A GENERIC SYSTEM OF PLANT IMPURITY BALANCE MODELS

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Abstract

Over the past several years, Alcoa World Alumina (AWA) has developed a generic system for modelling plant impurity (most particularly carbonate, sulphate and chloride) balances. Impurity balance models, built in this way, are now in place for all 9 AWA refineries. Their purpose is to give Plant, Technology Delivery Group and other Technical staff a unified methodology for predicting long term impacts of major process changes (e.g. changes in bauxite type or introduction of new or altered impurity removal processes). This paper outlines:

- Modelling objectives, scope and philosophy.
- The type of technical and process information required for this type of modelling.
- Implementation (in Speedup) and use (from Excel interfaces).
- Strengths and weaknesses. Relationships to other models.
- Example uses.

Although still relatively new, the models have already proven their value in a number of contexts. The talk will review some of these, and discuss future prospects for this type of modelling.

1. Introduction

In 1997, an Alcoa World Alumina (AWA) project was initiated, aiming to:

- Develop a generic system of models for evaluation of steady state impurity balances in AWA plant liquors.
- Provide an easy-to-use framework within which to evaluate effects on impurity concentrations from possible major changes in plant inputs, flowsheets or operating strategies.
- Incorporate the best practical understanding of Bayer process chemistry (a shared basis for the models).

The resulting system, which has now been deployed across 9 AWA refineries, demonstrates a viable approach to meeting these aims, and the value of doing so. The following discusses the many issues involved in achieving this outcome.

2. Overall Modelling Objectives and Scope

The overall scope of the impurity balance modelling project was to:

- Include steady mass balance models for H_2O, Al_2O_3, TC, Na_2CO_3, Na_2SO_4, NaCl, NaF, $Na_2C_2O_4$, non oxalate organic carbon, Ga_2O_3, P_2O_5 and SiO_2 (plus three other unnamed components, as placeholders for possible future needs).
- Provide model flowsheets for all 9 AWA plants, with options for trying known strategic flowsheet options (e.g. causticisation anywhere down the washer train).
- Ensure the models can be run without specialist programming skills, from any standard AWA workstation.
- Deploy the models to all major user groups (plant technical departments, and central technical support groups), with adequate training documentation.

Specific exclusions from the project's scope were:

- No dynamic modelling. All models to be solely for prediction of steady state solutions (e.g. no modelling of seasonal effects due to lake volume changes).
- No hydrate yield prediction (users to supply the A/TC ratios necessary to calculate this).
- No details of oxalate and TOC chemistry (e.g. users to tell the models the oxalate concentrations in oxalate removal process output streams).
- No fluoride chemistry.

Carbonate, sulphate and chloride were the priority impurity species, in terms of accurate prediction of concentrations allowing for known process chemistry. Other impurities were to be tracked correctly through splitting and mixing operations, in soluble losses and losses with product, but with little built in prediction of chemical reactions. Such prediction was to be left for possible inclusion in the future. Similarly, the other exclusions listed above are possibilities for inclusion in future developments of the models. To allow for these possibilities, the modelling environment was required to be flexible and provide a good framework for future extension or improvement.

3. Project History

Prior success with a carbonate model (developed by Gerald Roach and Zenon Olszewski, Technology Delivery Group, Alcoa World Alumina) provided the impetus to begin the broader impurity balance modelling project. Written in Lotus, but later converted to Excel, the carbonate model provided a generic tool for assessing strategic options with respect to plant TC/TA control (e.g. the effect of moving causticisation further down a washer train).

For purposes of modelling plant carbonate, sulphate and chloride balances, prediction of these impurities' exits with desilication product was recognised as important. As a result, the early part of the project included the joint work with CSIRO Minerals reported in [3] and [4]. Based on careful analysis of DSPs prepared under a wide range of formation conditions, this work provided the necessary equations for prediction of DSP composition from model liquor compositions in slurry storage and digestion.

In the early part of the project, emphasis was also placed on defining the requirements to be met by the model, then identifying and testing an appropriate software environment. The eventual choice was Speedup, the flowsheet modelling equation solver from Aspentech [1], linked to a user interface system developed in Excel using VBA. Further details

of this combination are described in Section 4. Its suitability was tested, in the first instance, by translating the Roach/Olszewski carbonate model into this software environment.

The next major step, completed in 1998, was to develop a full impurity balance model for a prototype plant (Kwinana). The late Dr David Binet, Alcoa World Alumina Technology Delivery Group, directed this work, and took overall responsibility for decisions re modelling strategies and assumptions. As well as giving further proof of project strategy, the prototype model defined the list of chemical and process assumptions used in the models, and provided a library of unit process models ready for use in other plant model flowsheets.

After further testing and refinement of the prototype Kwinana model in 1999, the project proceeded into its implementation stage, whereby impurity balance models (IBMs) were progressively completed, documented and deployed to all 9 Alcoa World Alumina refineries. This included a round of site visits, for purposes of finalising base case data, validating the models and providing training in their use.

4. Aspects of Model Implementation

4.1 *Use of Speedup*

As mentioned in Section 3, Speedup was chosen as the environment in which the models would be coded. The following features explain the reasons for this choice:

- Speedup solves large, user-supplied systems of equations. This provides great flexibility, but means that equations have to be written for all aspects of the mass balances and chemical reactions modelled in each unit operation.
- The heart of Speedup is a powerful, iterative equation solver, capable of coping with up to 100,000 simultaneous non-linear equations. This power is important when solving the AWA impurity balance models, which contain:
  - many more equations than the earlier carbonate model, due to the increased number of modelled species,
  - more links between species (e.g. the carbonate, sulphate and chloride balances are all linked through the equations for DSP composition),
  - broad closed loops around the plant and lake circuits, creating dependencies between the solutions for large groups of equations.
- Speedup is modular. Models are developed for unit operations, then joined up in appropriate configurations using the flowsheet section of the code for a plant model. The same library of unit operations models can be shared between all plants. This facilitates the development of a "generic" system of models, with all plant models based on the same set of equations for each relevant unit operation (e.g. the same mudwasher model is used to construct the washer trains in all AWA plant impurity balance models).
- Speedup has an external data interface, allowing user inputs to be imported from external files and export of model output files. This provides the basis for remote use of Speedup models, through Excel interfaces.

4.2 *Excel User Interfaces*

An Excel user interface was developed for each plant IBM. Although details of model flowsheets and variables differ between plants, the user interfaces for the different plants all work in exactly the same way, with the same "look and feel". This was achieved by exploiting the flexibility and power of Excel and Visual Basic for Applications, to develop a shared user interface system including:

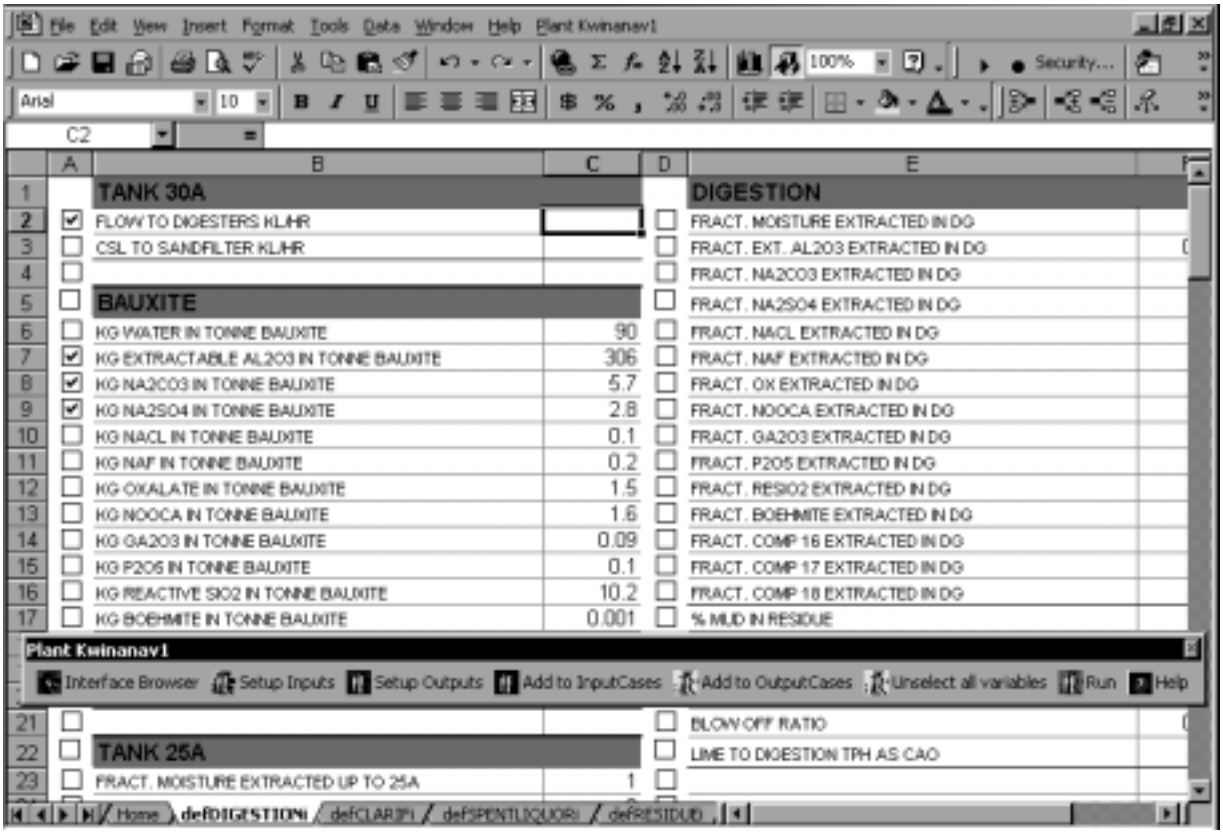

Figure 1 — A Snapshot from the Excel User Interface for a Plant Impurity Balance Model

- input and output data sheets, organised by plant area;
- pull down menus and a tool bar, for selecting between a comprehensive set of modelling and data management actions (setting up model runs, sending model runs to Speedup for solution, retrieval of Speedup outputs, review of calculated steady state flows and concentrations, saving and retrieving results, etc);
- user forms to select options and control the details of user interface actions;
- VBA routines to carry out these actions.

The Excel user interface system provides widespread access to the models without the need for Speedup programming knowledge. Another advantage is that it includes a convenient system for managing multi-run case studies, providing tables of results on user-selected output variables when user-selected input variables are varied according to the values in a table of cases previously set up by the user (in a multi-run input sheet). Compared with direct running of the models in the Speedup environment, the main disadvantage of the Excel interfaces is loss of flexibility over flowsheet design and in the selection of the variables to be set by the user.

4.3 *Centralised Model Management with Distributed Access*

A key project objective was to provide multi-site access to the plant models, across several continents, by any authorised user with a standard Alcoa World Alumina workstation. A requirement of equal long-term importance was provision for centralised model maintenance and updating, with change control and protection of model integrity. Figure 2 below illustrates the system design by which these two potentially competing objectives have been met. Important aspects of this are:

- The authorised version of the Speedup code for each plant model is kept in a secure area on a central modelling server (preventing unauthorised changes).
- Users are provided with accounts on this server, but do not have write access to the secure model storage area.
- Speedup also resides on the server. A licence manager handles Speedup use, queuing jobs as necessary to ensure the licensed number of simultaneous users is not exceeded.
- A copy of each plant's user interface is kept in a convenient area on a plant server. Users are encouraged to make their own copies of these interfaces, and customise them in various ways (setting up their own base case data, selecting particular multi-case variables, adding extra worksheet entries or whole worksheets to display calculations of particular interest).
- Users initiate model runs from Excel by employing the user interface facilities described in Section 3.2. For each run, the user interface sends a user input file through the Alcoa intranet to the user's account on the central modelling server.
- The user interface then starts up Speedup, solves the model with the user's input file, retrieves a result file to the user's central modelling server account and sends an email to the user giving notification of the completion of each run (plus a set of model run diagnostics from Speedup).
- The user can then run a user interface macro to retrieve the result files for their selection from their completed runs (once again through the Alcoa intranet).
- The first time a user initiates a run following a model version update, the updated versions of the model and converged base case data files are copied from the secure area to the user's account on the modelling server. This occurs prior to carrying out the first model run after a version change (providing a centralised method of version control).

4.4 *Technical Content*

An important aim when the structure of the models was being worked out was to include just enough detail for success with the main modelling objectives (evaluation of effects on impurity concentrations), but avoid anything more complex than this requires. Aspects of this included:

- The level of flowsheeting detail. Figure 3 provides an example of this. In most respects, the model flowsheets are much simpler than actual plant flowsheets (e.g. representing digestion as a single unit operation, no splits between parallel units, assuming a single addition point for all purge and packing water sent to the green liquor side of a plant). However, where useful for experimentation with new options, the model flowsheets sometimes contain extra elements

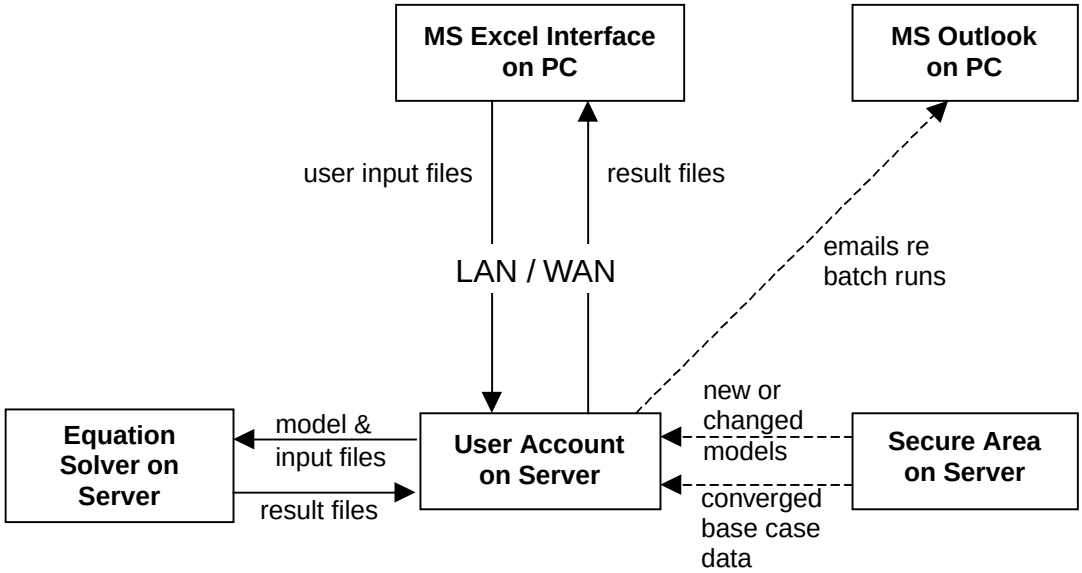

Figure 2 — Information Flows in a System for Widespread Access to a Centrally Managed System of Models

compared with the plants they are modelling (e.g. causticisers at all washer stages, for experimentation on effects of causticisation at different stages).

- Deciding which liquor components to model. As noted in Section 2, modelling the major inorganic impurity balances was the primary aim of the project. Because of its intrinsic complexity, a thorough model of plant total organic carbon (TOC) balances was not a primary aim. However, as some TOC decomposes to carbonate, a TOC balance (split into several components) became necessary for construction of an adequate carbonate balance. Similarly, models for plant soda and water balances were necessary because of their many effects on plant impurity concentrations. For example, these balances determine the caustic input to a modelled plant (calculated to maintain a user specified TA in liquor to precipitation), and hence also determine the major chloride input for the model, and a major dilution factor for other impurities.
- Deciding which residue components to model. Although separate tracking of different residue phases (e.g. different lime solids) could be useful for some purposes, the only distinction in the models is between residue originally from bauxite and residue arising from reaction products.
- Deciding not to model energy balances. Except for one or two instances, where user specified temperatures and basic heat balances determine injection steam use or evaporation, the model does not deal in any way with energy balances.
- Modelling of Chemical and Physical Processes. Reasonably detailed equations were included to predict the results of some chemical and physical processes with major impacts on impurity concentrations. For example:
  - the extent of impurity exits by incorporation in DSP, as determined by the correlations referred to in [3] & [4] (see Figure 4),

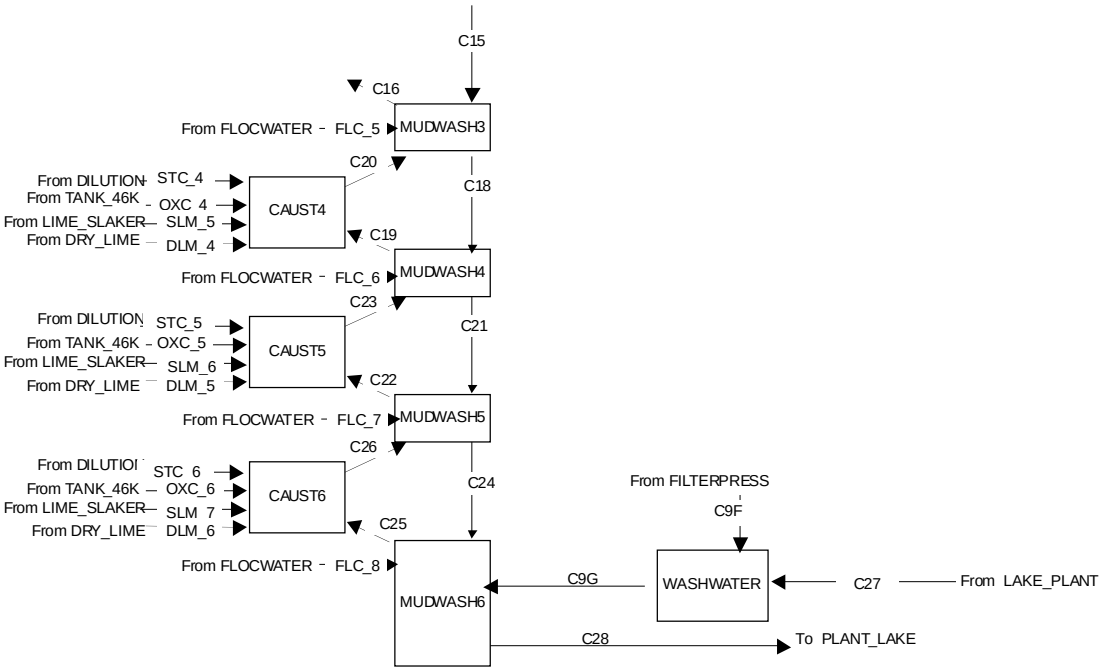

Figure 3 — Level of flowsheeting detail — example from model mud washing section

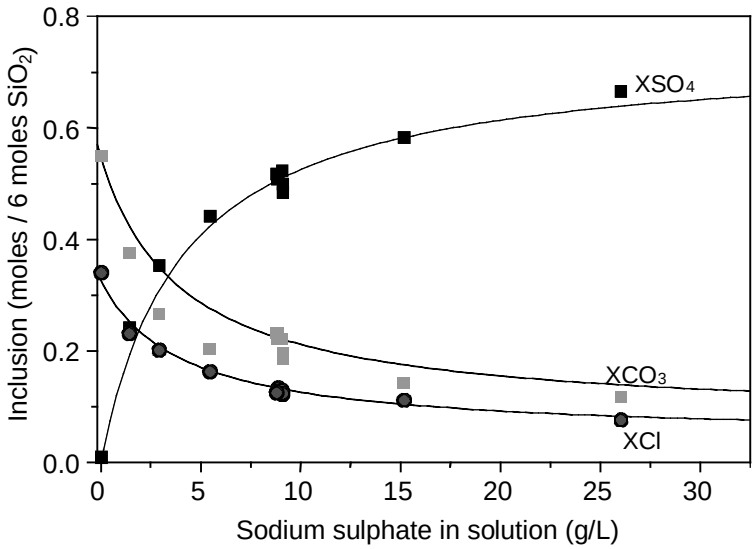

Figure 4 — Inclusion of equations to describe process chemistry: DSP composition example

- equilibrium TC/TA ratios in the presence of lime, using in-house correlations,
- soda adsorption to mud as a function of TA, using the equations reported in [5].

In other cases, users are required to tell the model the results of important chemical or physical processes. For example, oxalate concentrations on exit from the oxalate removal buildings in the models, or A/TC ratios on exit from digestion and precipitation.

An intermediate approach found suitable in some circumstances is for the models to be told simple percentages or ratios determining the extent to which a chemical or physical process occurs (e.g. %extractions from bauxite in 25A and digestion, or %conversions of TOC fractions to carbonate).

Mud washers were modelled as in [2], with user specification of washing efficiencies, underflow densities, and bypass fractions (to allow changes in assumptions re washer stage availability and utilisation).

A large effort went into assembling the chemical and process knowledge which now provides the technical basis of the models. Along the way, numerous assumptions and compromises had to be made, to cope with incomplete knowledge or avoid unnecessary detail. The reward from this effort is that all Alcoa World Alumina plant impurity balances have now been modelled from a common technical basis, with a well-documented list of chemical and process assumptions, using chemically or physically interpretable parameters (not fudge factors). There are some areas where improvements in the technical basis for the models would be worthwhile. When future advances in chemical or process knowledge make this possible, these improvements will be able to be shared between refineries, taking advantage of the generic approach to modelling Bayer process unit operations.

5. Initial Applications

Although the models have been deployed for a relatively short time, they have already been employed in a number of important case studies. These include work:

- impacts of bauxite changes on long term sulphate concentrations and TC/TA ratios,
- causticisation options,
- implications of residue carbonation,
- expansion options.

Some of these studies have involved flowsheet changes. In these cases, centralised support from Speedup modelling experts has been necessary. In other cases, where there were no flowsheet changes to consider, except those covered by flow switching variables built into the models (e.g. with causticisation), centralised support has not been necessary.

6. Future Prospects

The modelling system described above provides a good starting point from which to build more detailed plant models. Possible additions include:

- Equations to predict effects of impurity concentrations on hydrate yield.
- Equations to predict oxalate yield.
- Allowance for monthly lake system volume changes.

Updates may also occur following future improvements in our knowledge of the Bayer process chemistry already covered by equations in the model (e.g. for lime chemistry).

At the same time, use of the models should grow, and will most likely include studies where flowsheet changes need to be examined. Expert support will still be needed for these cases.

Conversion to Aspen Customer Modeller (Aspentech's recent major update to Speedup) will also be necessary within a year or two. This conversion will consume significant resources, but is necessary to ensure ongoing Aspentech support. It will also provide some important extra capabilities (e.g. a graphical user interface for constructing or modifying flowsheets, using the unit operations models in the library we have built).

7. Conclusions

Using the strategies outlined above, a generic system for predicting steady state plant impurity concentrations has been constructed. Impurity balance models, using a shared library of custom-built unit operations models, and remote access to a shared modelling server, have been successfully deployed to 9 refineries across Alcoa World Alumina's operation. This provides an important shared basis for studying effects of strategic options on impurity concentrations, with considerable scope for further application and enhancement.

Acknowledgements

Many people have contributed significantly to the impurity balance modelling project. Contributions from the AWA Technology delivery group, other AWA support groups, plant technical departments and external organisations have all been important. Although too numerous to list, the many contributors to the development of the models are all gratefully acknowledged.

References

Aspen Technology, Inc. (1994), *Speedup Release 5.4 User Manual.*

Binet, D.J., McClain, J.K. and Stone, R.J. (1977) CCD residue washing calculations using the resolved flow concept, *Proceedings of Chemeca 77, Canberra, 14–16 September, 1977*, 127–130.

Riley, G.W., Binet, D.J., Smith, P.G. and Pennifold, R.M. (1999) Plant impurity balances and impurity inclusion in DSP, *Proceedings of the Fifth International Alumina Quality Workshop, Bunbury, 21–26 March 1999*, 498–507.

Smith, P.G., Pennifold, R.M., Whittington, B.I. and Fletcher, B.L. (1998) *Measurement of inorganic impurity inclusions into desilication product: final report*, CSIRO Minerals Report DMR-705, 107 pp. CONFIDENTIAL.

Thornber, M. and Binet, D.J. (1999) Caustic soda adsorption on Bayer residues, *Proceedings of the Fifth International Alumina Quality Workshop, Bunbury, 21–26 March 1999*, 498–507.