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| Technical Report on CCSI’s Boiler Model | February 28  2014 | |
| This report describes the details of the hybrid 1-D reacting flow and 3-D radiation boiler model developed for DOE’s CCSI project. The theories and equations are described first followed by numerical algorithm software design in C++. The boiler model can be used to simulate both air-firing and oxy-firing configurations of pulverized-coal-fired boilers. The validation of the boiler model is also reported using the results from CFD simulations of two existing utility boilers | | Theory, implementation and validation |

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# Introduction

Oxy-combustion is a modern combustion technology that enables the capture of the green-house gas carbon dioxide (CO2). The design of an oxy-combustion system for CO2 capture involves the integration of multiple devices in the system including air separation unit, pulverized coal-fired (PC) boiler, flue gas cleanup and recirculation unit, flue gas compression unit, steam turbines, and electric generator. Thousands of design parameters for the entire system need to be optimized to achieve the lowest cost per kilowatt-hour of electricity generated. Modern optimization packages such as General Algebraic Modeling System (GAMS) enable the use of large scale nonlinear programming algorithms to efficiently optimize systems with 100,000+ variables, provided algebraic models are available. The radiant furnace of a PC boiler is a main device in the oxy-combustion system. Heat released from the combustion of the pulverized coal inside the radiant furnace is transferred to the water inside the tubes of the enclosure walls and to the steam inside the tubes of superheaters. The detailed physics of the turbulent multiphase reacting flow inside the furnace can nowadays be modeled using Computational Fluid Dynamic (CFD) software. However, the CFD model is very CPU intensive and, therefore, inappropriate for a system-wise large-scale optimization. On the other hand, over-simplified boiler models such as ideal reactor models found in commercial process modeling software usually do not fully consider the effects of the shape and the size of the radiant furnace, the locations of burners and over-fire air ports. It is highly desired that a first principle-based boiler model be developed for system optimization that is more sophisticated than the ideal reactor model but much faster than the CFD model.

Historically the designs of radiant furnaces by boiler manufacturers were carried out using company proprietary empirical correlations based on their previous installations. Those empirical curves are usually plotted or expressed in some forms of non-dimensional parameters based on the principle of similarities. The shapes and dimensions of the enclosure water walls and superheater walls of a radiant furnace should be designed to absorb the desired amount of heat while keeping the heat flux to the water wall tubes small enough to avoid excessive slagging and overheating of the boiler tubes and to keep the temperature of the flue gas leaving the furnace below the fusion temperature of the ash from the pulverized fuel such that the fouling on the downstream convective heat transfer surfaces can be minimized. The empirical correlations are valid for conventional firing configurations. However, when the firing configuration is dramatically changed as in the case of oxy-combustion, those empirical correlations are very likely invalid. Therefore, models based on the first principles have to be used.

The dimensions of a boiler determine the total heat transfer surface area, which determines the weight of the tube metals and the capital cost of the boiler. A boiler with a defined heating rate should be designed large enough to ensure a) the defined amount of heat can be transferred to the water walls and superheater walls, b) the complete combustion of fuel with minimum amount of oxidant and the highest possible boiler efficiency, and c) the minimum amount of pollutants formed. Traditionally boilers were designed to meet the first requirement. The second and the third requirements become also important nowadays due to the higher fuel prices and more stringent environmental regulations. Note that the first requirement is mainly related to the heat transfer while the other two requirements are related to the reaction kinetics. A good boiler model should accurately account for both the heat transfer and reaction kinetics.

The theory section of this report will describe the principles, assumptions and equations applied to the boiler model that has been developed. The numerical schemes and software implementation are discussed in implementation section along with the descriptions of C++ classes developed for the boiler model. The validation of the boiler model will be provided in the last section of the report.

# Theory

One-dimensional zonal method has been used to model pulverized coal-fired boilers and entrained flow gasifiers in the literature (Beijing Boiler Works, 1973; Gazzani et al., 2013). Since combustion flames are at very high temperatures and the ratio of wall surface area to furnace volume is quite low in a typical utility boiler, the radiation heat transfer is the dominant heat transfer mechanism in the radiant furnace. A zonal boiler model called Russian normative method was developed in 1970s to model the radiation heat transfer inside radiant furnaces firing pulverized coals. In that model, however, the radiation properties of both gas and particles were based on empirical correlations and the radiative heat exchange between two neighboring zones were also modeled based on empirical correlations. The radiant furnace was considered as optically thick and only the heat exchange between two neighboring zones was considered. Therefore, the model cannot be considered as the first principle model. Modeling of radiative heat transfer with gas and particle participating media has been dramatically improved since 1980s. Advanced models such as P-1 model and discrete ordinates (DO) model have been applied to commercial CFD software packages and implemented on discretized 3-D meshes (Fiveland, 1988; Chui and Raithby, 1993; Murthy and Mathur, 1998). The DO method can solve the radiation intensity in space and in predefined directions known as discrete ordinates. It can consider all terms in the radiative transfer equation including emission, scattering, and adsorption of participating media in both gas and solid phases. However, since the radiation takes place in 3-D space and in any directions, a 3-D mesh has to be used. To obtain an accurate prediction of the radiative heat transfer, a 3-D unstructured mesh is automatically generated in the boiler model with the mesh resolution defined by the user and used for radiative heat transfer calculations. This approach is similar to that applied to a 3-D CFD model. To limit the CPU time required to solve the 3-D radiation problem, a coarser mesh than that of a typical CFD model is used in the boiler model developed here.

While the radiative heat transfer is solved in 3-D in the boiler model, the reacting flow inside the furnace is solved in 1-D along the height of the furnace. Each zone is modeled as a well-mixed ideal reactor with uniform temperature and uniform flow properties except the radiative intensity. In other words, the detailed local fluid dynamics is not modeled and only the average velocities across horizontal cross sections are calculated. Chemical kinetics of heterogeneous reactions between char and gas species are modeled using the average residence time of each zone. Reaction kinetics, material balance and energy balance are modeled inside each zone with the assumption that the gas phase reactions always reach local chemical equilibrium in each zone.

The overview of the boiler model, the detailed model assumptions, and equations involved are described below.

## Boiler model overview and spatial discretization

Figure 1 shows a schematic of the boiler model for a typical pulverized coal-fired utility boiler with a hopper at the bottom and a nose near the flue gas exit. Note that flue gas exit plane here is defined as the vertical plane above the nose tip. The radiant platen superheaters as shown in Figure 2 in green are also included in the model as boundary walls while the convective superheaters usually downstream of the vertical exit plane are excluded from the radiant furnace model. The 3-D mesh is generated automatically after the shapes of boiler enclosure walls and the superheaters are specified as well as the number of zones along the furnace height and the number of cells in each zone in the height, depth and width directions. The 3-D mesh consists of unstructured hexahedron cells with top and bottom faces always in horizontal planes and the number of cells in each direction constant throughout the 3-D domain.

Figure 1. 3-D mesh and zones in the hybrid boiler model

Figure 2. Radiant platen superheater walls (in green) inside boiler model

The Cartesian coordinate system is used to define the dimensions of a boiler in the boiler model. As shown in Figure 2, X is in the depth direction pointing from the front wall to the rear wall with X=0 at the front wall. Y is in the height direction pointing from the bottom of the hopper to the roof with Y=0 at the bottom of the hopper. Z is in the width direction pointing from the left side wall to the right side wall with Z=0 at the left side wall. The shape of a superheater can be defined as a polygon in X-Y plane. Multiple panels of platen superheaters along the furnace width can be defined and all of them should be parallel to the side walls (in X-Y plane). Currently they are always evenly spaced along the width. The number of the cells in the width (Z) direction should be large enough such that there are at least two cells in the Z direction between two neighboring panels. In case there are wing walls or a partial division walls inside the furnace, they can be modeled in the way similar to a superheater panels using polygon shapes.

Note that other boiler designs such as arch-fired design are currently not allowed due to the complexity of the flow pattern. Tower unit with flue gas exit at the top can be modeled if the tip of the nose is set at the rear wall. The fuel and oxidant are fed to the furnace at different elevations through burners and overfire air ports. The gas mixture and the coal particles flow upward. The 1-D zones are numbered from the hopper to the roof of the furnace with the first zone always covers the entire hopper. The zones from hopper knuckle to the bottom of the nose (Zones 2 through 7 as in Figure 1) are usually the burner and overfire air zones. The number of zones in this region is defined by the modeler with a large number generally leading to a more accurate simulation result but longer computational time. The zones from the bottom of the nose to the nose tip are called the nose zones and the zones from the tip of the nose to the roof are called the upper zones. Again the numbers of zones in those regions are user inputs. Currently the roof is always in the horizontal plane and it becomes the exit plane if the tower unit option is selected.

Any cell in the 3-D mesh is assigned to a specific zone. The interaction between the 3-D cells and 1-D zones will be discussed in the equation section. Note that each cell has six faces and some of which are boundary faces. A cell that does not contain any boundary faces is an interior cell. Likewise, a face could either be an interior face or boundary face. There are two types of boundary faces, namely, the wall boundary face and the outlet boundary face. For a wall boundary face, the boundary conditions include wall emissivity, backside fluid (liquid water or steam) temperature, and overall thermal resistance for heat conduction through the slag layer and tube metal layer, and the heat convection from the inner tube wall to water or steam inside a wall tube. These wall boundary conditions can be specified as inputs for individual superheaters and for furnace enclosure water wall. For a sub-critical unit, the enclosure wall boundary conditions can be uniform throughout the entire enclosure wall since the temperature of the water and steam mixture is simply the saturation temperature at the operating pressure of the drum. For a super-critical unit, fluid temperature changes along the furnace height and the boundary conditions can be specified zone by zone. The inside wall temperature (the slag layer) of the furnace at each boundary face is actually calculated based on the energy balance at individual face (see the equation section). For the outlet boundary faces, only the emissivity and temperature of outside objects that receive the radiation are needed.

## Model assumptions

Seven main assumptions for the first principle boiler model are listed below.

1. Ignore uneven spatial velocity, temperature and other property distributions within a zone. Average uniform upward flow velocity is calculated based on continuity and ideal gas law. Average residence time is calculated likewise. Momentum equation is not solved.
2. Gas phase in each zone is in chemical equilibrium. In other words, the reaction kinetics of the homogeneous reactions in the gas phase is ignored. However, the amount of unreacted mass in the solid phase in each zone is calculated from char oxidation and gasification kinetics. Each zone is modeled as a well-mixed reactor.
3. Ignore the velocity difference between coal particles and the gas phase. Coal particles are assumed to have the same velocities as the gas mixture and hence the same average residence time as the gas mixture.
4. Temperatures of coal particles of all sizes are the same as the temperature of the gas phase in each zone.
5. The moisture evaporation and coal devolatilization are very fast processes and complete immediately after coal particles enter a zone in the radiant furnace. Ash from coal is inert and stays in the particle phase. Coal particles do not fragment.
6. Ignore convective heat transfer between boundary walls and the gas mixtures nearby.
7. Inner walls of the furnace including the superheaters are gray and diffuse.

The assumption of uniform properties in each zone (Assumption 1) is the simplification due to the limitation of a 1-D model. It is well known that pulverized coal burners are designed to generate swirling flows near the burner outlets to stabilize the coal flames and to reduce the generation of NOx. The 1-D model certainly cannot resolve the complicated flow field near coal burners and, therefore, cannot be used to help burner design. However, in terms of overall heat transfer rate along the furnace walls, this simplification is believed not to cause too much simulation errors. Actually the swirling flow could causes enhanced mixing between fuel and oxidant which make the well-mixed reactor a valid assumption.

Assumption 2 is generally valid since the temperatures in the radiant furnace are always very high, which causes gas phase chemical reactions to reach equilibrium. Actually most CFD models have the same assumption except that the equilibrium properties are calculated considering the effect of turbulence in terms of variance of mixture fractions. Since the boiler model developed here does not solve the turbulence, the turbulence effect on average equilibrium properties is not accounted for.

Assumption 3 is acceptable since pulverized coal particles are very small (<200 micron) and the slip velocity of a coal particle (the difference of velocities between a particle and its nearby gas) is very small, which can be verified by CFD models.

Assumption 4 is also acceptable. Based on CFD models, the maximum temperature difference between coal particles and the nearby gas mixture is usually less than 50 K, again due to small particle sizes.

Since the temperatures inside a radiant furnace are very high, both the convective and radiation heat transfer mechanisms will heat the particle very quickly. Assumption 5 is valid since the two processes complete in less than 100 milliseconds. Note that a high heating rate usually causes a higher volatile yield and, therefore, a volatile yield higher than that from coal proximate analysis should be used as the boiler model input.

For large-scale boilers, the ratio of the wall surface area to the volume of the furnace is very small and the convective heat transfer rate is relatively small compared to the radiative heat transfer rate. Based on CFD model simulations, radiative heat transfer rate accounts for more than 90% of total heat transfer rate. Therefore, the convective heat transfer can be ignored in the boiler model as indicated in Assumption 6. Slight increase in the model input of wall emissivity could compensate for the ignored convective heat transfer rate. It is recommended that only radiant platen superheaters be included in the boiler model and the convective superheaters be excluded. The boiler model exit plane is set at the vertical plane above the nose tip by default. Convective superheaters are usually located downstream of that exit plane.

Assumption 7 is usually valid since furnace tube walls are diffuse and its emissivity is usually not wavelength dependent.

## Equations

With the assumptions described in the previous section, the reacting flow and heat transfer in a radiant furnace can be modeled in a hybrid mode with radiative heat transfer solved using the 3-D mesh and the reacting flow solved in 1-D zones along the furnace height. The solution of the 3-D radiation heat transfer equations provides the heat losses of individual cells in a zone, which can be summed up to obtain the total heat loss of the zone. With the obtained total heat losses of individual zones, the total enthalpies of gas and solid leaving individual zones can be calculated and chemical equilibrium calculations can be performed to obtain the mixture temperatures and mole fractions of gas species at a given coal burnout for the zone. The coal burnout in each zone can be calculated from the char reaction kinetics based on the temperature and mole fractions of gas reactants in the zone using the average residence time of the zone. Meanwhile, the radiation properties of each zone for both gas and particle phases can be updated and assigned to all cells in the zone. All the equations related to radiative transfer, mass and energy balance, chemical equilibrium, and coal reaction kinetics can be solved numerically in an iterative manner.

Radiative heat transfer takes place in a particle-laden medium enclosed by boundary walls in all directions of steradian solid angle across the spectrum of all wavelengths. Since it is always 3-dimensional in nature, it has to be solved on the 3-D mesh. Radiative transfer equation as shown in Eqn. 1 describes the physics of the radiative heat transfer in a participating medium consisting of a gas mixture and solid particles.

Eqn. 1

where , and are respectively the radiation intensity, black body emission intensity, and the distance in the direction defined by the solid angle . and are the absorption and scattering coefficients of the radiation medium (gases and particles), respectively. is the phase function for the scattering from direction to the direction. The in-scattering term (the last term in Eqn. 1) contains the integration over steradian solid angle. Both gas and particle phases contribute to and . For example, is the sum of the gas phase absorption coefficient and the particle phase absorption coefficient as shown in Eqn. 2.

Eqn. 2

For the radiation in the infrared region as in a typical coal-fired boiler, the gas phase scattering can be ignored and the particle phase scattering is assumed to be forward scattering dominant. The weighted-sum-of-gray-gases model (WSGGM) is used to calculate . The radiation intensity in Eqn. 1 represents the overall intensity across entire spectrum. is related to local gas emissivity and optical mean beam length of the entire flow domain by Eqn.3.

Eqn. 3

The gas emissivity in the boiler model is calculated based on a narrow-band model (Grosshandler, 1993) developed at National Institute of Standards and Technology (NIST) in which absorptions of individual species including O2, N2, CH4, CO, CO2, and H2O over the entire infrared spectrum are integrated line by line to obtain the average emissivity. The modeled gas emissivity can be expressed as a function of the mole fractions of individual gas species, gas temperature , total pressure and mean beam length as shown in equation 4.

Eqn. 4

The optical mean beam length is related to the total volume of the flow domain and the total area of boundary faces by Eqn. 5.

Eqn. 5

This model is believed to be more accurate than the traditional Hottel chart model based on experimental data in typical air-firing conditions. NIST’s model can be used for oxy-combustion conditions in which CO2 and H2O concentrations in the gas phase are quite high.

in Eqn. 2 can be calculated based on the number densities of the particles, their diameters and their absorption efficiencies. If there are size bins of spherical particles, is expressed as

Eqn. 6

where , , and are the number density, diameter, and absorption efficiency for size , respectively. The contribution from each particle is based on the projected area. is a function of wave length and particle optical properties, which are functions of particle temperature. For spherical particles, it can be calculated based on Mie theory (Mie, 1908). Since the organic part of the char and the ash in a particle have different optical properties, two separate absorption efficiencies can be calculated for a particle with given diameter and temperature, one for the organic particle and the other for the ash particle. The absorption efficiencies at different wavelengths are convoluted over the entire infrared spectrum to obtain the average efficiency over the spectrum. In the boiler model, two separate tables are set up in the model initialization stage for the lookup of average efficiencies for organic and ash particles, respectively, at a given temperature and particle diameter. The value of in Eqn. 6 is actually calculated as the weighted average of the organic char and ash particles based on the mass fraction of dry-ash-free organic content and the ash content in a char particle. The number density can be calculated by the number flow rate of the particle , the residence time and the volume of the zone the particle travels through as shown in Eqn. 7.

Eqn. 7

Actually multiple time steps are used in the boiler model to track heterogeneous char/gas reactions through a zone. Therefore, the actual time step is used in place of in Eqn. 7 and the total for the zone are summed up over the multiple time steps.

After the radiation intensity in the radiative transfer equation is solved, the irradiance at a point inside a flow domain can be calculated from the radiation intensity by integration over the steradian solid angle.

Eqn. 8

When the radiation intensities are solved in discrete ordinates (directions) of the solid angle in the boiler model, the integration in Eqn. 8 is calculated as the summation of discretized intensity at a direction multiplied by the weight the direction represents in the solid angle.

The radiation heat loss per unit volume is the flux divergence considering both the absorption and emission of the participating medium and can be calculated as

Eqn. 9

where is the Stefan-Boltzmann constant (= W/m2-K4) and is the gas and particle mixture temperature at the zone the cell belongs to. The heat loss of a 3-D cell due to radiative heat transfer can be calculated by multiplying by the cell volume and the total heat loss in a zone can be calculated by summing up the heat losses of all cells in the zone as shown in Eqn. 10.

Eqn. 10

where and are the heat loss per unit volume and the volume of Cell in the zone, respectively. The summation is over total number of cells in the zone. This heat loss term for the zone is used to calculate the enthalpy of the gas and solid mixture in the zone.

The wall of a radiant furnace can usually be assumed as gray and diffuse (Assumption 7). The incident heat flux towards the wall surface can be calculated by integration over the steradian solid angle of the hemisphere facing the flow domain. In a spherical coordinate system, the incident radiation heat flux can be calculated from the radiation intensity along the azimuthal and polar angles.

Eqn. 11

where and are azimuthal and polar angles, respectively. Note that if the radiation intensity is isotropic (uniform in any directions), the incident heat flux integrated from Eqn. 11 will be . Also note that Eqn. 11 can be evaluated as a summation over the intensities and angles of all discrete ordinates in a hemisphere relative to the normal direction of a boundary face with weighting factors for individual directions. A good discretization scheme makes the summation very close to if the intensity in every direction is unity.

A gray and diffuse wall with an emissivity is able to emit radiation and reflect part of the incident radiation heat flux. The sum of the emitted and reflected radiation heat flux can be computed as

Eqn. 12

No transmission through the wall is considered in Eqn. 12. The net radiation heat transferred from the wall to the flow domain is

Eqn. 13

For a diffuse wall, the isotropic outward radiation intensity can be expressed as

Eqn. 14

The net radiation flux from the wall to the gas-solid mixture in the furnace is also used to calculate the wall temperature based on Eqn. 15.

Eqn. 15

where , , and are respectively the temperature of the fluid (water liquid or steam) inside the wall tube, the slagging layer wall temperature, and the overall heat transfer resistance including the heat conduction through the slagging layer and metal wall and the convective heat transfer between the inner tube wall and the fluid inside the wall tube. Note that the wall temperatures of wall boundary faces on the mesh have to be iteratively solved. From an initial guess of the wall temperatures, the radiative transfer equation can be solved and the incident heat flux in Eqn. 11 can be obtained and then the wall temperature can be solved for each wall face by combining Eqns. 12, 13 and 15 and using a root finding method such as Newton’s method.

Numerically, the radiative transfer equation (Eqn. 1) is discretized to a set of discrete ordinates and solved using the discrete ordinates (DO) method (Chui and Raithby, 1993; Murthy and Mathur, 1998). 20 discrete ordinates are used in the current boiler model with its directional cosines calculated based on 20 vertices in a regular dodecahedron, a special polyhedron known as Platonic solid as shown in Figure 3. The direction of a discrete ordinate can be defined by the unit vector pointing from the center of the dodecahedron to a vertex (a red dot in Figure 3). One important property of the discrete ordinates based on Platonic solid is that the weights for all ordinates are the same. For the 20 discrete ordinates based on the dodecahedron, the weight is . Historically 24 discrete ordinates known as S4 discretization scheme and 48 discrete ordinates known as S6 discretization scheme were used for structured meshes with non-uniform weights (Fiveland, 1988). Those schemes can make the summation based on Eqn. 11 exactly equal to when radiation intensity is unity for a boundary face perpendicular to either x, y, or z direction, which is the case for a structured mesh. For an unstructured mesh with wall faces’ normal directions not always pointing to x, y or z direction, that property for the S4 and S6 is no longer valid. It was found that the discretization scheme in the boiler model based on 20 vertices of a dodecahedron is reasonably accurate and is faster than the S4 discretization scheme.

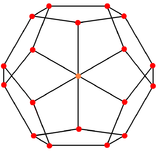
[](http://en.wikipedia.org/wiki/File:Dodecahedron_t0_A2.png)

Figure 3. A regular dodecahedron with 12 faces and 20 vertices

A special algorithm is used to solve the discretized radiative transfer equation in each direction. Spatially, the radiation intensity is solved at the centroids of all cells and the centroids of boundary faces on the unstructured mesh. Since the radiation intensity at any given direction is always positive and pointing from one side of the flow domain (upstream side) to the other side (downstream side) depending on the directional cosines of the discrete ordinate, the iterative algorithm is always applied from the upstream boundary faces to the downstream boundary faces through the cells in a special sequence. Actually all cells in the mesh are presorted based on the location of the cell centroid in the direction of the given discrete ordinate. There are 20 sorted cell lists, one for each discrete ordinate. Unlike the typical Gaussian-Seidel smoother or Jacobi smoother in which the solved value of a cell is calculated by all its neighbors including both downstream and upstream neighbors, the radiation intensity of a downstream cell is calculated by its upstream neighboring in the boiler model by taking advantage of the radiation physics involved. The sequence of the calculation of the intensity for the cells in the flow domain is in the presorted cell sequence. Therefore, the solving process is like marching from the upstream cells to the downstream cells in the direction of the discrete ordinate. This approach can reach a converged solution very quickly. One iteration sweep involves one set of iterations in individual discrete ordinates. After each sweep, the boundary conditions of Eqns. 12-15 are applied for all boundary faces and new wall temperatures of the boundary faces are solved. The iteration continues until the net flux and wall temperature on each boundary face converges.

The discretized radiative transfer equations described above are solved based on given flow field properties of individual zones including the temperature, gas and solid absorption coefficients, which are related to gas phase species mole fractions, particle sizes and particle compositions. These field properties are calculated by the mass and energy balances based on the assumptions made in the assumption section. In the boiler model, the mass balance of individual elements as well as ash is calculated zone by zone. The material leaving a zone contains both gas and solid phases. The leftover elements including C, H, O, N, S, and ash in the solid phase are those remained in char particles after coal moisture vaporization, coal devolatilization, and char reactions. The boiler model assumes that all the ash from the coal feed streams is inert and stays in the solid phase. In other words, no ash is vaporized and released to the gas phase. The total mass of an element contained in the gas species and in the unburned char particles that leave a zone is always conserved and can be calculated from the feed streams below the zone as shown in Eqn. 16.

Eqn. 16

where is the elemental mass flow rate of element from feed stream and is the number of feed streams below the top horizontal plane of the zone.

While the total elemental flow including the ash flow has nothing to do with the coal reaction kinetics, the amount of leftover element in the solid phase in each zone is dependent on coal and char kinetics. The leftover element mass flow rate from a specific feed stream and a specific solid size bin can be calculated by tracking the coal particle through individual zones above the feed stream inlet. The tracking algorithm is very similar to the Lagrangian discrete phase model (DPM) in some commercial CFD software packages except that the particle temperatures are assumed to be the same as zone temperatures and the energy equation for the particle along its trajectory is not solved. Before the particle tracking calculations, the average residence time of each zone or each well-mixed reactor is calculated based on the mass flow rate of gas phases leaving the zone and the mass of gas mixture in the zone calculated based on the volume of the zone and the gas density of the zone as shown in Eqns. 17 and 18.

Eqn. 17

Eqn. 18

In case a feed stream with coal particles enter the zone above the bottom horizontal plane of the zone, the residence time of the tracked particle in the zone is calculated as a fraction of the zone residence time. The fraction is the ratio of the distance it travels from the inlet to the top of the horizontal plane of the zone to the height of the zone as shown in Eqn. 19.

Eqn. 19

where , and are the heights of top and the bottom planes of the zone, and the height of inlet location of the feed stream, respectively.

The Lagrangian tracking of individual coal particle through individual zones on its path to exit is performed in the boiler model to calculate the amount of elements remained in the solid phase and the particle radiation absorption coefficient (see Eqn. 6). Since the fraction of unburned organic material in a char particle, its diameter and temperature change along the particle trajectory, the particle absorption coefficient needs to be updated at each integration time step. Based on the model assumption, the coal moisture vaporization and coal devolatilization reactions are assumed to be completed immediately upon a coal particle’s entry to the boiler, the mass of the fresh char particle upon the completion of the moisture vaporization and coal devolatilization can be expressed as:

Eqn. 20

where is the mass of the original coal particle, is the mass fraction of moisture in the original coal particle, and is the volatile content (mass fraction) in the original coal particle. can be calculated from the particle density and original particle diameter as shown in Eqn. 21.

Eqn. 21

The number flow rate of the particles from a feed stream in a specific size bin can be calculated by the particle mass flow rate in the size bin .

Eqn. 22

Note that the boiler model assumes no particle fragmentation and therefore, the number flow rate remains constant throughout the entire particle trajectory.

During coal devolatilization, the diameter of the coal particle could increase slightly, which is known as particle swelling. The swelling factor defined as the fraction of the increase in particle diameter from the original diameter depends on the coal type. For example, high volatile bituminous coals have a swelling factor around 0.1. The diameter of a fresh char particle after the completion of devolatilization is related to the swelling factor and original diameter by

Eqn. 23

The density of the fresh char particle can be calculated by the mass of the char particle from Eqn. 20 and the diameter from Eqn. 23.

Eqn. 24

After the moisture and the volatiles are released, the remaining char particle will undergo heterogeneous reactions with reactants in the gas phase including O2, H2O and CO2. The reaction with O2 is known as the oxidation or combustion reaction and the reactions with H2O and CO2 are known as the gasification reactions. During the heterogeneous reactions, the char particle usually shrinks and the density of the char particle also decreases. Eqn. 25 relates the particle density to the particle mass during heterogeneous char reactions.

Eqn. 25

where exponent is called the burning mode parameter. From Eqn. 25, the diameter of the char particle can be expressed as

Eqn. 26

The heterogeneous reaction between the char particle and a gas species involves the film diffusion of gas reactant to the external surface of the particle through the boundary layer, the pore diffusion of the reactant to the internal surface of the char and the reaction on the internal char surface. Some products of the heterogeneous reactions such as CO could also react in the boundary layer with other species in the gas phase. Depending on the reaction temperature, particle size and reactant concentrations in the bulk gas mixture, the reactions could fall in three reaction categories or zones, namely, the film diffusion controlling, the pore diffusion controlling, and the kinetics controlling zones. Different char reaction kinetics can be found in the literature considering the processes mentioned above. In the current boiler model, global kinetic models are used which expresses the reaction rate based on the reactant concentrations at the external surface of the particle and the external surface area. The concentrations of the reactants at the external surface of the particle are solved by equating the reaction rate calculated from kinetics to the rate of the mass transfer of the reactant through film diffusion. The three heterogeneous reactions considered in the boiler model can be expressed in a general form as in Eqn. 27

Eqn. 27

where , , and are the gas reactant and the two gas products of Reaction , respectively. The corresponding stoichiometric coefficients are , and . Table 1 lists the reactants, products, and the stoichiometric coefficients for the three heterogeneous reactions modeled.

Table 1. Reactant, products of char heterogeneous reactions and their stoichiometric coefficients

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Reaction |  |  |  |  |  |  |
| 1 | O2 | CO2 | CO |  |  |  |
| 2 | H2O | H2 | CO | 1 | 1 | 1 |
| 3 | CO2 | CO | N/A | 1 | 2 | 0 |

Note that the char oxidation reaction (Reaction 1 in Table 1) could form both CO2 and CO as the products. Usually more CO is formed when particle temperature is higher and film diffusion controls. The ratio of the stoichiometric coefficients of CO2 to CO is defined as parameter , which can be expressed as an Arrhenius function of particle temperature as shown in Eqn. 28.

Eqn. 28

where , , and are the pre-exponential factor, activation energy, and particle temperature, respectively. in Eqn. 28 is the universal gas constant. The bulk flow is outward for char reactions. The net outward molar flow per mole of C reacted for Reaction can be expressed as

Eqn. 29

The rate of heterogeneous reaction can be expressed in a general global rate form based on the unit external surface area for Reaction as

Eqn. 30

where is the reaction rate in kmol-C/m2s and double prime “” symbol indicates the rate based on the unit external surface area. and in Eqn. 30 are the pre-exponential factor and the activation energy for Reaction . is the exponent of temperature and is the reaction order. is the molar concentration of gas reactant at the external surface of the particle, which is related to mole fraction of the reactant and total molar concentration of the gas mixture

Eqn. 31

The total molar concentration can be calculated from total pressure based on ideal gas law as shown in Eqn. 31.

The half-order char oxidation reaction model reported by Hurt (Hurt and Mitchell, 1992) is used to model the first heterogeneous reaction in Table 1 along with his burning model (Eqn. 25) and CO2 to CO stoichiometric coefficient ratio model (Eqn. 28). The first-order kinetic models are used for char gasification reactions by H2O and CO2. Table 2 shows the temperature exponents and reaction orders for the three char reactions modeled.

Table 2. Temperature exponent and reaction order for char heterogeneous reactions

|  |  |  |  |
| --- | --- | --- | --- |
| Reaction | Gas Reactant | Temperature Exponent | Reaction Order |
| 1 | O2 | 0.5 | 0.5 |
| 2 | H2O | 1 | 1 |
| 3 | CO2 | 1 | 1 |

The mole fraction of reactant at external surface of a char particle is usually lower than that in the bulk of the gas mixture . If the reaction is kinetics controlling, they are very close to each other. If the reaction is film diffusion controlling, the surface mole fraction will be very close to zero. To consider a general condition where both the diffusion and kinetics are important, the surface mole fraction needs to be solved by the stoichiometric relationship of the C reactant and the gas reactant.

Eqn. 32

where is the molar flux of gas reactant of Reaction reached to the particle surface through mass transfer. can be expressed as

Eqn. 33

The first term on the right hand side of Eqn. 33 accounts for the diffusion of the gas reactant from the bulk gas mixture stream to the particle’s external surface and the second term accounts for the effect of convection due to net outward flow from the particle to the bulk stream. is the net outward molar flux of gas species leaving the char particle due to the three reactions.

Eqn. 34

in Eqn. 33 is the mole fraction based mass transfer coefficient, which can be calculated from the uncorrected concentration based mass transfer coefficient and a correction factor due to high mass transfer rate , also known as blowing factor.

Eqn. 35

Based on the film theory (Bird et al., 1960), the blowing factor is related to the flux ratio by

Eqn. 36

and flux ratio is defined as

Eqn. 37

The concentration based mass transfer coefficient can be calculated from Sherwood number, which is approximately equal to 2 when slip velocity between the particle and the gas mixture is ignored. Therefore,

Eqn. 38

where is the molecular diffusivity of the gas reactant of Reaction in the gas mixture and is the particle diameter. As an approximation, the diffusivity of the reactant (O2, H2O, or CO2) in N2 is used in the boiler model to avoid calculating complicated binary diffusivities in the mixture.

Combining Eqns. 30-33, the equation for solving the surface mole fraction of the gas reactant of Reaction can be expressed as

Eqn. 39

Note that at a given , the blowing factor and can be calculated based on Eqns. 35-38 and then the surface mole fraction in Eqn. 39 can be solved. For the two char gasification reactions in which the reaction order is 1, Eqn. 39 is a linear equation and can be solve in algebraic form. For the char oxidation reaction, the reaction order is 0.5, can also be solved using the quadratic equation formula. Since is unknown *a priori*, an iterative procedure has to be used. Initially it is set to zero and the surface mole fractions of three gas reactants are solved followed by the calculation of and . The new is used thereafter until a converged solution is reached, usually within 3 iterations.

The char reaction rate in term of mass loss per particle per unit time can be calculated after for each reaction is calculated.

Eqn. 40

where is the molecular weight of C. It is assumed that the remaining unreacted char still contains other elements (H, O, N, S) in addition to C and the proportion of those elements is still the same as that in the parent coal. The high heating value of the dry-ash-free part of the char is also assumed to be the same as that of the parent coal, which is used to calculate the enthalpy of the remaining char.

It needs to be mentioned that the char reaction rate calculations described above are performed for every time step during the particle trajectory calculation. Multiple time steps are used during the trajectory calculation for a coal particle from a feed stream in a given size bin. Particle mass and diameter are updated in each time step based on Eqns. 26 and 40. The particle radiation absorption coefficient is also updated for each time step.

With heat loss of each zone calculated from DO method and solid phase mass flow leaving the zone calculated from the coal particle tracking method mentioned above, the flow properties of each zone including temperature and species mole fractions in the gas phase are calculated by minimizing the Gibbs free energy of the gas and solid mixture at given solid phase composition (computed from particle tracking) and the given gas phase elemental composition. The gas phase elemental mass flow rate for each element is simply the total mass flow rate of the element calculated by Eqn. 16 minus its flow rate in the solid phase

Eqn. 41

The local chemical equilibrium calculation in the gas phase of each zone is carried out using Lagrangian multiplier’s method with mass conservation for each element as the constraints. The gas mixture is assumed to be an ideal gas mixture with partial molar Gibbs free energy of a species related to Gibbs free energy of the pure species and the mole fraction of the species in the mixture as shown in Eqn. 42.

Eqn. 42

The mole fraction of species is related to the specific mole defined as the kmoles of species in 1 kg of gas mixture.

Eqn. 43

where is the total number of gas species in the gas mixture. The total Gibbs free energy of the gas mixture can be calculated as

Eqn. 44

To solve the chemical equilibrium, the Gibbs free energy of the gas mixture shown in Eqn. 44 is minimized subject to the constraints of element conservation as shown in Eqn. 45.

Eqn. 45

where is the number of atoms of element in a molecule of species and is the kmoles of atoms of element in 1 kg of the gas mixture, which can be calculated from Eqn. 41.

A set of non-linear equation can be obtained based on the Lagrangian multiplier’s method to minimize in Eqn. 44 subject to the constraints in Eqn. 45. Actually, natural logarithms of the specific moles of individual species are solved as the independent variables. The logarithm transformation allows for accurate equilibrium solutions to minor species with specific moles very small. The non-linear equation set is solved using Newton’s method with initial guess based on the equivalence ratio of the mixture. It needs to be pointed out that the temperature of the zone is iteratively solved from the chemical equilibrium calculations at constant pressure and temperature to match the total enthalpy of the gas and solid mixture calculated by considering the heat loss from Eqn. 10.

The Gibbs free energy of a pure gas species as well as the heat capacity and enthalpy is calculated based on the Joint Army Navy and Air Force (JANAF) thermodynamic table. The boiler model currently considers 11 species including C(S), O2, N2, H2, CO, CO2, H2O, SO2, H2S, CH4, and Ar. Their JANAF table coefficients are built in the boiler model.

The properties of coal are calculated as the weighted averages of the moisture, dry-ash-free content, and ash. The heat capacities of moisture and ash in the parent coal are calculated as linear functions of particle temperature,

Eqn. 46

Eqn. 47

The heat capacity of the dry-ash-free part of the coal is calculated based on Merrick’ formula (Merrick, 1983).

Eqn. 48

where is the universal gas constant, is the particle temperature in K and as a function of is defined as

Eqn. 49

in Eqn. 48 is the average atomic weight of the dry-ash-free coal calculated from the mass fraction of individual element .and its atomic weight .

Eqn. 50

The summation in Eqn. 50 is over 5 elements in coal (C, H, O, N, and S).

The standard heat of formation for the dry-ash-free coal is calculated from high heating value (HHV) of the coal.

Eqn. 51

Where is the reference temperature at 298.15 K, is the mass fraction of Element , is the atomic weight of Element , and is the heat of reaction for burning Element to the combustion product. Note that the HHV in the proximate analysis is usually measured in constant volume condition and the second term on the right hand side of Eqn. 51 accounts for the conversion to constant pressure based enthalpy due to the difference between total moles of products and those of the reactants.

# Numerical Algorithm

Equations listed in the theory section are solved numerically in the boiler model. Figure 4 shows the work flow of the numerical algorithm.

Figure 4. Numerical solution procedure for the boiler model

The main function of the C++ code for the boiler model reads the input data from an input file and then calls a function called SolveBoilerModel(), passing the input data as the parameter to the function. The input data include the boiler geometry, wall and outlet boundary conditions, and data related to the feed streams including pressure, temperature, flow rate, and composition. For a solid feed stream, the data related to the size distribution, char reaction kinetics are also included in the input file. Within the SolveBoilerModel() function, an instance of the boiler model class is created and the input data are assigned to the member variables of the boiler model object. Then it calls a member function of the boiler model class called Solve() to solve the boiler model.

Within the Solve() function, an initialization function of the boiler model class is called first to check the consistency of input data, create the 3-D unstructured mesh, assign a zone number to each cell and each boundary face, create lookup tables for the particle absorption efficiency calculation, and create the discrete radiative transfer equations. Then some constant variables are calculated for each zone such as total molar flow rates of individual elements, total ash flow rate, total adiabatic enthalpy flow rate. To setup the initial guess for the variables to be solved, chemical equilibrium calculation assuming complete char reactions is performed for each zone. Initial guess for the temperature of each zone is assumed to be proportional to the adiabatic equilibrium temperature. The initial radiative properties (gas and particle absorption coefficients) for each zone are also calculated based on the composition at adiabatic condition and the estimated zone temperature. For the zones below the lowest feed stream, such as the hopper zone, gas composition of the nearby zone is used to calculate the gas absorption coefficient. The coal particles are assumed not to enter the “dead” zone and therefore, no particle radiation in the “dead” zone needs to be considered.

After setting up the initial guess for the variables, the Solve() function enters an iteration loop in which some model variables are updated, under-relaxed, and finally the convergence of those variables can be reached. The iteration loop starts from the Lagrangian tracking of coal particles from each feed stream and each size bin through the zones along their path to furnace exit. During the tracking process, the remaining mass of a particle is calculated in multiple time steps based on the char reaction kinetics and mass transfer and the diameter of the particle as well as its radiation properties are updated. After all particle from different feed streams and different size bins are tracked, the amount of unburned dry-ash-free part of the particles in each zone is updated and so is the particle absorption coefficient of the zone. They are actually under-relaxed for the purpose of convergence. The heat loss calculated for each zone from the solution of the discrete radiative transfer equation is also under-relaxed, which is used to calculate the actual enthalpy of the gas-solid mixture leaving the zone. With updated total enthalpy, elemental molar flows, and unburned dry-ash-free part in the solid phase, chemical equilibrium calculation for each zone is performed thereafter. The new temperature for each zone is obtained and under-relaxed. The new gas composition for the zone is also obtained from the equilibrium calculation and used to update the gas emissivity and gas absorption coefficient. With the updated zone temperatures and radiative properties, the discrete radiative transfer equation is solved again on the 3-D mesh and this concludes the steps of the iteration cycle. The zone temperatures are compared with the old values obtained in the previous iteration. If the maximum difference is less than 0.2 K, the model is considered as converged and the model exits the iteration loop.

After the convergence of the model is reached, the overall furnace performance data are calculated including the total heat transfer to the enclosure wall and those to individual superheaters. The properties of the feed water stream and the superheated steam streams are also updated based on the calculated heat duties. A detailed output array is also prepared by calling a member function of the boiler model. That output array is returned as a reference parameter in the SolveBoilerModel() function. If a flag in the input parameters of the SolverBoilerModel() for writing a 3-D Paraview file is true, the function will call the member function of the boiler model to write the 3-D results for visualization and post processing in Paraview. Likewise, an text file with the description of the variables in the result array returned by the SolverBoilerModel() function can also be written if a flag in the input parameters is set to true.

# Code Structure

The boiler model is developed in C++ which allows for faster execution compared with other languages. In case the boiler model needs to be integrated with other software packages or development environment such as MATLAB and python, the C function SolveBoilerModel() in the source code can be easily converted to a DLL or MEX library. Note that currently the driver function main() is included in the source code in C++, which reads an input file and then calls the SolveBoilerModel() function.

In addition to the two global functions SolveBoilerModel() and main(), there are 18 C++ classes in the source code. Physical constants including universal gas constants and the atomic weights of elements involved are defined in a header file called “Constants.h”, which is used by some classes of the boiler model. Following Microsoft’s conversion, a class name always starts with a capital “C”. For example, the class for the 3-D mesh is called “CMesh”. Each class has a header file with “.h” extension for class declaration and an implementation file with “.cpp” extension for class definition. The file name of a class is the class name with capital “C” removed. For example, the header file of class “CMesh” is called “Mesh.h” and the corresponding implementation file is called “Mesh.cpp”. Among the 18 classes, “CRadiantFurnace” is the most important class that represents a boiler while the other 17 classes are either the members of the “CRadiantFurnace” class or a helper class for the boiler model. The brief descriptions of the 18 C++ classes are given below.

1. CVertex: A class represents a vertex in the 3-D mesh with member variables declared for x, y, and z coordinates of the vertex.
2. CQuadFace: A class represents a quadrilateral face. Its members include the indices to 4 vertices of class CVertex, the unit vector of its normal direction, the x, y, and z coordinates of its centroid, the area of the face, and the indices of two cells sharing the face. If the face is a boundary face, it belongs to only one cell but contains a pointer to an object of CBoundaryFaceProperty that defines the boundary condition of the face. Interior faces do not have the boundary condition and hence the pointer is null.
3. CHexCell: A class represents a hexahedron cell. Its members include the indices to its 8 vertices of class CVertex, the indices to its 6 faces of class CQuadFace, the indices to up to 6 neighboring cells, the x, y, and z coordinates of its centroid, and the volume of the cell.
4. CMesh: A class represents the 3-D mesh that consists of a list of vertices, faces, and cells of class CVertex, CQuadFace, and CHexCell, respectively. Its members also include a list of indices to boundary faces and mean beam length of the entire flow domain.
5. CSuperHeater: A class represents the geometry of a superheater. Its members include the x and y coordinates of the vertices of a polygon shape in the x-y plane and the number of panels evenly distributed along the furnace width.
6. CBoundaryFaceProperty: A class represents the properties of a boundary face for heat transfer calculations. Its members include wall emissivity, overall heat transfer resistance from the slagging wall to the water or steam inside a tube, backside fluid (water or steam) temperature, slagging wall temperature, incident and net radiation heat fluxes. Each boundary face in the 3-D mesh contains an object of CBoundaryFaceProperty class. The emissivity, overall heat transfer resistance, and backside fluid temperature are user inputs and the other properties are calculated when the radiative transfer equation is solved.
7. CParticleRadiationProperty: A class represents the lookup tables for the particle absorption efficiencies for both dry-ash-free coal and ash. There are member functions to calculate the efficiencies based on Mie theory and convoluted over the infrared spectrum.
8. CPSD: A class represents the coal particle size distribution. Its members include the number of size bins, the average diameter and corresponding mass fraction in each size bin. Particle initial density is also a class member.
9. CCoalKinetics: A class represents the parameters for coal devolatilization and char reactions. Its members include particle swelling factor during coal devolatilization, burning mode parameter during char reactions, parameters for calculating the ratio of stoichiometric coefficient of the CO2 product to that of the CO product, and kinetic data (activation energy, pre-exponential factor, temperature exponent, and reaction order) for char oxidation and gasification by H2O and CO2.
10. CSolidFuel: A class represents a solid fuel such as a coal. Its members include proximate and ultimate analysis data, mass flow rate of the solid fuel, and molar flow rates of individual elements (C, H, O, N, and S). The indices to a CPSD object and to a CCoalKinetics object are also the class members which represent the size distribution of the solid fuel and the kinetic data of the solid fuel. Its member functions include the methods to calculate standard heat of formation from high heating value and heat capacity of the coal or char particle at a given temperature.
11. CLiquidFuel: A class represents a liquid fuel such as heating oil. Its members include high heating value and composition of individual elements (C, N, O, N, S, and ash). Mass flow rate and molar flow rates of individual elements are class members. The member functions include the methods to calculate enthalpy and heat capacity of the liquid fuel. Note that liquid fuel is assumed to vaporize immediately and enter to the gas phase immediately upon entry to the boiler.
12. CIdealGas: A class represents an ideal gas species. Its class members include the 14 constants in JANAF table that can be used to calculate state variables such as heat capacity, enthalpy, entropy, and Gibbs free energy of a pure ideal gas species. Its functions include the methods to calculate those state variables at a given temperature and the molecular viscosity, thermal conductivity, and diffusivity. CIdealGas class also contains a static member variable which is a list of CIdealGas objects representing all gas species used in the boiler model. The JANAF table constants for each species are built in the class.
13. CIdealGasMixture: A class represents a mixture of ideal gases which exist in the gas phase of each zone in the boiler model. Its member variables include the mass flow rate of the mixture, the molar flow rates of individual elements in the gas mixture, molar and mass fractions of individual gas species. Its member functions include those for calculating the state properties such as heat capacity, enthalpy, Gibbs free energy and those for calculating the chemical equilibrium by minimizing the Gibbs free energy of the mixture.
14. CWater: A class represents the water substream. Its members include mass flow rate of the water stream, the dryness of the stream, and the molar flow rates of C, H, and O elements. Its member functions include those to calculate the properties based on ASME’s steam table through a DLL.
15. CMaterialStream: A class represents a material stream that could contain up to four substreams including ideal gas mixture, liquid fuel, solid fuel, and water substreams which are represented by CIdealGasMixture, CLiquidFuel, CSolidFuel, and CWater objects, respectively. Its class members include the four substream objects, stream pressure and temperature, total mass flow rate, and total enthalpy flow rate. Any feed stream, product stream, and gas-solid mixture in each zone in the boiler model are represented by the corresponding CMaterialStream objects.
16. CUtilityFunctions: A class used to wrap the utility functions as the static functions of the class. The static functions include the sorting functions based on “quick sort” algorithm and the function for writing and reading string to and from a binary file.
17. CDiscreteOrdinateEquation: A class represents the spatially discretized radiative transfer equations in multiple discrete ordinates. Its member variables include the variables to be solved such as radiation intensity and wall temperatures and radiation heat fluxes. The cell temperatures and the gas and particle absorption coefficients are the inputs to the radiative transfer equation. Its member functions include the function to iteratively solve the radiation intensity in each direction and the function to solve the slagging wall temperatures based on the energy balance at any boundary wall face. After solving the radiative transfer equation, the net heat loss, the difference between the radiation energy emitted and that absorbed, can be calculated for each cell. Then the total heat loss for each zone can be calculated. Since the radiative transfer equation is discretized based on a 3-D mesh, the CSiscreteOrdinateEquation contains a pointer to a CMesh object.
18. CRadiantFurnace: A class represents a boiler. This is the class that contains everything required for modeling the radiant furnace of the boiler. Its member variables include the inputs for the geometry and boundary conditions of the boiler, an object of CMesh, a list of CSuperHeater objects, a list of CPSD objects, a list of CCoalKinetics objects, a list of feed streams as CMaterialStream objects that enter the boiler and participate in chemical reactions, a list of water and steam streams as CMaterialStream objects that pick up the heat, and the object of flue gas product stream and those exit water/steam streams. An instance of CDiscreteOridnateEquation is also a member of the CRadiantFurnace class and used for radiation heat transfer calculations. The main public member function of the CRadiantFurnace class is the Solve() function in which a solution algorithm as discussed in the previous section is implemented.

# Model Validation

The developed boiler model can be validated using the geometries and operating conditions of two existing utility boilers. The two boilers were chosen from a report by a NETL sponsored research project known as “Characterization of oxy-combustion impacts in existing coal-fired boilers.” (Adams et al., 2013) The project contracted to Reaction Engineering International (REI) includes CFD modeling of the two utility boilers in both air-firing and oxy-firing configurations. The first boiler is PacifiCorp’s Hunter Unit 3 and the second boiler is DTE Energy’s River Rouge Unit 3. The validation of the first unit has been completed and reported here.

## Validation of Hunter Unit 3

Hunter Unit 3 is a wall fired subcritical unit with 40 B&W HV-4Z low-NOx burners and 10 over-fired air (OFA) ports. A diagram of the geometry used by the CFD model reported by REI (Adams et al., 2013) is shown in Figure 5. Notice that the CFD model’s exit is at the vertical plane above the rear wall and therefore it includes both platen and pendant superheaters. The exit of the hybrid boiler model is at the vertical plane above the tip of the nose and includes only the platen superheater. The required user inputs for the geometry of the furnace enclosure wall and the platen superheater are listed in Table 3. Note that the English unit of the dimensions shown in Figure 5 is converted to SI unit shown in Table 3. The elevations in Figure 5 are converted to the Y coordinates with Y=0 set at the bottom of the hopper. Some dimensions not labeled in Figure 5 are estimated and listed in Table 3. Eleven platen panels were modeled in the CFD model and so were in the hybrid boiler model.

The fuel used for Hunter Unit 3 is Utah Skyline bituminous coal and its analysis data are listed in Table 4. Note that volatile matter is not listed in the original report. It is estimated based on typical values of high-volatile bituminous coals and is listed in Table 4. Note that 40% volatile yield on the as-received basis corresponds to 50% volatile yield on the dry-ash-free basis which is typical for a bituminous coal fired at very high heating rate as in a utility boiler.

The particle size distribution of the pulverized coal is listed in Table 5. Eleven size bins were used in both the CFD model and the hybrid boiler model.



Figure 5. Geometry of Hunter Unit 3

Table 3. Boiler model inputs for geometry of Hunter Unit 3

|  |  |  |
| --- | --- | --- |
| Description | Unit | Value |
| Number of Burner Levels |  | 4 |
| Number of Overfire Levels |  | 1 |
| Number of Superheater Panels |  | 11 |
| Number of Vertices of Superheater Polygon |  | 4 |
| Furnace Width | m | 15.8496 |
| Furnace Depth | m | 15.5448 |
| Furnace Height | m | 51.816 |
| X of Hopper Bottom of Front Wall | m | 6.7056 |
| X of Hopper Bottom of Rear Wall | m | 8.8392 |
| X of Nose Tip | m | 10.668 |
| Y of Hopper Knuckle | m | 9.144 |
| Y of the Bottom of Nose Slope | m | 33.6804 |
| Y of the Nose Tip | m | 36.8237 |
| X of Superheater Vertex 1 | m | 3.048 |
| X of Superheater Vertex 2 | m | 9.144 |
| X of Superheater Vertex 3 | m | 9.144 |
| X of Superheater Vertex 4 | m | 3.048 |
| Y of Superheater Vertex 1 | m | 38.7096 |
| Y of Superheater Vertex 2 | m | 38.7096 |
| Y of Superheater Vertex 3 | m | 51.816 |
| Y of Superheater Vertex 4 | m | 51.816 |
| Y of Burner Level 1 | m | 12.192 |
| Y of Burner Level 2 | m | 14.9352 |
| Y of Burner Level 3 | m | 19.2024 |
| Y of Burner Level 4 | m | 21.9456 |
| Y of Overfire Air Level 1 | m | 25.1206 |

Table 4. Fuel analysis data for Utah Skyline bituminous coal used by Hunter Unit 3

|  |  |
| --- | --- |
| Mass % of C | 64.49 |
| Mass % of H | 4.44 |
| Mass % of O | 9.25 |
| Mass % of N | 1.18 |
| Mass % of S | 0.64 |
| Mass % of Moisture | 8.86 |
| Mass % of Ash | 11.14 |
| Mass % of Voaltile | 40.0 |
| HHV (Btu/lb) | 11344 |

Table 5. Particle size distribution of Hunter Unit 3

|  |  |  |
| --- | --- | --- |
| Bin Number | Particle Diameter (Micron) | Mass Fraction |
| 1 | 9.1 | 0.025 |
| 2 | 16.3 | 0.05 |
| 3 | 22.1 | 0.075 |
| 4 | 28.6 | 0.1 |
| 5 | 37.1 | 0.15 |
| 6 | 50.2 | 0.2 |
| 7 | 68.8 | 0.15 |
| 8 | 89.8 | 0.1 |
| 9 | 116 | 0.075 |
| 10 | 155 | 0.05 |
| 11 | 230 | 0.025 |

A particle swelling factor of 0.1 is used in the boiler model, indicating 10% diameter increase during devolatilization. Half-order global char oxidation kinetics and first-order char gasification kinetics are used as shown in Table 2. The burning model parameter, activation energies, and pre-exponential factors for the three heterogeneous reactions are listed in Table 6. These data are typical for a high-volatile bituminous coal (Hurt and Mitchell, 1992). All values are in SI unit.

Table 6. Char reaction kinetic data used for Utah Skyline bituminous coal

|  |  |
| --- | --- |
| Burning Mode Parameter ( in Eqn. 25) | 0.1 |
| Activation Energy for CO2/CO Ratio |  |
| Pre-exponential Factor for CO2/CO Ratio |  |
| Activation Energy for Char Oxidation by O2 |  |
| Pre-Exponential Factor for Char Oxidation by O2 | 6.914 |
| Activation Energy for Char Gasification by H2O |  |
| Pre-Exponential Factor for Char Gasification by H2O | 208 |
| Activation Energy for Char Gasification by CO2 |  |
| Pre-Exponential Factor for Char Gasification by CO2 | 440 |

The inputs for the boundary conditions of enclosure wall, superheater wall and exit plane are listed in Table 7. The overall thermal resistance for both enclosure wall and superheater wall is set to 0.001 m2K/W, which is the typical value used by CFD models. The gas emissivity of both enclosure and superheater walls is set at 0.4. The backside fluid temperature for the enclosure wall is set to 623.15 K, which is the saturation temperature of water at drum pressure of 16.6 MPa. The backside fluid temperature for the superheater wall is set to 699.817, which is estimated as the average of the steam from the platen superheater’s inlet to its outlet. Emissivity of the exit plane is set to a low number of 0.1 to avoid heat loss or gain through the exit plane. The exit plane temperature is set to approximately 700 K. This temperature usually is not the gas temperature at the exit. When the emissivity of the exit plane is set to a low value, the heat loss through the exit plane is always very low and the exit plane temperature input is not important.

Table 7. Inputs for the boundary conditions of Hunter Unit 3

|  |  |  |
| --- | --- | --- |
|  | Unit | Value |
| Enclosure Wall Thermal Resistance | m2K/W | 0.001 |
| Superheater Wall Thermal Resistance | m2K/W | 0.001 |
| Enclosure Wall Emissivity |  | 0.4 |
| Superheater Wall Emissivity |  | 0.4 |
| Enclosure Wall Backside Fluid Temperature | K | 623.15 |
| Superheater Wall Backside Fluid Temperature | K | 699.817 |
| Exit Plane Emissivity |  | 0.1 |
| Exit Plane Temperature | K | 699.817 |

The operating conditions including flow rates and temperatures of coal, primary, and secondary air for the air-firing configuration of the boiler are listed in Table 8.

Table 8. Operating conditions of Hunter Unit 3 at air-firing configuration

|  |  |  |
| --- | --- | --- |
|  | Unit | Value |
| Total Coal Flow Rate | kg/s | 50.28 |
| Total Air Flow Rate | kg/s | 512.2104 |
| Primary Temperature | K | 338.71 |
| Secondary Temperature | K | 548.71 |
| Coal Flow Per Burner Level | kg/s | 12.5714 |
| Primary Air Flow Per Burner Level | kg/s | 24.7658 |
| Secondary Air Flow Per Burner Level | kg/s | 72.8268 |
| Overfire Air Flow | kg/s | 121.84 |

To model the radiant furnace of Hunter Unit 3, 9 zones are used along the furnace height with one zone for the hopper, 6 zones from the hopper knuckle to the bottom of the nose slope, one zone in the nose region and one zone in the upper furnace region. To generate the 3-D mesh for radiation calculation, each zone contains three to five cells in the height direction. 24 cells in both width and depth directions are used. Since there are 11 superheater panels, two cells in the width (Z) direction sit between two neighboring superheater panels.

The solution of the boiler model can be reached after about 45 macro iterations (the iteration loop shown in Figure 4). The entire simulation takes approximately 40 seconds on a 32-bit Windows XP computer at 1.87 GHz. Figure 6 shows the solved temperatures in individual zones on the 3-D mesh. The corresponding plot of zone temperature versus zone midpoint height is shown in Figure 7. The temperature of flue gas leaving the horizontal nose plane (Zone 8) is 1679 K, which is very close to the CFD modeling result of 1674 K reported. The maximum gas temperature is at 1888 K in Zone 5, which is at the top burner level. The overall trend of temperatures along the height is similar to the average temperature reported by REI. The temperature of the flue gas leaving the boiler model exit is 1573 K.

Figure 8 shows the solved wall temperatures at the boundary faces of the 3-D mesh. Notice that the wall temperatures at the water wall near the platen superheater is much lower due to the blocked radiation by the nearby superheater panels. The maximum wall temperatures are found in the burner zones at 815 K. Notice that the temperatures at four corner regions are lower even though uniform gas temperatures are assigned to all cells in each zone. The net radiation heat flux distribution at the boundary wall faces is shown in Figure 9. The maximum net heat flux is W/m2, which is close to the maximum value of W/m2 or 80000 BTU/hr-ft2 reported for the CFD model as shown in Figure 10.

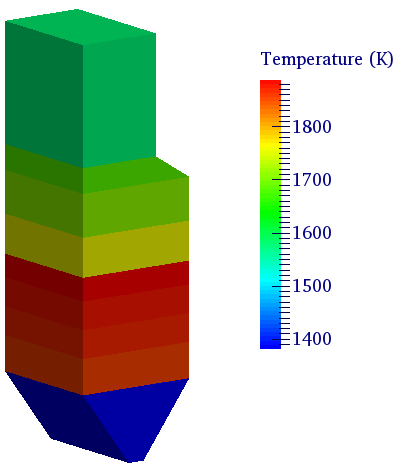


Figure 6. Solved zone temperatures for air-firing Hunter Unit 3



Figure 7. Zone temperature versus furnace height of air-firing Hunter Unit 3

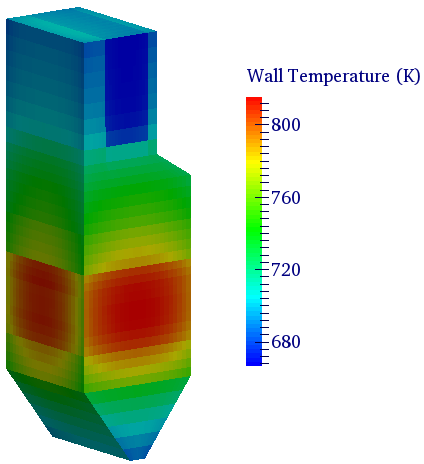


Figure 8. Solved wall temperatures on the 3-D mesh of air-firing Hunter Unit 3

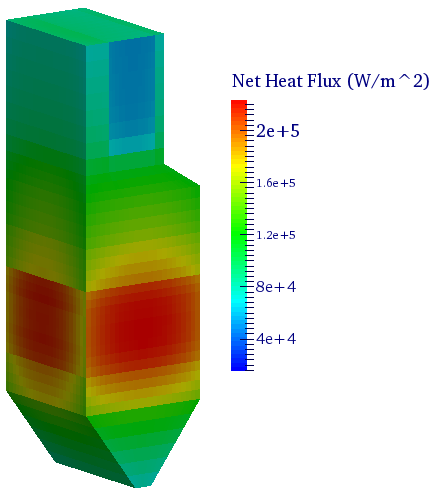


Figure 9. Solved net radiation heat flux of air-firing Hunter Unit 3 on the 3-D mesh



Figure 10. Net radiation heat flux from CFD of air-firing Hunter Unit 3

The total heat losses to the enclosure wall and to the platen super heater are listed in Table 9 along with the predictions by the CFD model reported by REI. Note that the CFD model includes a section of enclosure wall that is beyond the hybrid boiler model’s exit plane. Therefore, the boiler model result for the heat loss to the enclosure wall should be less than the reported CFD result as shown in Table 9. The heat loss to the platen superheater solved by the boiler model matches quite well with the CFD prediction.

Table 9. Heat losses to furnace enclosure wall and platen superheater

|  |  |  |  |
| --- | --- | --- | --- |
|  | Unit | Boiler Model | CFD Model |
| Enclosure Wall | W |  |  |
| Platen Superheater | W |  |  |

The unburned carbon of particles leaving the horizontal nose plane predicted by the boiler model is 1.74%. The unburned carbon in the fly ash leaving the boiler model is 0.8%, corresponding to a coal burnout of 99.86%. The CFD model prediction for unburned carbon is 1.7%, corresponding to a coal burnout of 99.70%. Therefore, the boiler model slightly over-predicts the coal burnout. Note that the kinetic data for Pittsburgh #8 coal is used for the Skyline bituminous coal fired at Hunter Unit 3.

The oxidation by O2 accounts for 87.7% of total char mass release due to heterogeneous reactions. The gasification reactions by H2O and CO2 account for 4.5% and 7.8%, respectively. This means coal gasification reactions should be included even in an air-firing case, as indicated by the REI report.

An oxy-firing case is also modeled using the boiler model developed here. The input data for the model is based on the input data described in the REI report for the oxy-firing case with O2 mole fraction at 0.26 after the flue gas is mixed with a pure O2 stream from an air separation unit. The corresponding recirculation ratio is 75%, meaning that 75% of the flue gas from the boiler exit is recycled and fed back to the boiler. Part of the recycled flue gas stream is fed to the mills as primary stream. That flue gas stream is cooled to 277.15 K and the water condensed out from the stream is removed. The operating conditions of the oxy-firing case are listed in Table 10. The mole fractions of primary and secondary streams after mixing the pure O2 stream with the recycled flue gas stream are listed in Table 11.

Table 10. Operating conditions of Hunter Unit 3 in oxy-firing configuration

|  |  |  |
| --- | --- | --- |
|  | Unit | Value |
| Total Coal Flow Rate | kg/s | 50.28 |
| Total O2 Flow Rate | kg/s | 102.44 |
| Primary Temperature | K | 355.37 |
| Secondary Temperature | K | 533.15 |
| Coal Flow Per Burner Level | kg/s | 12.5714 |
| Primary Stream Flow Per Burner Level | kg/s | 22.6285 |
| Secondary Stream Flow Per Burner Level | kg/s | 83.1027 |
| Overfire Stream Flow | kg/s | 83.7886 |

Table 11. Compositions of primary and secondary stream in oxy-firing configuration

|  |  |  |
| --- | --- | --- |
|  | Primary Stream | Secondary Stream |
| O2 Mole Fraction | 0.21049 | 0.26081 |
| N2 Mole Fraction | 0.00607 | 0.00438 |
| CO2 Mole Fraction | 0.77404 | 0.55876 |
| H2 Mole Fraction | 0.00652 | 0.17397 |
| SO2 Mole Fraction | 0.00288 | 0.00208 |

The boundary conditions and other inputs are specified using the same data as in the air-firing configuration. Figure 11 shows the solved temperatures in individual zones on the 3-D mesh. The corresponding plot of zone temperature versus zone midpoint height is shown in Figure 12.

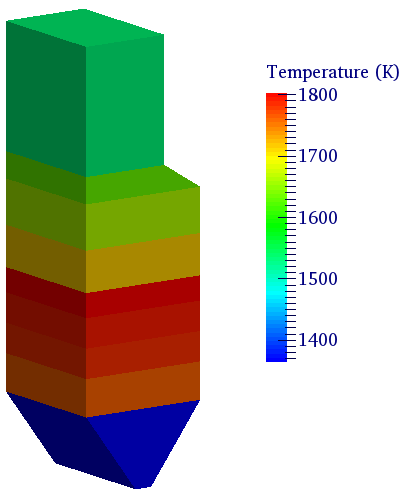


Figure 11. Solved zone temperatures for oxy-firing Hunter Unit 3



Figure 12. Zone temperature versus furnace height of oxy-firing Hunter Unit 3

The temperature of flue gas leaving the horizontal nose plane (Zone 8) is 1628 K, which is 28 K lower than the CFD modeling result of 1656 K. The maximum gas temperature is at 1802K in Zone 5, which is 86 K lower than that of the air-firing case. The overall trend of temperatures along the height is similar to the average temperatures reported by REI. The temperature of the flue gas leaving the boiler model exit is 1529 K.

Figure 13 shows the solved wall temperatures at the boundary faces of the 3-D mesh. The maximum wall temperatures are found in the burner zones at 800 K, which is 15 K lower than that in the air-firing case. The net radiation heat flux distribution at the boundary wall faces is shown in Figure 14. The maximum net heat flux is W/m2, which is also lower than that of the air-firing case. This trend can also be found in the CFD predictions.

The total heat losses to the enclosure wall and to the platen super heater are listed in Table 12 along with the values of the CFD models reported by REI. Again the CFD model includes a section of enclosure wall that is beyond the hybrid boiler model’s exit plane. Therefore, the boiler model’s result for the heat loss to the enclosure wall should be less than the reported CFD result as shown in Table 12. Compared with the air-firing case, both heat losses are slightly lower. Compared with the CFD model results, the heat loss to the platen superheater is under-predicted by 9% while the heat loss to the enclosure wall could be over-predicted considering the fact that less enclosure wall area is included in the boiler model.

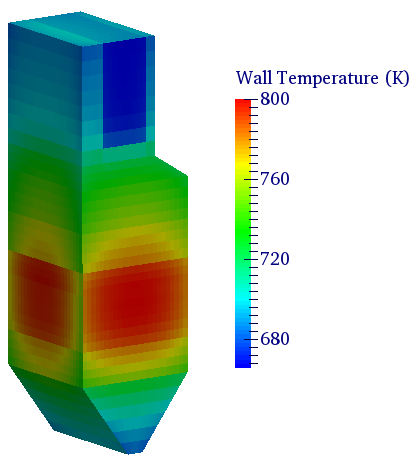


Figure 13. Solved wall temperatures on the 3-D mesh of oxy-firing Hunter Unit 3

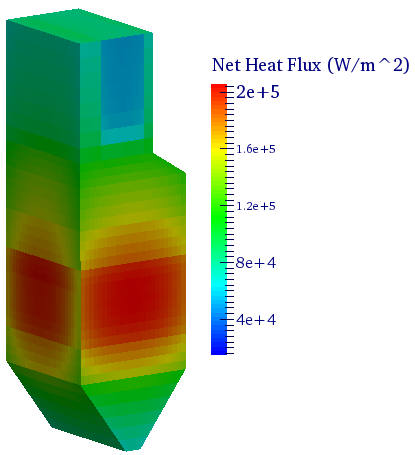


Figure 14. Solved net radiation heat flux of oxy-firing Hunter Unit 3 on the 3-D mesh

Table 12. Heat losses to furnace enclosure wall and platen superheater

|  |  |  |  |
| --- | --- | --- | --- |
|  | Unit | Boiler Model | CFD Model |
| Enclosure Wall | W |  |  |
| Platen Superheater | W |  |  |

The unburned carbon in the fly ash leaving the horizontal nose plane predicted by the boiler model is 1.15%. The unburned carbon in the fly ash leaving the boiler model is 0.53%, corresponding to a coal burnout of 99.9%. The CFD model prediction for unburned carbon is 1.1%, corresponding to a coal burnout of 99.8%. Compared with the air-firing case, slightly higher burnout is predicted. This trend is also found in the CFD model predictions. As in the air-firing case, the boiler model slightly over-predicts the coal burnout.

The oxidation by O2 accounts for 76.3% of total char mass release due to heterogeneous reactions. The gasification reactions by H2O and CO2 account for 5.6% and 18.1%, respectively. The contribution by CO2 gasification increased significantly due to high CO2 mole fractions in the furnace.

## Summary of Hunter Unit 3 validation

By modeling the Hunter Unit 3 in both air-firing and oxy-firing configurations and comparing the results to those from CFD simulations, the hybrid boiler model was found to give very reasonable predictions in terms of flue gas temperatures in the upper furnace, heat loss to platen superheater and enclosure wall, and coal burnout. The overall pattern of the net heat flux along the furnace height and the maximum net heat flux match the CFD predictions. The trend of unburned carbon predictions in the two firing configurations also matches the CFD results. Overall the air-firing case matches the CFD case better. The differences in gas temperature at the horizontal nose plane and the heat losses to enclosure wall and superheater wall between the CFD and hybrid boiler models are slightly higher in the oxy-firing configuration. Note that those results are obtained when identical wall boundary conditions for the two firing configurations are used. In reality, the boundary conditions such as slagging wall emissivity could change from air-firing configuration to oxy-firing configuration. Fine tuning of the user inputs related to wall boundary conditions could increase the accuracy of the oxy-firing case.

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# Appendix A. An Example of Input for Boiler Model

The text input file for modeling Hunter Unit 3 boiler in the oxy-firing condition is listed here.

0 //flag for creating Paraview files "boiler\_model.vtk" and "boiler\_model\_bnd.vtk"

1 //flag for creating output variable discription file "boiler\_model\_output\_description.txt"

4 //number of burner levels

1 //number of OFA levels

1 //number of zones between OFA and nose zone

1 //number of zones in exit region

24 //number of cells in depth direction x

24 //number of cells in width direction z

6 //number of cells in zone 1: hopper zone

4 //number of cells in zone 2

3 //number of cells in zone 3

3 //number of cells in zone 4

3 //number of cells in zone 5

4 //number of cells in zone 6

4 //number of cells in zone 7

3 //number of cells in zone 8

8 //number of cells in zone 9

11 //number of panels for superheater 1

4 //number of vertices for polygon shape of superheater 1

11 //number of size bins for coal particle size distribution

0 //flag indicating if enclosure wall property depending on zone, 0=No

15.8496 //width in z

15.5448 //depth in x

6.7056 //x coordinate of the point of hopper bottom at front wall

8.8392 //x coordinate of the point of hopper bottom at rear wall

10.668 //x coordinate of the point of nose tip

51.816 //furnace height in y direction

9.144 //y coordinate of hopper knuckle

33.6804 //y coordinate of the bottom of the nose slope

36.8237 //y coordinate of the nose tip

13.5636 //y coordinate at the top of zone 2, 1st burner zone

17.0688 //y coordinate at the top of zone 3, 2nd burner zone

20.574 //y coordinate at the top of zone 4, 3rd burner zone

23.4696 //y coordinate at the top of zone 5, 4th burner zone

28.3464 //y coordinate at the top of zone 6, 1st OFA zone

3.048 //x coordinate of point 1 of superheater 1

38.7096 //y coordinate of point 1 of superheater 1

9.144 //x coordinate of point 2 of superheater 1

38.7096 //y coordinate of point 2 of superheater 1

9.144 //x coordinate of point 3 of superheater 1

51.816 //y coordinate of point 3 of superheater 1

3.048 //x coordinate of point 4 of superheater 1

51.816 //y coordinate of point 4 of superheater 1

12.192 //y of burner level 1

14.9352 //y of burner level 2

19.2024 //y of burner level 3

21.9456 //y of burner level 4

25.1206 //y of OFA level 1

9.1e-006 //diameter of size bin 1

0.025 //mass fraction of size bin 1

16.3e-006 //diameter of size bin 2

0.05 //mass fraction of size bin 2

22.1e-006 //diameter of size bin 3

0.075 //mass fraction of size bin 3

28.6e-006 //diameter of size bin 4

0.1 //mass fraction of size bin 4

3.71e-005 //diameter of size bin 5

0.15 //mass fraction of size bin 5

5.02e-005 //diameter of size bin 6

0.2 //mass fraction of size bin 6

6.88e-005 //diameter of size bin 7

0.15 //mass fraction of size bin 7

8.98e-005 //diameter of size bin 8

0.1 //mass fraction of size bin 8

11.6e-005 //diameter of size bin 9

0.075 //mass fraction of size bin 9

15.5e-005 //diameter of size bin 10

0.05 //mass fraction of size bin 10

23.0e-005 //diameter of size bin 11

0.025 //mass fraction of size bin 11

1350 //desnsity of coal particle

0.1 //particle swelling factor during devolatilization

0.1 //burning mode parameter alpha, denp/denp0 = (mp/mp0)^alpha

1.25e8 //activation energy for CO/CO2 molar ratio

4e4 //pre-exponential factor for CO/CO2 molar ratio

1e8 //activation energy for O2 combustion, half order model

6.914 //pre-exponential factor for O2 combustion, half order model, kmol-C reacted

2.4e8 //activation energy for H2O gasification, 1st order model

208 //pre-exponential factor for H2O gasification, kmol-C reacted

2.51e8 //activation energy for CO2 gasification, 1st order model

440 //pre-exponential factor for CO2 gasification, kmol-C reacted

355.37 //temperature

101325 //pressure

22.6285 //gas mass flow rate

0 //mole fraction of C(S)

0.210491 //mole fraction of O2

0.00607252 //mole fraction of N2

0 //mole fraction of H2

0 //mole fraction of CO

0.774035 //mole fraction of CO2

0.00652362 //mole fraction of H2O

0.00287786 //mole fraction of SO2

0 //mole fraction of H2S

0 //mole fraction of CH4

0 //mole fraction of Ar

12.5714 //mass flow rate of coal

0.6449 //mass fraction of C

0.0444 //mass fraction of H

0.0925 //mass fraction of O

0.0118 //mass fraction of N

0.0064 //mass fraction of S

0.0886 //mass fraction of moisture

0.1114 //mass fraction of ash

0.4 //mass fraction of volatile

2.63597e+007 //high heating value

533.15 //temperature

101325 //pressure

83.10275 //gas phase mass flow rate

0 //mole fraction of C(S)

0.26081 //mole fraction of O2

0.0043836 //mole fraction of N2

0 //mole fraction of H2

0 //mole fraction of CO

0.558763 //mole fraction of CO2

0.173966 //mole fraction of H2O

0.0020774 //mole fraction of SO2

0 //mole fraction of H2S

0 //mole fraction of CH4

0 //mole fraction of Ar

83.7886 //mass flow rate of OFA level 1

400 //feed water temperature

1.68928e+007 //feed water pressure

200 //feed water mass flow rate

10000 //feed water pressure drop through water wall

700 //steam inlet temperature

1.6548e+007 //steam inlet pressure

200 //steam mass flow rate

1e5 //steam pressure drop through superheater

0.4 //wall emissivity

0.001 //thermal resistance from ash layer to water

623.15 //boiling water temperature, saturation temperature for sub-critical unit

0.4 //wall emissivity

0.001 //thermal resistance from ash layer to water

699.817 //average steam temperature in the superheater

0.1 //exit plane emissivity, use a small number to avoid radiation leak

699.817 //exit plane back side temperature for radiation calculation