A GENERIC SYSTEM OF PLANT IMPURITY BALANCE MODELS: FURTHER IMPROVEMENTS

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Abstract

This paper presents an update on improvements to the generic system of plant-wide impurity balance models (IBMs) discussed in the last International Alumina Quality Workshop (Riley et al. 2002). Following the successful initial global deployment of the Alcoa plant-wide model, to ensure ongoing support from the software vendor, we have converted the original models to a new platform. In the process, these converted models have been further enhanced, not only to include precipitation yield prediction but also inclusion of a number of important improvements in knowledge of Bayer process chemistry, and development of a semi-dynamic mode of operation (for modelling effects of lake volume changes). A new model interface system has also been developed as part of the software conversion project. The enhanced Alcoa generic system of plant-wide IBMs has gained significantly wider usage, from regular and advanced model users.

1 Introduction

Over the last eight years, Alcoa World Alumina (Alcoa) has been developing and using a generic system of plant-wide impurity balance models (IBMs) to support detailed expansion and greenfield studies of its alumina refineries, improve product quality, reduce operating costs and help process troubleshooting. With the advent of powerful computers, user-friendly commercial process simulation packages and improved knowledge of Bayer process chemistry, engineers within Alcoa are able to build and use more detailed plant models and leverage on the system to predict the complex and difficult process behaviour more accurately and obtain quicker solutions. A project to further improve the Alcoa generic system of plant-wide IBMs was initiated in 2003 with the following objectives:

- Conversion of the generic system of plant-wide IBMs from SpeedUp® to Aspen Custom Modeller™
- Incorporation of updated Bayer process chemistry into the library of models
- Incorporation of Alcoa precipitation yield model into the plant-wide IBMs to allow direct prediction of precipitation yield
- Development of a new graphical user interface.

2 Conversion of Alcoa models from SpeedUp® to Aspen Custom Modeller™

2.1 *Withdrawal of SpeedUp® and Alcoa decision*

With the imminent withdrawal of software licenses and technical support for SpeedUp® from AspenTech and the introduction of Aspen Custom Modeller™ (ACM) by the software company, the Alcoa plant-wide modelling team faced two major problems. Firstly, once the SpeedUp® licenses expired, we risked losing access to the know-how built into the plant-wide IBM process system, which includes Alcoa's best practical understanding of Bayer process chemistry. Significant efforts, knowledge and engineering man hours had been devoted to developing the SpeedUp® models which would be useless once SpeedUp® licensing was withdrawn. Secondly, site engineers in the nine Alcoa refineries using the plant-wide models would not be able to conduct regular what-if studies for plant troubleshooting or plant expansion studies once the licenses expired. It is also worth noting that SpeedUp® was used under the UNIX operating system, which is not Alcoa's preferred standard operating system. The modelling team commissioned a study, led by Ali Nooraii, to carefully explore a number of options to convert the original SpeedUp® models to a suitable platform, while still keeping the existing models accessible by site engineers until an agreed licence withdrawal deadline was reached. On the basis of the study, it was decided that the team should convert the models to the ACM software. The benefits of this were seen as production of more readable models, taking advantage of new software features and securing a guarantee of continued technical support by the software vendor. These benefits outweighed the associated risks and according to the investigation report (Nooraii, 2001), the ACM option was superior to other options investigated.

2.2 *Use of ACM*

Like its predecessor, ACM is an equation-oriented process simulation package capable of simultaneously solving a model containing many balance equations, and is predominantly used to model continuous chemical or minerals processing plants. The following features differentiate ACM from SpeedUp®:

ACM is an object-oriented software package that runs under the Microsoft® Windows® operating system. The ACM graphical users interface (GUI) is an important enhancement that allows ease of use such as the ability to drag and drop objects and visually construct flowsheets from a library of unit operation models, custom models or the built-in system library. Conceptually, the ACM modelling language does not significantly differ from SpeedUp® and in fact, AspenTech has provided SpeedUp® 5 Source Converter software (Aspen Technology, 2001) to allow computer-aided conversion of a SpeedUp® model to an ACM model. However from experience, conversion of large SpeedUp® models such as the plant-wide IBMs is not a straightforward exercise, requiring an iterative process and often produces programs that are not readable or require significant pre-treatment to a SpeedUp® 5 text file prior to a conversion. In order to alleviate this problem, and to take advantage of the new features in ACM, it was found to be preferable to rewrite most of the original SpeedUp® code.

One of the useful features of ACM frequently used by the Alcoa modelling team is the concept of inheritance. Writing a unit operation model which uses another model not only simplifies programming work but the converted model is much neater and readable. Another feature of the ACM language, considered an advanced function, used by the team is a containing model. A multi-stage mud washer train containing model in ACM allows sub-models of single mud washers to be lumped together and shown as a single object, eliminating the need to drag, drop and connect individual objects of the mud washer unit operation model within an ACM flowsheet. In the development of the Clarendon plant-wide IBM, we engineered a containing model for causticisation with sub-models of causticiser selector, high efficiency causticiser (HEC), mud slurry separation and mixing resulting in reduced flowsheet complexity. The disadvantage of developing a flowsheet with this approach in the current version is that graphically, the connectivity of sub-models within a containing model is not shown and it therefore may not be as easy for a non ACM specialist to visualise the overall process scheme.

For a plant-wide model as complex as that of an alumina refinery, the ACM hierarchy model, when used, is particularly beneficial in terms of readability of the process flowsheet. Although a flowsheet outside the hierarchy level in the ACM GUI is virtually not readable, flowsheets for buildings inside of a hierarchy are readable. To enhance readability of an ACM plant-wide model, we employ a standard colour coding and thickness to differentiate stream types. Figure 1 shows examples of the ACM GUI outside the hierarchy level (Left) and inside of a hierarchy respectively (Right). Hierarchies in Figure 1 (Left) are shown as square boxes.

2.3 *Documentation*

In any software development project, maintenance costs are often cited as a significant contributor to the overall cost. With an overall expectation that the outcome of the SpeedUp® to ACM software conversion project would have a long-term impact on the performance of Alcoa's refineries, the modelling team has placed importance on the provision of standardised documentation. Consequently, we need to ensure that the ACM codes we develop are usable, understandable and maintainable, not just by the original developer, but by anyone who needs to continue development of the plant-wide IBMs. This demands that we produce documentation at all levels, from source through to end user (White, 2004a). To automate the production of the documentation as much as possible, particularly at the code level, the modelling team employed Robodoc (2005). This open source code is designed to use specially formatted documentation headers within the source, which can be converted to a variety of formats, including HTML, PDF and RTF. By maintaining the documentation within the source code, it is easier to keep the documentation up to date.

3 Updating Bayer chemistry and precipitation yield modelling in ACM

In the ACM version of the IBMs, we have included apatite production chemistry for lime reactions in the lime slaker, causticiser and digestion models. Improvements have also been made in other aspects of the lime chemistry assumptions built into the models. Precipitation is the rate-controlling step within a Bayer alumina refining process and production capacity is therefore determined by precipitator performance. In addition, product quality, measured in terms of both crystal size distribution and impurity levels, is largely determined by conditions within precipitation. Consequently, modelling of the alumina precipitation process can play an important role in identifying critical precipitation operating variables that often compete and incrementally change the costs of refining by their impact on yield. Alcoa has a long history of developing and using computer-aided precipitation yield modelling (e.g. Swansiger, 1992; White, 1995) to support design studies and development of operating strategy to optimise yield and improve alumina product consistency. More recently, White (2004b) has incorporated particle size distribution calculation into Alcoa's precipitation yield model or 'YieldMod' using a population balance approach. The modelling team has decided to incorporate the yield-only precipitation model within the plant-wide ACM model. Users are required to assemble and connect individual precipitation tanks and we compute precipitation yields in a separator block after the last precipitation tank. Finally, the completed precipitation flowsheet is connected to the Bayer liquor circuit which allows for direct prediction of precipitation yield within the plant-wide IBMs in ACM.

4 ACM modelling of semi-dynamic IBM

It is not enough to know only the equilibrium or steady-state concentration of an impurity or water input/output within an alumina refinery. A dynamic understanding of water and impurities in the lake system is essential to have an effective planning and budgeting process within the refineries. Some of the identified applications of semi-dynamic modelling are:

- Forecasting not only the ultimate impurity concentration after a change in Bauxite quality or addition/modification of an impurity removal process, but how long it will take to equilibrate.
- Forecasting not only the total fresh water required for an extended period of time but with reasonable accuracy when it will be required.
- For plants increasing in production or introducing residue drying beds, site engineers could predict and monitor plant exposure to dry summers or wet winters that may threaten storage capacity at one extreme or the other.

This need has motivated modelling of lake dynamics at Alcoa's Wagerup refinery and a system has been in used for nearly 20 years (Phegan, 2001) to predict lake volume changes, water, soda, and organic over a period of user-specified time. As part of the conversion project, the modeling team has included a provision to modify the plant-wide, steady-state IBMs to allow prediction of lake volume changes, water and the identified impurities. This is similar to Wagerup's lake dynamics modeling system but includes all individual impurities identified by Riley *et al*. (2002). Furthermore, in order to model the dynamics of multiple lakes, we developed a dynamic lake model

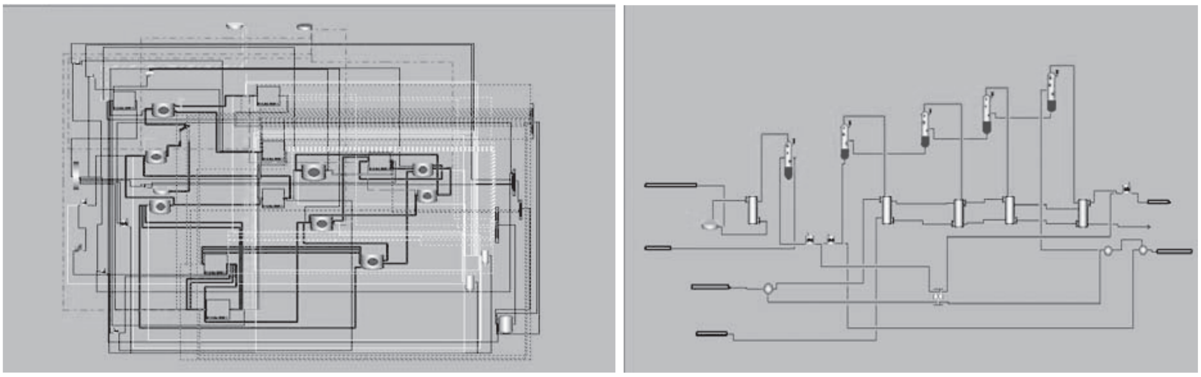

Figure 1. Flowsheets of an alumina refinery plant-wide model (Left) and a heat interchange hierarchy (Right)

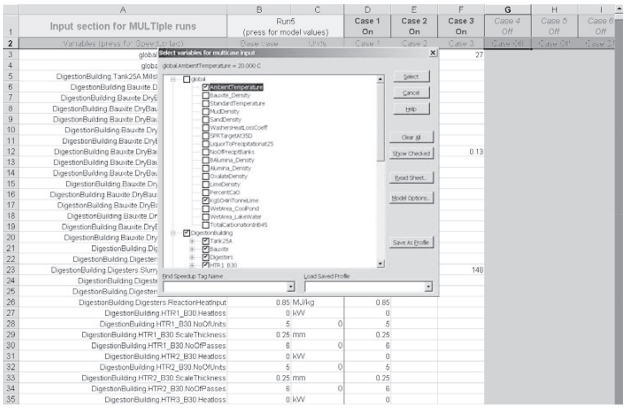

Figure 2. An example of Excel interface for AWA plant-wide IBM

using a finite difference approach (Nooraii, 2003). This model calculates the average impurity concentrations for a given time step as an approximation for the outlet concentration and assumes constant density within a lake. In a pilot project, the modeling team has successfully converted the original Wagerup dynamic lake system from TK Solver to ACM. Further validation of the converted model with the Wagerup residue engineer has been necessary due to inclusion of additional impurities not accounted for in the original TK Solver model.

5 ACM Excel Interface

An Excel interface has been developed to allow users to run ACM models on the modelling server from their desktops, in a similar manner to that formerly used to run SpeedUp® models. An interface is required because there are only a limited number of licences to the ACM software and it is targeted at site engineers who only wish to run the ACM plant-wide models and obtain results. The interface is generic in the sense that it can be used to run any ACM model, although it is tailored towards plant-wide IBMs and mass and energy balance models (MEBs).

The interface consists of a number of different Excel workbooks and other files that reside on the user's PC, and several workbooks and a custom-written executable program that are used on the modelling server. The graphical user interface is menu-driven and employs a number of dialog boxes (user forms) to guide the user. Context-sensitive help is available at all stages. Variable selection differs from that used for the SpeedUp® interface. Variables are selected from a directory-style structure within a dialog box. The interface can allow access to all variables within the model. Entry of case values for input variables is into a normal worksheet, similar to the SpeedUp® interface. The starting point or base case of a run can be selected from: the default case, special cases that may have been created, or any successful previous case created by a user. Users are allowed to run up to 30 cases simultaneously. Figure 2 shows an example of the generic ACM Excel interface developed as part of the SpeedUp® to ACM conversion project. To facilitate ease of access by site engineers, a globally-accessible intranet site was created, from which the ACM Excel interface can be downloaded once access has been granted to the modelling server.

6 Application of plant-wide models in ACM

Deployment of the plant-wide models at some Alcoa refineries occurred much earlier than the anticipated project completion due to the demand for plant-wide models to support plant expansion process design studies. The modelling team worked closely with the process design teams in developing plant-wide models for these expansion studies, thus giving them the vital lead time in producing a suitable model to study various design options; leading to optimised process flow sheets and the process data required for equipment sizing. Using the completed library of unit operation models, design team members trained by the modelling group were able to quickly construct and investigate flow sheet options with sufficient detail directly in ACM. This was done prior to committing to major business decisions, and with minimal need for central modelling support. A significant increase in the usage of the plant-wide models in terms of number of simulations made either via the ACM Excel interface or ACM directly indicated an early success for the AWA modelling team.

7 Conclusions

The following are concluded from this study:

- The Alcoa system of plant-wide IBMs in ACM has been successfully converted from SpeedUp® and deployed to all nine Alcoa refineries globally. Site engineers from Alcoa refineries globally are able to access the models via a centralised modelling server which resides at the Kwinana refinery.
- The system has attracted significant interest from site engineers; not only from ordinary model users who only want to run the models and obtain simulation results via the ACM Excel interface, but also advanced model users who are capable of doing flowsheet changes and developing custom models within ACM directly.
- The original system of plant-wide IBM in SpeedUp® was enhanced by the inclusion of precipitation yield modelling flowsheet in each of the IBMs. This allows direct prediction of precipitation yield.

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