

Research Article

A Reduced Order Model for the Design of Oxy-Coal Combustion Systems

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Received 2 July 2015; Accepted 7 October 2015

Academic Editor: Satyanarayanan R. Chakravarthy

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Oxy-coal combustion is one of the more promising technologies currently under development for addressing the issues associated with greenhouse gas emissions from coal-fired power plants. Oxy-coal combustion involves combusting the coal fuel in mixtures of pure oxygen and recycled flue gas (RFG) consisting of mainly carbon dioxide (CO_2). As a consequence, many researchers and power plant designers have turned to CFD simulations for the study and design of new oxy-coal combustion power plants, as well as refitting existing air-coal combustion facilities to oxy-coal combustion operations. While CFD is a powerful tool that can provide a vast amount of information, the simulations themselves can be quite expensive in terms of computational resources and time investment. As a remedy, a reduced order model (ROM) for oxy-coal combustion has been developed to supplement the CFD simulations. With this model, it is possible to quickly estimate the average outlet temperature of combustion flue gases given a known set of mass flow rates of fuel and oxidant entering the power plant boiler as well as determine the required reactor inlet mass flow rates for a desired outlet temperature. Several cases have been examined with this model. The results compare quite favorably to full CFD simulation results.

1. Introduction

The anthropogenic emission of greenhouse gases (GHG) from the combustion of fossil fuels for the generation of electrical power has been considered as one of the driving factors for global climate change [1]. In order to meet future targets for the reduction of GHG emissions, a number of developing technologies for carbon capture and storage are currently under development; including pre- and postcombustion capture and oxy-fuel combustion [2].

Oxy-fuel combustion utilizes a combination of pure oxygen and recycled flue gas (RFG) as an oxidant for the combustion of the fuel source, producing a gas that consists mostly of CO_2 and water vapor [2]. The high concentrations of CO_2 in the flue gas enable easier and more economical CO_2 separation and compression and have been shown to reduce gaseous emissions of NO_x and SO_x from pulverized coal (PC) power plants [3]. Because of the higher specific heat of CO_2 as opposed to nitrogen in conventional air-fired combustion, oxy-coal combustion has been found to lead to significant

changes in flame temperatures, chemical species concentrations, and radiation heat transfer within the combustor [3].

As a consequence of this, many researchers have turned to CFD modeling of oxy-combustion as a design tool for the design of new power plants and retrofitting of existing facilities utilizing oxy-coal combustion [3–7]. These simulation tools are capable of providing detailed information about the flow field, turbulent mixing, temperature, and species concentration profiles within a reactor. However, these simulations depend upon a number of model parameters and assumptions. More importantly, each of these simulations requires a considerable amount of time investment and computational costs [7]. If the purpose of the simulations is to obtain a set of operating conditions such as fuel and oxidant flow rates that will lead to reactor temperatures within a certain narrowly defined range, then a large number of simulations may be required, multiplying the costs by a significant margin.

In an effort to reduce the time and effort that must be spent to determine acceptable reactor operating conditions,

a simplified reduced order model (ROM) has been developed. The ROM utilizes a combination of a commercially available coal devolatilization model based upon lattice percolation theory, a chemical equilibrium code developed by NASA, and an iterative energy balance calculation spreadsheet using Microsoft Excel. Each of these elements will be described in greater detail in the following sections, as well as a comparison between the ROM predictions and CFD simulations using the Ansys-Fluent software package.

2. Description of the Reduced Order Model

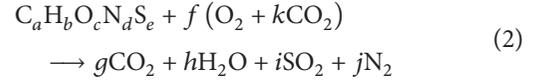
For a given coal feedstock, the ultimate and proximate analysis data and higher heating value are used to calculate the required flow rates of fuel (coal) and oxidant (as a mixture of O_2 and CO_2) for a desired level of input energy, expressed in kW, and equivalence ratio, where the equivalence ratio is expressed as the ratio of available oxygen to that required for stoichiometric combustion. In order to account for the devolatilization of the coal as it is heated, ultimate and proximate analysis data for the selected coal feedstock, as well as a heating rate, is provided as inputs to the Chemical Percolation Devolatilization (CPD) model software developed at Brigham Young University [8–10]. The CPD software enables prediction of the mass fractions of the coal tar and volatile gasses that are released when the coal is heated. The model also predicts the mass fraction of the remaining solid material, which is assumed for the purposes of the ROM to consist of pure carbon (graphite). These mass fractions are then converted into flow rates (moles/s) and, along with the molar flow rates of fuel and oxidant, are provided as inputs for the NASA Chemical Equilibrium Applications (CEA) software. The CEA software is then used to determine the adiabatic flame temperature, total enthalpy, and equilibrium concentrations of the combustion products. This information is then used to calculate an energy balance which accounts for the energy contained within the outlet gas and the energy transferred to the ash materials, as well as an assumed amount of heat lost to the surroundings. The mass and energy balance equations lead to an iterative process in which the CEA software is run repeatedly at different specified temperatures until the energy and mass conservations are satisfied, resulting in an average outlet temperature and mass fractions of prescribed species. In what follows, each of the steps discussed above are described in greater detail.

2.1. Fuel/Oxidant Stoichiometry Calculations. The first step in determining the required stoichiometric amounts of oxidant required for complete combustion is to calculate the mass flow rate of fuel (or coal) that is needed to produce the desired amount of power output during the combustion process. This is done by solving (1), where \dot{m}_f is the mass flow rate of fuel in kg/s, H_{HV} is the higher heating value of the feedstock in kJ/kg, and PO is the power output in kW:

$$\dot{m}_f = \frac{PO}{H_{HV}}. \quad (1)$$

Once the mass flow rate of the fuel is known, it is necessary to calculate the required mass flow rate of oxidant for complete

combustion. This is done by solving for the stoichiometric coefficients of the coal combustion reaction shown in (2) for a single kg of coal:



where f , g , h , i , and j are stoichiometric coefficients, and the subscripts a , b , c , d , and e are the number of moles of carbon, hydrogen, oxygen, nitrogen, and sulfur present in the coal (as found by dividing the dry ash-free percent mass of each element, determined via ultimate analysis, by the molecular weight of each element). The number of moles of oxygen per mole of fuel required to complete combustion is equal to the value of f . Finally, k is the number of moles of carbon dioxide required to obtain a desired percentage of oxygen in the total oxidant and is calculated from

$$k = \frac{100 - \%O_2}{\%O_2}. \quad (3)$$

In order to determine the required mass flow rate of the oxidant, the number of moles of oxidant per kilogram of dry, ash-free (daf) fuel must then be multiplied by the molecular weight of the oxidant and the total mass flow rate of the fuel:

$$\dot{m}_{ox} = fM_{ox}\dot{m}_f(1 - \%_{moisture} - \%_{ash}), \quad (4)$$

where the expression in parentheses accounts for the difference between the “as-received” and “daf” coal. It should be noted here that the mass flow rate of oxidant obtained via (4) is that required by stoichiometry for complete combustion. If instead a fuel-lean (or fuel-rich) mixture is desired, then the right-hand side of (4) can be multiplied by the equivalence ratio, λ , to obtain the desired conditions, where

$$\lambda = \frac{\text{actual moles of oxygen}}{\text{stoichiometric moles of oxygen}}. \quad (5)$$

An equivalence ratio less than one signifies that the combustion will occur in a fuel-rich environment and greater than one will be fuel-lean, and a ratio of one signifies stoichiometric combustion.

2.2. Coal Devolatilization Model. The devolatilization characteristics of the coal are modeled using the Chemical Percolation Devolatilization (CPD) model developed by Fletcher et al. [8–11]. Utilizing the ultimate and proximate analysis data of a given type of coal and a specified heating rate, the CPD model is able to predict the evolution of volatile gases, tars, and residual solids during coal pyrolysis (which is considered to be one of the early stages of coal combustion). The CPD model outputs the mass fractions of CO, CO_2 , CH_4 , water vapor, (unspecified) tars, solids (i.e., carbon and ash generating materials), and other (unspecified) volatile gases as a function of time and temperature.

For the purposes of the ROM, it is then assumed, for brevity, that the tar consists mainly of phenol (C_6H_5OH) and that the balance of the released gasses not in the form of CO, CO_2 , CH_4 , or water vapor (i.e., the unspecified gases referred to above) will consist of the following gas species:

TABLE I: Coal properties (Decker Coal).

| Proximate analysis (wt% as received) | | | VM (% daf) | Ultimate analysis (wt% daf) | | | | | HHV |
|--------------------------------------|-----|--------------|------------|-----------------------------|-----|-----|-----|------|---------------|
| Moisture | Ash | Combustibles | | C | H | N | S | O | H_i (MJ/kg) |
| 10.2 | 5.0 | 84.8 | 59.4 | 69.9 | 5.4 | 0.6 | 1.0 | 23.1 | 20.9 |

C_2H_6 (ethane), H_2S , SO_2 , O_2 , N_2 , and H_2 . The amounts of these individual gas species are then estimated by calculating an elemental mass balance based upon the mass fractions of carbon, hydrogen, nitrogen, sulfur, and oxygen provided by the ultimate analysis of the coal. The selection of the assumed gas and tar species listed above is primarily driven by the available selection of fuel and oxidant compounds within the NASA CEA software, as described below.

2.3. Chemical Equilibrium Calculations. The ROM utilizes the NASA Chemical Equilibrium with Applications (CEA) computer code [12] for the calculation of combustion-related parameters, such as adiabatic flame temperature, total enthalpy, and equilibrium gas compositions. The CEA code was developed by the NASA Glenn Research Center and contains modules for constant-pressure or constant-volume combustion, rocket performance based on finite- or infinite-chamber-area models, shock wave calculations, and Chapman-Jouguet detonations. In addition, the code contains databases of thermodynamic and transport properties for more than 2000 chemical species. The CEA code is available both as a web-based application and as downloadable source code written in the Fortran programming language. The CEA code is first used to determine the adiabatic flame temperature, as well as the total enthalpy and chemical composition of the reactor flue gases. This is done using the “combustion” module, in which the reactor pressure and molar flow rates and inlet temperatures of the previously determined fuel and oxidant species are specified as inputs. Unless otherwise specified, the temperature of the calculated oxidant is assumed to be at standard conditions, while the temperature of the devolatilization products is specified at the final temperature specified during devolatilization of the coal via the CPD model. The resulting flame temperature, enthalpy, and gas composition are then recorded and used as the inlet conditions for the energy balance calculations that will be discussed in the next section.

Additionally, during the iterative steps of the energy balance calculations, the CEA code is run again with the specified flow rates, but at specified temperatures and pressures. This step is completed in an iterative manner (with changing temperature) until the energy balance calculations, described below, are satisfied.

2.4. Energy Balance Calculations. For the energy balance calculations component of the ROM, the oxy-combustion reactor is treated as a control volume over which a steady-state energy balance is performed. In this treatment, the specified inlet conditions used with the NASA CEA code provides the total enthalpy (energy) entering the control volume. It is assumed that there is no change in energy within the control volume so that the energy leaving the control

volume must equal that which is entering the control volume. The total energy leaving the control volume is a combination of the temperature-dependent enthalpy contained within the flue gas, conduction heat transfer losses through the walls of the theoretical reactor, and the energy required to raise the temperature of the remaining solids (ash) to the outlet temperature. The first iteration uses the adiabatic flame temperature data, and subsequent iterations gradually reduce temperatures until the difference between the inlet and outlet energy values is negligibly small, thus satisfying the principle of conservation of energy.

3. Results and Discussion

A number of simulations were carried out using the ROM and the results of these simulations were then compared to previously validated CFD simulations for similar combustion conditions. In these simulations, coal and various mixtures of O_2 and CO_2 are fed into a 100 kW downfired oxy-coal reactor (currently being designed by the authors), assuming an overall heat loss of 25 kW, and the predicted outlet temperatures provided by the ROM and CFD simulations are compared. In total, three different operating conditions are considered; these conditions correspond to the oxidant consisting of 25%, 50%, and 75% O_2 , with the remaining balance consisting of CO_2 . The coal properties for each case are shown in Table 1.

3.1. CFD Simulations. As previously stated, the reactor used for the comparison of the CFD simulations and the ROM predictions is currently being developed by the authors. This Very High Temperature Entrained Reactor (VHTER) is a vertical downfired design with a combustion chamber that is 150 mm in diameter and 2 m in length. The burner is composed of two concentric ports. The first port is for injection of pulverized coal using a small portion of the oxidant gas as carrier. The remaining balance of oxidant is injected through a second port, which is swirled with a fin angle of 45° . In addition, a pair of tangential injection ports can be used for injection of chemical reagents for desired chemical processes within the reactor. Schematics of this reactor are shown in Figure 1.

For each of the simulations used in this comparison, an assumed power input of 100 kW, corresponding to a mass flow rate of $4.78e - 03$ kg/s of pulverized coal, is used. In addition, three different O_2/CO_2 mixtures, with O_2 concentrations of 25, 50, and 75%, were considered. These cases are named OF25, OF50, and OF75, respectively. The heat losses through the wall were assumed to be 25% of the power input, or 25 kW. The mass flow rates of oxidant were calculated using an equivalence ratio of 0.85 and are shown in Table 2. The coal and oxidant are assumed to enter the reactor at standard

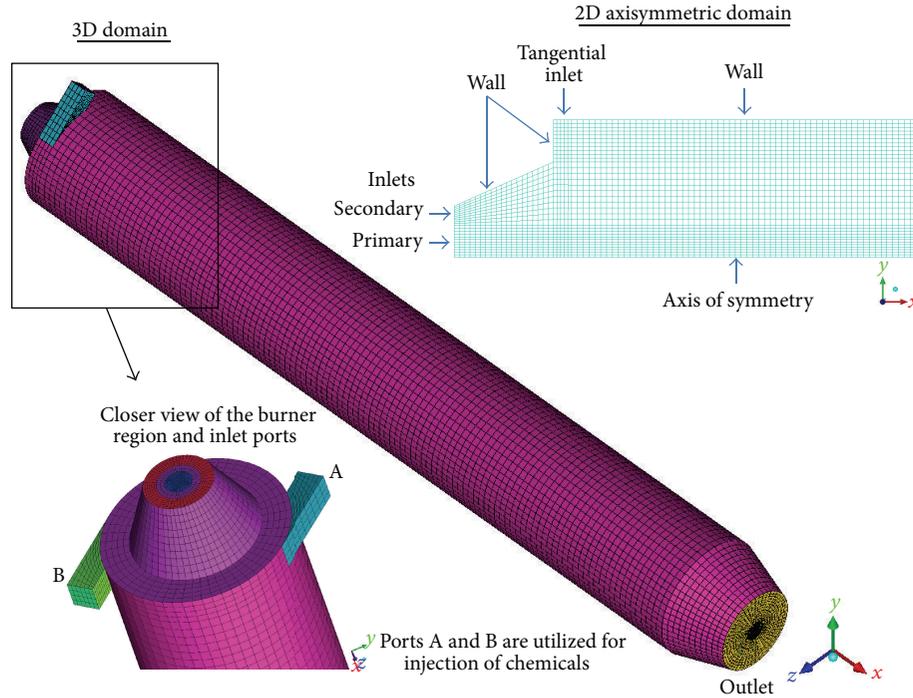


FIGURE 1: CFD computational domain for the VHTER reactor design.

TABLE 2: CFD simulation flow rates (kg/s).

| CASE | O ₂ | CO ₂ | Coal |
|------|----------------|-----------------|------------|
| OF25 | $8.70e-03$ | $3.59e-02$ | $4.54e-03$ |
| OF50 | $8.70e-03$ | $1.20e-02$ | $4.54e-03$ |
| OF75 | $8.70e-03$ | $3.99e-03$ | $4.54e-03$ |

conditions. Finally, the tangential injection ports were not used in these simulations.

3.1.1. Solution Method (CFD). The simulations were performed using the ANSYS-Fluent software package. The SIMPLE scheme [13] was used for pressure-velocity coupling in conjunction with the PRESTO scheme [14] for pressure coupling as it is recommended for swirling flows [15]. Turbulent flow, transport of species, and radiative heat transfer equations were solved using the first order UPWIND scheme [13]. The governing equations for turbulent flow, combustion, heat, and mass transfer for the continuous and discrete phases are solved using the finite volume method in structured grid systems. Both 2D and 3D axisymmetric domains were used; however, only the results for the 2D axisymmetric domain are presented here.

The combustion process is modeled using the Eulerian-Lagrangian approach for the continuous and discrete phases, respectively. The flow dynamics of the continuous media is determined by solving the Navier-Stokes equations by using the Reynolds Average approach (RANS). The Reynolds stresses are modeled by utilizing the standard $k-\epsilon$ model of Launder and Spalding [16]. The modeling of turbulence close to the wall region is performed by using standard wall

functions for near-wall treatment from Launder and Spalding [17].

Combustion and species transport for the gas phase is modeled using the well-known time averaged energy equation and species transport equations.

The energy equation is formulated in terms of the specific energy accounting for conduction, convection, and viscous dissipations with effective thermal and diffusive properties modified by turbulent effects. The effect of combustion, radiation heat transfer, and additional sources are also included. The Radiative Transfer Equation (RTE) is solved by using the Discrete Ordinates (OD) Radiation Model (Siegel et al. [18]), which can account for the effect of radiation exchange between the gas and particle phases as well as for scattering. For turbulent-chemistry interaction the turbulent-chemistry model of Hjertaer and Magnussen [19] is assumed, that is, the Eddy-dissipation model.

Coal devolatilization is modeled using the single kinetic rate devolatilization model of Badzioch and Hawksley [20], where the volatiles are defined by a two-step reaction mechanism where the species “volatiles” is a generic hydrocarbon obtained from the proximate and ultimate analysis of coal. Finally, the oxidation of char is modeled by utilizing the kinetics/diffusion-limited surface reaction model of Baum and Street [21] and Field [22]. The models utilized in these simulations were tested for oxy-coal combustion in the exploratory study performed by the coauthors [23].

The boundary conditions for the primary and secondary ports were set as inlet flow conditions. For the secondary port, a swirling flow component was given in order to model the 45° fins swirler. The walls were modeled assuming a constant heat transfer rate and a constant emissivity of 0.5.

TABLE 3: Outlet gas composition (mole fraction).

| Case | Volatiles | O ₂ | CO ₂ | H ₂ O | CO | SO ₂ | N ₂ |
|------|-----------|----------------|-----------------|------------------|----------|-----------------|----------------|
| OF25 | 4.29e-06 | 3.59e-02 | 8.58e-01 | 1.04e-01 | 2.80e-05 | 3.98e-04 | 1.17e-03 |
| OF50 | 2.51e-04 | 6.63e-02 | 7.38e-01 | 1.92e-01 | 5.95e-04 | 7.28e-04 | 2.09e-03 |
| OF75 | 6.93e-04 | 1.05e-01 | 6.30e-01 | 2.60e-01 | 1.09e-03 | 1.00e-03 | 2.21e-03 |

TABLE 4: Reduced order model (ROM) case study NASA CEA inputs.

| | Species | Feed rate (mole/s) | | |
|---------|---|--------------------|--------------------|--------------------|
| | | 25% O ₂ | 50% O ₂ | 75% O ₂ |
| Fuel | Carbon (graphite) | 0.1681717 | 0.1681717 | 0.1681717 |
| | CH ₄ | 0.0110667 | 0.0110667 | 0.0110667 |
| | C ₆ H ₅ OH (phenol) | 0.0037952 | 0.0037952 | 0.0037952 |
| | C ₂ H ₆ | 0.003525 | 0.003525 | 0.003525 |
| | H ₂ | 0.0 | 0.0 | 0.0 |
| | H ₂ S | 0.0 | 0.0 | 0.0 |
| | N ₂ | 0.0014144 | 0.0014144 | 0.0014144 |
| | SO ₂ | 0.0004807 | 0.0004807 | 0.0004807 |
| Oxidant | O ₂ | 0.2724017 | 0.2724017 | 0.2724017 |
| | CO ₂ | 0.817942 | 0.2732708 | 0.0918949 |
| | CO | 0.003273 | 0.003273 | 0.003273 |
| | H ₂ O | 0.0824674 | 0.0824674 | 0.0824674 |

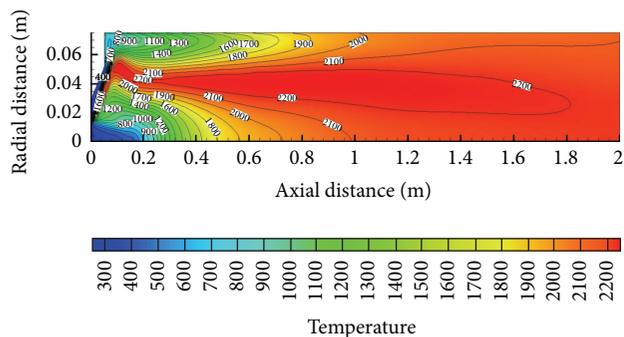


FIGURE 2: Predicted temperature contours for OF50 case.

The outlet condition is set as pressure outlet with standard pressure and back flow temperature close to the average outlet temperature.

3.1.2. Simulation Results. Results for combustion of coal indicate that a complete coal devolatilization and char burnout percentages close to 99% are attained in all cases. Results for a typical temperature contour are shown in Figure 2. The predicted outlet gas composition in mole fractions is shown in Table 3. The predicted outlet temperatures from the CFD simulations are given in Table 5.

3.2. ROM Predictions. The three simulation cases described in the previous section were also considered with the reduced order model (ROM) approach. Following the process described previously, the products of coal devolatilization and the corresponding required amount of oxidant were broken down into molar flow rates for each of the various individual chemical compounds and used as input for the NASA CEA code. The resulting values for each of the three

TABLE 5: Comparison of CFD and ROM results for average outlet temperature.

| Case | Outlet temp K (CFD) | Outlet temp K (ROM) | Difference | % error |
|------|---------------------|---------------------|------------|---------|
| OF25 | 1459 | 1412 | 47 | 3.22 |
| OF50 | 2140 | 2074 | 66 | 3.08 |
| OF75 | 2497 | 2410 | 87 | 3.48 |

simulation cases are provided in Table 4. As can be seen in the table, all of the values are constant across each case except for the molar flow rate of CO₂, which is used as a diluent for regulation of reactor temperature. For these ROM cases, the oxidant is assumed to be entering the reactor at room temperature, while the products of the coal devolatilization are considered to be entering at a temperature of 2000 K. The predicted outlet temperatures are given in Table 5. As expected, as the concentration of oxygen in the oxidant gas stream increases the average outlet temperature decreases due to the reduced amount of diluent CO₂.

The resulting outlet gas composition for each of the three cases, calculated through Gibb's free energy minimization by the NASA CEA code, is shown in Table 6. Once again, as expected, the mole fraction of CO₂ in the product gas decreases with increasing oxygen percentage within the initial oxidant gas injected into the reactor. These results will be discussed in greater detail in the following section.

3.3. Comparison to CFD Simulations. The temperatures obtained from the ROM were compared to the average outlet temperatures obtained from CFD simulations. The resulting comparisons are shown in Table 5. As can be seen from Table 5, the CFD and reduced order model ROM exhibit close agreement with respect to the estimated outlet gas

TABLE 6: ROM-predicted outlet gas composition (mole fractions).

| Gas species | OF25 | OF50 | OF75 |
|------------------|---------|---------|---------|
| CO | 0.00001 | 0.00679 | 0.04083 |
| CO ₂ | 0.85825 | 0.73049 | 0.58303 |
| H | 0.0 | 0.00005 | 0.00090 |
| HO ₂ | 0.0 | 0.0 | 0.00001 |
| H ₂ | 0.0 | 0.00036 | 0.00293 |
| H ₂ O | 0.10550 | 0.19008 | 0.24832 |
| NO | 0.00001 | 0.00026 | 0.00077 |
| N ₂ | 0.00117 | 0.00202 | 0.00252 |
| O | 0.0 | 0.00029 | 0.00289 |
| OH | 0.00003 | 0.00336 | 0.01566 |
| O ₂ | 0.03463 | 0.06556 | 0.10116 |
| SO | 0.0 | 0.0 | 0.00001 |
| SO ₂ | 0.00040 | 0.00073 | 0.00097 |

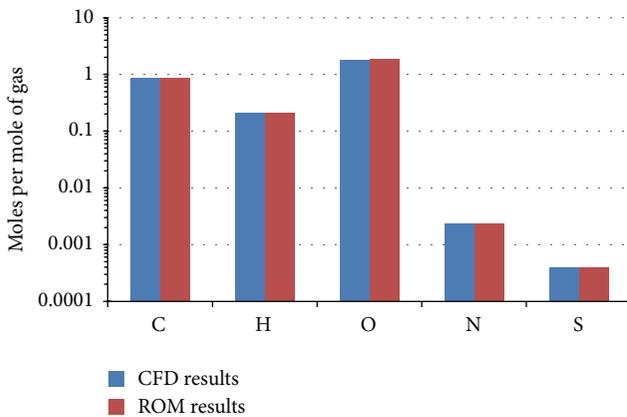


FIGURE 3: Elemental Balance for OF25.

temperature. For each of the cases presented, the percent error between the ROM and CFD results falls within the range of 3.0 and 3.5 percent.

A comparison of the outlet gas composition predicted by the ROM (Table 6) and the Fluent CFD simulations (Table 3) shows fairly close agreement with respect to some of the chemical species of interest, while showing significant difference in others. For example, the resulting mole fractions of CO₂, H₂O, N₂, and O₂ for both models show good agreement, whereas the ROM predicts CO concentrations that are approximately an order of magnitude larger than that seen in the CFD results. The authors attribute this, at least in part, to the fact that the NASA chemical equilibrium code considers a far larger set of chemical species than what is considered in the Fluent CFD simulations. For instance, the NASA code also includes H, HO₂, NO, O, OH, and SO in its determination of chemical equilibrium, whereas Fluent lumps all of the “extraneous” chemical species into a single generic volatile compound of the form C_{1.17}H_{2.90}O_{0.75}N_{0.0635}S_{0.0107}.

Because of this difference between the two, it is important to check to make sure that the results from both simulations incorporate a similar amount of each element present (i.e., C, H, O, N, and S) in a single mole of exhaust gas. The results of this analysis are shown in Figures 3–5, and it can be seen

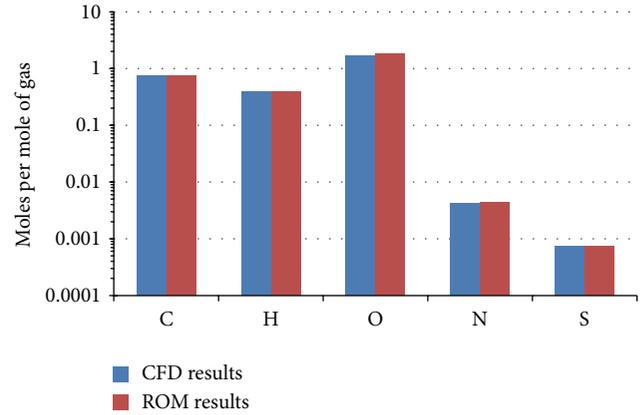


FIGURE 4: Elemental Balance for OF50.

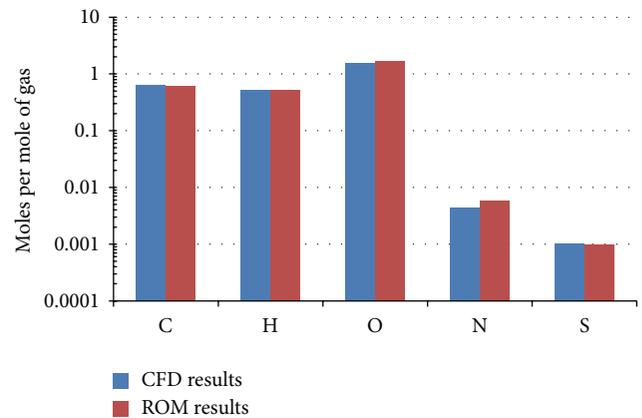
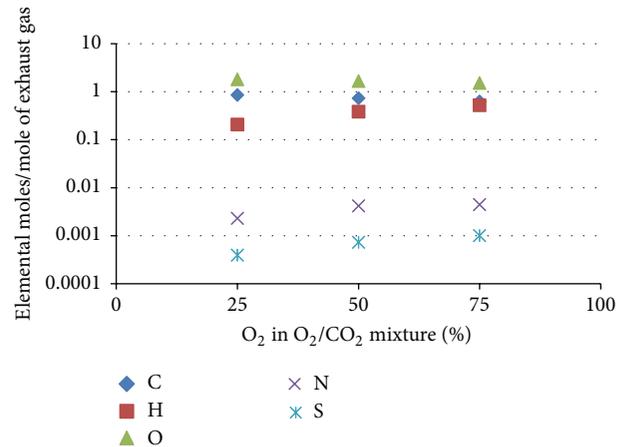


FIGURE 5: Elemental Balance for OF75.

FIGURE 6: Effect of O₂ percentage in oxidant mixture on outlet gas composition (CFD simulations).

from these figures that there is good agreement between the two methods.

Finally, Figure 6 depicts the behavior of the composition of the predicted exhaust gas composition as a function of the percentage of oxygen in the oxidant mixture for the CFD cases. For the simulations discussed in this work, the flow rate

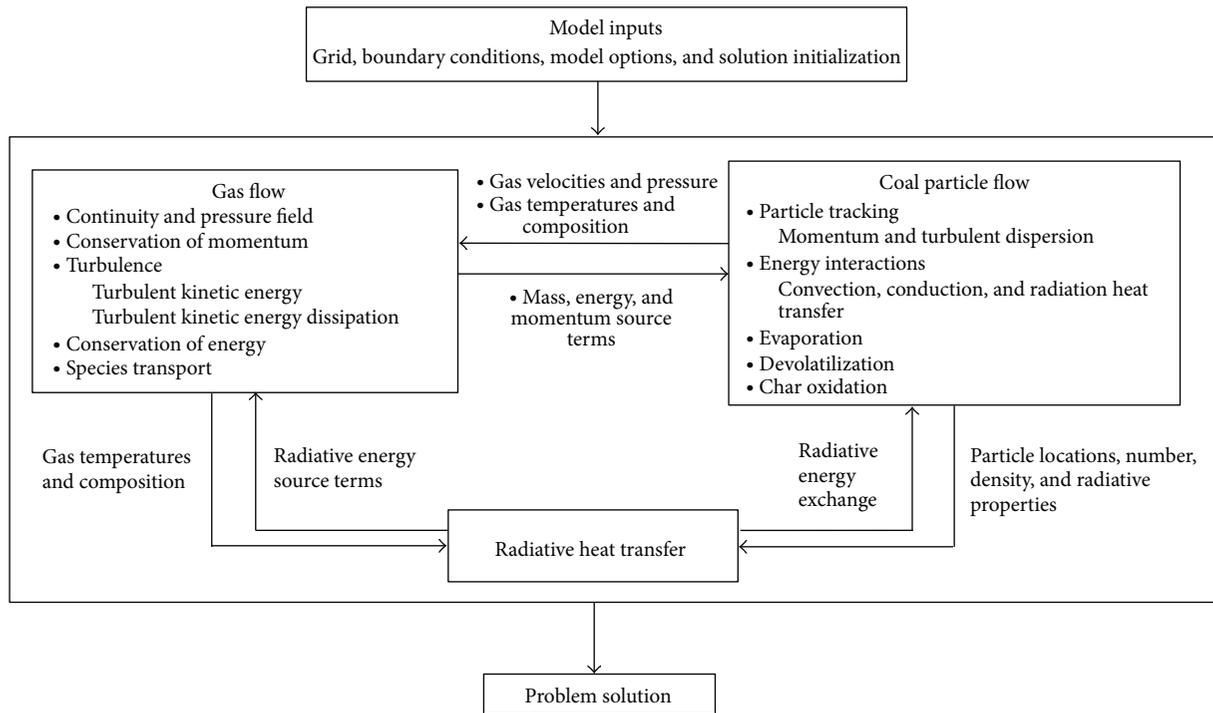


FIGURE 7: CFD model flowchart.

of oxygen was held constant, and the oxygen percentage was obtained by varying the amount of carbon dioxide added to the oxidant. Therefore, increasing percentages of oxygen in Figure 6 are the result of reducing the amount of carbon dioxide. As a consequence, Figure 6 shows a decrease in oxygen and carbon with increasing O_2 percentage, as expected. By comparison, there are slight increases in hydrogen, nitrogen, and sulfur with increasing O_2 percentage. This is also to be expected, due to the fact that higher O_2 percentages mean that there is less oxidant overall to act as a diluent. While not provided here, similar trends can be seen if one looks at the outlet gas composition of the ROM cases as well.

4. Conclusions

A reduced order model (ROM) for oxy-coal combustion has been presented. This model, which utilizes the Chemical Percolation Devolatilization (CPD) model developed by Fletcher et al. and the freely-available NASA Chemical Equilibrium with Applications (NASA CEA) code can be quickly used to help identify the outlet gas temperature and chemical composition for an oxy-coal combustion reactor without the requirement of exhaustive CFD simulations. The main advantage of this model is that it provides reactor designers and operators with the ability to quickly obtain preliminary estimates of the required flow rates of fuel and oxidant for a desired operating condition, or a quick estimate of the outlet gas temperature and composition for a given set of initial flow rates. The fact that it can do so without the need for time-intensive CFD simulations can lead to reductions

in computational cost and time requirements. However, it should be noted that CFD simulations will still be required for prediction of gas composition and temperature variations within the reactor vessel itself.

Appendix

In response to reviewer comments, a brief discussion on CFD and ROM model complexities is included. Figure 7 shows the components integral to the CFD simulations. These simulations consist of gas and solid phase models, as well as a radiative heat transfer model. The flowchart in Figure 7 lists all of the submodels that make up each of the primary models, as well as the interactions between them. The models presented in this study were carried out utilizing the NIFTY computer cluster at West Virginia University, which consists of 96 GB RAM, 2TB Network Storage 6 Dual Quad-Core Xeon 2.66 GHz Processor Nodes, each node containing a total of 8 processors. A single simulation case running on a single one of these nodes took approximately 10 hours of computational time to complete. In comparison, the reduced order model (ROM) presented in this work can be carried out on a single personal computer, in this case a Dell Inspiron Laptop with an Intel i5 2.5 GHz processor with 8 GB RAM, in approximately 30 minutes. In addition, if the flow rates of fuel (i.e., coal) are held constant, and only the flow rates of the oxygen/carbon dioxide oxidant mixture are varied, different cases can be computed in approximately 10–15 minutes. In either case, this represents significant resources savings over full-blown CFD simulations. A flowchart depicting the complexity of the ROM procedure is shown in Figure 8.

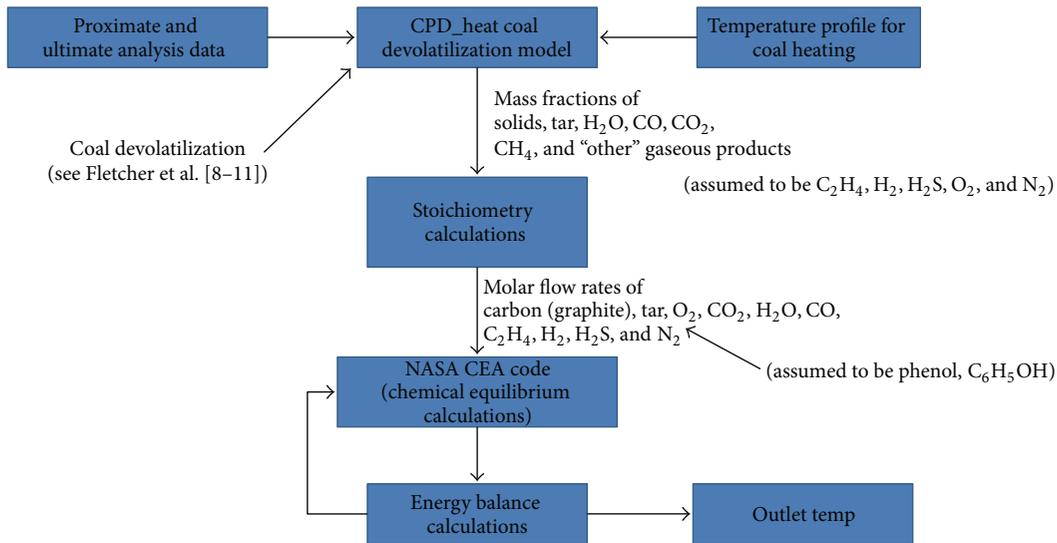


FIGURE 8: Reduced order model (ROM) computational flowchart.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

Acknowledgment

This technical effort was performed in support of the US-China Clean Energy Research Center–Advanced Coal Technology Consortium’s (CERC-ACTC) ongoing research in clean coal conversion processes under the DOE Contract DE-PI0000017.

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