AA13 - CFD Modeling of Gas Suspension Calciner in an Alumina Refinery

Sai Hitesh Bhandaru[1], Kumaresan Thangaraj[2], Vilas Tathavadkar[3], Subha Banerjee[4], Kiran Kumar Kondala[5] and Kausikisaran Misra[6]
1. Scientist
2. Lead Scientist (Domain Leader)
3. Senior Vice-president (Function Head)
Aditya Birla Science and Technology Company Pvt. Ltd, Navi Mumbai, Maharashtra, India
4. Senior Engineer
5. Senior Manager
6. General Manager – Technical
Utkal Alumina International Limited, Rayagada, Odisha, India
Corresponding Author: kumaresan.t@adityabirla.com

Abstract

Calcination of gibbsite to alumina is an important energy intensive final stage of Bayer alumina refinery process. Approximately, 30 % of the total energy consumption is alone used for the calcination stage. Thus, improvement of energy efficiency plays a crucial role in minimizing cost of production and emissions. The aim of this study is to investigate combustion efficiency of heavy fuel oil (HFO) atomized with steam inside the gas suspension calciner of alumina refinery. The combustion model was developed using species transport model with addition of all possible combustion reactions. Discrete phase lagrangian approach model was incorporated for studying HFO and alumina hydrate particle trajectories in combustion and holding vessel zones. Turbulence has been modeled using SST – K-ω turbulence model and P1 method was used for accounting radiative heat transfer equation. Post combustion efficiency investigation with respect to the mole fractions of carbon dioxide, carbon monoxide, unburnt O_2 emissions, this work also aims to focus on introducing routes (such as optimization of Air to fuel ratio) for reduction of fuel consumption less than the design consumption and to build an optimum curve for best fuel efficiency with respect to throughput satisfying operation limits.

Keywords: Alumina calcination, alpha alumina, combustion efficiency, CFD modeling, fuel consumption.

1. Introduction

Bauxite ore consists of gibbsite, boehmite, diaspore, bayerite, nordstrandite, tohdite, kaolinite and doyleite as aluminum containing phases along with calcium, iron and silica phases viz., hematite, anatase and quartz. Among the minerals present in bauxite, gibbsite, bayerite, nordstrandite and doyleite are aluminum tri-hydroxides while boehmite, diaspore and tohdite are aluminum oxide hydroxides. The detailed alumina minerals with their compositions depicted in Table 1 were given by Wefers et al., (1987) [1]. Properties, minerology, type, amount of alumina content and other impurities vary widely in bauxite depending on its geographical location. Aluminum containing phases in bauxite are widely used to produce smelter grade, specialty grade and high purity alumina in alumina refineries across the globe using conventional Bayer Alumina process. Along with these applications, alumina also finds applications as a flame retardant and paper additive while, boehmite is used as a catalyst support and in the production of ceramic pieces [2], [3]. Due to these wide applications and properties, alumina has achieved a great significance industrially and in the new technology development.

Table 1. Comparison of different oxides of Aluminum [1].

S.No	Name of alumina mineral	Chemical composition	Crystallographic formula
1	Gibbsite	Aluminum tri-hydroxide	γ-$Al(OH)_3$
2	Bayerite	Aluminum tri-hydroxide	α-$Al(OH)_3$
3	Nordstrandite	Aluminum tri-hydroxide	$Al(OH)_3$
4	Boehmite	Aluminum mono-hydroxide	γ-$AlOOH$
5	Diaspore	Aluminum mono-hydroxide	α-$AlOOH$
6	Corundum	Aluminum oxide	α-Al_2O_3

Among these minerals, gibbsite ($Al(OH)_3$) is the pre-dominant phase available in the Eastern Ghats bauxite present at Utkal Alumina International Limited (UAIL). This mineral composite is widely used for production of smelter grade alumina from raw bauxite ore which is an energy intensive process that uses substantial amounts of caustic soda for extraction of gibbsite.
In alumina refineries, bauxite ore is processed using the Bayer process to extract alumina tri-hydroxide (gibbsite). Calcination of gibbsite or $Al(OH)_3$, to alumina occur via an endothermic thermal decomposition reaction which is given by

$$2Al(OH)_3 \xrightarrow{1000°C} Al_2O_3 + 3H_2O,\ \ \Delta H° = +185.2\ \text{kJ/mol} \quad (1)$$

Equation 1 which seems to be a simple one step reaction happens at over 1000 °C to produce desirable alumina phase with an LOI less than 1%. Alumina calcination process involves various stages viz., unbound moisture removal, phase and structural transformations in which hydroxides are converted to oxides. Residual hydroxide content starts to decrease with temperature and time in a calcination process. Most of the reduction in free moisture present in the feed hydrate was observed in temperatures lower than 250 °C after which at a reduced rate of LOI, phase and structural transformations takes place.

Phase transformations play a crucial role in an alumina calcination process for producing desirable alumina phase. During the calcination process, alumina has a significance of existing in various metastable forms including γ, χ, κ, δ, η, θ and in the final stable α-alumina phase. The reaction pathway to several alumina phases are majorly characterized by particle sizes and heating rates. On-set of phase transformation to alumina mono hydroxide (Boehmite) from gibbsite starts at temperatures lower than 250 °C after which several phase transformations based on heating rates and particle sizes to χ and desirable γ-alumina takes place at temperatures between 300 to 800 °C. Stable alpha alumina formation occurs at temperatures greater than 1000 °C.

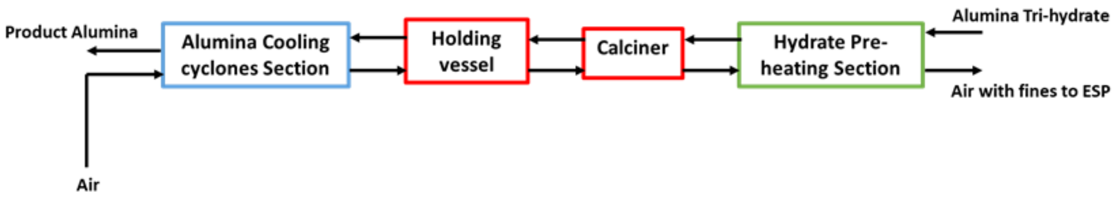

Figure 1. Block diagram of calcination process in an alumina refinery.

In modern day Gas suspension calciners (GSC), gibbsite particles were fed into a series of pre-heaters maintained at around 300-500 °C for removing moisture and initiating the conversion of aluminium tri-hydroxide to mono-hydrated alumina (boehmite) and transition alumina. In the calciner furnace and holding vessel sections, production to a desirable smelter grade alumina is less than minimum fluidization velocity. It was observed that for a higher A/F (22.8) where recirculation's were higher, slightly higher number of particles were found to be in the fluidization regime. From the lab scale XRD analysis, it was identified that particle sizes (<75 μ) had a higher tendency to form alpha phase from desirable γ-alumina. The aluminium hydrate sample were collected from the inlet to calcination circuit and experimented in a laboratory muffle furnace for different sets of temperature and heating rate before carrying out XRD analysis. For the sake of brevity, details of XRD results are not shown in this work. Hence, for the quantification study, retention times of finer fractions of alumina particles (<75 μ) in each velocity regime at higher temperatures (>1000 °C) were extracted [11]. Using the lab scale predictions by C.P. Steiner et al., (1971) [12], analysis was carried out to segregate particles spending time in temperatures greater than 1000 °C to understand and validate possible chance for alpha phase formation. It was particularly noticed that when a finer fraction of particles (<75 μ) spends time inside calciner and holding vessel at higher temperatures (>1000 °C), chances to form α-alumina are greater due to an enhanced heat transfer and shorter diffusion distance for reaction products for finer particles to further transform into undesirable α-alumina. From the literature by C.P. Steiner et al., (1971), a linear dependency between percentage of alpha alumina and retention time was observed following zero-order kinetics [12]. Thus, the correlation for alpha content with temperature and residence time was used to understand and validate the formation of alpha alumina from CFD simulations. Table 4 shows the quantitative results in which correlation of percentage alpha phase with retention times spent by alumina particles at three velocity regimes and at a temperature 1000 °C was depicted. The predictions of alpha phase by mapping CFD flow pattern results along with the lab scale phase transformation experiments was found to be in good agreement with plant data (Table 4).

Table 4. Quantitative particle information from CFD analysis.

Air to Fuel	Velocity Zone	Temperature (%)	Retention time (sec)	% Particle size (<75μ)	Actual alpha content	Alpha from simulation
22.8	Above terminal velocity	T between 1000 - 1100	10-40	4.5	5.97	5.58
		T > 1100	15-150			
	Between terminal & minimum fluidization	T between 1000 - 1100	10-60	0.9		
		T > 1100	50 -350			
	Below minimum fluidization	T between 1000 - 1100	15-145	0.2		
		T > 1100	30-430			
		T > 1100	30 - 430			
26.5	Above terminal velocity	T between 1000 - 1100	4-15	0.6	4.24	4.33
		T > 1100	2-12			
	Between terminal & minimum fluidization	T between 1000 - 1100	4-20	2		
		T > 1100	4 -70			
	Below minimum fluidization	T between 1000 - 1100	5-20	0.3		
		T > 1100	10-700			

4. Conclusions

The present study mainly focused on the detailed investigation pertaining to calciner and holding vessel section. CFD analysis was carried out to understand the flow phenomena of gas-solid hydrodynamics along with the distribution of temperature predicted. Along with that, fluidization analysis was carried out to understand the particle retention time and velocity and its effect on alpha phase transformation.

1. The lower A/F ratio (22.8) demonstrated a biased flow pattern with non-uniform mixing pattern leading to poor combustion efficiency in the calciner section whereas the higher A/F ratio (26.5) predicted a non-biased flow pattern with good swirl flow mixing of fuel oil and air leading to better combustion efficiency.
2. The non-biased flow in the higher A/F ratio (26.5) along with the effective combustion of fuel predicted a uniform reduction in temperature gradient starting from the calciner entry till the holding vessel exit.
3. The non-biased flow in the higher A/F ratio (26.5) reduced the recirculation vortices and thus in turn provides an optimum retention time for the desired phase transformation of particles.
4. The biased flow in the lower A/F ratio (22.8) and non-biased flow in the higher A/F ratio (26.5) produced alpha phase formation by ~6 % and ~4.5 % respectively. A difference of 1.5 % was identified between two A/F ratios.

5. Future Work

1. The present work was limited to combustion and holding vessel zones of gas suspension calciner. CFD simulation of the whole gas suspension calciner unit, which includes cooling cyclones and pre-heater sections would be carried out for optimization of Heavy fuel oil (HFO) consumption for different variations of feed rates.

2. In the upcoming CFD simulations, both SO_x and NO_x reactions will be included.

6. References

1. K. Wefers and M. Chanakya, Oxides and hydroxides of aluminum, Pittsburgh: *Alcoa Laboratories*, 1987.
2. I. Jones, J. Victoria, C. S. Robert, D. Thomas, W.S.C. Jennifer, and S. Sylvain, Dehydroxylation sequences of gibbsite and boehmite: study of differences between soak and flash calcination and of particle-size effects., *Journal of Materials Chemistry,* Vol. 6, No. 1, pp. 73-79, 1996.
3. J. A. Jiménez, P. Isabel , L. Aurora , F. Laila and L. Sol , Characterization of the aluminas formed during the thermal decomposition of boehmite by the rietveld refinement method., *International Journal of Applied Ceramic Technology,* Vol. 12, pp. 178-186, 2015.
4. C. Marsh, "CFD Modelling of Alumina Calciner Furnaces," *CSIRO Australia,* pp. 9-11, 2009.
5. D. J. Gunn, Transfer of heat or mass to particles in fixed and fluidised beds., *International Journal of Heat and Mass Transfer,* Vol. 21, No. 4, pp. 467-476, 1978.
6. S. Morsi and A. J. Alexander, An investigation of particle trajectories in two-phase flow systems., *Journal of Fluid mechanics,* Vol. 55, No. 2, pp. 193-208, 1972.
7. C. L. Wu, K. Nandakumar, A. S. Berrouk and H. Kruggel-Emden, Enforcing mass conservation in DPM-CFD models of dense particulate flows., *Chemical engineering journal,* Vol. 174, No. 1, pp. 475-481, 2011.
8. Versteeg, K. Henk and M. Weeratunge , An introduction to computational fluid dynamics: the finite volume method., Pearson education, 2007.

9. T. Kumaresan, S. Thakre, B. Basu, B. Jain, K. Pandey, R. Singh and R. Somani, Design Optimization of the De-duster to reduce Alumina carry over load on the dry scrubbing system, *International Conference on CFD in Oil & Gas, Metallurgical and Process Industries*, Trondheim, Norway, 2008.
10. O. Levenspiel, Chemical reaction engineering, *Industrial & engineering chemistry research,* Vol. 38, No. 11, pp. 4140-4143, 1999.
11. O. Levenspiel, Chemical Reaction Engineering, New York, NY: Wiley, 1999.
12. C. P. Steiner, D. Hasselman and R. M. Spriggs, Kinetics of the Gamma-to-Alpha Alumina Phase Transformation, *Journal of American Ceramic Society,* Vol. 54, No. 8, pp. 412-413, 1971.