Predicting Ash Deposition During Oxy-Coal Combustion

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Abstract:

An ability to predict and control ash deposition are crucial to effective heat extraction from pulverized fuel (pf) units. Computation Fluid Dynamic (CFD) simulations in conjunction with fuel characterization data have been used in recent years to develop sub-models to predict slagging propensities under various operating conditions. A common methodology is to use particle and wall temperature predictions in conjunction with particle Weber numbers (obtained from Lagrangian tracking methods) to assess the slagging and fouling tendencies. However, a Weber number based capture criterion requires as inputs important slag properties like the critical sticking viscosity and surface tension that are needed to estimate the Weber number. Given that there is no consistency in reporting the values of critical sticking viscosity (with values as low as 1 Pa-s to higher than 10^9 Pa-s been reported in the literature), it is clear that a few key performance parameters (such as ash transport and sticking propensities such as the Weber number criterion) could be "tuned" to match the observations. Another inherent limitation of Lagrangian tracking methods is their inability to track changes to the ash composition and particle-size distribution (PSD) within the combustor which can subsequently impact the ash partitioning and deposition characteristics. This is attributed to the fact that the ash formation is a complex physio-chemical process consisting of: vaporization, condensation, melting, fragmentation, nucleation and coagulation of the mineral matter and organically bound metals in the parent fuel. In spite of these complexities, there are representative scenarios (depending on the location of ash deposition within the boiler) where its deposition rates can be predicted reasonably accurately based on simple Stokes number criterion. This is demonstrated here based on simulations of oxy-coal combustion in a 100 kW down-fired combustor where the deposition rate predictions of the "outer layer" of ash deposits are shown to agree reasonably well with experimental measurements.

1. Introduction

Oxy-combustion processes for power generation is a promising technology for CO_2 reuse and sequestration using essentially conventional equipment. During oxy-fuel combustion, fuel is burnt in a stream of O_2 and recycled flue gas (to regulate combustion temperatures) instead of air as the primary oxidant [1]. This results in the generation of a CO_2-rich flue gas stream. Although many aspects of oxy fuel combustion for coal systems have been well researched, there are notable challenges that still need to be overcome and understood, before oxy-combustion can be fully scaled up to a commercial scale [2]. Understanding the ash formation and deposition processes and their subsequent impact on wall heat transfer under these novel operating conditions remains one such challenge. This is attributed to the fact that the ash formation is a complex physio-chemical process consisting of: vaporization, condensation, melting, fragmentation, nucleation and coagulation of the mineral matter and organically bound metals in the parent fuel. This results in a distinct tri-modal distribution of the ash particles [3]. Recent experimental studies have shown that a correlation exists between the rate of deposition of the tightly bound "inner" deposit layer adjacent to the heat transfer surfaces and the concentrations of the submicron aerosols in the flue gas [4]. Thermophoresis is the mechanism that mainly governs the deposition rates of this "inner" deposit later. A follow on study has shown that the deposition rates of the "outer" deposit layer appears to be proportional to the concentration of Na + K in the flue gas [5]. Therefore, the long-term objectives of this

project are to develop validated models and methodologies that can predict and uncover the mechanisms governing the ash deposition rates during pulverized fuel combustion. While the incorporation of ash deposition models in Computational Fluid Dynamic (CFD) simulations is not new, most of current CFD modeling efforts of ash deposition are all based on bulk ash composition and do not consider ash partitioning (vapors and liquid/solid particles) during the deposition process. Due to the resulting differences in ash composition during the ash partitioning process, the deposition criteria (ash transport, sticking, growth, and sintering (strength development) that are based on bulk ash properties will result in erroneous CFD predictions. To offset these errors, key modeling parameters such as critical transport, sticking, growth, and sintering parameters are often "tuned" to match experimental/field observations [6].

For instance, a common methodology is to use particle and wall temperature predictions in conjunction with particle Weber numbers (obtained from Lagrangian tracking methods) to assess the slagging and fouling tendencies. However, a Weber number based capture criterion requires as inputs important slag properties like the critical sticking viscosity and surface tension that are needed to estimate the Weber number. Given that there is no consistency in reporting the values of critical sticking viscosity (with values as low as 1 Pa-s to higher than 10^9 Pa-s been reported in the literature), it is clear that a few key performance parameters (such as ash transport and sticking propensities such as the Weber number criterion) could be "tuned" to match the observations. In spite of these complexities, there are representative scenarios (depending on the location of ash deposition within the boiler) where its deposition rates can be predicted reasonably accurately based on simple Stokes number criterion. This is demonstrated here based on simulations of two oxy-coal flames (OXY 27 and OXY 70) in a 100 kW down-fired combustor where the deposition rate predictions of the "outer layer" of ash deposits are shown to agree reasonably well with experimental measurements. The numerical simulations in this study are based on measurements of rates of inner and outer ash deposition layers for a wide range of fuels in a down flow laboratory combustor (shown schematically in Figure 1) made by Wang et al [5].

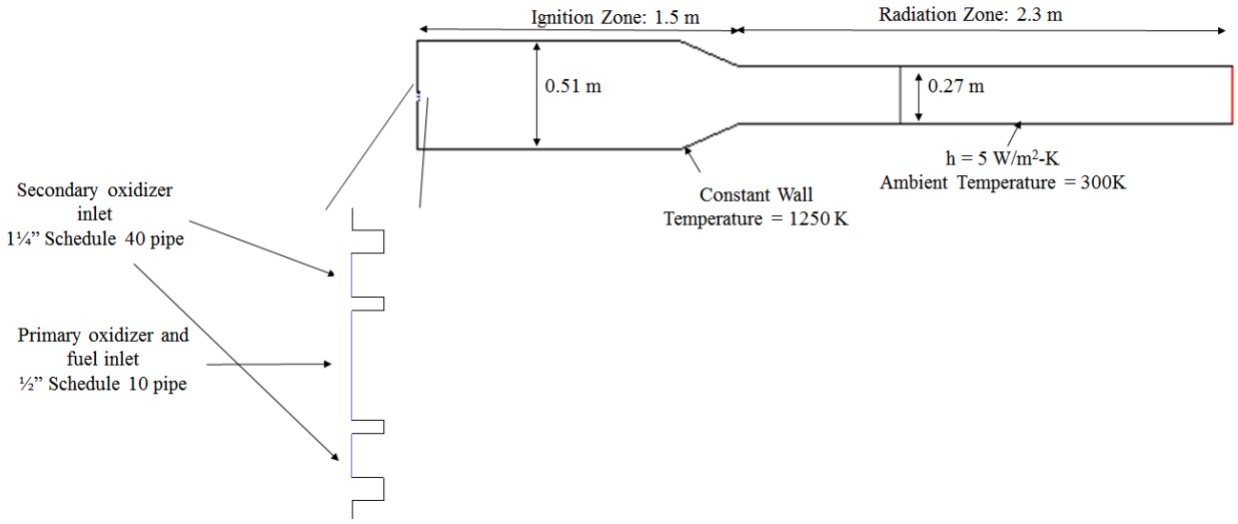

Figure 1: 2D, axisymmetric geometry designed to replicate the experimental 100 kW combustor.

2. Methods

CFD simulations for the two oxy-combustion flames were completed using commercial software ANSYS Fluent 16.2 [7]. Sufco coal, a Utah sub-bituminous coal, was used as the fuel for oxy-combustion. Table 1 contains the proximate and ultimate analysis for this coal.

Table 1: Proximate and Ultimate Analysis of Sufco coal

Proximate Analysis (wt. %)		**Element Analysis (wt. %)**	
Fixed Carbon	47.04	C	67.87
Volatiles	38.49	H	5.45
Ash	8.36	N	1.09
Moisture	6.11	S	0.36
HHV (BTU/lb.)	11,899	O (by difference)	16.87

Al_2O_3	CaO	Fe_2O_3	MgO	MnO	P_2O_5	K_2O	SiO_2	Na_2O	SO_3	TiO_2
8.34%	18.21%	5.25%	2.84%	0.05%	0.01%	0.33%	48.85%	3.09%	5.96%	0.64%

Boundary conditions, contained within Table 2, were obtained from the University of Utah and employed in the simulations to recreate experimental trials.

Table 2: Primary and Secondary Oxidizer Stream Specifications for the OXY27 and OXY70 Flames

	Oxy27	**Oxy70**
Mass flow rate (kg/h)		
Fuel	3.46	3.46
Primary	6.22	5.26
Secondary	31.8	6.63
Inlet gas temperature (K)		
Primary	480	480
Secondary	480	480
Species concentration of primary inlet (mol %)		
O_2	21	21
H_2O	0	0
CO_2	79	79
N_2	0	0
Species concentration of secondary inlet (mol %)		
O_2	28.2	100
H_2O	0	0
CO_2	71.8	0
N_2	0	0

A 2D, axisymmetric geometry was built in ANSYS Workbench to the specifications of the combustor used in Utah as shown in Figure 1. The length of geometry is 3.8 meters. The length and diameter of the ignition zone are 1.5 meters and 0.51 meters, respectively. The length and diameter of the radiation zone are 2.3 meters and 0.27 meters, respectively. For reference, the location where the ash deposition measurements were taken during the experimental trials are shown by a vertical line in the radiation zone in Figure 1. Thermal boundary conditions were set for the walls in the ignition and radiation zone. The

ignition zone walls were set to a temperature of 1250 K. The radiation zone walls were set to a heat transfer coefficient of 5 W/m^2-K and a surrounding fluid temperature of 300 K.

The single-rate model was chosen to model devolatilization. This model assumes that the rate of devolatilization is first-order with respect to the volatiles [7]. After release of the volatiles during the volatile pyrolysis process, the remaining char reacts with the surrounding gas phase. Gaseous combustion between the fuel volatiles and oxidant was simulated using a two-step mechanism. Initially, volatiles are oxidized and release CO. Then, CO is oxidized to CO_2. The heterogeneous and homogenous reactions modeled in these studies are contained in Table 3.

Table 3: A summary of reactions and kinetic parameters modeled in this study.

	A	**Ea, J/kmol**	**Reference**
Heterogeneous reactions			
Devolatilization	382000*	7.4e+07	[10]
Char combustion: $2C_s + O_2 \rightarrow 2CO$	0.86**	1.13e+08	[8]
Homogeneous reactions			
Volatile combustion: $vol \rightarrow 1.05CO + 1.96H_2O + 0.0283N_2 + 0.0082SO_2$	2.119e+11*	2.027e+08	[11]
CO oxidation: $2CO + O_2 \rightarrow 2CO_2$	2.239e+12*	1.7e+08	[9]
*Pre-exponential factor, A, units: *(1/s) , **(kg/m^2 s Pa)*			

Table 4 provides a complete summary of the different modeling options invoked in this study. Additionally, non-gray effects of gas radiation and the variations in the radiative properties of the solid phase during combustion were implemented as user-defined functions.

Table 4: A summary of modeling options invoked in this study

Physics being modeled	**CFD Framework (ANSYS Fluent)**
Multiphase hydrodynamics	DPM
Turbulence	SST k-omega
Coal devolatilization	Single-rate
Gas-phase chemistry	Finite rate/Eddy dissipation
Heterogenous chemistry	Kinetic based char oxidation (with O_2)
Drag law	Morsi-Alexander
Particle radiative property	Variable K_{abs} and K_{scat} [12]
Particle scattering phase function	Anisotropic (forward scattering)
Gas-phase radiative property	Perry (5gg) [13]

The sieve mass fractions of the parent fuel were fit to a Rosin-Rammler distribution function (which was subsequently split into 100 intervals) and then employed in the simulations (Figure 2).

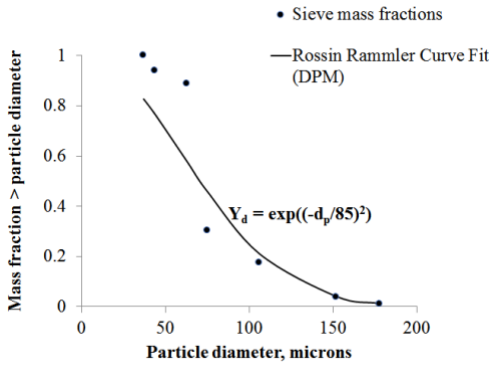

Figure 2: The Rosin-Rammler distribution function used to represent the PSD of the parent fuel.

3. Results and Discussion

Figure 3 shows the predicted temperature contours in the OXY27 and OXY70 flames. Due to an increase in the oxygen concentration in the oxidizer, higher peak temperatures are seen in the OXY 70 flame. Nevertheless, the gas temperatures in both flames are in the 1100 K – 1200 K range at the location where the ash deposition measurements were made.

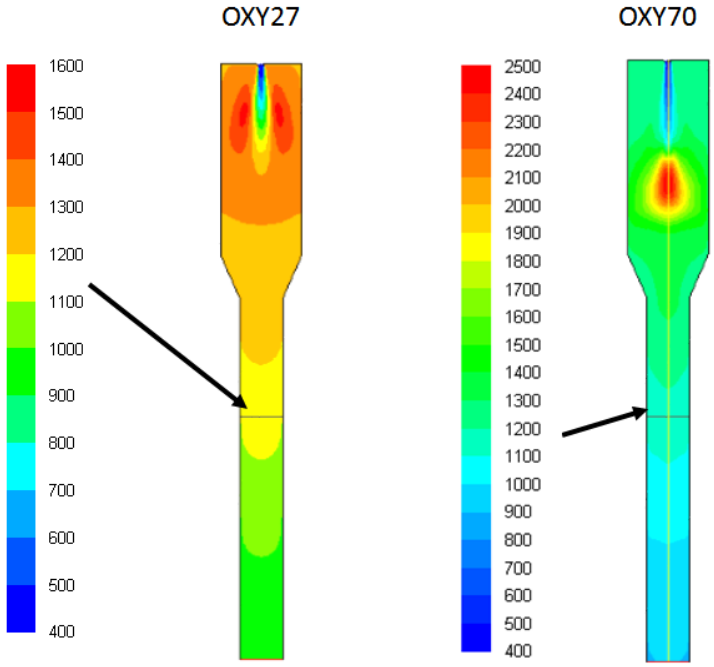

Figure 3: Predicted temperature contours in the OXY27 and OXY70 flames

Figure 4 shows the predictions in the axial gas temperature variations in both flames. The corresponding thermocouple based measurement data in Port-6 (where the ash deposition measurements

were made) are also shown. The predictions are within 100 K of the thermocouple based measured temperatures which may be deemed to be adequate at this stage.

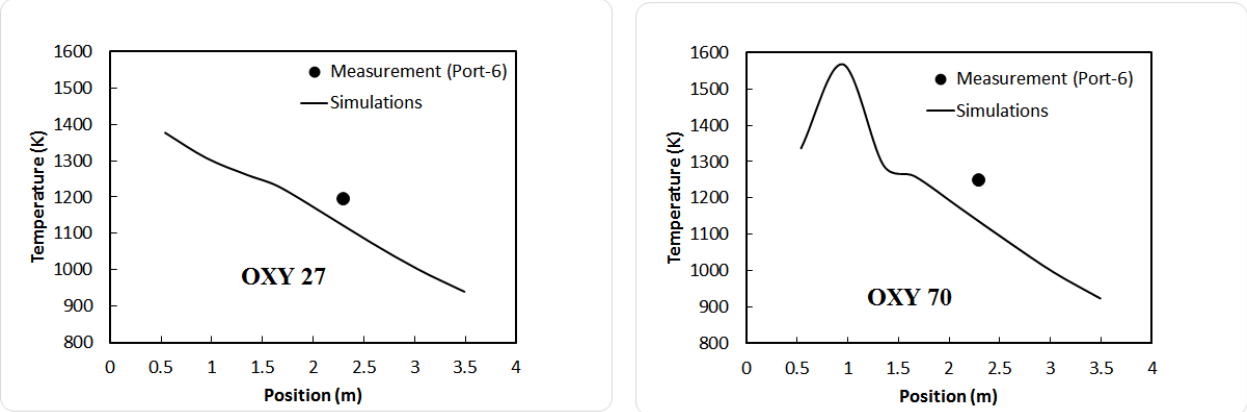

Figure 4: Axial temperature variations.

Table 5 compares and summarizes the primary variables that have an impact on the deposition rates. Based on the predicted mass flux of ash at port-6, a Stokes number based deposition criterion was employed to determine the capture efficiency of the ash particle and subsequently determine the rate of deposition of the "outer" layer at port-6. To do this, the Stokes number (St) for all the individual particles were first determined as:

$$St = \frac{u_p \rho_p d_p^2}{9 \mu d_c}$$

The subscript "p" in the above equation corresponds to the particle properties and d_c corresponds to the diameter of the collection probe. Based on the predicted Stokes number, an impaction efficiency (denoting the probability that the particle will be captured/deposited) was determined [14]. The predicted impaction efficiency is reported in Table 5. The predicted total mass flux of ash at port-6 was then multiplied by this impaction efficiency to determine the ash deposition rate. A comparison of the measured and predicted ash deposition rate show that such a simple criterion has been useful towards predicting the rates of "outer" ash layer in this configuration given that the collection probe is at a location where the gas temperatures are 1100 to 1200 K and the flow is laminar.

Table 5: Summary of experimental conditions and predictions

	OXY27		OXY70	
	Measurements	Predictions	Measurements	Predictions
Coal input rate (kg/hour)	3.46	3.46	3.46	3.46
Energy input (kw)	27	27.1	27	27
O_2 fraction in dry flue gas (vol.%)	3	2.51	3	2.93
Flue gas flow rate (m^3/hour @ standard condition) - outlet	22.41	22.94	8.96	9.07
Calculated ash concentration at port 6 (g/m^3)	2.43	2.86	5.82	5.87
ash mass flux at port 6 (g/(m2-hr))		4752.0		3879.1
Impaction efficiency		0.05		0.15
ash deposition rate at port 6 (g/(m2-hr))	**250**	**238**	**700**	**582**

4. Conclusions

Two oxy-combustion flames were investigated in this article. These scenarios were representative of experimental measurements carried out at the University of Utah. Methodologies in ANSYS FLUENT were refined to replicate the conditions observed in the scenarios. The paper demonstrates that in spite of the complexities governing the ash deposition process, there are representative scenarios (depending on the location of ash deposition within the boiler) where its deposition rates can be predicted reasonably accurately based on simple Stokes number based criterion. This is demonstrated here based on simulations of oxy-coal combustion in a 100 kW down-fired combustor where the deposition rate predictions of the "outer layer" of ash deposits are shown to agree reasonably well with experimental measurements.

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