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CFD Modelling of Alumina Calciner Furnaces

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ABSTRACT

Developing CFD models of calciner furnaces requires careful consideration of the relevant physical processes including the gas flow, turbulence, flow of solids particles, fuel combustion and the pyro-metallurgical process. All these processes are closely coupled and the interaction between the phases must be correctly considered in order to produce realistic simulations.

By considering the physical processes coupled together within one model, the complex behaviour of the calciner furnace can be modelled. These furnace models greatly enhance the design process by providing information on calcination rates and particle composition exiting the furnace, interaction between the combustion zone and calcination reaction and identifying high temperature regions responsible for NOx production.

NOMENCLATURE

A	Pre-exponential factor
E	Activation energy
k	Rate constant
R	Gas constant
T	Temperature

INTRODUCTION

The calcination process is used in many industries such as the cement, alumina and petrochemical industries. The process of calcination is carried out at high temperatures within furnaces or kilns of various designs including shaft furnaces, rotary kilns, fluidized bed reactors or gas suspension calciners.

This paper covers the modelling approach used to simulate a furnace within a gas suspension alumina calciner. Alumina calcination is the last step in the Bayer process, where bauxite ore is processed to extract the alumina hydrate in the form of $2Al(OH)_3$. To produce the end product of alumina, the hydrate must be heated to high temperatures to drive off the water producing alumina, Al_2O_3.

The control of the calcination process and the design of the associated process equipment has a direct influence on the alumina crystalline phases that are produced and the degree of particle breakage. This affects the quality of the product which in turn has implication in the cost aluminium production and pollution control.

Creating a numerical simulation of an alumina calciner furnace is a complex problem as there are many physical processes occurring simultaneously including the gas flow, flow of solids particles, fuel combustion and the pyro-metallurgical calcination process. All these processes are coupled together and must be considered within one integrated model to provide accurate and meaningful results.

A typical calciner furnace layout is described in this paper and consists of vertical cylindrical furnace section with preheated combustion air entering axial at the bottom. The combustion zone is positioned at the base of the furnace with radial burners around the circumference. The alumina hydrate is introduced to the combustion zone in a steady stream and the combustion air suspends the solids carrying the product to the top outlet.

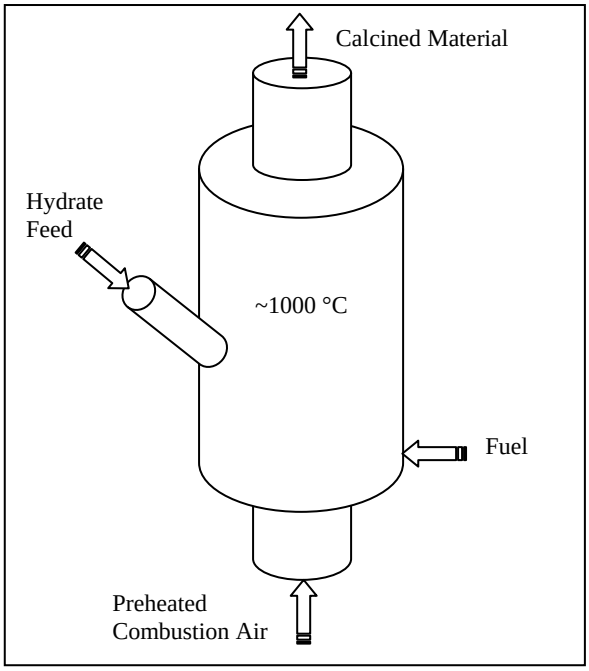

Figure 1 Outline of Gas Suspension Calciner Furnace

Background

Only limited publications have been found relating specifically to the alumina calcination process, with no previous examples of complete CFD simulations found. There are early examples of water based experiments, however most recent publications relate to the reaction kinetics such as Rozic [2001] and Wang [2006]. There are examples of CFD simulations of cement furnaces, Fidaros [2007], which do have similarities with alumina calciners. The main point of difference is the particle size which determines which multiphase models can be used.

MODEL DESCRIPTION

The CFD code employed was ANSYS FLUENT version 12 with this work capitalising on the latest advances within the multiphase models. The Eulerian Granular Model (EGM) was used for the flow of alumina and the Discrete Phase Model (DPM) for the injection of fuel. A number of different species where defined to model the processes of combustion and calcination. The realizable k-ε was used to model turbulence on a per-phase basis.

Combustion

The fuel used within alumina calciners is generally heavy fuel oil, natural gas or a combination of the two. In the example presented here the atomisation, devolitization and combustion of heavy fuel oil was modelled. The discrete phase model (DPM) was used to model the trajectory of the evaporating droplets. There are a number of empirical models available to determine the droplet size distribution leaving the burner nozzle such as plan orifice atomization or air-blast atomization models.

The fuel oil properties include of two primary chemical species allowing the evaporation of the principle hydrocarbon and the remaining non-volatile components to tracked through the furnace.

The combustion process is modelled by defining a volumetric reaction between species, with the rate determined by the degree of local turbulence using the Eddy-Dissipation rate equations, Magnussen (1976).

Granular Solids Flow

Two modelling approaches could be used to model the solids flow within the furnace, including the Discrete Phase Model (DPM) and the Eulerian Granular Model (EGM). Both models have their merits, however several localised regions of high solids concentrations necessitate the use of the EGM for this particular design.

In the EGM, the solids phase is regarded as a continuum and is treated as a second continuous interpenetrating fluid. In this model, the solids phase has properties similar to those of a fluid with specific terms to describe solid-solid interaction and the kinetic energy of the particles (termed granular temperature), Gidaspow (1992).

Calcination Reaction

The alumina particles undergo a significant phase change within the furnace from gibbsite to an amorphous phase. Additional scalar terms are used to define the amount of water left within the crystal structure and the resulting phase composition.

Experiments performed by Rozic [2001] show the reaction rates for dehydration can be correlated with the Arrhenius equation with respect to the remaining water content of the solid material as per equation 1. The activation energy E was determined to be 66.5 kJ/mol and pre exponential factor equal to 8850 s^{-1}.

$$k = A \exp\left(\frac{E}{RT}\right) \quad (1)$$

More recent experimental research by Wang [2006] reveals that the reaction can be more closely described as a multi-step reaction with the activation energy dependant on the extent of the reaction steps. Either of these reactions can be incorporated within the CFD simulation, the choice depending on the overall objective of the particular simulation.

Experimental Validation

Reaction rates and formation enthalpies were implemented through the use of a user defined subroutine. The experiments performed by Rozic [2001] were simulated using this subroutine to provide a level of validation. The experiments consist of a preheated air supply, vibrating gibbsite feed, cooling air and cyclone/bag filter. The experiment allowed the particle residence time to be varied and the resulting particle composition to be determined.

Figure 2 shows the comparison between the measured particle composition and the simulated values, indicating very good agreement.

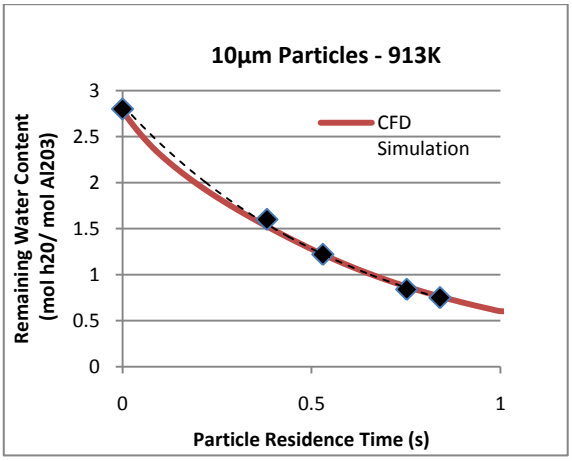

Figure 2 Comparison between experiment and simulation.

The local gas temperature has a significant effect on the rate of the calcination reaction as illustrated in Figure 3. Lower temperatures greatly extend the required residence time within the furnace.

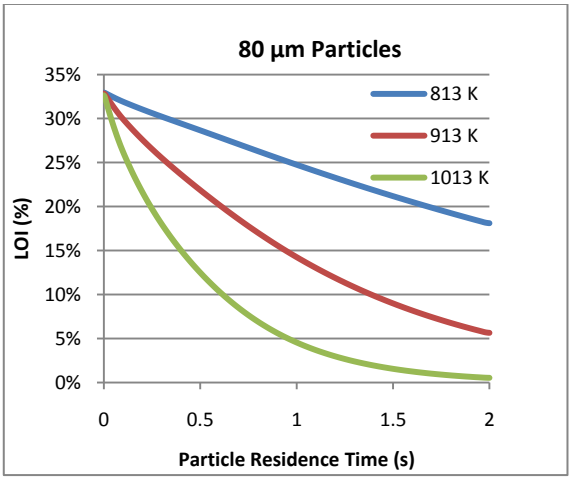

Figure 3 Temperature effect on calcination reaction rates.

IMPLEMENTATION

The number of different processes occurring simultaneously within this numerical model result in an inherently unstable solution. There is strong coupling between the energy released from the combustion process and the energy absorbed from the calcination reaction.

There is also a large momentum exchange between the solids falling into the furnace and the incoming combustion air. A number of solution strategies are required to maintain stable solution throughout the transient simulation.

The simulation was run on an HPC IBM cluster consisting of 16 compute nodes. This example took approximately 4 days to reach a quasi-steady state and was continued for another 3 days to provide transient and time averaged data.

RESULTS

The results of the furnace simulations are highly transient in nature with the solids and temperature profiles oscillating rapidly over time. The momentum of the incoming stream of solids carries the alumina against the air flow into the combustion zone at the base of the furnace as shown in Figure 4. The solids stream is dispersed as it strikes the wall of the furnace and is then entrained within the air stream.

Solids Distribution

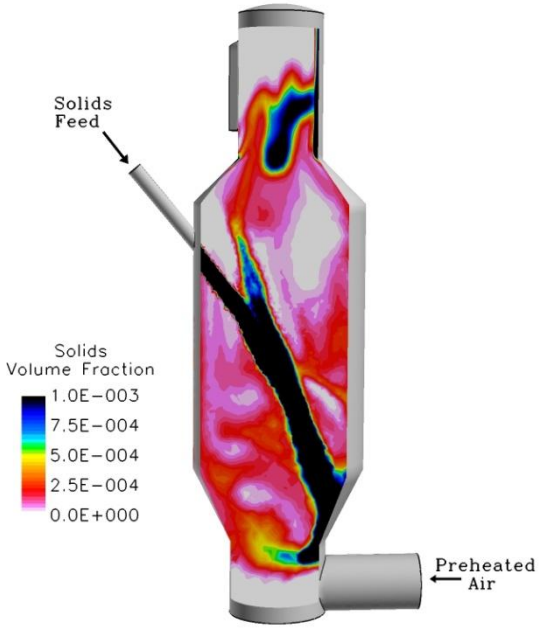

Figure 4 Solids distribution through the furnace.

Combustion Zone

This example models the combustion of heavy fuel oil which is influenced by several parameters including the size distribution of the fuel spray, local gas temperature and the cooling effect of the incoming solids. The incoming solids and the endothermic calcination process rapidly cools the combustion gases and as shown in Figure 5. Correct burner placement and the solids distribution are critical factors in achieving consistent product quality and low NOx emissions.

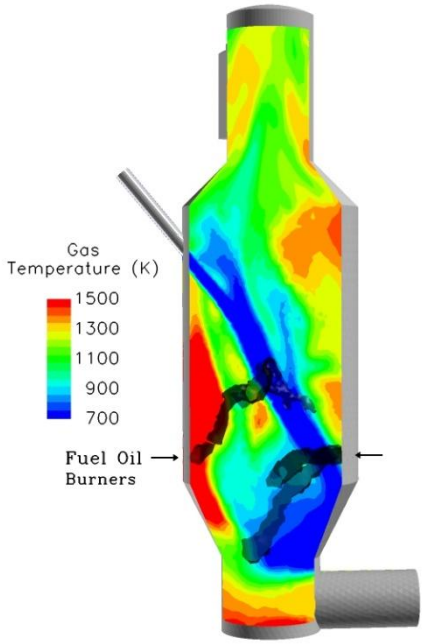

Figure 5 Temperature profile through the furnace.

Calcination Process

The calcination process is very energy intensive with approximately 25 MW required to remove the remaining water molecules from the partially calcined material entering the furnace in this example. The amount of water remaining in the alumina is termed “Loss On Ignition” (LOI). In this example the alumina enters the furnace with 18% LOI as shown in Figure 6. As the alumina is dispersed across the base of the furnace there is a rapid drop in LOI with the high rate of energy transfer. Some of the material entering the furnace is immediately entrained in the air flow and carried straight to the outlet. This short-circuiting can be seen at the top of Figure 6 and can have an impact in product quality.

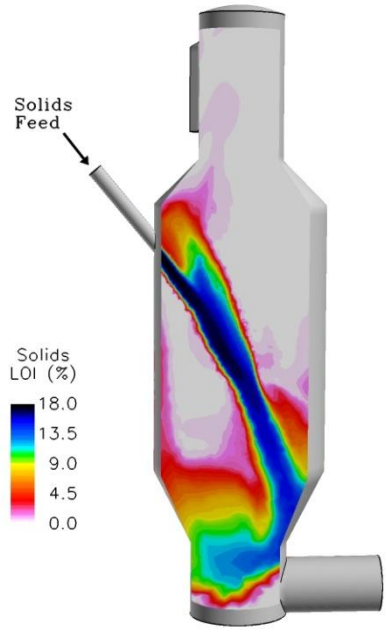

Figure 6 Calcination process within the furnace.

Reviewing these results shows how closely coupled the processes are within the furnace. Figure 7 shows how the solids circulate within the furnace, reducing in LOI as solids are dispersed. The solids influence on the gas flow is very apparent and a key consideration with respect to burner placement and the combustion process.

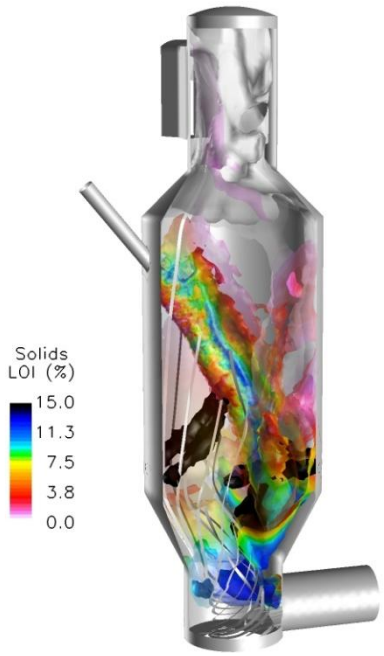

Figure 7 Flow of solids, gas and fuel oil.

INDUSTRIAL APPLICATIONS

Present computing capabilities already make these simulations very accessible to design projects, with run times typically completed in several days. This allows a range of operating scenarios or design concepts to be readily investigated, well within the time frame of most projects.

Furnace designs can be optimised for particular fuel types, which must include consideration of the rate of combustion, the solids/temperature profile and the processes the particles undergo. This can provide added value to new designs, quantity the effects of changing fuel types on existing units or help achieve capacity increases.

The appropriate furnace size can be determined for the required unit capacity by investigating the particle residence times, heat transfer to solids and the rate of calcination, with a well designed furnace achieving consistent particle composition, even at turn down. As part of a new or modified furnace design the optimum burner placement for the fuel selected can also be determined.

Determining the optimum furnace design and burner position has several benefits, including an improved understanding of the processes within the furnace, reduced risk, minimal commissioning time, improved product quality, and reduced NOx and refractory damage.

CONCLUSION

High temperature industrial processes are difficult problems to simulate with numerical models as the often involve reacting multiphase flows, several simultaneous reactions and transport of multiple species. Recent advances within the CFD framework now allows these processes to be considered on an industrial scale within one coupled model.

The results shown in the example presented here demonstrate how CFD is now a viable and often vital design tool for the further development of this type of industrial process. The results provide clear insights into the operation of existing facilities and allow rapid development of more efficient industrial furnaces with lower emissions and improved efficiencies.

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