# Optimizing Alumina Production Utilising Spreadsheet Models Based on Limited Data

# Denis R. Audet,

Director Audet Process Audit, Brisbane, Queensland, Australia Corresponding author: denis audet@hotmail.com

#### 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.

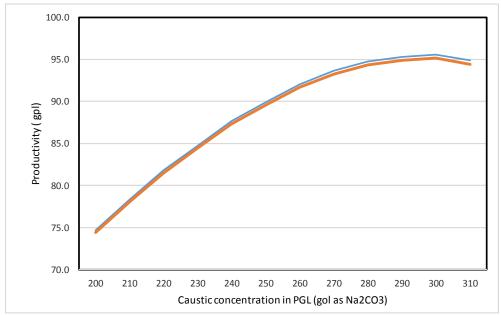


Figure 2. Optimum Caustic curves for a simple flowsheet using two of the generated equations (D in red and F in blue)

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.

## 7. References

- 1. C. Misra and E.T. White, "Kinetics of Crystallization of Aluminium Trihydroxide from Seeded Caustic Aluminate Solutions", *Chem. Eng. Progr. Sympos.* Ser., 110, 53, 1970.
- 2. A. Lectard and F. Nicolas, "Influence of Mineral and Organic Impurities on the Alumina Trihydrate Precipitation Yield in the Bayer Process". *Light Metals*, p123, 1983.

- 3. W.R. King., "Some Studies of Alumina Trihydrate Precipitation Kinetics", *Light Metals*, 551, 1973.
- 4. T.T. Overbey and C.E. Scott, "Characterization of Bayer Plant Liquors and Seeds, Utilizing a Mathematical Model for Precipitation", *Light Metals*, 163, 1978.
- 5. Jacques Mordini and Benoit Cristol, "Mathematical Model of Alumina Trihydrate Precipitation from Bayer Aluminate Liquors", *Paper presented at the 4th Yugoslav International Symposium of Aluminium*, Titograd, April 1982.
- 6. E.T. White and S.H. Bateman, "Effect of Caustic Concentration on the Growth Rate of Al(0H3) Particles", *Light Metals*, 157, 1988.
- 7. Stephane Veesler and R. Boistelle, "Growth kinetics of hydragillite Al(OH)3 from caustic soda solutions", *Journal of Crystal Growth*, 142, pp177-183, 1994.
- 8. W.J. Crama and J. Visser, "Modelling and Computer simulation of Alumina trihydrate precipitation", *Light Metals*, pp73-82, 1994.
- 9. Denis R. Audet and Jacques E Larocque, "Plant trial of a new Precipitation Line Up based on ...", *Alumina Quality Workshop (AQW)*, Sept 1993.
- 10. Jan J. Kotte, "Bayer digestion and predesilication reactor design", *Light Metals*, pp45-81,1981.