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CFD Modeling of Combustion and Calcination Reaction in Cement Calciner

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Cement Clinker is produced by calcination of limestone, $CaCO_3$. The calcination reaction is endothermic in nature and releases pollutants like CO, CO_2 and NO_x. The Calcined lime stone then undergoes fusion, melting, solidification reactions in rotary kiln. The energy required for both these steps reaction is supplied by the combustion of fossil fuels like coal. This makes cement industry one of the largest CO_2 emitting and most energy intensive industry. It is imperative for the cement industry to be energy efficient and control pollutants. The combustion efficiency can be improved by efficient mixing of fuel and air. There are primary and secondary measures to reduce NOx. The primary measures of NOx reduction, (NOx reduction at source) are more favourable as it does not involve additional operating cost. The concept of Nox reduction in primary measure is to feed lime stone in hot region under reduced (oxygen limited) conditions. Computational Fluid Dynamics is the best tool to analyze mixing, predict the extent of coal combustion, understand temperature profiles, and hence understand the optimal location of lime stone injection in Calciner. In this work, a full 3D CFD model has been developed on a typical industrial scale Calciner. The model involves coal combustion and calcination of lime stone. As a first step, we validated the coal combustion model, and pollutant formation mechanisms with the experimental data for the International Flame Research Foundation (IFRF) furnace no. 1. The developed CFD model of combustion is used on the industry-scale cement calciner to analyze the combustion and calcination processes. The results obtained by the simulations give the in-depth understanding of the calciner processes which can be used for the optimization of the air feeding location, injection of limestone, improve combustion efficiency and lower the pollutant formation.

***Keywords*:** Combustion, Calciner, Calcination, Modeling

1. Introduction

The calciner is an integral part of the modern cement industry. The introduction of calciner in the cement industry has reduced the fuel consumption to a considerable amount. The major problems related to the performance of a calciner are handling the combustion of fuel, dust loading and formations of solid deposits due to the condensations of volatile matters, higher NOx. The extent of fuel combustion and calcination depend on the interaction of air, coal particles and cement raw meal particles ($CaCO_3$) and their residence time. The flow patterns and temperature profiles inside the calciner drive the performance of calciner. Also, the pollutants reduction is possible by maintaining the right mixing, proper residence time and temperature profile in the calciner. The CFD is the best tool to analyse mixing, predict the extent of coal combustion, understand temperature profile, and extent of calcination.

In this work, the combustion and the calcination reactions were simulated by using CFD codes (Fluent) to analyse the calciner performance. Due to the Combustion process and Calcination, a large amount of pollutants (CO, CO_2, NO_x and SO_x) are released. CFD analysis of Calciner will help to predict the pollutant formation. The in-depth understanding of flow patterns and temperature profiles can help us to decide the optimal injection locations of the air, fuel and raw meal to maximize fuel combustion efficiency, calcination and reduce pollutant formation.

In context to this more robust and accurate a mathematical or numerical model is required with a level of confidence with which such models can be applied to the industrial situation to represent the real world. Hence in this work, the non-premixed coal combustion is simulated in ANSYS Fluent code and the validation of the CFD combustion results is done with the experimental data given in [1] for International Flame Research Foundation (IFRF) furnace no. 1. as shown in Fig. 1 and Fig.2.

The developed CFD model of combustion is used in the industry-scale typical cement calciner as shown in Fig.3 with the operating conditions as given in Table. 1 to analyse the combustion and calcination processes in it. The results obtained by the simulations give an in-depth understanding of the calciner processes which can be used for the optimization of the calciner's geometry, to have a more efficient production of cement, to lower the pollutant formation and subsequently reduce the greenhouse gases emission.

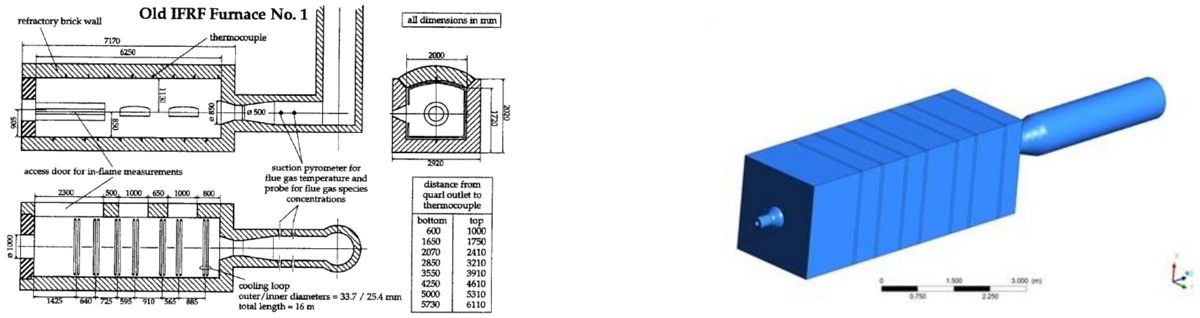


Fig.1: a) IFRF Furnace No.1.[1] and b) A 3D computational domain of IFRF furnace no.1

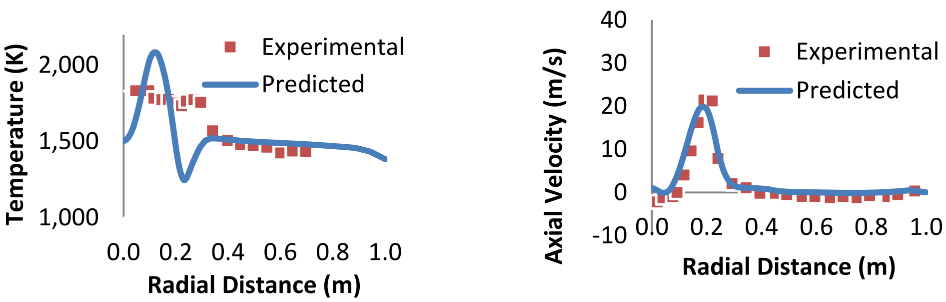


Fig. 2: Comparison of CFD results with experimental data of IFRF furnace for temperature and axial velocity.

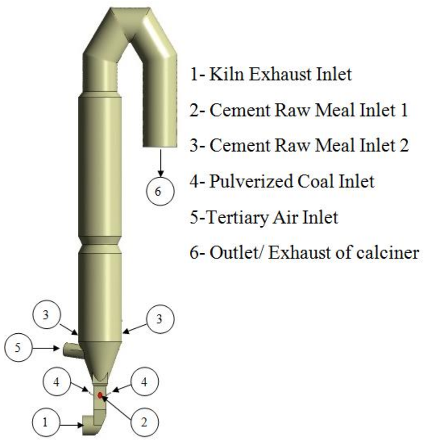


Fig. 3. Calciner Geometry

Table 1. Operating conditions of calciner

Location	Air (m^3/kg)	Coal (TPH)	Raw (TPH)
1	678843 (1150 ^{0}C)	-	-
2	-	-	80
3	-	-	320
4	6627 (40 ^{0}C)	16	-
5	688743 (946 ^{0}C)	-	-

2. Mathematical Model

The combustion of pulverized coal is modeled as two-phase by considering a volatile matter, carbon monoxide, carbon dioxide, oxygen, nitrogen and water vapour as continuous gaseous phase while char is considered as a dispersed solid phase. The governing equations for the gaseous phase and solid phase are solved in Eulerian and Lagrangian way respectively.

2. 1. Continuity Equation

The general Continuity equation is given as,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = S_m \tag{1}$$

The term S_m takes care of mass added to continuous gaseous phase from dispersed phase char due to Devolatization of volatile matter.

2. 2. Momentum Balance Equation

The momentum balance equation for the continuous phase is written as,

$$\frac{\partial}{\partial t}(\rho \vec{V}) + \nabla \cdot (\rho \vec{V}\vec{V}) = -\nabla p + \nabla \cdot (\bar{\bar{\tau}}) + \rho \vec{g} + F \tag{2}$$

In this equation the term F is the external body forces arises from the interaction with a dispersed phase

2. 3. Energy Balance Equation

The energy equation has the following form

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot \left(\vec{V}(\rho E + p)\right) = \nabla \cdot (k_{eff} \nabla T - \sum_j h_j \vec{J}_j + (\bar{\bar{\tau}}_{eff} . \vec{V})) + S_h \tag{3}$$

In the above equation, S_h indicates the heat of a chemical reaction.

2. 4. Species Transport Equation

The general form of species transport equation is

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{V} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \tag{4}$$

Above equation is solved for (N-1) species where N is the total number of fluid phase chemical species present in the system. The mass fraction of N^{th} species is given by one minus summation of mass fractions of (N-1) species.

2. 5. Particle Force Balance

According to Rusas, if the fluid to particle density ration is less than 10^{-3}, then only drag and gravity forces are considered. Hence by neglecting other types of forces, the force balance equation is written as

$$\frac{d\vec{u}_p}{dt} = F_D(\vec{u} - \vec{u}_p) + \frac{\vec{g}(\rho_p - \rho)}{\rho_p} + \vec{F} \tag{4}$$

By integrating the above equation, the trajectories of the particles can be determined which is written in a Lagrangian reference frame.

2. 6. Heat Transfer with Coal Particles.

As the coal particle size is very small, by neglecting internal particle temperature gradient

$$m_p c_p \frac{dT_p}{dt} = hA_p(T_\infty - T_p) + \varepsilon_p A_p \sigma(\theta_R^4 - T_p^4) \tag{5}$$

The particle heat balance is written by considering convection and radiation at the particle surface. The heat transfer coefficient, *h*, is evaluated using the correlation of Ranz and Marshall.

2. 7. Devolatization Model

The constant Devolatization model assumes that volatiles is released at a constant rate.

$$-\frac{dm_p}{dt} = A_0 f_{v,0}(1 - f_{w,0}) m_{p,0} \tag{5}$$

Where the term A_0 is a rate constant.

2. 8. Reaction Model (Volatile Matter Combustion Model)

The controlling parameter of volatile combustion is the turbulence. Hence the Eddy Dissipation model is used. In this model, the rate of reaction is limited to a minimum of net rate production of species due to the reaction and it is given by,

$$R_{i,r} = v'_{i,r} M_{w,i} A\rho \frac{\varepsilon}{k} min_R \left(\frac{Y_R}{v'_{R,r} M_{w,R}} \right) \qquad R_{i,r} = v'_{i,r} M_{w,i} AB\rho \frac{\varepsilon}{k} \frac{\left(\sum_p Y_p\right)}{\left(\sum_j^N v''_{j,r} M_{w,j}\right)} \tag{6}$$

2. 9. Char Combustion Model

The kinetic/diffusion rate model is used which assumes that the surface reaction rate is determined by either by kinetics or diffusion rate. The Particle size distribution is assumed as a Rosin Rammler type.

2. 10. Calcination Model

The rate of calcination depends on the a) heat transferred from surroundings to the particle surface, b) heat conduction through the reacted layer to the reaction zone, c) kinetics of chemical reaction occurs in the reaction zone. The reaction happens in the following way

$$\mathrm{CaCO_3(s)} \longrightarrow \mathrm{CaO(s)} + \mathrm{CO_2(g)} + 178\ \mathrm{kJ/mol}$$

The reaction rate at the interface is expressed as follows, Borgwardt

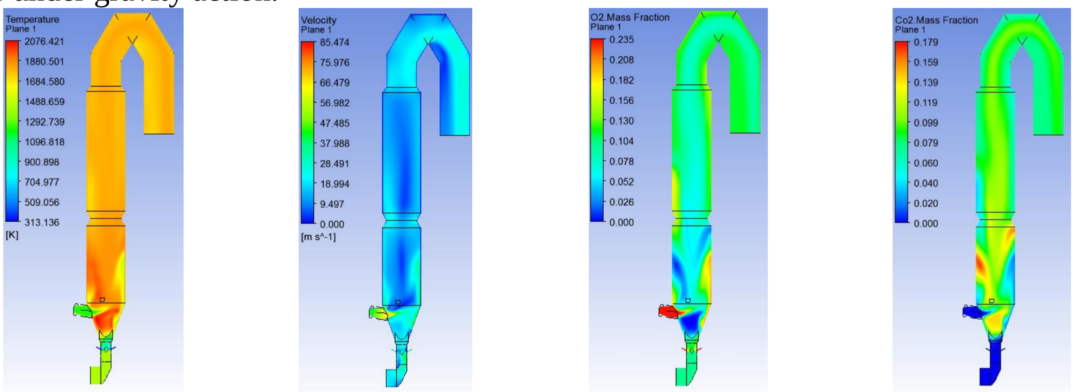
$$Rate = -k_s * A_{CaCO_3} \tag{7}$$

Where, $k_s = A * \exp(\frac{-E_a}{RT})$ (8)

The E_a is the activation energy in the range 165-205 kJ/mol. [2, 3]

3. Results and Discussion

The calciner is taken for the analysis, Fig. 1, consisting of two cylindrical portions with four kinds of inlets. The kiln exhaust inlet supplies the exhaust gasses coming from the kiln to calciner. The coal inlet carries the coal particles to calciner with the help of carrying air. There are two raw meal inlets are provided with a different mass flow rate. The raw meal enters the calciner under gravity action.



Temperature | Velocity | O_2 Mass Fraction | CO_2 Mass Fraction

Fig. 2. contours Plots for Different Parameters

The Fig.2 show the contours for different parameters. The temperature is maximum in the bottom cylindrical section of calciner because actual combustion is happening at that place. The flame is not centrally placed because of the flow effect of kiln exhaust inlet and tertiary air inlet. The flow velocity in the central portion of the calciner is very less as compared to a velocity near the wall. The blue colours in the O_2 mass fraction mean that all O_2 form that place is consumed in combustion. The O_2 mass fraction at the outlet is 0.11, which indicates the presence of excess air in the inlet supplies. The CO_2 mass fraction at the outlet is 0.08.

The Fig.3 shows the predicted temperature along the centre of calciner measured from the coal inlet position to exit of the upper cylindrical portion. There is a sudden drop in the temperature because at the point coal and raw meal enter the calciner at room temperature which absorbs the heat. After that, the sudden increase in the temperature indicates combustion. The process of combustion is completing within approximately 10 m from the coal inlet. After that, the temperature of the gas remains constant at 1800 K approximately.

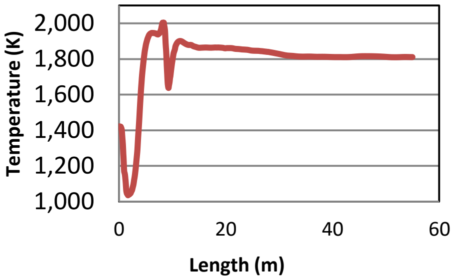
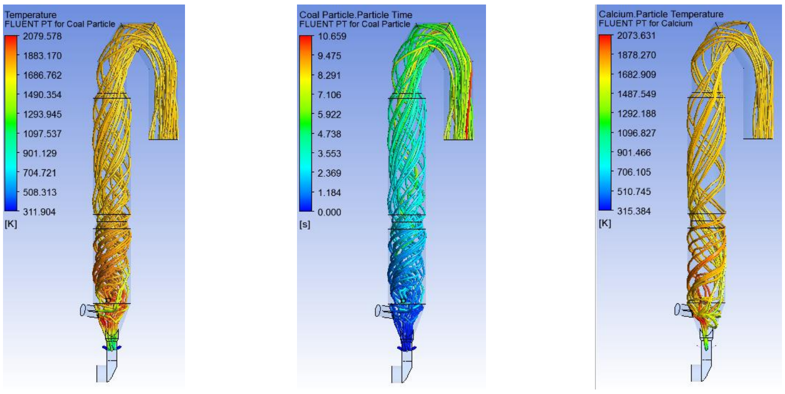


Fig. 3 Temperature profile along the calciner

Fig. 4 shows the coal particle temperature variation where it enters the calciner at room temperature i.e. 300K. The temperature rises to Devolatization temperature. At that temperature volatile matter is evolved from coal particles. The coal particle temperature rises to approx. 2000K and becomes equilibrium with surrounding gas temperature.

The average residence time of coal particles in the calciner is around 9 seconds which is sufficient for complete coal combustion. The temperature variation of $CaCO_3$ is also shown in Fig. 4. Due to the tertiary air, the major part of $CaCO_3$ mass is bypassing without entering through the combustion zone.



Coal Temperature Variation | Coal Particle Residence Time | $CaCO_3$ Temperature Variation

Fig. 4. contours Plots for Different Parameters

4. Conclusion

The CFD model used in the calciner is can predict the mass fractions, trajectories, velocities and temperatures of gas phase and discrete phase at all locations in the calciner. Some circulations are present in the calciner near coal inlet and tertiary air inlet which increases the residence time of coal for proper combustion. Some of the $CaCO_3$ particles are bypassed due to tertiary air. So some attention needs to pay towards the location of the tertiary air inlet. The total CFD analysis helps to redesign or modification in the calciner. Although the model needs to be validated with the actual measurement, which can be stated as a future scope of this work.

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