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ONE-DIMENSIONAL MODELING OF OXY-FUEL FLUIDIZED BED COMBUSTION FOR CO2 CAPTURE

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ABSTRACT

A one-dimensional model has been developed with the aim of investigating oxyfuel circulating fluidized bed (CFB) combustion for CO_2 capture with the main focus of assessing the heat balance of the CFB loop. For different oxygen concentrations in the gas flow fed to the furnace, the model calculates the external solids recirculation and the heat load in the furnace and in external particle coolers.

INTRODUCTION

Oxyfuel combustion is a promising combustion technology for Carbon Capture and Storage (CCS). In oxyfuel combustion, the fuel is burnt in a mixture of pure oxygen and recirculated flue gas. The oxygen is produced in an Air Separation Unit (ASU), i.e. which removes the nitrogen from air. Since nitrogen is removed, the resulting flue gas contains almost only CO_2 and water, and the water can be removed in a condenser. Flue gas recirculation (FGR) is applied in order to control the temperature. If a Pulverized Coal (PC) fired oxyfuel plant is to mimic air-like conditions, around 2/3 of the flue gas has to be recirculated, which corresponds to around 27% oxygen in the oxidizing gas, see (1). This means that the flue gas flow downstream of the recirculation point is 1/3 of that under air firing. Although it is likely that the FGR can be reduced for PC oxyfuel boilers, the high heat capacity of the bed in a Circulating Fluidized Bed (CFB) may offer a possibility to apply higher oxygen concentrations (lower FGR flow) compared to PC oxyfuel combustion. This would then facilitate a more compact unit as well as lowering the excess oxygen (losses) while maintaining combustion temperature at 850 ºC.

In addition to the possibility of lowering the RFG flow, CFB oxyfuel combustion may have additional advantages similar to those under air firing such as fuel flexibility and possibility for in-bed sulphur capture. Yet, little information is available from operation of fluidized bed under oxyfuel conditions and most of literature and reports on oxyfuel combustion focuses on PC furnaces. Especially what happens at high oxygen concentrations (low FGR flows) is not known. This is both with respect to the combustion process itself (i.e. if there may be local hot spots resulting in agglomeration problems as well as the fate of NO_x and SO_x) and with respect to how to allocate heat transfer surfaces in the furnace and in external particle coolers which is the topic of this paper, *i.e.* how to close the heat balance.

In CFB oxyfuel combustion, use of high oxygen concentration (*i.e.* low FGR) and the limited heat extraction area in the furnace results in that a much larger fraction of the heat extraction must take place in external particle coolers placed in the return leg (*i.e.* loop seals), which imposes a challenge with respect to design, heat transfer and fluid dynamics and requirements on a high enough external solids flux (i.e. from furnace to external particle cooler). In addition, additional in-furnace heat transfer surfaces may be required to close the heat balance.

There is not yet any large size (cross section of several meters in width) oxy-fuel CFB pilot plant built. At present, experience and results reported in literature are from small test units (see (2), in which a unit of a riser diameter of 0.167 m was used). As a support for design of pilot plants (and later full scale units), it is of importance to establish models which using available knowledge on the fluidized bed combustion can provide first estimates on what behaviour can be expected in oxyfuel combustion. Thus, the aim of the work presented in this paper has been to establish a first version of a process model for oxyfuel CFB combustion, which can serve as a simple tool to assess possible range of operational conditions for oxyfuel fired CFB boilers. The model, which is developed from a previous model for air fired conditions, describes the fluid dynamics, combustion and heat transfer, closing the heat and mass balance of the CFB loop. The paper presents results from air-fired combustion used for validation of the model and thereafter extrapolates results for the heat extraction under oxyfuel combustion conditions for different oxygen concentrations.

THEORY

Based on a comprehensive, semi empirical 3-dimensional (3D) process model for CFB combustion, developed previously by the authors (3), the 1.5-dimensional (1.5D) model has been designed in order to reduce complexity and minimize calculation time, providing a simple tool for modeling and assessment of oxyfuel CFB boilers under a wide range of operating conditions. The model is 1.5D in the sense that the furnace (riser) is divided into a number of vertical cells, but with a horizontal division in the furnace freeboard to represent the core/annulus characteristics of the flow. Similar to the 3D model, the 1.5D model is divided into three major modeling modules: fluid dynamics, heat transfer and combustion, all briefly described below. For simulation of the oxyfuel cases, the model must be provided with additional features compared to the original model for air-fired conditions. Most importantly, FGR needs to be included. This requires an extra iterative procedure in the code; since flue gas is assumed to be recirculated at the same temperature as it leaves the cyclone (which is an output of the model). Oxygen can be considered to enter at ambient or preheated temperature.

Fluid Dynamics

The fluid dynamics are modeled by a 1.5D semi empirical model developed by the authors (4), which accounts for two solid phases in the freeboard: a cluster phase dominating the splash zone in the lower freeboard and a dispersed phase establishing a core-annulus flow structure in the upper freeboard.

Combustion

Solid fuels are characterized by their content in moisture, volatile matter, char and ash. In the current modeling, a sub model previously developed by the authors (3) is used for the description of the fuel concentration and fuel release (*i.e.* moisture, volatiles) fluxes in a CFB unit. The volatile composition is calculated according to the model presented in (5) and is assumed to contain four combustible volatiles, namely H_2, CO, $C_{1.16}H_4$, $C_6H_{6.2}O_{0.2}$. Char combustion, γ, is expressed as.

$$C + O_2 \rightarrow (2-2\gamma)CO + (2\gamma-1)CO_2 \qquad (1)$$

where γ depends on particle size and temperature (6). The resulting CO can be further oxidized to CO_2. While the loop seals and the cyclones are assumed to be perfectly mixed reactors, the mixing in the furnace cannot be approximated as perfect mixing. At typical temperatures in the furnace of a CFB boiler, mixing can be assumed to control the volatile combustion, i.e. combustion is assumed not to be limited by kinetics (*i.e.*, assumed infinitely fast), see (3). Char combustion, however, is limited by both the gas-solids mixing and the kinetics of char combustion (with kinetic rates from (3)). The mixing rate expresses, in each cell of the furnace, the fraction of reactants that will be effectively mixed (*i.e.* that will meet). Such a mixing rate, is here defined to be directly proportional to the residence time of reactants in each cell (τ), *i.e.* K_{mixing}

$$K_{mixing} = \Psi * \tau \qquad (2)$$

The constant Ψ is adjusted so that the modeled oxygen concentration at the top of the furnace matches that one given by measurements under air fired conditions (typically, values around 5% are obtained).

Heat Transfer

In fluidized beds, the heat transfer is typically divided into radiation and convection. In this context, convection includes gas and particle convection, as well as conduction by direct contact of the fluidized solids with the walls. Radiation to the heat transfer surfaces increases significantly in more dilute solid suspensions. Heat transfer by radiation and by convection obviously has to be modeled separately.

Breitholtz et al. (7) investigated convection and radiation in three large-scale CFB units and proposed the following correlation for the convective heat transfer coefficient:

$$h_{conv} = 25.C_S^{0.58} \qquad (3)$$

As indicated above, heat transfer by radiation is strongly influenced by the solids concentration. Solids are absorbing the radiation and yield a shadowing effect preventing gas radiation from core to wall in CFB reactor systems. The shadowing effect was studied in (8) in which the following expression was used for the absorption effect of the solids suspension (shadowing effect):

$$\alpha_c = \exp\left(-\frac{1.5.C_{v,s}.L}{d_s}\right) \qquad (4)$$

The present model accounts for radiation between the following three items: the gas-solids suspension in the core region, the wall layers and the water walls. Figure 1, illustrates the treatment of net radiative heat transfer in the gas-solids suspension in the core. Similar patterns apply for the rest of the radiative terms including wall radiation to core and water walls. The radiative heat flux from the core region of the furnace to the water walls accounting for the shadowing effect of the wall layer solids is calculated as:

$$q = \epsilon.\sigma.(1-\alpha_c).\left(T_{core}^4 - T_{waterwall}^4\right) \qquad (5)$$

Thus, in the lower part of the freeboard, where the solids concentration in the wall layers is relatively high, radiation plays a minor role while it becomes the dominant heat transfer mechanism in the upper freeboard where solid concentrations are low. The radiative heat absorbed by the wall layer can be expressed as:

$$q = \epsilon.\sigma.\alpha_c.\left(T_{core}^4 - T_{wall}^4\right) \qquad (6)$$

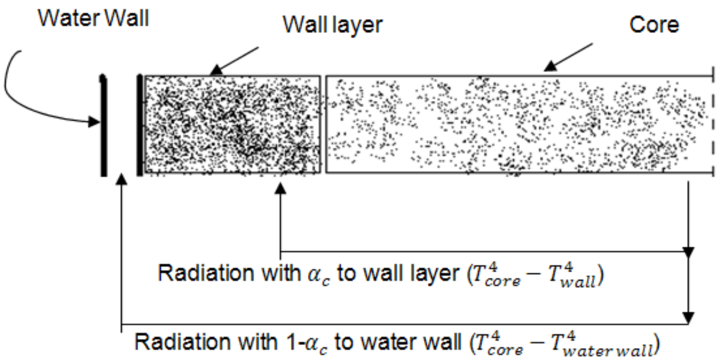

Figure 1: Radiation route from core to the wall layer and water walls

RESULTS

Validation of the model has been made against measurements from large-scale CFB boilers ranging up to 287 MW, in general with a good agreement under air fired operation. A summary of this validation is given in (4). Figure 2 exemplifies the agreement between experimental (9) and modeled vertical solids concentration profiles for a 226 MW CFB boiler. In the present work, the experimental results used are new and from a state-of-the-art CFB boiler of 278 MW_{th} for which no experimental data is yet published (but made available for the authors). This boiler is here used both for the air case and oxyfuel modelling (but experimental data obviously only available in air case). The furnace has a height of 37 m with a cross section of 15 x 6 m at the furnace top. The fuel used in the calculations is hard coal.

Figures 3 and 4 show modeled results for the air case. As can be seen in Figure 3, vertical profiles of O_2 and CO_2 concentrations experience steep gradients in the lower part of the furnace, where fuel concentration is high. Figure 3 also shows that in the lower part of the furnace, where volatile release dominates over volatile consumption, the concentration of CO increases. However, after a certain height, the sharp decrease in fuel concentration leads to that the volatile consumption gets larger than the volatile release, thus leading to a decrease in CO concentration. This trend is also predicted for volatile species other than CO.

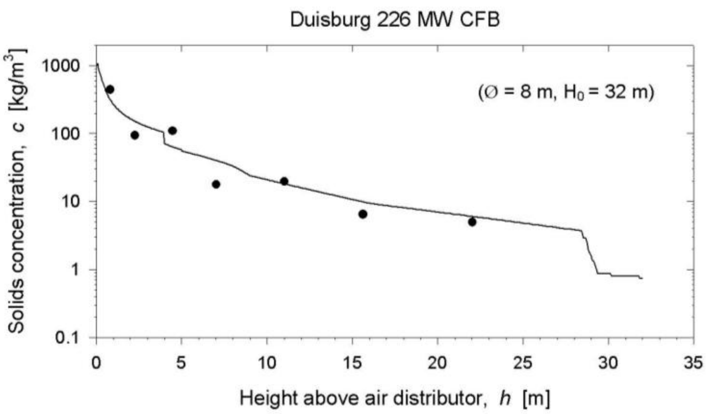

Figure 2: Vertical profile of solids concentration. Experimental data from Werdermann (9) compared to submodel results.

The modeled temperature field in Fig. 4 illustrates the effect of heat extraction panels in order to allow for additional heat extraction in the furnace than that provided by the water walls, a usual situation in large-scale CFB boilers. The model is implemented in such a way that, given an average temperature in the furnace, the heat flow to be extracted from these extra panels is calculated. In a CFB boiler, this heat flow is then adjusted by activating more or less of the heat extraction panels located in the furnace. Typically, in order to optimize different phenomena such as combustion, sulphur capture, corrosion and emissions, a furnace temperature of 850 C is is aimed for (also applied in this work). Table 1 shows the different heat extraction sources in two air-fired cases: with and without extra panels in the furnace respectively. When no panels are used, the average temperature in the furnace raises to 915 C (air case 2), while an extra heat extraction of 35 MW is required to keep the average temperature at 850 C (air case 1).

The oxyfuel simulations have been performed using different oxygen concentrations applied to the same furnace geometry as used in the air cases. Thus, additional heat transfer surface required to close the heat balance under oxyfuel conditions can be estimated from the modelling for different oxygen concentrations. Based on the required heat extraction in the loop seal, the necessary external solid circulating from furnace to the loop seal is calculated and compared to that under air firing (the original air fired net solids flow is 170 kg/s, corresponding to a net solid flux of 1.9 $kg/m^2 \cdot s$). By adjusting the fuel feeding rate, the gas velocity (and thereby fluid dynamics of the unit) has been kept constant for all cases. The results are presented in Table 1 and Fig. 5. In oxyfuel combustion at high oxygen concentrations, the heat extraction in the furnace is limited by the available area for additional heat extraction panels. The available area for additional in-furnace heat transfer surfaces is assumed limited to the same area as that of the water wall heat extraction area. With this, Fig. 5 shows that an oxygen concentration of 29% is the highest for which heat transfer surfaces in the furnace (walls and additional in-furnace heat transfer surfaces) are large enough to maintain the furnace temperature at 850ºC. Thus, for higher oxygen concentrations, additional heat extraction in the loop seals (external particle cooler) is required to maintain the average furnace temperature at 850 C.

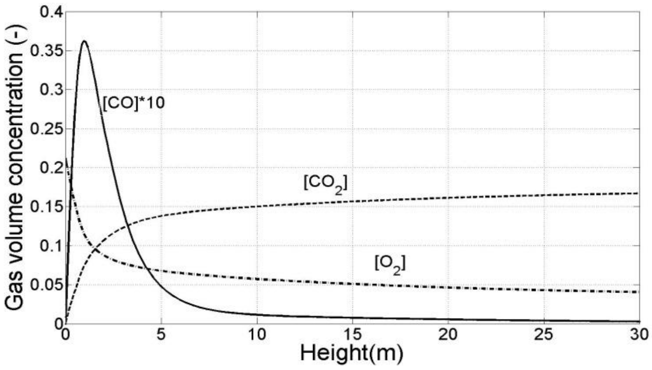

Figure 3: Oxygen, CO2 and CO volume concentration in the air fired case (note the difference in scale for CO).

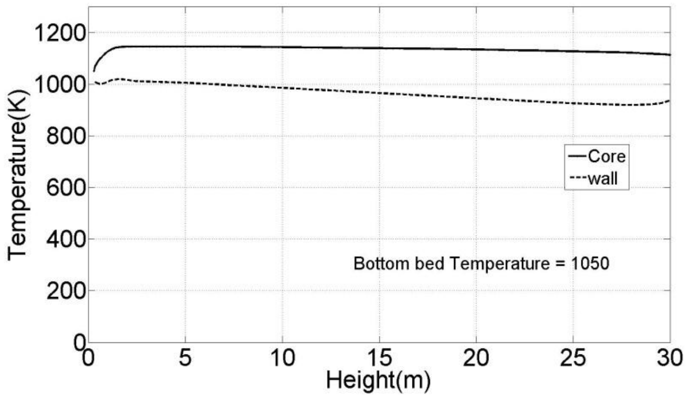

Figure 4: Temperature profile in the air fired case

Table 1: Model results. H [MW], F [kg/s], G [kg/m²s]

Γ_{oxy}	P_{th}	H_{WW}	H_{panel}	H_{flue}	H_{seal}	F_{circ}	G_{circ}
Air Case 1	257.3	139.3	35.1	82.1		170	1.9
Air Case 2	257.3	161.2	0.0	89.7		170	1.9
Oxy 24%	257.3	142.9	87.5	26.9		170	1.9
40%	440.1	141.4	139.8	42.5	116.5	463.5	5.2
60%	672.5	137.7	139.8	59.8	335.2	1 ,334.1	14.8
80%	900.8	137.3	139.8	76.1	547.7	2 ,179.8	24.2
99%	1, 118.0	139.5	139.8	91.0	747.7	2, 975.7	33.1

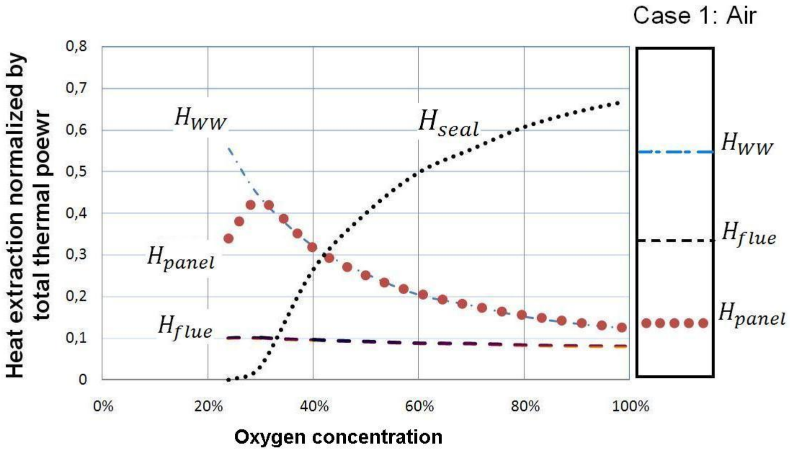

Figure 5: The share of different heat extraction terms normalized by the total thermal power.

Therefore, exceeding 29% oxygen concentration in the FGR flow, heat must be extracted from the externally recirculated solids flow. In this work, it is assumed that solids cannot be cooled down to temperatures below 690 C before being re-fed into the furnace. The model gives that for oxygen concentrations exceeding 34%, the net solids flow of the boiler design used is too low to provide the required heat extraction from the circulating loop while maintaining a furnace temperature of 850 C. Table 1 gives the modelled external solids flow values required for different oxygen concentration (in the FGR flow) and it can be seen that values around 30 kg/m^2s are required for the highest oxygen concentration investigated (99%), *i.e.* significantly higher than typical values in air-fired CFB boilers (usually between 0.1 and 10 kg/m^2s). Operation with high net solids fluxes requires other design than the one used in this work, *i.e.* geometry must be different (*i.e.* smaller furnace cross section or finer bed material in order to increase the gas carrying capacity). Yet, net solids flow of up to 200 kg/m^2 have been applied in tall and narrow CFB units for chemical applications (*cf.* (10)) and some 30 kg/m^2s should therefore be possible to apply, but such conditions need to be investigated further. As can be seen from Fig. 5 the share of heat recovered from flue gas in the convection pass increases with an increase in oxygen concentration (obviously, since the lower FGR makes a higher fraction of flue gas available for heat extraction). The share of heat extraction in the seal increases dramatically with oxygen concentration, and for oxygen concentrations exceeding 55%, heat extraction in seal becomes larger than that given by water walls and heat panels in the furnace. This imposes significant changes in the design and dimensions of loop seals for oxy-fired CFB boilers compared to those of air-fired units. The water wall heat extraction depends on oxygen concentration since this influences the temperature profile along the furnace.

CONCLUSION

A 1.5-dimensional model has been developed in order to assess oxyfuel combustion in large-scale CFB units. The model gives an estimate of the external solids recirculation required for different concentrations of oxygen in the FGR. The shares of heat extraction from water walls, extra heat panels, loop seal heat exchangers and convection pass is determined by the model. The model predicts that for the highest oxygen concentration applied, the net external solids flux is significantly higher than typical values in air-fired CFB boilers.

ACKNOWLEDGMENT

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NOTATION

C	Solids Concentration [kg/m^3]	α_c	Bouguer transmissivity[-]
d	Particle diameter [m]	L	Length[m]
F_{circ}	Net Solid flow needed [kg/s]	P_{th}	Total thermal power [MW]
G_{circ}	Net Solid flux needed [kg/m^2.s]	q	Heat flow[w]
h	Heat transfer coefficient [w/m^{2}K]	T	Temperature[K]
H_{ww}	Heat extracted by water wall[MW]	ϵ	Emissivity [-]
H_{panel}	Heat extracted by additional panels in furnace [MW]	Γ_{oxy}	Oxygen concentration[%mass]
H_{flue}	Heat extracted from flue gas recovery [MW]	$Hseal$	Heat extracted from loop seal [MW]

Subscripts

conv	Convection	*susp*	Suspension
rad	Radiation	v	Volumetric
s	Solids		

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