Optimizing Alumina Production Utilising Spreadsheet Models Based on Limited Data

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Abstract

Computer models to predict heat & mass balances have been used to optimize production in Alumina refineries since modern data processing capabilities have allowed it. But for refineries that have poor or no experimental data or knowledge, a major roadblock is that published models are usually dated and as a result, have more uncertainty in the predictions for their processes. This is particularly true for the precipitation area where the model development requires considerable effort, while the best and newest published models do not always disclose the parameters of the equations to protect IP. However, there is an approach that enables casting older models into newer equation types using little or no experimental data. This kind of model is not accurate enough for rigorous flowsheet models such as SysCAD or Aspen, but are accurate enough to provide optimization using spreadsheets and the Excel Solver Add-in.

Keywords: 1; Optimization 2; Alumina 3; Production 4; Precipitation 5. Modeling.

1. Introduction

In the early 80's when computing power was becoming widely accessible, many companies embarked on a journey to improve the operation of their refinery by building models of their process as faithfully as possible. Many programmers, scientists and engineers were involved in building these models, but in the early stages of computer programming and in the absence of commercial platforms, these big models were mostly made from first principles and attempted to model Heat & Mass Balances to explain or optimise operations. Eventually, models were migrated to known platforms like Aspen, Speedup, SysCAD, etc., when they started to exist.

However, none could be exempt from the first law of process modelling: "Thou shall not enter erroneous hypotheses and expect divine intervention to save your predictions" or more simply "Garbage in, Garbage Out".

The limitation of models based on poor knowledge of theoretical phenomena became very apparent, and extensive projects to determine more appropriate equations followed.

2. Traditional approach to model building

Because of the involved nature of Bayer process simulations, the usual approach is to minimize the number of experiments required to obtain a good model. This is often done using a statistical experimental design. However, this approach does not well discriminate between different model types; the multivariable regression cannot evaluate well the power of a coefficient for a variable if it is not varied enough. This explains why published models are so diverse in style.

Another reason for differences between equations published by different authors can be related to experimental approach: the precautions taken to minimize the effect of the speed of reaction and during and after sampling (ongoing reaction) for instance can create bias and then difference in derived models.

2.1. Availability of powerful PC and spreadsheet programing

The extent to which PC processing power has increased since their beginning is nothing short of phenomenal, increasing the number of equations per sec processed by several order of magnitude from a PC in 1984 to Pentium 7 today. Many of the newer desktop or laptop processors have several "core" which multiply this number even more for the software that can take advantage of this.

As a consequence, spreadsheets which used to be for very simple models, are now able to handle far more complex tasks at a very high speed, particularly if compiled Add-ins are used. These give the advantage of replacing the slow interpreted language in Visual Basic for Application (VBA) by fast compiled codes.

Spreadsheets have the bonus of familiarity with its user-friendly interface by almost everybody. A lot of features come by default and automatically available such as input validation and error checking. Finally, Microsoft have made available an optimizer that is quite user-friendly: the "Solver" Add-in.

3. Casting Existing Equations into a Known Model Type

3.1. Current trends in alumina industry technical publication

Prior to the 1990s, technical papers in Alumina Industry generally shared large amounts of information, often including the complete form of the equations developed, and sometimes base data. It was then possible for refineries to use published equations to utilise and develop their own refinery specific models.

The more recent trend in technical paper publication is to divulgate the methodology and to present only the shape of the equation, avoiding disclosure of constant values, for example, making it difficult to use these equations effectively.

A perfect example which is also very important to model for Bayer plant optimization is the precipitation process, and which will be used for the demonstration in this paper.

3.2. Status of current precipitation models

Although there is a large body of papers and studies on this topic, a unified or 'agreed" model for the alumina precipitation rate is not discoverable. There a few things on which studies do agree, such as the effect of supersaturation being a power square as a numerator, and also that for the denominator there should be a parameter related to caustic and/or impurity concentrations or more recently, Ionic strength.

Past researchers also had the tendency to cover a narrower range of conditions, deemed appropriate at that time for the operation of the refineries for which they were developed. This is certainly one of the reasons accounting for the differences in the published models.

Those who covered a sufficiently wide range of conditions have found the need to account for the effect of liquor composition either "free caustic", impurity concentrations (such as Ionic strength), or caustic concentration.

Hence the generalized rate of precipitation could be represented by the following expression:

$$\frac{dC}{dt} = \frac{kS(Supersaturation)^2}{liquorStrenght^a} \tag{1}$$

Where *dC/dt* is the precipitation rate,

k the kinetic constant,

S the total seed surface area

a the exponent for liquor or caustic strength (close to 2 generally)

More recently, due to interest in population balance modelling, the precipitation rate has been replaced by an equation for particle growth rate (*G*), where the precipitation is simply calculated using the corresponding equation.

$$\frac{dC}{dt} = S * G * \rho \frac{102}{156} \tag{2}$$

Where G is the growth rate

ρ is the density of the seed

3.3. The main precipitation driving force: alumina supersaturation

Regarding the type of supersaturation term to be used, there has been a fair variation, and no consensus. There are mainly three types of supersaturation that can be used whether absolute or relative:

- The simpler one is the difference between the actual concentration, and the solubility in grams per liter or moles of alumina in solution

$$Supers = \mathrm{C} - C_\infty \tag{3}$$

- the difference between the actual concentration and the solubility divided by the solubility; with this representation, the supersaturation goes toward zero as the reaction proceeds.

$$\beta = \frac{\mathrm{C}}{C_\infty} \tag{4}$$

- the actual concentration divided by the solubility; with this representation, the supersaturation goes toward 1 as the reaction proceeds.

$$\sigma_S = \frac{(\mathrm{C} - C_\infty)}{C_\infty} \tag{5}$$

- Another form was proposed for the particular case of gibbsite precipitation, which is much more complex.

$$\sigma = \frac{(\frac{\mathrm{C}}{\mathrm{FC}} - \frac{C_\infty}{FC_\infty})}{\frac{C_\infty}{FC_\infty}} \tag{6}$$

Where C is the alumina concentration
C_∞ the alumina solubility,
FC is the Free Caustic
FC_∞ is the Free Caustic at solubility

3.4. Equations selected to generate the data to be cast into new equations

As mentioned earlier, there have been considerably more equations published, but the absence of details like the value of the coefficients make these impossible to use directly without more information from the authors. [1 to 8]

Three equations that have been referenced abundantly in papers will be used for this demonstration: from Misra & White [1], King [3] and White & Bateman [6].

Firstly, the Misra & White equation:

$$G = 1.96x10^6 \exp\left(\frac{-14300}{(T+273)}\right)(C - C_\infty)^2 \tag{7}$$

Then King's equation,

$$G = 2.87x10^8 \exp\left(\frac{-6257}{(T+273)}\right)\frac{(C - C_\infty)^2}{(C_{caus} - C*106/102)} \tag{8}$$

Finally, White & Bateman's equation:

$$G = 6.5x10^{12} \exp\left(\frac{-8400}{(T+273)}\right)\frac{(C - C_\infty)^2}{C_{caus}^{2.5}} \tag{9}$$

Generally, all of the models published make sense, making it even more difficult to choose one as the best for a given study. For optimisation exercises, this is definitely the first stumbling block, particularly if the refinery doesn't have resources to do this kind of literature review or the funds to buy modelling technology or support.

4. How to cast new model type using older functions

In essence, recasting models consists of generating sufficient data using a known equation, covering the desired range of conditions (as long as they are inside the range of validity of the equation), followed by a multi-parameter regression on the generated data. This is achieved by defining and limiting the type of equation to the desired form.

When the data is generated experimentally, there is often a need to minimize the number of simulations and measurements using a statistical design. Using the recasting approach, generating more data is not much more work, and consequently, there is no real constraint on generating a large number of data points.

In Excel, there is a random number generator that can easily be used for this task, being aware that the generator is not perfect but gets better when a large number of points are needed.

4.1. Generation and comparison of a series of equations for alumina growth rate

For this comparison, the three models mentioned previously were used as generation sources and 2 model types were used to cast them into: one using the relative supersaturation with free caustic with no denominator (10) and the second type, the simple supersaturation with Ionic strength to the power of 2 as denominator (11).

$$G = K \exp\left(\frac{E}{R\,(T+273)} \right) \quad \sigma^2 \tag{10}$$

$$G = K \exp\left(\frac{E}{R\,(T+273)} \right) \frac{(C - C_\infty)^2}{I_{caus}^2} \tag{11}$$

Table 1 gives a summary of the equation coefficients found:

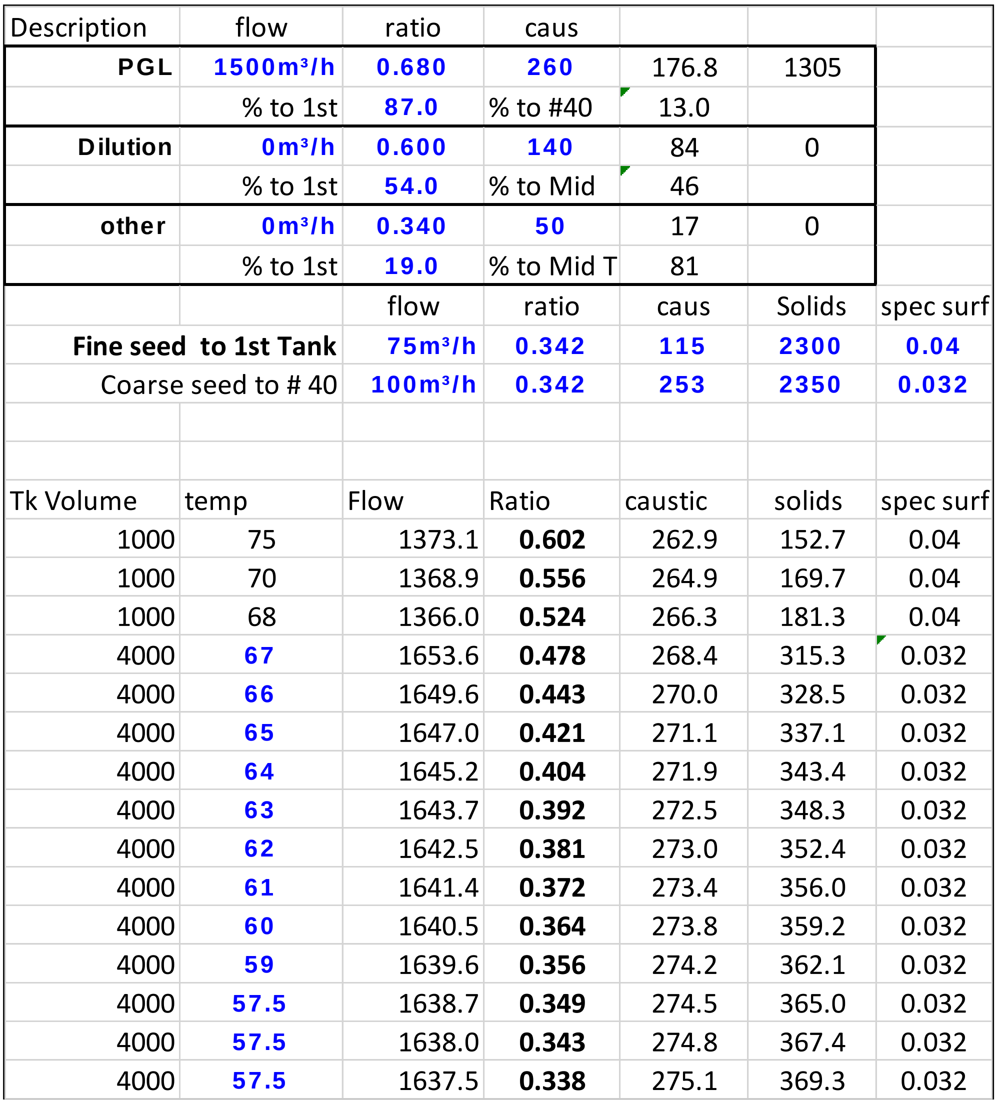
Table 1. Coefficients of the two equations generated:
Equation 10 type for A,B,C and Equation 11 type for D,E,F.

	Equation used to generate data	Supersation type	Denominator	K constant	E/R coefficient
A	Misra & White	Relative FC	none	2.218E+10	-8195.4
B	King	Relative FC	none	2.016E+16	-12710.0
C	White & Bateman	Relative FC	none	7.797E+11	-9366.2
D	Misra & White	GPL supers	Ionic St ^{2}	22306717	-7182.6
E	King	GPL supers	Ionic St ^{2}	4.638E+13	-11995.0
F	White & Bateman	GPL supers	Ionic St ^{2}	932222028	-8415.2

The first observation is that the coefficients E/R for the equations generated using Misra & White, and White & Bateman, are not too different, but those from King equation are markedly different.

4.2. 3. Comparison of results using the equations generated

To evaluate and compare the difference in the modelled parameter caused by using any of these equations versus another, a simple flowsheet (published previously [9]), was used. Figure 1 below is a screen capture of a typical scenario run for this study.



Description	flow	ratio	caus			
PGL	**1500m^3/h**	**0.680**	**260**	176.8	1305	
	% to 1st	**87.0**	% to #40	13.0		
Dilution	**0m^3/h**	**0.600**	**140**	84	0	
	% to 1st	**54.0**	% to Mid	46		
other	**0m^3/h**	**0.340**	**50**	17	0	
	% to 1st	**19.0**	% to Mid T	81		
		flow	ratio	caus	Solids	spec surf
Fine seed to 1st Tank		**75m^3/h**	**0.342**	**115**	**2300**	**0.04**
Coarse seed to # 40		**100m^3/h**	**0.342**	**253**	**2350**	**0.032**
Tk Volume	temp	Flow	Ratio	caustic	solids	spec surf
1000	75	1373.1	**0.602**	262.9	152.7	0.04
1000	70	1368.9	**0.556**	264.9	169.7	0.04
1000	68	1366.0	**0.524**	266.3	181.3	0.04
4000	**67**	1653.6	**0.478**	268.4	315.3	0.032
4000	**66**	1649.6	**0.443**	270.0	328.5	0.032
4000	**65**	1647.0	**0.421**	271.1	337.1	0.032
4000	**64**	1645.2	**0.404**	271.9	343.4	0.032
4000	**63**	1643.7	**0.392**	272.5	348.3	0.032
4000	**62**	1642.5	**0.381**	273.0	352.4	0.032
4000	**61**	1641.4	**0.372**	273.4	356.0	0.032
4000	**60**	1640.5	**0.364**	273.8	359.2	0.032
4000	**59**	1639.6	**0.356**	274.2	362.1	0.032
4000	**57.5**	1638.7	**0.349**	274.5	365.0	0.032
4000	**57.5**	1638.0	**0.343**	274.8	367.4	0.032
4000	**57.5**	1637.5	**0.338**	275.1	369.3	0.032

Figure 1. Simulation of a precipitation circuit using a spreadsheet model.

Five scenarios have been used for this comparison:

1. the effect of residence time created by removing 1 tank
2. removing 2 tanks (out of service for cleaning for example)
3. the effect of a 10 g/L PGL caustic concentration increase
4. increasing the seed charge by 50 g/L
5. and increasing the seed charge by 100 g/L

The summary results in Table 2 below are the variation in productivity from a Base Case for the equations A to F for each of the 5 scenarios.

Table 2. Productivity variations versus Base Case for the 5 scenarios studied.

	Loosing 1 tank	Loosing 2 tanks	Caustic inc. 10 gpl	50 gpl seee inc	+50 extra gpl seed inc.
A	1.26	2.8	0.95	0.88	0.70
B	1.08	2.37	1.15	0.78	0.63
C	1.21	2.67	1	0.86	0.68
D	1.29	2.84	1.56	0.99	0.77
E	1.07	2.33	1.69	0.86	0.68
F	1.22	2.69	1.6	0.95	0.74

At first glance, the results are not vastly different even though some choices regarding the model had an impact on some of the scenarios. The last 3 models using Ionic Strength as a denominator, for example, predict a larger impact for the increase in caustic concentration. Of interest also is that the equations A, C and D and F have predicted similar impacts in each scenario, except for the effect of caustic concentration, where the difference is as explained earlier. The 2 other equations (B and E) were both based on the King equation as data source.

5. Comparison of two equations for an Optimum Caustic evaluation

For most refineries, when there is a need for increased production, the question of the optimum caustic concentration for the precipitation area usually arises. There are a few ways to calculate this optimum, but an easy estimation can be done in a spreadsheet using the simple flowsheet model that has been illustrated above for a typical Alcan design. As part of the evaluation, there is a need to decide on the strategy for increasing the digestion ratio with increasing caustic concentration. In the current evaluation, for lack of better published data, the curves from the J. Kotte paper [10] were used with a 60 ratio point margin. Figure 2 shows the curves obtained using the D and F equations. The two curves are quite close and it’s clear that the choice of one or the other shouldn’t affect the choice of the caustic concentration. Because of the shape of the optimum caustic curve, it does not appear practical to target it, as it plateaus slowly towards the optimum.

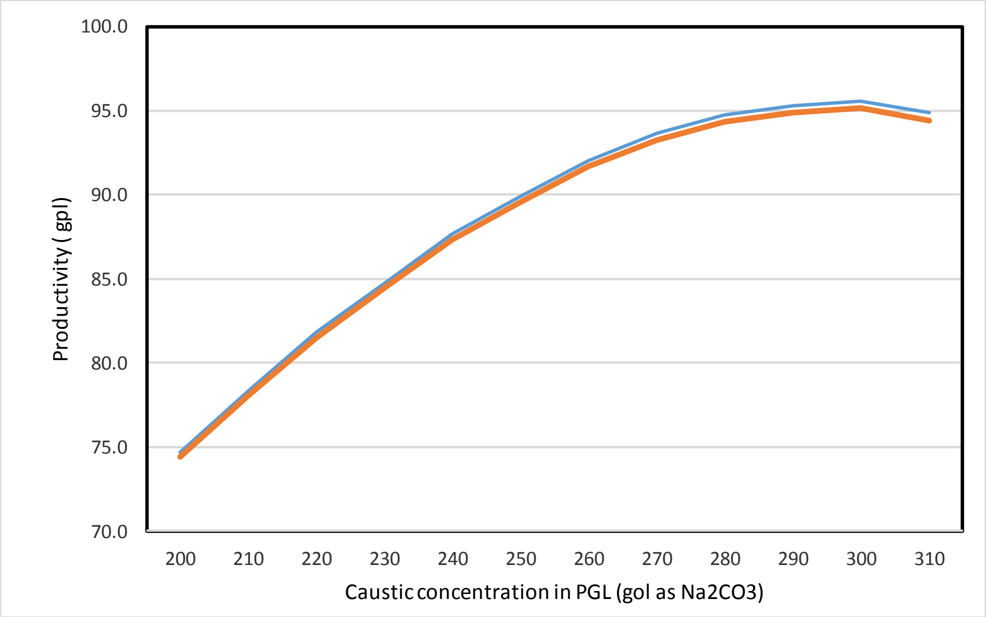


Figure 2. Optimum Caustic curves for a simple flowsheet using two of the generated equations (D in red and F in blue)

The main reason to limit a refinery to a value below its optimum is that at some point, other parameters will be adversely affected by this caustic concentration increase, with a poor net result on productivity as the asymptote is approached. The behavior of the sodium oxalate comes to mind as one that is quite sensitive to caustic increases. Finally, in the process of increasing the caustic concentration, other variables will inevitably fluctuate, making the progression to the optimum more erratic and potentially unproductive.

6. Conclusions

It has been demonstrated in this paper that it is possible to transform an existing model into a different equation form that has a stronger theoretical basis without using any new experimental data. The demonstration has also showed that the final equations don’t have a critical role in the final result, and that they can be accurate enough for some optimization studies, such as looking at seed charge response, specific surface changes, and residence time modifications.

However, there are studies for which the actual A/C ratio at various point of the circuit is of importance and the choice of the model will then make important differences. These circumstance would be for instance, the selection of an optimum temperature profile or other secondary phenomena related to the ratio profile like oxalate supersaturation behavior, occluded soda in product, nucleation, etc. For these situations, the approach to selecting the best model would be to carry out sampling of a whole precipitator row and use this profile as a basis for the selection.

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