DIGESTER DESIGN USING CFD

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Abstract

In the Bayer process, dissolution of gibbsite and kaolinite occur in the digester train. Understanding the hydrodynamics of the digester is key to improving the extent of dissolution, and thus the extraction of alumina and re-precipitation of silica. Deviation from ideal plug flow results in a miscalculation of the slurry retention time. The outcome may be a loss of undigested alumina to the red mud with a consequent reduction in extraction efficiency.

To address this issue, the hydrodynamics of a digester train were modeled using computational fluid dynamics (CFD). The impact of column aspect ratio and inlet configuration on the slurry residence time distribution (RTD) was investigated. The RTD was used to estimate reaction extents and evaluate the effect of design parameters on performance. The modeling approach allows the inclusion of the digestion chemistry to directly evaluate the yield. Results show that the choice of slurry inlet configuration significantly impacts performance.

Introduction

Globally, the Bayer process is the established method for the production of alumina from bauxite that has been in use for over a century. With large quantities of bauxite being processed and a highly competitive marketplace, incremental process improvements resulting in minor increases in efficiency have a significant benefit to the overall operating costs.

A 2001 review of the alumina industry, sponsored by industry leaders and the governments of Australian and the USA [1], advised that both continuous improvement through incremental changes and major advances through innovative step changes will be required for the alumina industry to remain viable over the next several decades. A number of technology initiatives were identified to bring these changes to fruition, including Computational Fluid Dynamics (CFD) modeling. To maximize the benefits of CFD, it should be employed to investigate "what-if" scenarios during the earliest possible stages of the design process [2].

In recent years, CFD has been widely used to understand and optimize process steps in the hydrometallurgical and, more specifically, the alumina industry [3,4,5]. The use of powerful and reliable modeling techniques as a supplement to traditional engineering practices allows process engineers to virtually prototype equipment. Process or geometry changes to unit operations can be applied to optimize the equipment design and process configuration. In this way, capital and operating costs may be reduced by reducing over-design. Although CFD simulation of process equipment or unit operations is becoming more widespread, no previous CFD study of bauxite digesters could be found in the literature.

For optimal reactor performance of the digester column, based on the characteristics of the digestion reactions, the flow field should approach plug flow. In ideal plug flow, the fluid moves in an orderly front through the vessel without any axial mixing along the flow path. This paper presents a case study for digester design using CFD to determine the flow characteristics of bauxite slurry within the digester vessel. CFD analysis can identify dead spots in which the digester volume is poorly utilized. By evaluating the residence time distribution (RTD) of the bauxite slurry the effect of the vessel aspect ratio and inlet configuration on the digester performance was quantified. The RTD results are then used to estimate the extent of the digestion in the train.

Bauxite Digestion

During the digestion process, alumina in the bauxite is dissolved in the Bayer liquor in the form of sodium aluminate. Gibbsite bauxites are digested at 140-150°C in a series of vertical, cylindrical pressure vessels. The iron mineral impurities are sparingly soluble, but another common impurity, kaolinite, dissolves. Gibbsite and kaolinite dissolution may be represented by the following equations [6]:

$$a\ NaOH + b\ Al_2O_3{\cdot}3H_2O \rightarrow c\ NaAlO_2 + d\ H_2O \qquad (1)$$

$$e\ NaOH + f\ Al_2O_3{\cdot}2SiO_2{\cdot}2H_2O \rightarrow g\ Na_2O{\cdot}SiO_2 + h\ NaAlO_2 + i\ H_2O \qquad (2)$$

Kaolinite dissolution is accompanied by reprecipitation of the silicate as a complex sodium aluminoslicate, known as desilication product (DSP). This reaction occurs at a much slower rate than the gibbsite dissolution and therefore controls the required digestion time [6]. Although most refineries attempt to deal with this issue by pre-desilication in holding tanks ahead of the digestion train, a digester train sized to accommodate the slow kinetics of kaolinite dissolution and reprecipitation as DSP ensures sufficient retention time for alumina digestion.

Digesters used in the Bayer process are typically sized based on throughput and digestion time under the assumption of plug flow. If the flow though the digester deviates from plug flow, then a quantity of slurry arrives at the digester outlet either earlier or later than the ideal retention time. If the slurry arrives early, then the bauxite digestion is premature, leading to losses of undigested alumina in the red mud and autoprecipitation in the washing train. If the slurry arrives late, then the column is over-sized. Each condition leads to increased operating or capital costs of the digester units. By applying CFD to the design of digesters, the hydrodynamics can be examined and design modifications can be made to approach plug flow conditions.

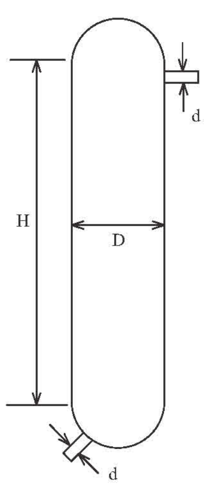
Deviation from the plug flow assumption is assessed by examining the residence time distribution (RTD) in response to a pulse input to the model. CFD has been previously shown to be an effective tool for predicting RTDs [7,8]. For the present case of the bauxite slurry flow through the digester, a homogeneous, non-settling slurry is assumed. Work is underway to incorporate a multiphase modeling approach, which is required to predict the flow of both the liquor and the bauxite, including the bauxite particle size distribution.

Digester Configuration

The digester configuration is of typical design — a vertical, cylindrical vessel with hemispherical heads. Alternate geometries (e.g. tube digesters) were not considered in this study. In the present configuration, the inlet slurry feed nozzle is located at the top and the outlet nozzle is located at the bottom of the vessel.

A single digester is studied to assess the impact of two geometric variables — the height-to-diameter ratio of the vessel and the slurry inlet configuration — on the performance indicator, the RTD. Two different height-to-diameter vessel aspect ratios are considered: 4:1 and 7.5:1. The volume of the digester is held constant (see Figure 1) for the applied throughput. Additionally, three slurry inlet configurations are considered: normal, central, and tangential, as shown in Figure 2. A deflector plate is added below the central inlet to distribute the slurry in the head of the vessel and reduce short-circuiting of the feed to the outlet at the bottom of the vessel. To predict the performance of the digestion train, a series of three digesters is also modeled.

The hydrodynamics of the digester are complex with turbulent, multiphase flow and liquid-solid reactions. These key complexities are not considered in the usual black-box approach of flow sheet simulation and can introduce uncertainty and risk into the process design. By employing CFD to investigate the hydrodynamics and to predict the performance of a digester during the initial design, many of these complexities are taken into account. The technical risks are mitigated and areas for design improvement can be readily identified and introduced to the design cycle project earlier rather than later.



Aspect Ratio	4:1	7.5:1
H, m	23	33.3
D, m	5.2	4.44
d, m	0.6	0.6
Deflector*, m	1.52	1.30
V, m^3	562	562

*Applies to Central inlet configuration only. See Figure 2.

Figure 1:Digester column geometry and dimensions.

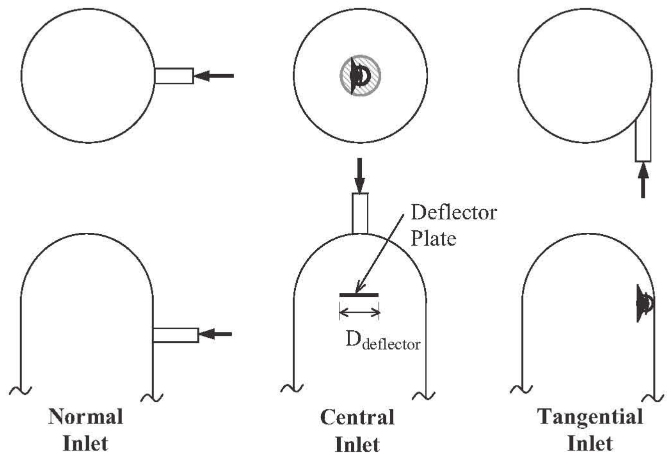


Figure 2: Schematic of the three slurry inlet nozzle configurations considered.

Modeling Methodology

In the first stage of modeling, the slurry hydrodynamics are studied to assess the influence of the vessel aspect ratio and inlet configuration leading to selection of preferred vessel geometry. In the second stage, the analysis was extended to estimate the digestion extent based on the RTD. A time-dependent, tracer technique is applied to find the RTD of the flow field. A pulse of a neutrally buoyant tracer is injected at the inlet to the digester and the concentration of the tracer is monitored at the outlet. The transient discharge profile is compared to the expected profile for ideal plug flow. The mean and variance of the concentration curve are used to quantify the deviation of the digester column from plug flow.

Numerical Methods and Boundary Conditions

The commercial code, FLUENT version 6.2, was used in this study. The 3D computational grid of the digester model consisted of approximately 200,000 hexahedral cells with symmetry applied for the normal and central inlet configurations. The grid size for the tangential inlet configuration was 400,000 hexahedral cells. Turbulence was modeled using the realizable k-ε turbulence model in the normal and central inlet digesters. For the tangential inlet configuration, the Reynolds stress turbulence model was applied due to the high degree of rotational, i.e., swirling, in the flow. The inlet slurry flow rate was 2840.5 m^3/h with an average slurry density of 1280 kg/m^3. The liquor has a specific gravity of 1.17 and the solids have a specific gravity of 2.98. The inlet slurry contains 6wt% solids. The inlet velocity boundary condition is 2.81 m/s. The outlet boundary was set to system pressure.

Slurry Hydrodynamics

The flow patterns with digester aspect ratios of 4:1 and 7.5:1 are shown in Figure 3 for the normal inlet configuration. The flow fields are similar, with large recirculation zones along the digester wall, below the inlet nozzle. These large recirculation zones indicate significant back-mixing within the digester and substantial deviation from plug flow. For the 4:1 aspect ratio, the recirculation zone extends along the full height of the column and into the bottom head. Increasing the aspect ratio increases the length that is available for the flow to recover downstream of the inlet. For the higher aspect ratio of 7.5:1, the flow becomes more aligned with the column geometry in a downward direction just upstream of the outlet. The digester was modeled without a vapor space in the vessel head contrary to typical digester operation. Neglecting the small headspace volume will not significantly alter the overall vessel circulation and the conclusions of the present study.

Figure 4 compares the flow fields in the 4:1 column for the three slurry feed nozzle configurations. Note that the flow patterns in the 7.5:1 columns with central and tangential inlets are similar to those shown for their 4:1 column counterparts. The inlet configuration greatly influences the flow patterns in the digester. As described above, the normal inlet nozzle leads to a large recirculation zone inside the digester. With a central inlet nozzle, a deflector plate was included to distribute the slurry jet and prevent short-circuiting through the vessel to the outlet. A recirculating wake develops immediately downstream of the deflector, but the flow develops into nearly uniform further downstream. The tangential inlet configuration gives rise to swirling flow throughout the height of the vessel with two counter-rotating vortices: an inner vortex traveling from the bottom upwards and a second vortex traveling back down the center of the digester.

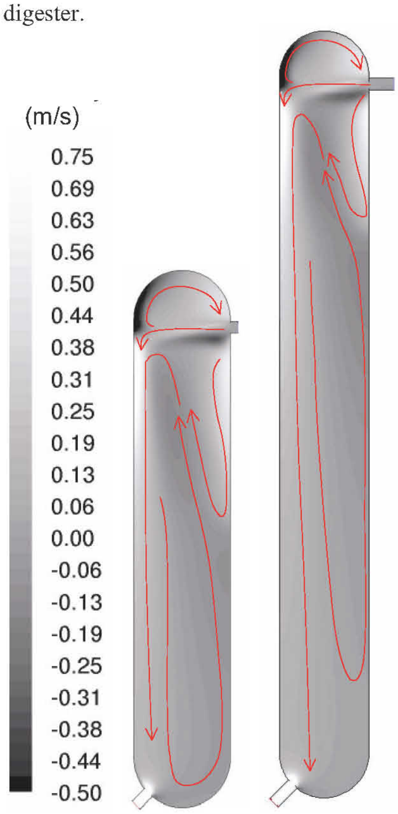


Figure 3: Comparison of axial velocity and the characteristic flow patterns in the digester for aspect ratios of 4:1 and 7.5:1.

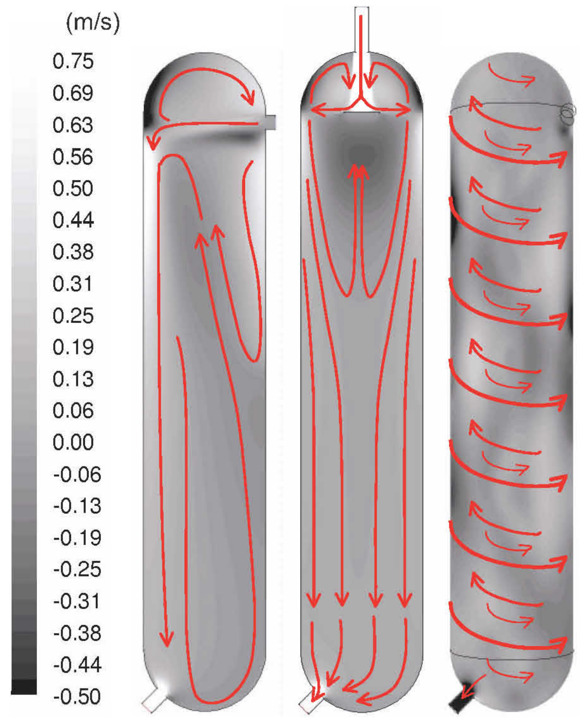


Figure 4: Comparison of axial velocity and the characteristic flow patterns in the digester with a normal, central, and tangential slurry inlets.

Figure 5 and Figure 6 show the tracer residence time distribution for digester column aspect ratios of 4:1 and 7.5:1, respectively. Based on the slurry throughput of 2840 m^3/h and a digester volume of 562 m^3, the mean retention time of the digester column is 712 s. The central inlet produces an RTD with a peak near the mean retention time. The normal inlet configuration produces an early, indistinct peak with a long tail that decays slowly indicating that some slurry short-circuits while the remainder is held up in the large region of recirculation. The tangential inlet RTD shows sharp peak followed by a very long tail indicating that most of the material short circuits to the outlet and the remaining material is held up in the swirling flow in the center of the digester. The column diameter decreases with an increase in aspect ratio, increasing the time for the slurry to swirl down the wall of the digester resulting in a long retention time.

Table I summarizes the mean time and variance for the RTD plots shown in Figure 5 and Figure 6. The lower variance for the central inlet configuration is an indication of less axial dispersion.

The bauxite particles exhibit single-particle terminal settling velocities exceeding the liquor superficial velocity in the digester. The residence times of the solid phase will likely differ from the liquid phase as the solid particles are expected to settle faster than the liquid flowing down the vessel. A multiphase simulation of the liquid and bauxite particle flow through the digester train (3 vessels) is required to predict hindered settling. Work is underway to include this effect and thereby obtain a more representative assessment of the bauxite (kaolinite) conversion

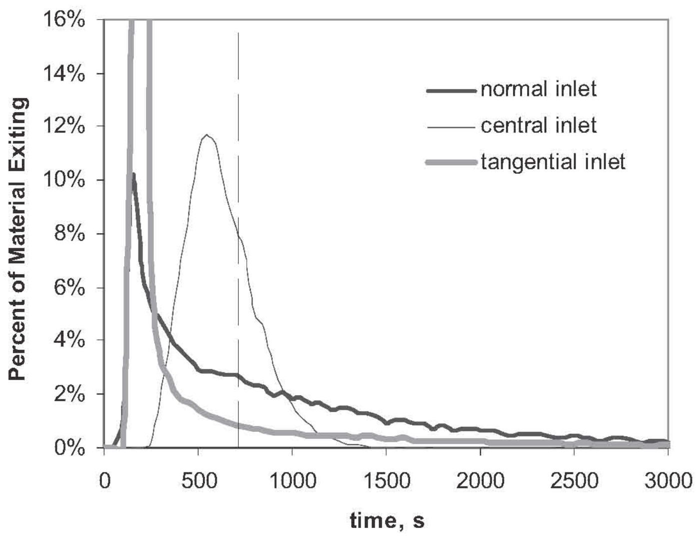


Figure 5: Single digester RTD. Aspect ratio = 4:1.

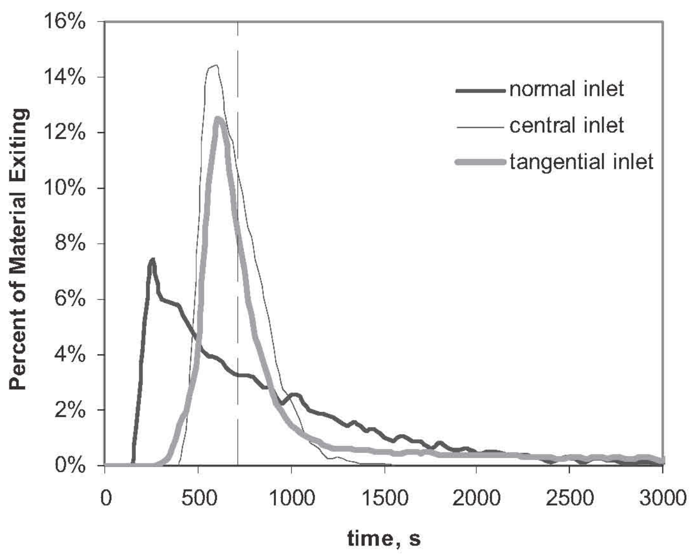


Figure 6: Single digester RTD. Aspect ratio = 7.5:1.

Table I: Influence of column aspect ratio and inlet nozzle configuration on mean residence time $\bar{t}$ and variance of the RTD (Results are for a single vessel).

	Aspect Ratio 4:1		Aspect Ratio 7.5:1	
Inlet.	$\bar{t}$, s	σ^2, s^2	$\bar{t}$, s	σ^2, s^2
Normal	940	856,000	830	420,000
Central	647	48,600	665	25,000
Tangential	505	691,000	1280	2,340,000

Extent of Digestion

The hydrodynamics and RTD of the digesters are related to the extent of dissolution of the silica-containing kaolinite to assess the extent of digestion and the performance of the vessel configurations. Compared to gibbsite dissolution, it is the slower desilication rate that controls the digestion time. A simple axial dispersion model [9] is used to estimate the extent of the kaolinite dissolution reaction based on the axial dispersion. The deviation from plug flow is characterized by the dispersion number *D/uL* where *D* is the axial dispersion coefficient, *u* is the superficial velocity and *L* is the characteristic length of the reactor/digester and is determined from:

$$\sigma_\theta^2 = \frac{\sigma^2}{\bar{t}^2} = 2\left(\frac{D}{uL}\right) - 2\left(\frac{D}{uL}\right)^2\left(1 - e^{-uL/D}\right) \tag{3}$$

The variance σ^2 and the mean residence time $\bar{t}^2$ are determined from the RTD (See Table I). The extent of the reaction, also known as the conversion, can then be determined from:

$$X = 1 - \frac{4a \cdot \exp\left(\frac{1}{2}\frac{uL}{D}\right)}{(1+a)^2 \cdot \exp\left(\frac{a}{2}\frac{uL}{D}\right) - (1-a)^2 \cdot \exp\left(-\frac{a}{2}\frac{uL}{D}\right)} \tag{4}$$

where $a = \sqrt{1 + 4k\tau(D/uL)}$
k = reaction rate constant
$\tau = V/Q$ = retention time of the column

The conversion of the kaolinite dissolution reaction can be estimated based on the following assumptions and simplifications:

1. The dispersion number is within the range $0.1 < D/uL < 1$. When the dispersion number is greater than 1, deviation from plug flow is large and the axial dispersion model is less accurate.
2. The reaction is first order with an estimated reaction rate constant, k, of 0.002 s^{-1}, based on laboratory studies of the bauxite digestion. The rate constant is a function of many variables including the bauxite ore, particle size distribution and morphology, and the digestion conditions: temperature and pressure. Though the relationship between the rate constant and the conversion in non-linear, the conversion is sensitive to the magnitude of the reaction rate.
3. Ideal plug flow is assumed in the pipes connecting the vessels. This assumption is reasonable because of the relatively small pipe diameter and the high-velocity flow.
4. The reaction is not mass-transfer limited, and relatively independent of the kaolinite concentration, because the reaction rate constant is small.
5. There is an availability of liquor (NaOH) for dissolution.

Table II and Table III show the reaction extent through a single vessel for different aspect ratios. Cases for which $D/uL > 1$ fall outside of the appropriate range for this conversion model. Conversions tabulated for $D/uL > 1$ are included for comparison purposes only. The superior hydrodynamic performance of the central slurry inlet nozzle configuration translates into improved digester performance with kaolinite conversion well above the other configurations.

Table II: Extent of the kaolinite dissolution reaction after one digester vessel. Aspect ratio = 4:1.

	Aspect Ratio 4:1		
	Normal Inlet	Central Inlet	Tangential Inlet
σ_θ^2	0.97	0.12	2.7
Dispersion, *D/uL*	10.4	0.062	9.5×10^8
Extent of Reaction, *X*	59%	73%	59%

Table III: Extent of the kaolinite dissolution reaction after one digester vessel. Aspect ratio = 7.5:1.

	Aspect Ratio 7.5:1		
	Normal Inlet	Central Inlet	Tangential Inlet
σ_θ^2	0.610	0.0565	1.43
Dispersion, *D/uL*	0.586	0.0291	6.5×10^7
Extent of Reaction, *X*	65%	75%	59%

RTD of Individual Solid Particles – Effect of Settling

The above analysis has assumed that the bauxite particles in the slurry follow the liquor flow. To assess the effect of solid settling on the extent of digestion, discrete particles were tracked through the digester in a Lagrangian frame of reference. The size distribution of the bauxite particles is shown in Table IV. Particles representing each diameter range were tracked through the 4:1 digester with central inlet. Figure 7 shows the RTD for the selected particles sizes. The RTD for the non-settling slurry is also plotted for comparison. The 100 μm particles, representing 50% of the solids by weight, follow the liquor closely. The larger particles begin to settle out of the liquor and exit the digester early.

Table IV: Slurry solid particle size distribution.

Diameter (μm)	wt%
100	50
450	30
600	10
800	5
1000	4

On the basis of the RTD of each particle size, the extent of the kaolinite dissolution was estimated once again. The overall, mass-weighted, kaolinite conversion is 89%. Based on this analysis, the settling solids decrease the conversion by nearly 10%. The influence of particle-particle collision has been neglected in the Lagrangian multiphase approach and could possibly overpredict the RTD's for the solids. A dense multiphase approach is being investigated to more accurately predict the transport of the solids phase through the digester. Additionally, the heterogeneous reactions between the caustic liquor and the bauxite ore will be incorporated to model the digestion reactions directly while coupled with a full multiphase, non-isothermal, hydrodynamic analysis to present a complete picture of the digester operation.

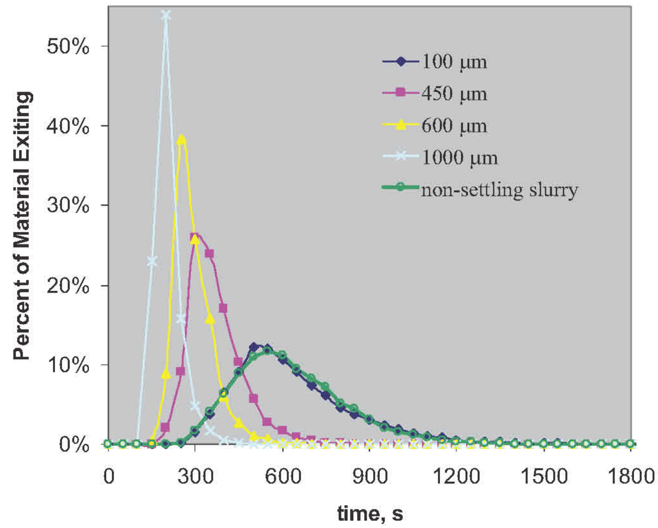


Figure 7: Solid Particle RTD (central inlet, Aspect ratio = 4:1).

Summary

CFD has been shown to be a valuable tool for the design of a bauxite digester by providing a cost-effective way to experiment with vessel design towards determining an optimal vessel configuration for digestion. The traditional black box approach does not account for effects of geometry such as the slurry inlet nozzle configuration or vessel aspect ratio. The inlet configuration has been shown to have a strong influence on performance in terms of the kaolinite conversion extent. The central inlet results a flow field most closely approaching plug flow and offers the best performance.

Further work is underway to extend CFD modeling methodology to include both multiphase representation of the slurry liquor and solid and the heterogeneous liquid-solid dissolution reactions. By modeling the multiphase hydrodynamics with reactions, the performance may be predicted with fewer assumptions and the design uncertainty may be further reduced.

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