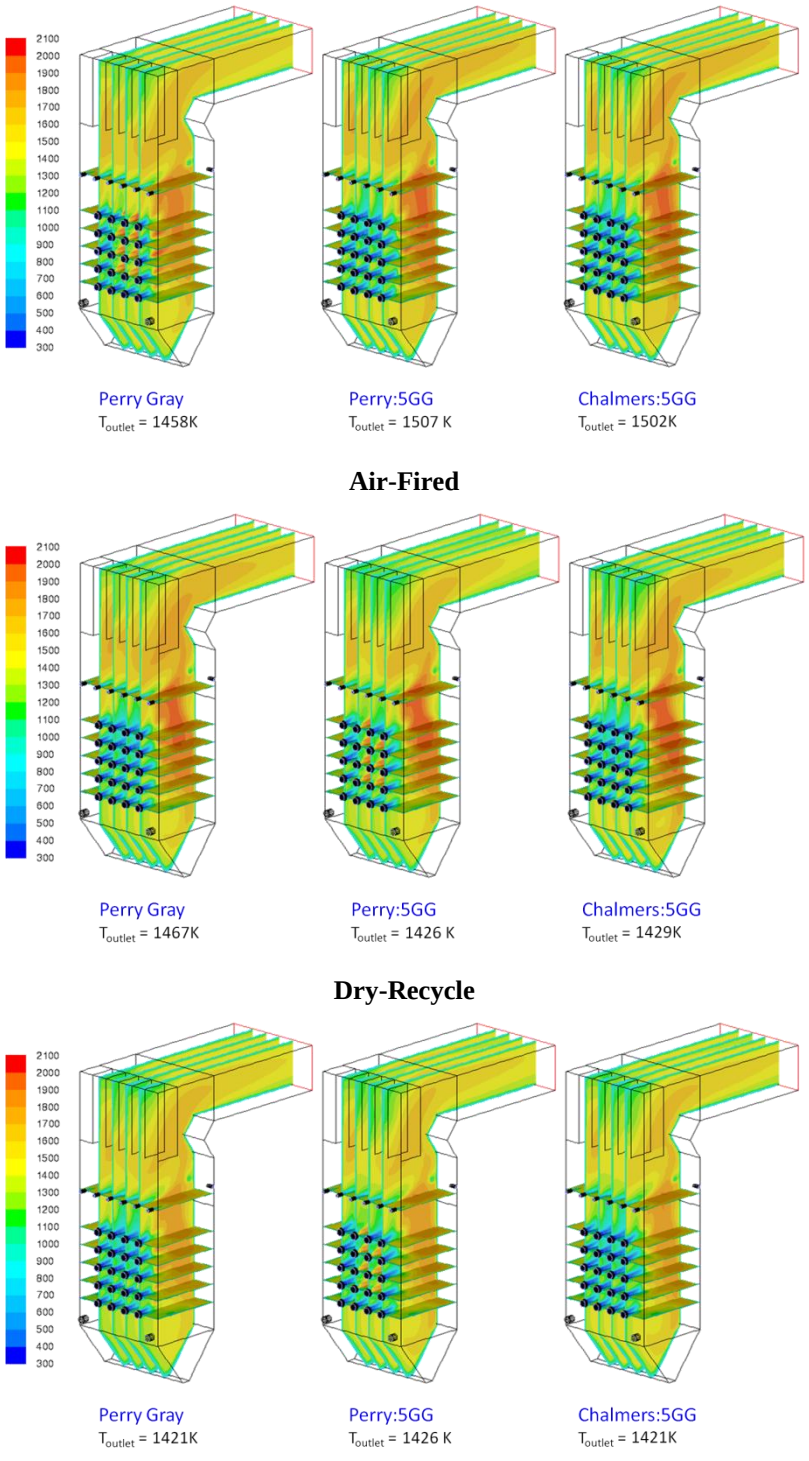

Figure 6. *Temperature Contours within the Full Scale Boiler for Air-Fired and Oxy-Fired with recycled Flue Gas Scenarios*

Table 3. *Summary of WSGG Models Examined in This Study*

Source	Model Notation	Radiative Property Database
Hottel et al. [36], Krishnamoorthy et al. [24]	Perry (gray)	Hottel charts and SNB RADCAL (Hottel et al. [36], Grosshandler [29])
Krishnamoorthy [34]	Perry (5 gg)	Hottel charts and SNB RADCAL (Hottel et al. [36], Grosshandler [29])
Johansson et al. [25]	Chalmers (5 gg)	EM2C SNB (Soufiani and Taine [30])

4. CONCLUSION

In this paper, a review of application of Computational Fluid Dynamics (CFD) in gasification and oxy-fuel combustion and important considerations while selecting sub-models for CFD simulations are presented. Volatile break-up and gasification reaction schemes needs to be selected and specified correctly to be able to predict accurate syngas temperature and species composition in gasification simulations. In oxy-fuel combustion, while retrofitting, temperature in the furnace can be reproduced similar to air fired scenario by adjusting the quantity of recalculating flue gas. Further, radiation heat transfer properties are significantly altered in case of oxy-fuel combustion. This needs careful selection of radiation property models to be able to predict radiation heat transfer accurately. Recently suggested Weighted Sum of Gray Gas model based on five non gray bands have shown promising results in terms of accuracy with modest increase in computation cost.

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