Development and Utilization of Detailed Process and Technology Models at RUSAL Alumina Refineries

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Abstract

RUSAL is completing the development of detailed steady-state mathematical models of the process technology in its alumina refineries in the current year. Models have been developed for refineries based on different technologies: Bayer process, parallel Bayer-Sinter and stand-alone Sinter processes. Each model includes equipment specifications for the production sites, mud disposal and Combined Heat and Power Plants (CHPP). The control logic of the models reproduces a refinery control system. Particular attention was paid to the creation of kinetic relationships for digestion processes, which help to predict recovery of alumina and soda, as well as the thermodynamic equilibrium of impurities in liquors. A large number of laboratory studies have been performed for the development of these thermodynamic and kinetic models. Several types of problems are solved using these mathematical process models, such as sensitivity investigations, "What-if" analyses, production optimization, business planning and estimation of capital investment efficiency. RUSAL has organized departments for mathematical modeling at their refineries and a central development team in its St. Petersburg office. Refinery specialists monitor the production process and perform routine daily calculations. They propose solutions for managing the production process to achieve maximum refinery efficiency based on their experience and modelling results.

Keywords: Mathematical modeling, alumina refinery optimization, process modelling.

1. Software for Process Simulation

RUSAL is developing a new unified approach to efficiency assessment, business planning and optimal process technology management at the enterprise level in the framework of its alumina refinery development program. This approach will allow the production of alumina of the required quality and at the minimum cost.

There are many conditions in solving for alumina production optimization. It is necessary to take into account the capability and the condition of equipment, resource portfolio, transport logistics, prices of energy carriers and auxiliary materials, climate change and weather. The optimum quality or cost of alumina is not an exceptional set of values for production parameters, but a sequence of dynamically changing states, since these factors are variable in time. The cost and quality of alumina ultimately depends on finding this dynamic optimum and maintaining it.

The unified approach to the assessment of process efficiency at all RUSAL's refineries is based on the use of SysCAD software, a product of the Australian company KWA Kenwalt Pty Ltd. SysCAD is a specialized software environment for the development of detailed Bayer process alumina refinery models. Although we were aware of the availability of alternative software environments (Table 1), and having similar software developed in-house, we nevertheless

settled on SysCAD [1, 2]. The highly specialized orientation of this product, the competitive cost and the recommendations of other users influenced our choice.

Table 1. Software for process simulation.

Software*	External thermodynamic databases**	Solvers ***	Scripting language	Compatibility Interfaces	Technologies where software is more often applied
Aspen Plus	OLI	SS, D	Fortran, VBA Excel	OPC, Excel, Word	chemical technology, metallurgy, energetics
Hysys		SS, D	Fortran, VBA Excel	OPC, Excel, Word	oil and gas treatment
SysCAD	HSC	SS, D	SysCAD	DDE, OPC, Excel, DXF, DLL	production of alumina, potash, sugar
ProSimPlus	DIPPR, User defined DLL	SS	Excel, VBA, C++, Fortran	Excel, DLL	oil and gas treatment, biochemistry, food industry
IDEAS	OLI, Gibbs	SS, D		OPC, DDE, Excel	pulp-and-paper production, oil-sand mining and treatment, oil transportation, heap leaching
METSIM	FactSage	SS, D	APL	DDE, Excel, DXF	mining, crushing, separation and classification
HSC Chemistry	-	SS, D	Excel	Excel, OPC, COM	crushing, separation and classification
UniSim Design	Hysys, DIPPR	SS, D		OLE	oil and gas treatment, chemical technology
JKSimMet	-	SS	-	-	crushing, separation and classification
JKSimFloat	-	SS	-	-	flotation
PRO/II	OLI, HTRI, DIPPR, Koch-Glitsch Spiral CrudeSuite	SS	Excel		oil and gas treatment, chemical technology
USIM PAC	DIPPR	SS, D			crushing, separation and classification
Math Designer	-	SS	VB, C#	Excel, OPC, COM, DXF, DLL	alumina production, building materials production

* All names of software products and trademarks mentioned in the table belong to registered owners; ** Except of built-in expanded database; *** SS – Steady-State solver, D – Dynamic solver.

The first steady-state models of RUSAL alumina refineries were created with the involvement of outside specialists. Since 2012, a subsidiary company, RUSAL-Australia has joined the development of models for Bayer refineries for non-Russian locations. RUSAL-Australia independently created models for refineries in Jamaica and Ukraine. An important decision to develop models for Russian refineries was taken in 2014. It should be noted that Russian alumina is produced from bauxites by parallel Bayer-Sinter processes and from nephelines by the Sinter method. There were no examples of SysCAD models to describe such flowsheets, but it was decided not to change the software platform, but to combine the skills of RUSAL-Australia specialists with the experience of the RUSAL Engineering and Technology Center in St. Petersburg to jointly develop these models. The current year is important for the project, because development of basic steady-state mathematical models for RUSAL alumina refineries will be completed in 2017. In total, this work has taken 7 years.

2. Models of RUSAL Refineries

Each mathematical model is a complete description of the material and heat flows, equipment specifications and control algorithms of an individual refinery. Material flows are characterized by consumption, chemical and mineralogical composition, aggregate state, particle size distribution, pressure and temperature. The production equipment is described both with the use of typical software units, and with the help of specially developed models for some technology elements that are not a part of the SysCAD software library. The control system logic of a real refinery is accurately reproduced in the model.

The model interface is in the form of the flow sheet diagram, each sheet refers to one of the refinery's areas (Figure 1). One of the modeling tasks was the compilation of integrated balances of alumina, soda, chemical impurities, water and energy. Taking into account all return flows, models included not only process areas, but also a combined heat and power generation facility, the residue storage area and water distribution system. The Ural and Bogoslovsky refineries operate according to the parallel Bayer-Sinter processes. Their models also contain peculiar areas, such as charge preparation, sintering kilns, sinter leaching units and production of soda-sulphate mixtures. The Achinsk Alumina Refinery produces alumina from alkaline and alumina-containing raw materials by sintering. Their flowsheet does not contain a Bayer refinery. They produce a number of by-products: monohydrate and anhydrous soda, potassium sulfate, and raw material feed for cement production. Against the background of other sites its model describes specific areas for soda production: soda evaporation areas, a facility for potassium sulphate crystallization, and by-product dryers.

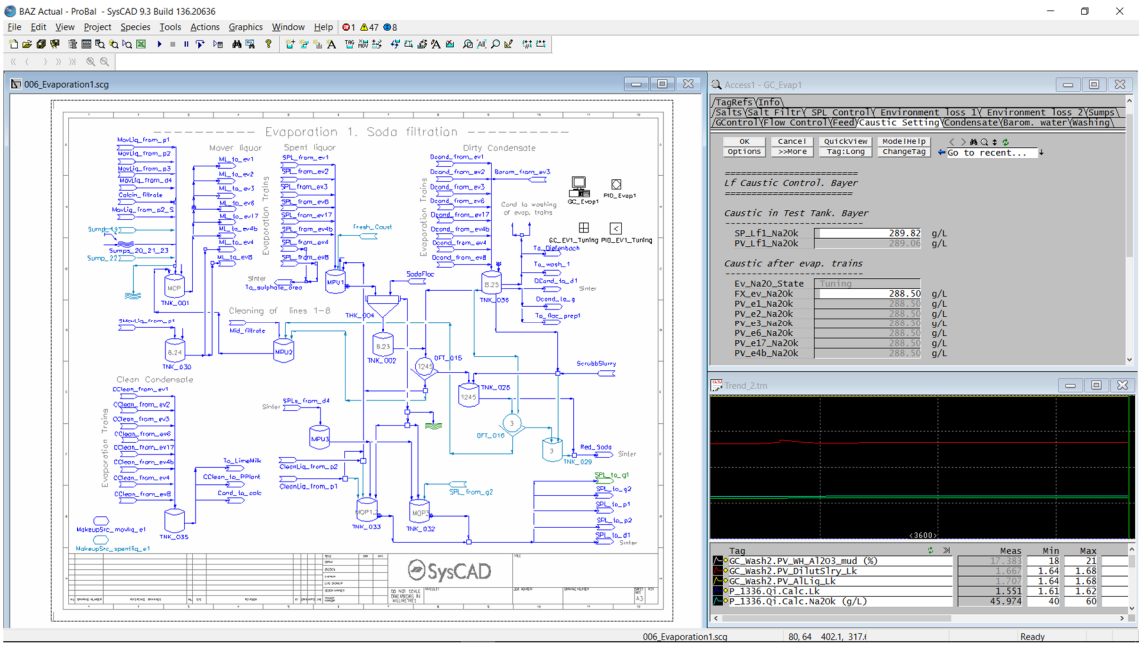


Figure 1. Tanks of mother and spent liquor of an evaporation area.

The technology of any refinery acquires unique features due to the different raw material composition and equipment used. These features need to be preserved during model development, if the final product model is not to lose its predictive power. The composition and properties of liquors, solubility of key compounds, chemical kinetics of leaching, digestion, desilication, precipitation, and crystallization of impurities must be described most accurately for the conditions of a particular refinery. A special program of laboratory tests and industrial measurements was developed to achieve this goal. Samples of bauxites, slurries and liquors from active processes were selected and used in these tests. Execution of the program was entrusted to the refinery laboratories and sites.

The test program included fitting of equation coefficients: Malloy-Donaldson equation for the liquor density, the Rosenberg-Healy equation for the equilibrium solubility of alumina, kinetic functions of alumina crystallization and occluded soda precipitation. Ores which are processed at RUSAL refineries can contain aluminum in two dozen compounds, including various forms of iron, silicon, sodium, potassium, phosphorus and sulfur. All process significant compounds were identified, their thermodynamic properties were found and loaded into the databases connected to the models (Figure 2).

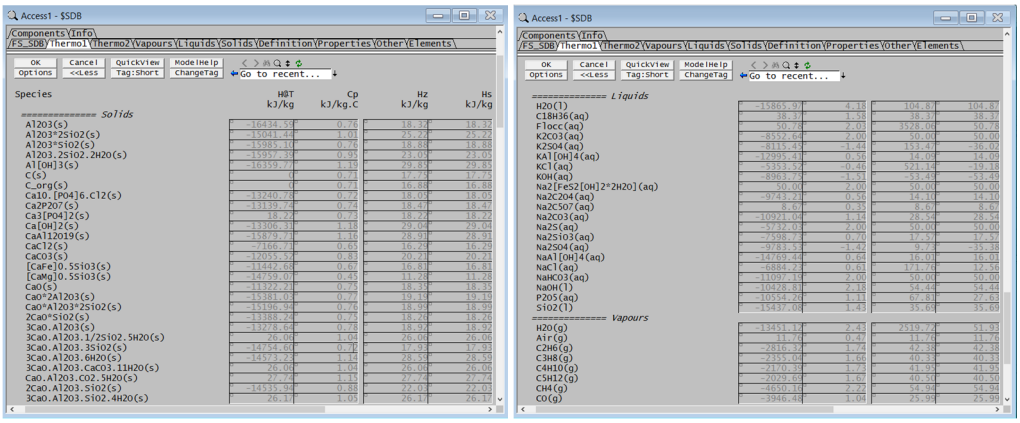


Figure 2. Part of the thermodynamic database for a Sinter refinery model.

With the joint presence of potassium and sodium in solution, their ions cannot be identified independently by titration, and atomic spectroscopy only allows separately determining elemental potassium and sodium content. Due to these measurement difficulties, independent accounting of sodium and potassium in liquors is not practiced, and it is usual to present their sum as R_2O. However, up to 30% of alkaline metals in liquors of the Achinsk Alumina Refinery is potassium. Studies have shown that solutions containing potassium are less stable [2, 3]. The Rosenberg-Healy equation and kinetic equations for alumina precipitation from soda liquor are not correct in this case. Another difficulty connected with potassium is the standard model for Bayer liquor in SysCAD software does not take into account the presence of potassium, so the built-in correlations for density and boiling point elevation cannot be used. The model for the nepheline sintering flowsheet has received significant improvements which have overcome these limitations. These changes were implemented using the scripting language and designed in the form of classes and functions that replaced the build-in software modules.

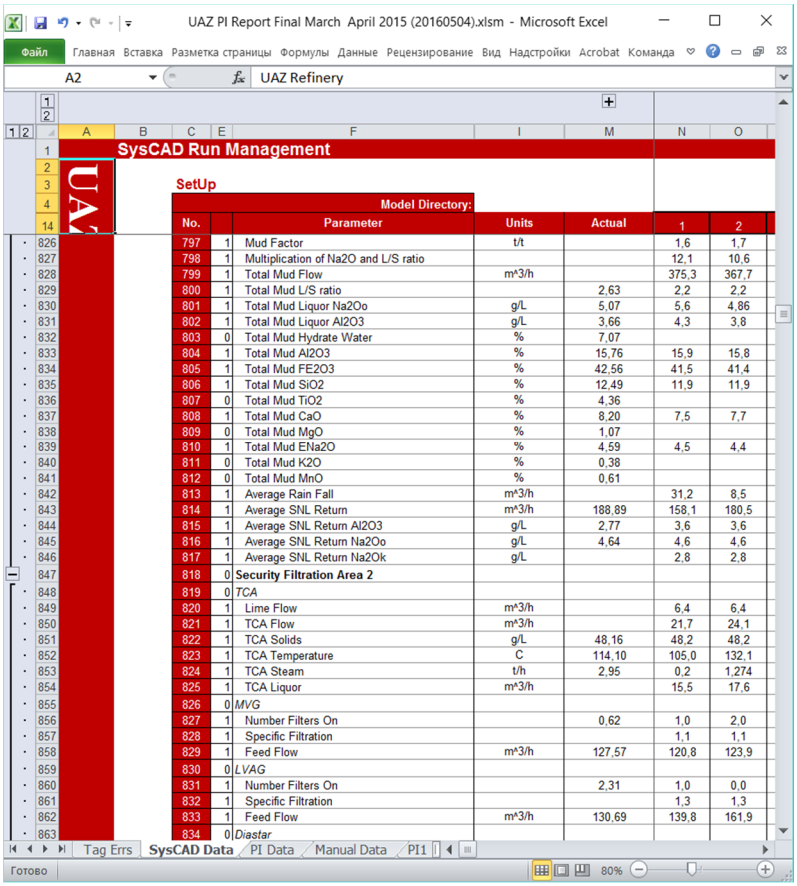
The kinetics of alumina extraction by digestion is determined by the mineralogy of alumina and silica, temperature, composition of spent liquor and particle size distribution. Variation of these factors in an operating process is small, and the degree of alumina extraction is relatively stable. Interest in the chemical kinetics arises when performing numerical calculations with goal to study influence of single or a group of parameters or global performance indicators of a refinery.

Studies of alumina digestion kinetics in hydrochemical technology, as well as alkalis in the Sinter process were carried out for all refineries, where these processes take place. Tests for total available alumina, alumina extraction from bauxite at equilibrium conditions and extraction kinetics were performed using real liquors for all bauxites entering the refineries. The results of experiments were processed to obtain kinetic relationships and integrated into the SysCAD models. This eliminates the necessity to make assumptions about degree of alumina extraction from tested bauxites due to deviations of temperature, residence time, concentration of the spent liquor and other process parameters from the standard values. This value is calculated by the model for each raw material.

Liquors at Sinter and Bayer-Sinter refineries are characterized by low concentrations of oxalates and carbon, but contents of carbonates and sulfur are increased. Crystallization of sulfur and carbonates begins in last stages of the evaporation trains and continues during the subsequent pipework and vessels exposed to evaporated liquor. Slurry with settled impurities is filtered and sent to the sintering area. Massive crystallization of impurities from the evaporated liquor reduces the productivity of lines, causing difficulties in servicing, affects the capacity of soda settlers, and it also impacts on the productivity of the sinter line. The investigation of

equilibrium concentrations of soda and sulfur in refinery liquors at different concentrations of total alkali and residence temperature was also one of tasks posed to refinery laboratories. Collected data on the equilibrium concentration of sulfur and soda are also processed and integrated into models.

Periodic updating of models should be carried out to bring the model into line with current refinery parameters. This procedure is very expansive because the number of fitting parameters is close to a thousand. Customization controllers in SysCAD and standardized Excel forms for uploading reports were created to simplify model updates. These tools allow semi-automatic collection and filtering of real data, their sending to SysCAD tuning controllers, automatic adjustment of the model, and the uploading of fitting results into the report. With these tools in place, it is now easy to compare calculated and actual values, and achieve their maximum compliance using Excel forms (Fig. 3).



No.		Parameter	Units	Actual	1	2
797	1	Mud Factor	t/t		1,6	1,7
798	1	Multiplication of Na2O and L/S ratio			12,1	10,6
799	1	Total Mud Flow	m^3/h		375,3	367,7
800	1	Total Mud L/S ratio		2,63	2,2	2,2
801	1	Total Mud Liquor Na2Oo	g/L	5,07	5,6	4,86
802	1	Total Mud Liquor Al2O3	g/L	3,66	4,3	3,8
803	0	Total Mud Hydrate Water	%	7,07		
804	1	Total Mud Al2O3	%	15,76	15,9	15,8
805	1	Total Mud FE2O3	%	42,56	41,5	41,4
806	1	Total Mud SiO2	%	12,49	11,9	11,9
807	0	Total Mud TiO2	%	4,36		
808	1	Total Mud CaO	%	8,20	7,5	7,7
809	0	Total Mud MgO	%	1,07		
810	1	Total Mud ENa2O	%	4,59	4,5	4,4
811	0	Total Mud K2O	%	0,38		
812	0	Total Mud MnO	%	0,61		
813	1	Average Rain Fall	m^3/h		31,2	8,5
814	1	Average SNL Return	m^3/h	188,89	158,1	180,5
815	1	Average SNL Return Al2O3	g/L	2,77	3,6	3,6
816	1	Average SNL Return Na2Oo	g/L	4,64	4,6	4,6
817	1	Average SNL Return Na2Ok	g/L		2,8	2,8
818	0	**Security Filtration Area 2**				
819	0	*TCA*				
820	1	Lime Flow	m^3/h		6,4	6,4
821	1	TCA Flow	m^3/h		21,7	24,1
822	1	TCA Solids	g/L	48,16	48,2	48,2
823	1	TCA Temperature	C	114,10	105,0	132,1
824	1	TCA Steam	t/h	2,95	0,2	1,274
825	1	TCA Liquor	m^3/h		15,5	17,6
826	0	*MVG*				
827	1	Number Filters On		0,62	1,0	2,0
828	1	Specific Filtration			1,1	1,1
829	1	Feed Flow	m^3/h	127,57	120,8	123,9
830	0	*LVAG*				
831	1	Number Filters On		2,31	1,0	0,0
832	1	Specific Filtration			1,3	1,3
833	1	Feed Flow	m^3/h	130,69	139,8	161,9
834	0	*Diastar*				

Figure 3. Report with results of model adjustment.

3. Model Features

Steady state mathematical models of refineries allow solving of six types of problems:

- Sensitivity studies with focus on strength of relationship between selected control parameter and other process indicators;
- "What-If" analyses to play scenarios involving multiple technology changes;
- Business planning for calculation of production indicators, unit costs of raw materials and energy for the next reporting periods;

- Evaluation of capital investment effectiveness for expansion projects and equipment modernization, for debugging of technologies, for production of new products, for research and development projects;
- Staff training on calculated examples, which help site personal to understand better and deeper how their work reflects in the performance of other sites and the efficiency of the enterprise as a whole;
- Production optimization.

The solutions for global refinery optimization is one of the priority directions for further work. This is expected to involve the use of SysCAD together with algorithms to search for optimum in various metrics. This automated method will make possible a rapid search of global optima in alumina productivity and cost, taking into account all limitations inherent in the refinery processes, equipment capabilities, environmental standards, etc.

4. Organizational Structure

The delivery of mathematical model development was accompanied by the creation of process modeling groups at each refinery. The Refinery groups consist of the most trained and experienced technologists. Their supplementary training in the methods of modeling and calculation of technological processes was organized (Fig. 4). One of the software developers was invited and university professors were involved in training. Refinery employees acquired their first experience of work in their new position during the creation of refinery models, providing developers with active help in collecting initial data, clarifying the features of process parameter regulation, organizing laboratory work and testing models.

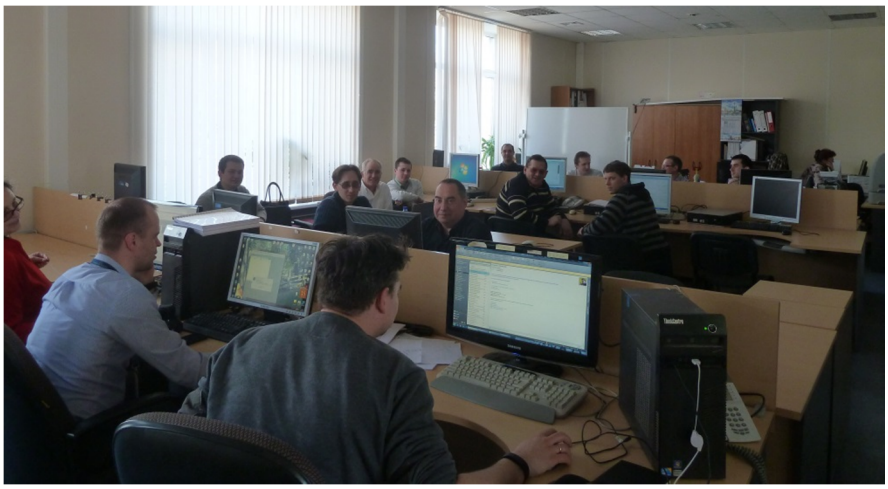


Figure 4. SysCAD Training in St. Petersburg.

The structure of the RUSAL team which supports the development of alumina refinery process models in SysCAD and performs calculations includes a central development team at the St. Petersburg Engineering and Technology Center, and process modeling groups at the refineries. The total staff of these teams today is 15 people, who are engaged in mathematical modeling in SysCAD on a daily basis.

Among tasks that were most often solved using SysCAD, are the following:

- studies of sensitivity to changes in the concentration of spent liquor and concentration of aluminate liquor;
- distribution of spent liquor and optimal concentration regime for a group of evaporation trains;

- calculation of the best pressure profile for flash train of digestion lines;
- playing scenarios for saving soda;
- reduction in water consumption;
- study of options for recycling secondary steam.

Model calculations are often performed within the framework of business planning. This type of calculations is used to study the implementation efficiency for a group of changes simultaneously. As a rule, the total effect of several measures is not additive, and sometimes it turns out to be the opposite of that expected. In this way, technological specialists at RUSAL are now achieving the optimum efficiency of alumina refineries with the support of their experience and modeling activities.

5. Conclusions

At their Engineering and Technology Center, RUSAL creates detailed models using SysCAD and our own software solutions and applies them to a wide range of scientific and engineering problems, including solutions for alumina production by the hydrochloric acid process, solving environmental problems, and for example, the development of a method for utilization of spent refractory from aluminum electrolysis. Separate processes and equipment that require special attention are optimized by computational fluid dynamics.

Further efforts to develop detailed process and technology models will focus on improving their quality and ease of use. Creation of dynamic models for individual areas and units, optimization calculations and the use of mathematical models in refinery control systems loops are also areas of priority for further development.

The utilization of dynamic models for individual areas and units provide additional opportunities to alumina refineries. Dynamic models can be used for optimal control of both ultrafast and slow-flowing processes. For example, using a detailed dynamic model, it is possible to accurately predict the particle size of hydrate and productivity of the precipitation area with a horizon of up to 3 months, and approximately estimate the long-term consequences of the actions taken with the horizon up to 12 months [4, 5]. In a series of predictions, various scenarios for adjusting seed ratio, temperature regime, concentration of aluminate liquor, and holding time can be considered, and then the results used to define the operational actions to undertake regulation the process. Dynamic models can be used to train operators, configure control systems, including pre-tuning and real-time tuning of advanced process control systems [6-8].

Today, the possibilities of using detailed models at alumina refineries is quite wide and the scope of their application will expand. This is because mathematical modeling is a source of a deep understanding of process fundamentals, and a tool for objective analysis of their efficiency.

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