MATHEMATICAL MODELING OF THE KINETICS OF GIBBSITE EXTRACTION AND KAOLINITE DISSOLUTION/DESILICATION IN THE BAYER PROCESS

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Abstract

An unsteady-state mathematical model incorporating the rates of external mass transfer, intraparticle diffusion and chemical reaction has been developed to describe the extraction of gibbsite from bauxite particles allowing for the competitive reactions - gibbsite and free caustic, and kaolinite and free caustic accompanied by the reprecipitation of the dissolved silica (as sodalite). The governing partial differential equations have been reduced to ordinary differential equations by the method of orthogonal collocation and solved using a standard variable step integration algorithm in terms of two parameters characteristic of the nature of the bauxite. The usefulness of the model is demonstrated by providing examples of cases where it has been applied to elucidate process performance under conditions that are envisaged for the future, or to gain an insight into reasons for certain apparently anomalous trends in process stream quality in terms of silica concentrations.

Introduction

There is a considerable body of literature on desilication during digestion (see for example, Oku and Yamada(1)), and before digestion (see for example, Cousineau and Fulford(2) and Cousineau et al(3)), but there does not appear to be any systematic discussion on issues relating to the modeling of simultaneous dissolution of gibbsite and kaolinite in the digester, accompanied by the controlling step, namely desilication. Desilication or controlled reprecipitation of silica in Bayer liquor may be realized in the digester by prolonging the time that the pregnant liquor spends in that unit beyond the two to five minutes typically required for the near-complete extraction of the gibbsite from bauxite to as long as an hour. This essentially means that the "digestion time" in a typical low-temperature (~140°C) digester is controlled by the considerably slower desilication rate of the pregnant liquor.

The reactive silica component, typically kaolinite, in bauxite, is an important source of caustic loss in Bayer process. In addition, the uncontrolled reprecipitation of the dissolved silica as sodium aluminosilicate is a major cause of fouling of the heat exchanger surfaces, with the net result being a decreased process energy recovery. While it is true that the effective way to manage caustic consumption in the Bayer process is to use bauxite(s) with low levels of silica, such resources are increasingly becoming rare. It is therefore important to identify the process conditions that might help to reduce the unproductive consumption of caustic and also alleviate the problem of scaling due to the uncontrolled deposition of the desilication product.

In order to be able to derive cost related benefits from efficient usage of caustic and the available capacities of the digester, and improved energy recovery through reduced scaling problems, it is necessary, as a first step, to construct an overall desilication model incorporating the kinetic behaviours of kaolinite dissolution and

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silica reprecipitation during digestion. The present work discusses an effort in that direction.

Development of the Mathematical Model Simultaneous Dissolution of Gibbsite and Kaolinite in the Digester

The chemical reactions responsible for the extraction (dissolution) of gibbsite and kaolinite from a bauxite matrix may be represented by the following equations:

$$\mathrm{p\,NaOH + q\,Al_2O_3.3H_2O \rightarrow s\,NaAlO_2 + v\,H_2O} \tag{1}$$

$$\mathrm{yNaOH + zAl_2O_3 \cdot 2SiO_2 \cdot 2H_2O \rightarrow eNa_2O.\,SiO_2 + fNaAlO_2 + gH_2O} \tag{2}$$

The governing coupled partial differential equations for the particulate phase that would describe the extraction (dissolution) process described by equations (1) and (2) above in a solid-liquid reactor may be written based on the following assumptions:

1. The bauxite particles are spherical in shape, with a known median for the size distribution.
2. The overall size of the bauxite particles does not change during extraction.*
3. Gibbsite and kaolinite are uniformly distributed throughout the bauxite matrix.
4. The reaction is isothermal in nature.
5. The effective diffusivity of caustic in bauxite does not change during the course of the extraction.**
6. Resistance to mass transfer in the bulk fluid phase is negligible.***

The first-principle based formulation of the mass transport equations for heterogeneous chemical reactions are treated adequately by authors such as Bird, Stewart and Lightfoot(4) and Carberry(5), and the present modeling effort draws considerably from this prior knowledge. In what follows, we present the governing equations that represent the situation that is of specific interest to us, namely the simultaneous extraction of gibbsite and kaolinite from bauxite.

A number of different reaction rate expressions for gibbsite extraction and kaolinite (or reactive silica) dissolution were considered in the model and these are shown in Table I. In an earlier model which considered only the extraction of gibbsite, the rate expression $R = k\,C_A^{0.5}$ (C_A being the free-caustic (as NaOH) concentration) for gibbsite extraction proved to be the one leading to an excellent agreement between experimental kinetic data for four different bauxites (Trombetas-Brazil, Hope-Jamaica, Boke and Weipa-Australia). Similarly, a limited study on the modeling of the kinetics of silica dissolution from a Jamaican bauxite at temperatures in the region of 100°C indicated that the rate expression, $R = k\,C_A C_K$ (C_A and C_K respectively being free-caustic (as NaOH) concentration and kaolinite concentration in the bauxite matrix) would adequately represent the experimental data. Therefore, based on these findings, the governing equations may be written as follows:

$$\varepsilon_p \frac{\partial C_A}{\partial t} = D_e\left\{\left(\frac{\partial^2 C_A}{\partial r^2}\right) + \left(\frac{2}{r}\right)\left(\frac{\partial C_A}{\partial r}\right)\right\} - k_1 C_A^{0.5} - k_2 C_A C_K \tag{3}$$

$$\frac{p}{q}\frac{\partial C_G}{\partial t} = -k_1 C_A^{0.5} \tag{4}$$

$$\frac{y}{z}\frac{\partial C_K}{\partial t} = -k_2 C_A C_K \tag{5}$$

Table I The various reaction rate expressions considered in the model.

Gibbsite Extraction	Kaolinite Dissolution
$R = k\,C_A\,C_G$	$R = k\,C_K$
$R = k\,C_A^{0.5}\,C_G$	$R = k\,C_A$
$R = k\,C_A\,C_G^{0.5}$	$R = k\,C_K^2$
$R = k\,C_A^{0.5}\,C_G^{0.5}$	$R = k\,C_A\,C_K$
$R = k\,C_A$	
$R = k\,C_A^{0.5}$	
$R = k\,C_G$	
$R = k\,C_G^{0.5}$	
$R = k\,C_A^2$	
$R = k\,C_G^2$	
$R = k\,(C_G - C_G^*)$	

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* It is considered that particle breakdown does not occur under the low-temperature predesilication conditions and, in the case of higher-temperature (130-150°C) gibbsite digestion/silica dissolution any breakdown which does occur happens in the flashing process.

** The effective diffusivity may be considered an average value after taking into account the creation of any straight-through and tortuous pores due to the removal of the gibbsite crystals (in the case of higher-temperature digestion/desilication) from the bauxite matrix, and the change in free-caustic concentration during the course of extraction. Any attempts to rigorously account for the change in effective diffusivity due to changes in particle porosity and bulk fluid phase free-caustic concentration would considerably add to the complexity of the model.

*** In order to keep the solids in suspension in a real or digester, the degree of agitation has to be so violent that convective mass transfer reduces the liquid-phase mass transfer in the bulk of the liquid to a negligible part of the total resistance.

The relevant initial and boundary conditions are:

$$t=0:\quad C_A=0;\quad C_{AB}=C_{AB0};\quad C_G=C_{G0};\quad C_K=C_{K0} \tag{6}$$

$$r=0:\ \frac{\partial C_A}{\partial r}=0 \tag{7}$$

$$r=R_p:\ D_e\frac{\partial C_A}{\partial r}=k_g\left(C_{AB}(t)-C_A\right) \tag{8}$$

In equation (8) above,

$$C_{AB}(t)=\frac{(C_{AB0}\cdot V_{L0}-2.x_G(t)\cdot C_{G0}\cdot V_B-6.x_K(t)\cdot C_{K0}\cdot V_B}{V_L(t)} \tag{9}$$

The liquor volume, V_L in equation (9) varies as a function of time due to the release of water from the two competing reactions, and is estimated from the following relationship:

$$V_L(t) = V_{L0}+\{(\text{Dilution factor}_1.x_G(t).C_{G0}.V_B.MW_G)+ (\text{Dilution factor}_2.x_K(t).C_{K0}.V_B.MW_K)\} \tag{10}$$

In equation (10), the Dilution factor_1 is equivalent to a value of 0.59 cm^3/(gramme of gibbsite dissolved) as experimentally determined by Halvorson(6), and in the absence of a similar experimentally determined value, Dilution factor_2 is estimated to be 0.14 cm^3/(gramme of kaolinite dissolved); MW_G and MW_K are respectively the molecular weights of gibbsite ($Al_2O_3.3H_2O$) and kaolinite ($Al_2O_3.2SiO_2.2H_2O$).

The amount of unprecipitated silica remaining in solution at any given time is given by the algebraic expression

$$S=\frac{[k_3t_{ds}(S_0-S_{eqb})S_{eqb}]+S_0}{1+k_3t_{ds}(S_0-S_{eqb})} \tag{11}$$

The above expression was obtained by integrating the following rate expression originally derived by Oku and Yamada(1) for desilication in Bayer liquor through the formation of sodium aluminosilicate:

$$\frac{dS}{dt_{ds}}=-k_3(S_0-S_{eqb})^2 \tag{12}$$

In equations (11) and (12)

$$k_3=\exp\left(a-bC_{Al_2O_3}-\frac{d}{T}\right) \tag{13}$$

where, according to Oku and Yamada(1)

$a = 26.376$, $b = 1.444 \times 10^{-2}$, and $d = 10{,}960$, (T.in °K)

The dimensionless form of equations (3)-(8) is as follows:

$$\psi\frac{\partial U_A}{\partial\tau}=\left(\frac{1}{\phi^2}\right)\left(\nabla^2U_A\right)-\left(U_A^{0.5}+\frac{RXN2}{RXN1}U_AU_K\right) \tag{14}$$

$$\frac{\partial U_G}{\partial\tau}=-U_A^{0.5} \tag{15}$$

$$\frac{\partial U_K}{\partial\tau}=-\frac{1}{\theta}U_AU_K \tag{16}$$

$$\tau=0:\ U_A=0;\ U_{AB}=1;\ U_G=1;\ U_K=1 \tag{17}$$

$$\eta=0:\ \frac{\partial U_A}{\partial\eta}=0 \tag{18}$$

$$\eta=1:\ \frac{\partial U_A}{\partial\eta}=Bi\left(U_{AB}(\tau)-U_A\right) \tag{19}$$

where:

$$Bi = \text{Biot Number} = \frac{k_gR_p}{D_e} \tag{20}$$

$$RXN1=k_1C_{AB0}^{0.5} \tag{21}$$

$$RXN2=k_2C_{AB0}C_{K0} \tag{22}$$

$$U_A=\frac{C_A}{C_{AB0}} \tag{23}$$

$$U_{AB}=\frac{C_{AB}}{C_{AB0}} \tag{24}$$

$$U_G=\frac{C_G}{C_{G0}} \tag{25}$$

$$U_K = \frac{C_K}{C_{K0}} \tag{26}$$

$$\theta = \left(\frac{q}{p}\right)\left(\frac{y}{z}\right)\left(\frac{C_{K0}}{C_{G0}}\right)\left(\frac{RXN1}{RXN2}\right) \tag{27}$$

$$\psi = \varepsilon_p\left(\frac{q}{p}\right)\left(\frac{C_{AB0}}{C_{G0}}\right) \tag{28}$$

$$\tau = \text{Dimensionless Time} = \frac{q}{p}\left(k_1\frac{C_{AB0}^{0.5}}{C_{G0}}\right)t \tag{29}$$

$$\phi = \text{Thiele Modulus} = R_p\sqrt{\frac{k_1 C_{AB0}^{0.5}}{D_e C_{AB0}}} \tag{30}$$

$$\eta = \frac{r}{R_P} \tag{31}$$

$$\nabla^2 = \text{Laplacian operator} \tag{32}$$

It must be stressed that throughout this paper, the term "caustic" concentration refers to the concentration of free, unreacted NaOH in solution only as NaOH, and is not used in the usual Bayer process sense of the sum of the free caustic plus the caustic equivalent of the dissolved sodium aluminate, expressed as equivalent Na_2CO_3 or Na_2O, which would greatly complicate the modeling.

Solution of the Model Equations

The method of solution involves reduction of the relevant model equations to ordinary differential equations by the method of orthogonal collocation, as described by Villadsen and Stewart(7) and Raghavan, et al.(8) followed by integration using a standard variable step algorithm. Accuracy of the solution was verified by progressively increasing the number of collocation nodes used for the purpose of reducing the partial differential equations to ordinary differential equations, and obtaining a solution until no significant further change in solution was found for a given set of parameter values.

Application of the Model to Bayer-Process Plant Operating Situations

The validity of the model was demonstrated by obtaining a good agreement between predicted and laboratory experimental gibbsite extraction/kaolinite dissolution/desilication kinetics for gibbsitic bauxites of Jamaican, Australian and Brazilian origin. Figures 1 and 2 show the kind of agreement obtained with Trombetas bauxite for the case of 143 °C digestion temperature and 92.5 g/L starting free-caustic concentration on NaOH basis (~200 g/L total caustic as e.Na_2CO_3). For this bauxite, model predictions for 110 °C and 127 °C digestion temperatures and 92.5 g/L starting free-caustic concentration on NaOH basis were also very good in comparison to experimental results, but are not shown here.

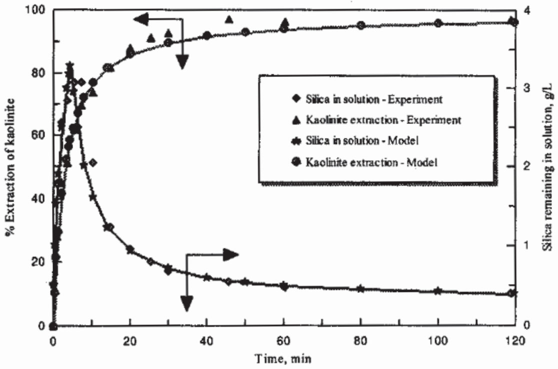

Figure 1: Silica Dissolution and Desilication – Caustic = 200 g/L e·Na_2CO_3, Temperature = 143 °C (Trombetas Bauxite).

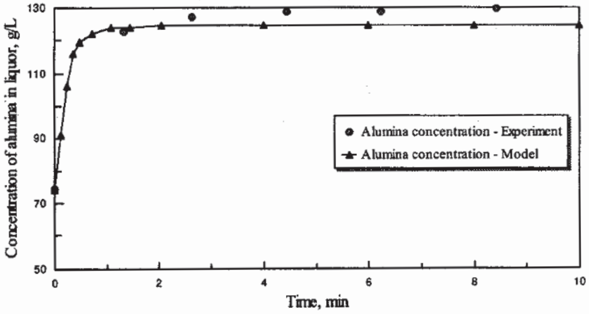

Figure 2: Gibbsite Extraction – Caustic = 200 g/L e·Na_2CO_3, Temperature = 143 °C (Trombetas Bauxite).

In view of the model's ability to be a useful tool in predicting the gibbsite extraction/kaolinite dissolution/desilication behaviour, it was decided to apply it to elucidate plant-process performance under conditions that are envisaged for the future, or to gain an insight into certain apparently anomalous trends in process stream quality in terms of silica concentrations. Specifically, the model has already been employed for the following purposes:

1. Prediction of desilication behaviour under certain modified plant operating conditions.

2. Prediction of desilication behaviour and associated issues under conditions leading to substantially increased production capacity.

3. Simulation of the silica profile in the digester train of an existing plant.

4. Evaluation of the effect of free-caustic concentration on silica dissolution to identify conditions under which a major amount of reactive silica may be left unextracted in the red mud in a low-temperature digest.

5. Prediction of silica extraction behaviour in a reactor configuration similar to a tube digester.

Here we describe two of the above five cases in some detail.

Desilication under Conditions Leading to Increased Production

A number of simulations were performed so as to be able to predict the concentration of silica in solution under a set of operating conditions perceived for a possible future production increase in an existing plant. The operating conditions took into account bauxite and liquor throughputs, reactive silica concentration in bauxite, caustic concentration during predesilication and digestion, and starting and ending ratios for predesilication and digestion. In essence, based on the flowsheet shown in Figure 3, the following two cases were simulated:

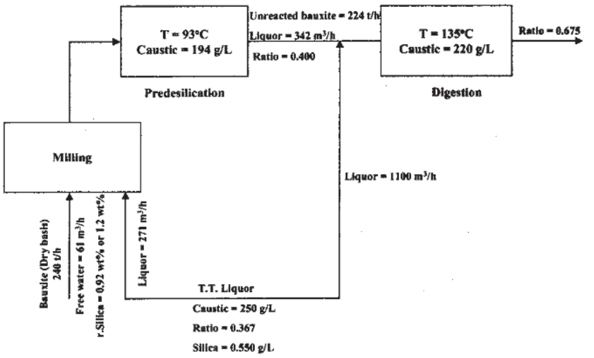

Figure 3: Flow sheet describing bayer plant operating conditions after production expansion.

1. 75% of the 0.92 wt% reactive SiO_2 is extracted during predesilication at 93°C and the remaining 25% is extracted during digestion. Desilication obeys the Oku-Yamada kinetics during both predesilication and digestion.

2. 75% of the 1.2 wt% reactive SiO_2 is extracted during predesilication at 93°C and the remaining 25% is extracted during digestion. Desilication obeys the Oku-Yamada kinetics during both predesilication and digestion.

For the cases studied, two different digestion temperatures, viz. 135°C and 142°C, were considered for the purpose of studying the effect of temperature on blow-off liquor silica. As seen from Table II, raising the temperature from 135°C to 142°C for a fixed predesilication time of 12 h would result in a reduced level of silica supersaturation in the digester blow-off liquor. Assuming that heater scaling rates are proportional to the square of silica supersaturation, it could be shown that an increase of 7°C in digestion temperature would result in a significant reduction in scaling rate. The simulation results also showed that, for the chosen bauxite containing 0.92wt% reactive silica supersaturation in the case of increased production (mainly achieved by increasing digestion caustic concentration) would be considerably higher than that with the current production capacity which is currently ~0.12 g/L SiO_2.

Digester Silica Profile

A number of numerical simulations were carried out to gain insight into the nature of the silica profile in the digester train under the present operating conditions of a Bayer plant. The simulations were based on the model, with parameter values (specific rate constants for gibbsite extraction and kaolinite dissolution, particle porosity and caustic diffusivity into bauxite particle pores) previously determined for Trombetas bauxite by matching the alumina (and silica) concentration **vs** time curves obtained in carefully controlled experiments with numerically simulated curves. In particular, the following cases for the simulation of the digester train for operating conditions shown in the flowsheet in Figure 4 were considered:

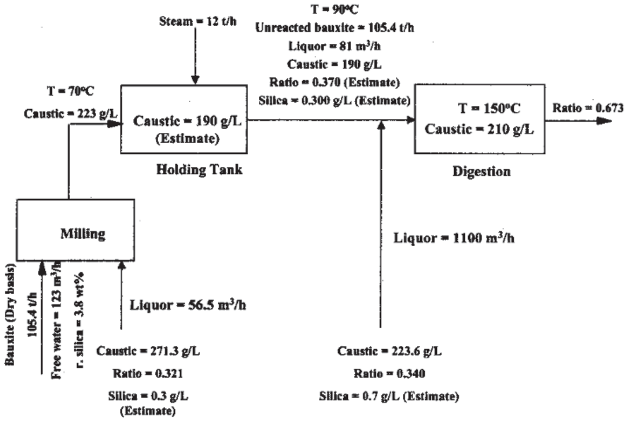

Figure 4: Flowsheet describing operating conditions of Bayer plant for which digester train silica profile is simulated.

1. Gibbsite digestion, kaolinite dissolution and desilication would occur simultaneously in the digester at 150°C. Desilication product was **carbonate sodalite** and the kinetics (of desilication) could be represented by the **Oku-Yamada** expression.

2. As described under item 1 above, except that the desilication product was **hydroxy sodalite.**

3. As described under item 1 above, except that the desilication product was **sulphate sodalite**.

For all of the above cases the assumption that no gibbsite or silica dissolution occurred in the holding tank was made in view of the potentially very short residence time there.

Table II Bayer plant production expansion: results of digestion/desilication simulation (0.92 wt% reactive SiO_2).

Stage	Conditions			SiO_2 in Exit Liquor, g/L (Based on Oku-Yamada kinetics)								
	Temp., °C	Caustic Concn., ($e{\cdot}Na_2CO_3$) g/L (at end of stage)	SiO_2 in Liquor, g/L (to stage)	Time (min)								
				15	20	30	40	60	360	480	720	960
Predesilication	93	194	0.550 [b]	--	--	--	--	--	0.527 (0.289)	0.453 (0.215)	0.384 (0.146)	0.349 (0.111)
Gibbsite Digestion (After 6 h predesilication)	135	220 [a]	0.545 [c]	0.735 (0.219)	0.725 (0.209)	0.704 (0.188)	0.684 (0.168)	0.653 (0.137)	--	--	--	--
Gibbsite Digestion (After 8 h predesilication)	135	220	0.527	0.725 (0.209)	0.718 (0.202)	0.698 (0.182)	0.680 (0.164)	0.651 (0.135)	--	--	--	--
Gibbsite Digestion (After 12 h predesilication)	135	220	0.511	0.716 (0.200)	0.709 (0.193)	0.693 (0.177)	0.675 (0.159)	0.648 (0.132)	--	--	--	--
Gibbsite Digestion (After 16 h predesilication)	135	220	0.502	0.709 (0.193)	0.703 (0.187)	0.688 (0.172)	0.672 (0.156)	0.645 (0.129)	--	--	--	--
Gibbsite Digestion (After 12 h predesilication)	142	220	0.511	0.703 (0.187)	0.689 (0.173)	0.664 (0.148)	0.644 (0.128)	0.617 (0.101)	--	--	--	--

Note: Numbers within parentheses are silica supersaturation values, given by (SiO_2 in Liquor - Equilibrium SiO_2)

a Before flashing

b Test Tank Liquor (TTL)

c Weighted average of liquor to first digester from live-steam heater and desilication

Figure 5 contains the measured silica profile (measured by the plant personnel) and the simulated profiles for cases 1-3. As seen from Figure 5, when hydroxy sodalite was assumed to be the product of desilication, the agreement with the experimentally measured profile was quite good. This is reasonable to expect since the causticity of the liquor at the time in question was quite high (>98 %) and it was also not contaminated with sulphates. It is worth pointing out here that the experimentally measured silica concentration at the plant blow-off and that predicted by the model were respectively 0.74 g/L and 0.78 g/L (assuming hydroxy sodalite formation) at the outlet of the last digester, for a total residence time of 55 min. This is a reasonably good agreement whereas, we see (Figure 5) that when sulphate sodalite was assumed as the product of desilication, there was no agreement between the measured and predicted silica profiles. It is also interesting to note here that heater scale samples obtained from the plant at that time were found to be hydroxy sodalite.

Based on this model-based study and assuming that the plant-silica-profile was representative of the actual profile that existed under normal operating conditions, it was concluded that the product of desilication was probably hydroxy sodalite and so the silica supersaturation in the blow-off liquor could be considered to be within acceptable limits from the point of view of silica in the product and heater scaling rates. This is in view of our separate experimental finding that under the conditions of hydroxy sodalite formation, the equilibrium solubility of silica in plant liquor conditions would be about 0.70 g/L.

Results and Discussion

The present work is an attempt towards developing theoretical models to describe the dissolution of kaolinite (reactive SiO_2) and desilication, both during gibbsite digestion. The experimental data considered in the modeling work were generated over a temperature range of 105°C - 146°C.

The dissolution behaviour of kaolinite has been adequately represented by the rate expression indicating a first order dependency on free-caustic concentration and a first order dependency on kaolinite concentration in bauxite matrix. It is useful to note that, according to Roach and White(9), a linear relationship exists between free caustic concentration in the liquor and the dissolution rate of reactive silica in bauxite. In the case of gibbsite

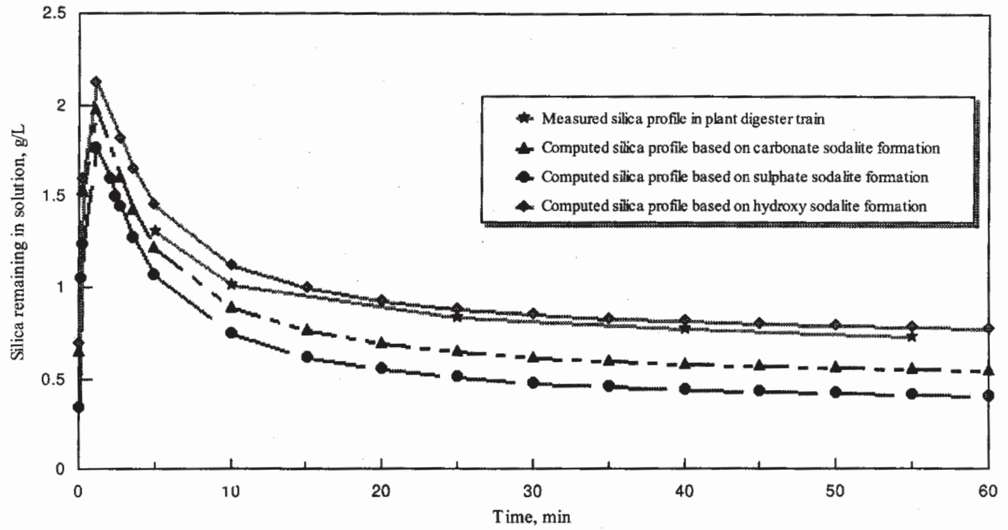

Figure 5: Experimentally measured and numerically simulated liquor-silica concentration profiles in Bayer plant digester train – Caustic = 210 g/L e·Na_2CO_3, Temperature = 150°C (Trombetas bauxite).

extraction, as already shown in Table I, the more logical rate expression, $R = k\ (C_G - C_G^*)^2$ which is the modified Pearson(10) rate expression for alumina hydrate precipitation in Bayer process, was also considered in the model. In this expression, C_G and C_G^* are respectively the number of gmole of gibbsite in unit volume (cm^3) of bauxite at any time and at the end of digestion when the upper limit for the digestion of gibbsite as dictated by the solubility considerations at the given temperature and caustic concentration has been reached. Although good agreement between experiment and model prediction could be obtained with this rate expression for three of the four bauxites studied, the specific rate constant k did not show the expected trend of increase with an increase in temperature. On the other hand, in some cases, the k value actually decreased with an increase in temperature. On the basis of this finding, it was concluded that, although the incorporation of the modified Pearson type expression in the model would lead to a reasonable representation of the experimental results for certain bauxites, it was not satisfactory.

In the model, the effect of gibbsite dissolution on kaolinite dissolution kinetics is allowed for through the competition of both reactions for free caustic soda. Although the present work shows that the simultaneous kinetics of bauxite digestion and desilication may be predicted with a reasonable degree of accuracy, it does not rule out the need for some preliminary experimental work whenever a new bauxite is being considered as a source of alumina. It would still be necessary to carry out a few digestion experiments under carefully chosen conditions in order to be able to determine (based on the present model) the manner in which the model parameters vary as a function of temperature and particle size. Once this is done, it would be possible (and indeed appropriate) to use the model to predict the digestion kinetics under other operating conditions of interest for the given bauxite. It is worth mentioning here that the present model has been successfully extended to take into account the whole real-life particle size distribution in a digester by assigning a distinct Thiele modulus value to each narrow-size range and solving the required number of sets of the coupled partial differential equations (each set of partial differential equations representing a known narrow-size range).

For model-based determination of liquor-silica concentration as a function of time, the specific rate constant for desilication is a critical model parameter. At present, the expression proposed by Oku and Yamada (1) is the one that is widely used for generating this constant. The rate constant, k, in the Oku-Yamada desilication expression is a lumped parameter and does not account specifically for the change in seed surface area (arising from auto nucleation) as a function of time. The lumped parameter, k, at present considers the seed surface area to be a constant, and does not provide for the possibility of a faster auto nucleation and increased levels of seed surface area when predesilication (or digestion without a predesilication stage) is carried out on a bauxite that has a higher reactive SiO_2 content compared to one that is poor in reactive SiO_2. In other words, it is not necessary that the value of the desilication rate constant, k, is independent of the amount of reactive SiO_2 in bauxite or its morphology. It is likely that both these factors determine the surface area of sodalite seed being formed. To improve on the present model, it would be necessary to obtain a better estimate of the lumped parameter, k, (real specific rate constant (k') x seed surface area (a)) for a given bauxite of specific reactive silica content. This may be done by matching the time vs silica-in-solution curves with those generated using the model with a desilication rate expression (which may be similar to the one proposed by Oku and Yamada) with constants that are bauxite (and reactive silica content) specific.

Another aspect of desilication that needs to be studied in some detail is the determination of the concentration of silica in solution at which desilication autonucleation actually begins to occur in plug flow under various conditions of temperature and liquor caustic concentration. Some work has already been done in this area at temperatures up to about 100°C, but the experimental set-up needs to be redesigned to enable tests at typical digestion temperatures.

Results of the simulations with respect to the plant present operating conditions and future plans have already been discussed elsewhere in the paper. Work to extend the modeling approach to cover boehmite and quartz extraction kinetics at high temperatures is also in progress.

Conclusion

The proposed model for kaolinite dissolution and desilication during gibbsite digestion will predict the liquor alumina and silica concentrations adequately, and could be used for estimating the blow-off liquor concentrations of alumina, and more importantly silica, for various plant operating conditions

Nomenclature

C_A = Concentration of free, unreacted caustic (NaOH) in the particle pore, gmole/cm^3
C_{AB} = Concentration of free-caustic in the bulk fluid phase, gmole/cm^3
C_{AB0} = Initial concentration of free-caustic (NaOH) in the bulk fluid phase, gmole/cm^3.
$C_{Al_2O_3}$ = Concentration of alumina (Al_2O_3) in liquor, g/L
C_G = Concentration of gibbsite in bauxite, gmole $Al_2O_3.3H_2O$/cm^3
C_{G0} = Initial concentration of gibbsite in bauxite, gmole $Al_2O_3.3H_2O$/cm^3
C_K = Concentration of kaolinite in bauxite, gmole $Al_2O_3.2SiO_2.2H_2O$/cm^3
C_{K0} = Initial concentration of kaolinite in bauxite, gmole $Al_2O_3.2SiO_2.2H_2O$/cm^3
D_e = Effective intraparticle diffusivity of caustic in bauxite, cm^2/s
k_1 = Reaction rate constant, (gmole/cm^3)$^{0.5}$.(1/s)
k_2 = Reaction rate constant, (cm^3/gmole).(1/s)
k_3 = Reaction rate constant, cm^3/(g.s)
k_g = Fluid film mass transfer coefficient, cm/s
p,q = Stoichiometric coefficients of reactants for the first reaction (equation (1))
s,v = Stoichiometric coefficients of products for the first reaction (equation (1))
y,z = Stoichiometric coefficients of reactants for the second reaction (equation (2))
e,f,g = Stoichiometric coefficients of products for the second reaction (equation (2))
r = Radial co-ordinate in particle, cm
R_p = Particle radius, cm
S = Concentration of silica (SiO_2) in liquor, g/L
S_0 = Initial concentration of silica (SiO_2) in liquor, g/L
S_{eqb} = Equilibrium concentration of silica (SiO_2) in liquor, g/L
t = Extraction (dissolution) time, s
t_{ds} = Desilication time, s
U_A = Dimensionless concentration of free, unreacted caustic (NaOH) in the particle, C_A/C_{AB0}
U_{AB} = Dimensionless concentration of free, unreacted caustic (NaOH) in the bulk fluid phase, C_{AB}/C_{AB0}
U_G = Dimensionless concentration of gibbsite in the particle, C_G/C_{G0}
U_K = Dimensionless concentration of gibbsite in the particle, C_K/C_{K0}
V_B = Total volume of bauxite particles, cm^3
V_L = Volume of liquor, cm^3
V_{L0} = Initial volume of liquor, cm^3
x_G = Fractional extraction of gibbsite from bauxite
x_K = Fractional extraction of kaolinite from bauxite
τ = Dimensionless time, $\{(q/p)\,(k_1\,C_{AB0}{}^{0.5}\,/\,C_{G0})\,t\}$
η = Dimensionless radial distance in particle, r/R_p
∇^2 = Laplacian operator
ϵ_p = Particle porosity
ϕ = Thiele modulus, $R_p\,\{(k_1\,C_{AB0}{}^{0.5})/(D_e\,C_{AB0})\}^{0.5}$
ψ = $\epsilon_p\,(q/p)\,(C_{AB0}/C_{G0})$

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