**Pressurized oxy-combustion with low flue gas recycle:
computational fluid dynamic simulations of radiant boilers**

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Abstract

Oxy-fuel combustion is considered a promising technology for carbon capture, utilization, and storage (CCUS). One of the primary limitations on full-scale implementation of this technology is the significant increase in the cost of electricity due to a large reduction in plant efficiency and high capital costs. Recently a new concept, namely staged, pressurized oxy-combustion, has been developed in which the flue gas recycle is reduced significantly by means of fuel-staged combustion. At higher pressure the latent heat of condensation of the moisture in the flue gas can be utilized in the Rankine cycle, further increasing the plant efficiency. As determined through ASPEN Plus modeling, this approach increases the net plant efficiency by more than 6 percentage points, compared to first-generation oxy-combustion plants.

The early stages of the system involves burning coal in high oxygen concentration, which means the flame temperature is extremely high. New boilers designs are required to handle these extreme conditions. In the present paper, a unique burner and boiler has been designed via computational fluid dynamics (CFD) to effectively and safely burn coal under conditions of elevated pressure and low flue gas recycle. The enclosed jet theory was used to design a combustion system with slow mixing and no external recirculation, which helped minimize flame impingement and ash deposition. A cone-shaped geometry was utilized to minimize the effects of buoyancy in the down-fired, axial-flow system. A 1540 MWth SPOC system was simulated based on this design and the results showed that a relatively uniform distribution of wall heat flux can be achieved and the peak wall heat flux was under a manageable level even though local gas temperature are extremely high.

Keywords: oxy-combustion; coal combustion; oxyfuel; fuel-staged combustion; pressurized combustion; computational fluid dynamics

44 1. Introduction

45 Increasing concern over climate change has made the development of technologies for
46 carbon (CO₂) capture, utilization, and storage (CCUS) an urgent requirement. Oxy-combustion is
47 considered by many to be promising among these technologies [1-4]. The process typically
48 entails burning the fuel in a mixture of O₂ and recycled flue gas instead of air as the primary
49 oxidant. By eliminating the use of air, this process avoids the large volume of N₂ gas that would
50 normally be present in the boiler and in the flue gas clean up processes; hence, a nearly pure
51 stream of carbon dioxide can be produced after the removal of water and trace gases. The “first
52 generation” oxy-combustion approach requires a large volume of flue gas (mainly carbon dioxide)
53 to be recycled back into the combustor so that combustion gas temperatures and wall heat flux
54 can emulate that of existing air-fired boiler designs. A significant amount of energy is consumed
55 in the air separation unit (ASU), flue gas recycle (FGR), and the compression & purification unit
56 (CPU), which leads to a low efficiency for first-generation oxy-combustion. This, along with the
57 added capital investment required, leads to an excessive cost of electricity (COE).

58 The fact that the CO₂ captured must ultimately be pressurized for geo-sequestration or
59 enhanced oil recovery (EOR) enables pressurized oxy-combustion to be implemented at no net
60 pumping cost because the energy to compress oxygen is comparable to that to compress CO₂.
61 Earlier studies have indicated that overall plant efficiency can be improved by as much as 3
62 percentage points by pressurizing the oxy-coal combustion process [5-7]. The primary benefits
63 of pressurized oxy-combustion are: (1) recovering latent heat from flue gas moisture; (2)
64 reducing the size and cost of equipment; (3) avoiding air ingress; and (4) increasing the
65 convective heat transfer for a given mean velocity.

Recently, a novel approach to pressurized oxy-combustion has been proposed to further improve efficiency and cost over first-generation technologies [8, 9]. This approach is referred to as Staged, Pressurized Oxy-Combustion (SPOC). In the SPOC process, pulverized coal is combusted at high-pressure with near-zero recycle. Normally, burning fuel in oxygen without dilution from inert gases, as compared to combustion in air, would lead to a dramatic increase in both the temperature and the rate of radiant heat transfer to the boiler tubes [10]. In the SPOC process, this problem is at least partially circumvented by staging the delivery of fuel so that both combustion products and excess O_2 are utilized for dilution. The concept of fuel staging is depicted in Fig. 1. As shown on the left, only a fraction of the total fuel for the plant is supplied in the first stage, but most of the oxygen is supplied, which means there is an over-supply of oxygen. This implies that the stoichiometric ratio is much greater than unity, where the stoichiometric ratio is defined as the ratio of the mass of oxygen supplied to the mass of oxygen required for stoichiometric combustion of the fuel supplied in this particular stage. The large amount of excess O_2 effectively acts as a diluent to control the mean temperature of the combustion products and thus moderates the heat transfer. Heat is extracted from the first stage and is transferred to the Rankine steam cycle, which reduces the flue gas temperature. The products of combustion from Stage 1, including the excess O_2 , are passed to Stage 2, where additional fuel is injected and more O_2 is consumed. This process continues in subsequent stages until nearly all of the O_2 is consumed.

It is important to note that the total coal and oxygen supplied in the SPOC process is equivalent to the case in which the coal and oxygen are combusted in nearly stoichiometric proportion in a single stage; i.e. there is very little net addition of dilution gases. The total oxygen supplied is slightly higher than the amount required for stoichiometry to ensure that the oxygen concentration at the exit of the final stage is sufficiently high to ensure complete char burnout. In

all stages, coal is fed with a pneumatic dry feeder using a very small amount of recycled flue gas as motive gas.

The SPOC process is able to capture carbon dioxide and produce electricity at significantly higher efficiency and lower cost, compared to “first-generation” oxy-combustion. Gopan et al. [8] showed that the net efficiency of this process, as determined through ASPEN modeling, is more than 6 percentage points higher than first-generation oxy-combustion technologies. The reasons for this increase in efficiency are many, and include the latent heat recovery associated with flue gas moisture condensation at high temperature, capture and integration of waste heat from the auxiliary systems (e.g. ASU), and the auxiliary load reduction and reduced exergy loss due to minimal flue gas recycle [8, 11] . In addition, the cost of SO_x and NO_x removal is significantly reduced by using an integrated flue gas cleanup process [8]. The bulk of the SO_x and NO_x is removed during the cooling of flue gas in a direct contact column. This conversion of gaseous SO_x and NO_x into weak acids in the column is enabled at elevated pressures, and is described by others [8, 12-16]. This integrated approach significantly reduces the cost of cleanup.

While flowsheet simulations showed that the SPOC process is very promising, new designs for the combustion boiler are required to handle coal combustion in atmospheres of elevated pressure and high oxygen concentration. Although fuel staging can reduce the flue gas temperature to a similar value as in air-fired combustion, the local flame temperatures can still be quite high because the local stoichiometric ratio at the flame location is close to 1. The goal of this study is to develop a nonconventional pressurized burner/boiler that has been designed specifically for pressurized oxy-combustion. This effort involves computational fluid dynamics (CFD) simulations to model the combustion processes in pressurized boilers, and to determine the effects of operating conditions on the radiative and convective heat transfer in the boilers. The specific objective is to understand and control the heat flux to the wall and maximize the

uniformity of wall heat flux while not exceeding the maximum allowable heat flux for boiler tube materials.

2. Boiler design methodology

2.1 Key design considerations

The pressure in each boiler in the SPOC system is 16 bar, which was determined to be optimal from a techno-economic analysis [8]. Nonetheless, a major issue with burning coal when there is limited flue gas recycle lies in how to limit radiative heat flux to the boiler tubes, due to the extremely high local flame temperatures that can be realized. In this conceptual approach, the gas temperatures for the fully mixed gases (post-flame temperature) are controlled by excess oxygen (c.f. Fig. 1, the first three stages) but the local temperatures can still be much higher than those in air-fired systems or oxy-combustion systems with full (~ 70%) FGR. To address this issue, a unique coal burner & boiler have been designed. The thought process for this design is described below for a case study of a 550MWe plant. The major design criteria for the boilers are to 1) optimize radiative wall heat flux, 2) avoid flame impingement, and 3) minimize particle deposition to avoid slagging, fouling, and corrosion.

First we will discuss the rationale for the staging approach as described in Fig. 1. NASA chemical equilibrium with applications (CEA) was used to calculate the overall adiabatic flame temperature for the supplied gases as a function of stoichiometric ratio, when coal is combusted in pure oxygen at constant pressure. The result is shown in Fig. 2. For a stoichiometric ratio of 1, the overall adiabatic temperature is approximately 3260 °C. The overall adiabatic temperature decreases with increasing stoichiometric ratio because the excess oxygen acts as a diluent. At a stoichiometric ratio of 4, the overall adiabatic flame temperature is approximately 2141 °C, which

is comparable to that of oxy-coal combustion with an O_2/CO_2 ratio of 30/70 vol.% [17], as shown in Fig. 2. It is worthwhile to note that reducing the overall adiabatic flame temperature by operating under high stoichiometric ratio, i.e., excess oxidizer, is also what is done to control gas temperatures in gas turbines. In that case, the temperature is controlled because excess air acts as a diluent.

By supplying all of the oxygen in the first stage, but only one-fourth of the coal, the stoichiometric ratio is 4 for this stage and the overall temperature is manageable. Four stages were therefore selected for the fuel staging approach, and as will be shown, the basis of selection has been verified by CFD results.

The first stage presents a unique challenge because, while the overall adiabatic flame temperature is manageable by excess oxidizer, the local temperatures can be quite high, which suggests that radiative heat fluxes could be excessive. As will be shown, to address this requires a novel design of the burner and boiler.

As the system is pressurized, the first constraint to the boiler design comes from the intrinsic shape of pressure vessels. They are generally cylindrical in shape with large aspect ratios (length-to-diameter). The cost of fabricating such vessels can rise dramatically if they are fabricated on site and transportation requirements limit the maximum size for pre-fabricated pressure vessels to approximately 61 m (200 ft) in length and 4.6 m (15 ft) in outer diameter. Such a vessel can be transported by rail. For the purposes of this study, this size will be considered the maximum size, although this constraint can be relaxed if the economics support on-site fabrication.

For the typical boiler material used in construction of the membrane wall in power plants, the peak heat flux is approximately $400 kW/m^2$, which ensures a safe peak operating wall temperature of around $450^\circ C$ [18]. Advanced alloy boiler tube materials can withstand fluxes up

to approximately 650kW/m^2 [19]. With this constraint, and assuming that the heat exchange surface area is approximately equal to the surface area of the inside wall of the pressure vessel, we can approximate the total length of pressure vessel needed. For the 4.6 m diameter vessel it is assumed that the internal diameter of the boiler would be 3.96 m (13 ft) in diameter. Based on the SPOC process simulation [8], the total heat transfer requirement in the radiant boilers is around 1300 MWth. Assuming an average wall heat flux of 400kW/m^2 , the required boiler tube surface area dictates that the length of reactor vessel should be roughly 244 m (800 ft). Of course, interior tubes can be added to reduce this length but this result suggests that since the maximum vessel length is 61 m, four separate vessels should be utilized for the case study. Therefore, for each stage, a separate pressure vessel is employed.

To minimize the heat transfer surface area that is needed, it is desirable to produce an optimal and relatively uniform radiative heat flux over the length of the vessel. This suggests that distributed heat release, as opposed to concentrated heat release, is desired for pressurized coal combustion and that the heat release should occur over a scale of approximately 30.5 m (100 ft). In high swirl [20] or flameless (or MILD) combustion [21] the mixing rates are fast. Here mixing rates should be slow in order to distribute the heat release, reduce global temperature, and obtain a more uniform radiative heat flux to the walls.

To avoid slagging, the flame and the ash particles must remain away from the walls because of the very high flame temperature, particularly in Stage 1 where the oxygen concentration is the highest. From a simple understanding of gaseous flame structure, a stoichiometric ratio of unity would require that the flame eventually come in contact with the wall as a consequence of the stoichiometric demand for oxygen [22]. In contradistinction, the high stoichiometric ratio in the first few stages ensures that the flame does not reach the walls.

In the subsequent stages, the oxygen is diluted by the products of combustion of the previous stages, so control of heat flux is less challenging. Nonetheless, the excess oxidizer in Stages 2 and 3 continue to be important to assist in the control of wall heat flux, flame impingement, and ash deposition/slagging.

2.2 Minimization of external recirculation

As mentioned above, minimization of ash deposition becomes especially important for the design of SPOC reactors. Any radial velocity component caused by recirculation could increase the tendency of collision of particles with the wall. Thus, enclosed jet theory was applied to design a combustor that avoids recirculation in the boiler [23]. The Thring-Newby parameter [24] was used to determine conditions leading to the onset of recirculation. The Thring-Newby parameter θ is given by

$$\theta = \frac{d_0'}{d_1} \left(\frac{\rho_0}{\rho_1} \right)^{0.5} \frac{m_0 + m_1}{m_0}, \quad (1)$$

where m_0 and m_1 refer to the mass flow rates, ρ_0 and ρ_1 the densities, and d_0 and d_1 the equivalent diameters for the primary (PO) and secondary (SO) oxidizer, respectively. External recirculation can be avoided by ensuring that the Thring-Newby parameter is greater than 0.9. The Thring-Newby parameters for all stages of SPOC boilers are higher than 26, leading to jet diffusion flames without recirculation. The Thring-Newby parameter represents a design tool to estimate appropriate dimensions and flow rates for the SPOC burners. It allows for a design that can 1) slow down mixing to yield a longer flame and thus a slower heat release, enabling a lower flame temperature (due to heat loss) and more uniform wall heat flux; and 2) eliminate external recirculation zone to avoid ash deposition.

2.3 Design geometry

As described previously, the approach to the preliminary design was to determine the number of stages required so that the mean temperature of each stage is similar to that of a conventional system. The combustion gases of each stage are cooled to 700 °C by heat transfer to the boiler tubes prior to entering the next stage. Four stages were determined to be optimum. Down-fired burners/boilers are assumed, and the products of combustion from each stage pass on to the next stage by means of a riser, as shown in Fig. 3.

The approximate geometry of the burner was estimated with the Thring-Newby parameter. The Richardson number, which represents the importance of natural convection relative to forced convection, was also considered in determining the appropriate geometry, so as to avoid buoyant flows, which could lead to recirculation. The Richardson number (Ri) is defined as

$$Ri = \frac{g\beta(T_{hot} - T_{ref})L}{V^2}, \quad (2)$$

where g is gravity acceleration, L is the characteristic length for natural convection, which can be considered the boiler height in our case, V is characteristic gas velocity, and β is the thermal expansion coefficient, where $\beta = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_p$. For an ideal gas, $\beta = -\frac{1}{T}$. When Ri is less than 0.1 the fluid dynamics is controlled by forced convection. On the other hand, when Ri is greater than 10, natural convection dominates.

By taking into account the overall boiler size limitations, the required gas and fuel flow rates, and the criteria to avoid recirculation and strong buoyancy effects, the burner and combustion chamber dimensions may be estimated. The final geometry presented here was determined after several iterations of CFD simulations, to achieve a desirable flame shape and heat flux distribution. As shown in Figure 4, the PO/SO inner diameters are 0.254/1.32 m and the furnace length is 53.34 m (175 ft) for all stages. The furnace diameter changes gradually from 1.32 m to

3.96 m over a length of 19.8 m. The same geometry is used for all stages for convenience of boiler construction.

2.4 Operating and boundary conditions

The properties of PRB coal used in this study are listed in Table 1. The total thermal input for a 550 MW_e plant was determined to be 1540 MW_{th} [8]. As a first step, the case in which the total thermal input is distributed evenly in each stage (385MW each) is considered. Because the earlier stages have high oxygen concentrations, it is expected that the flame temperatures and peak wall heat fluxes in these stages are higher than those in the later stages. Shifting some of the thermal input (coal) from the early stages to the later stages is one way to obtain similar wall heat fluxes in all four stages. In the present work, studies in which coal has been equally (uniformly) distributed among the four stages and non-uniformly distributed are presented. Table 2 shows the boundary conditions for all four burner inlets for the uniformly distributed thermal input study. A comparison of the thermal inputs between the uniformly and non-uniformly distributed cases is provided in Table 3.

Because radiation is the dominant mode of heat transfer in SPOC, the emissivity of wall plays an important role in determining the wall heat flux. After long periods of operation, certain amount of ash particles would inevitably deposit on the boilers tubes. In coal boilers, the emissivity of the ash deposits on the boiler tubes depends, not only on the ash composition, but also the temperature and characteristics of the ash deposits. Emissivities between 0.38 and 0.67 have been reported for powdery deposits, and values between 0.76 and 0.93 for sintered or fused deposits [25]. A higher emissivity means that the wall is less reflective and thus the net heat flux to the boiler tubes will be higher. Simulation showed that as the wall emissivity varied from 0.9 to 0.4, the wall heat flux dropped by about 50%. In the current study, a relatively conservative

value of 0.8 was chosen for the emissivity of the wall. To enhance flame stability, 25vol.% O₂ is used in the PO, while the majority of the transport gas is CO₂ for safety reasons. A unique burner design has also been proposed to enhance flame stability for this axial (non-swirl) mode of burner operation. Since the focus of this paper is on controlling wall heat flux, detailed information on the burner design is not presented.

3. Numerical methods

ANSYS FLUENT version 13.0 was used to simulate the designed boiler above. The flow field was modeled applying the Reynolds Averaged Navier Stokes (RANS) equations with the Semi-Implicit Method for Pressure Linked Equations (SIMPLE) algorithm to address pressure-velocity coupling. RANS has been used extensively to study the flame behaviors of pulverized fuel [26-28]. Up till now, none of the solid fuel combustion submodels has been validated for pressurized oxy-combustion environment. In the present work, the sub-models that have been extensively validated under atmospheric pressure oxy-coal combustion environment are used [4, 29-34]. It has been shown that RANS is able to provide reasonable agreement between experiments and CFD simulations under atmospheric pressure oxy-combustion conditions.

3.1 Turbulence and turbulent interaction models

In turbulent combustion simulations, modeling the turbulence is one of the most significant considerations. Serious limitations have been observed for the k - ε model in the near-wall region. The model overpredicts turbulence scales for flows with adverse pressure gradients, which leads to higher heat transfer rates and wall shear stress [35]. It is beneficial to use the ω -equation in the near-wall region, however, the solution of the standard k - ω model is strongly sensitive to the free stream values of ω outside the boundary layer [36]. The shear stress transport (SST) k - ω model

was developed to address the problems associated with the standard $k-\varepsilon$ and standard $k-\omega$ models, [37]. The SST $k-\omega$ model combines the best of the two eddy-viscosity models and is used in this simulation.

The interaction between chemistry and turbulence is modeled by using a finite rate/eddy dissipation model in which the reaction rate is defined by taking the minimum of the chemical reaction rate and the turbulent mixing rate. This model has been extensively used in oxy-coal combustion modeling studies [38-40][28-30]. The chemical properties of the volatile matter species were approximated from the ultimate and proximate analyses. A two-step global reaction mechanism was used to capture the gaseous volatile reaction, including a global mechanism for volatile oxidation and the conversion of CO to CO₂.

More detailed reaction mechanisms [41] together with a more advanced reaction model, i.e. eddy dissipation concept (EDC) model have also been tested. The EDC model takes account of the CO₂ and H₂O dissociation and thus give a lower flame temperature and slightly lower peak wall heat flux than the finite rate/eddy dissipation model. In this work, the more conservative results from the finite rate/eddy dissipation model are presented.

3.2 Coal combustion models

The particles trajectories were computed in the Lagrangian frame and are coupled to the gas phase, which is in the Eulerian frame. With this approach, mass, momentum, and energy are exchanged between the two phases. All discrete particles were assumed to be spherical. The pulverized coal particle size was assumed to follow the Rosin-Rammler distribution, with an

average diameter of 65 μm . The effect of turbulence on the particle trajectories was accounted for with the Discrete Random Walk (DRW) model.

3.2.1 Coal devolatilization model

The Chemical Percolation Devolatilization (CPD) model [42] was used to calculate the thermal decomposition rate of the coal particles. NMR chemical structure parameters were calculated according to the correlations in [43]. Ultimate and proximate analyses were applied to determine the chemical properties of volatile matter. The oxidization of volatile gases was modeled using a two-step reaction mechanism with wet combustion [44].

3.2.2 Coal char combustion model

A multiple-surface-reaction char model was employed to simulate solid particle (char) surface oxidation. Reactions between char and the oxidizers oxygen, carbon dioxide and water vapor were assumed to occur as the oxidizers diffused to the particle surface and into the pores. The global kinetics for the consumption of char particle surface species was represented by Arrhenius reaction rate expressions based on the activation energies, reaction orders, and pre-exponential factors assumed in Toporov et al.,[45] and Crowe et al. [46].

3.3 Radiation model

For high-temperature, particle-laden flows radiation is the dominant mode of heat transfer. Since the interaction of the emitted radiation with the surrounding coal, char, and ash can significantly influence radiation heat transfer, absorption and scattering were included in the radiative transfer equation (RTE) [47]. The average emissivity of the particles was set to be 0.4 [48]. The Discrete Ordinates (DO) [49, 50] radiation model was used in this simulation to solve the RTE, with each octant being discretized into 4x4 solid angles. Gaseous absorption was considered by a domain-based Weighted Sum of Gray Gases model (WSGGM) [51].

3.4 Solution strategy

The 3-D double precision pressure-based solver in FLUENT 13.0 was used for the RANS simulation with the second-order upwind scheme. During the simulation, the cold flow field was obtained first, followed by the ignition patch with the injection of coal particle and activation of reactions applying the finite rate/eddy dissipation model. After a converged solution was obtained, the DO radiation model with particle radiation interaction as well as the second order scheme for the momentum, turbulence, species transport, energy, and radiation equations were applied to obtain the final converged solution.

4. Numerical results and discussion

Based on the burner and boiler geometry, a 3-D 30-degree sector model was built, which took advantage of the axisymmetric character of this case. Periodic boundaries were applied on the two axisymmetric surfaces. The mesh size was determined from a grid sensitivity test. The simulation results of cases with 805,000 and 1,567,000 cells were compared, and negligible differences of velocity, temperature and heat transfer were observed. Moreover, an additional case with 362,600 cells was calculated to estimate the discretization error using the Richardson extrapolation (RE) method [52]. The grid convergence index (GCI) for the case with 805,000 cells was 0.16%, as found by comparing key variables on the three computational meshes. Thus the mesh with 805,000 cells was used for the CFD model.

The burner outlet was specified as a pressure outlet and the wall of the combustion chamber was maintained at 700 K. Sensitivity studies showed that wall temperature had a minor effect on the peak wall heat flux in the SPOC boilers. As wall temperature increased from 100 K to 1000 K, the peak wall heat flux change was less than 50 kW/m^2 (i.e. relative difference about 8%). A one-dimensional heat transfer calculation was also carried out for membrane wall with cooling water

at 573 K. Results showed that when the wall heat flux is 600kW/m^2 , the surface temperature of the wall could be controlled in the range of 700 K which is an acceptable value for standard boiler tube materials. Therefore, 700 K was chosen as the wall temperature in the simulation. For this simulation it is assumed that the ash particles exiting each stage have been removed before entering the next stage.

4.1 Temperature distribution and wall heat flux

Figure 5 shows the temperature distribution for all the four stages when the thermal input is uniformly distributed among the stages. The temperature contours exhibit flame patterns typical of jet flames. The maximum local flame temperature is 2997 K in the first stage. This drops to 1857 K in the fourth stage due to lower oxygen concentration. This resulting temperature profile leads to rather uniform heat transfer to the wall, as demonstrated in Fig. 6, which shows the wall heat flux profiles for the four stages. The wall heat flux distributions correspond closely to those of temperature. For example, in Stage 1 the maximum wall heat flux of 690kW/m^2 is obtained in the region near the maximum flame temperature. The maximum wall heat flux also decreases from Stage 1 to Stage 4, as the maximum flame temperature decreases. The long and thin flames obtained in these four stages result in relatively uniform wall heat fluxes, and they are within manageable levels, even in Stages 1 and 2. The peak heat flux in Stage 2 is close to that in Stage 1 because, while the peak temperature is less, the temperature of the SO in Stage 2 is higher, as shown in Table 2, which enhances the convective heat transfer over that of the first stage.

By adjusting the distribution of thermal input among the four stages the peak wall heat fluxes in Stages 1 and 2 can be further reduced, as shown in Fig. 7. This distribution, which is termed the non-uniform distribution case, leads to a maximum heat flux of less than 600kW/m^2 for every stage. These results indicate that with an appropriate burner/boiler design, similar flame

sizes and manageable and relatively uniform wall heat fluxes can be achieved for all four stages. An additional reason that manageable wall heat fluxes can be achieved, even under extremely high temperatures, can be explained by a mechanism called “radiative trapping”. This phenomenon can occur in high-temperature systems that are optically dense [53], such as the SPOC boilers, and is described in [54, 55]. Since this is not the focus of this paper, detailed information is not presented here.

4.2 Buoyancy effects

The characteristic velocity is inversely proportional to pressure under the same mass flow rate and boiler geometry. Thus, due to the inverse of V^2 in the Ri number (Eq. (2)), it is imperative to study the effects of buoyancy on the flame characteristics in this pressurized system. To fully understand the effects of buoyancy, numerical modeling was performed with and without buoyancy (g), using a simpler burner design than that described in Section 4.3 above. The geometry has a PO/SO inner diameter of 0.3/3.96 m and a furnace length of 53.34 m. In this case, the SO outer diameter is the same as the furnace diameter. The case with buoyancy was carried out under down-fired conditions.

Figures 8 and 9 show a comparison between these two cases. It can be seen in Fig. 8 that case (a) has a shorter and wider flame than that of case (b) because of buoyancy. This shorter and wider flame enhances radiation, which accounts for the significant difference in wall heat flux for cases (a) and (b), as shown in Fig. 9. The case with buoyancy has a much higher maximum wall heat flux and less uniform wall heat flux along the axis than that of the case without buoyancy.

Moreover, backflow of hot gas into the SO stream is observed in case (a) of Fig. 9 and this is due to buoyancy. The Richardson number of this burner is around 200 at the inlet, which implies the flow is buoyancy dominated particularly in the upstream region near the inlet where

the temperatures are not uniform. Figure 10 shows the velocity vector diagrams for cases (a) and (b). The recirculation inside the secondary tube, which is caused by hot gas backflow, is clearly shown in case (a) of Fig. 10. On the contrary, in case (b) of Fig. 10, uniform flow is observed in the secondary stream and extends downstream to give a longer and thinner flame located in the center of the furnace.

The design described in Section 2.3 of this paper minimizes the effects of buoyancy through appropriate choices of burner and boiler geometry. With this geometry the Richardson number is reduced to 2.8. Also, the higher momentum in this system helps to keep the flame centered, and results in a manageable wall heat flux.

Based on the above discussions, two major advantages are obtained with the cone-shape boiler design. First, compared to the cylinder-shape boiler, the cone-shape can lead to a higher local axial velocity, and thus a lower Ri number, which minimizes the effects of buoyancy. In the entrance of the boiler the diameter is smallest and thus the velocity is highest to minimize buoyancy. Downstream, the volume flow rate increases for two reasons: the gas temperature increase and gaseous species are being produced, as the solid fuel is combusted. Thus the Ri number can remain low even as the diameter increases. A second advantage of the cone-shape can be seen in Fig. 8. The flame in the near-burner zone is thinner than that downstream. The cone-shape of boiler means that the boiler tubes are closer to the flame and thus there is a higher wall heat flux as indicated in Fig. 9. Thus, the boiler tube surface is more effectively used for the SPOC design with cone-shaped boiler.

6. Conclusions

Staged, pressurized oxy-combustion (SPOC) is a promising technology that boasts a considerably higher efficiency compared with first generation oxy-combustion systems and post-

combustion capture. The first stage of the system involves burning coal in a nearly pure oxygen environment at high pressure. In order to handle these extreme conditions, a new burner and boiler design is proposed in this study. The enclosed jet theory is used to design a combustion system with slow mixing and no external recirculation, which helps minimize flame impingement and ash deposition. A cone-shaped geometry is utilized to minimize the effects of buoyancy in the down-fired, axial-flow system. 3-D CFD simulations were performed based on this design to simulate a 1540 MWth SPOC system.

Simulation results show that with the new burner/boiler design, a long and relatively thin flame is created in the combustion system without an external recirculation zone, and buoyancy effects can be significantly reduced due to the low Richardson number resulted from the cone-shaped boiler design. Relatively uniform heat flux distributions on the walls can be achieved for all four stages with this design. If the thermal inputs are equal for all four stages, the peak wall heat flux in Stages 1 and 2 are about 690kW/m^2 . After optimizing the thermal input distributions among the four stages, a peak wall heat flux lower than 600kW/m^2 can be achieved for each stage.

The boiler described here is fundamentally different from traditional boilers in the power generation industry, which typically employ high mixing rates and result in complex flow fields. The application of this traditional approach should not be expected to succeed in a pressured boiler having a high aspect ratio and lower volume. The approach described herein can be employed to overcome many foreseeable challenges associated with pressurized oxy-combustion, such as particle deposition and radiative heat exchange. Besides being applied to SPOC system, the unique design concept can also be applied to pressurized oxy-combustion boilers with substantial flue gas recycle.

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588 **Figure captions**

589 Figure 1. Concept of staged combustion, showing four stages.

590 Figure 2. Overall adiabatic flame temperature at different stoichiometric ratios, when coal is
591 combusted in pure oxygen (solid line), and in typical oxy-coal environment (star).

592 Figure 3. Flow diagram for SPOC process.

593 Figure 4. Geometry of the burner of SPOC.

594 Figure 5. Temperature (K) distributions of SPOC design for Stages 1- 4.

595 Figure 6. Wall heat flux for Stages 1- 4 with uniformly distributed thermal input.

596 Figure 7. Wall heat flux for Stages 1- 4 with non-uniformly distributed thermal input.

597 Figure 8. Temperature (K) contours of Stage 1 for (a) with buoyancy (b) without buoyancy.

598 Figure 9. Wall heat flux for cases (a) with buoyancy, and (b) without buoyancy.

599 Figure 10. Velocity vector (m/s) profiles for cases (a) with buoyancy, and (b) without buoyancy.

600

601

Table 1. Properties of PRB coal.

Proximate analysis (% wet)				Ultimate analysis (% daf)					HHV
Moisture	VM	FC	Ash	C	H	O	N	S	(MJ/kg)
27.42	31.65	36.43	4.5	73.81	5.01	19.91	0.95	0.32	20.47

Table 2. Summary of operating conditions.

		Mass flow rate (kg/s)	O ₂ (vol. %)	CO ₂ (vol. %)	H ₂ O (vol.%)	Temp. (K)
Stage 1	Coal	18.81				
	Primary stream	4.2	25	75	0	458
	Secondary stream	110	100	0	0	458
Stage 2	Coal	18.81				
	Primary stream	4.2	25	75	0	458
	Secondary stream	132.2	63.8	21.3	14.8	873
Stage 3	Coal	18.81				
	Primary stream	4.2	25	75	0	458
	Secondary stream	154.3	37.3	36.8	25.7	873
Stage 4	Coal	20.52				
	Primary stream	4.2	25	75	0	458
	Secondary stream	176.5	17.1	48.7	34.0	873

Table 3. Comparison between studies with uniformly distributed and optimized distribution of thermal input among the four stages.

	Stage 1	Stage 2	Stage 3	Stage 4
Uniform distribution	385 MW	385 MW	385 MW	385 MW
Optimized (non-uniform) distribution	340 MW	302 MW	385 MW	513 MW

Figure1

Figure2

Figure3

LEGEND

ASU: Air Separation Unit
BFW: Boiler Feed Water
SC: Steam Cycle

Figure4

Figure5(color)

Figure6

Figure 7

Figure8(color)

Figure9

Figure10(color)