Process simulation in VM-CBA alumina refinery

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Abstract

Modelling of chemical processes has been developed since the seventeenth century with several authors expressing mathematical relationships between system properties. More recently, with the development of modern computational capabilities and by applying process models in numerical simulations, it has been possible to make predictions and evaluate ideas prior to making any modifications in the operation. Along with these advancements it was possible to control and optimize processes, to evaluate process improvement projects and also to train operators. The current work presents process modelling development and results of process simulation in Votorantim Metais - Companhia Brasileira de Alumínio (VM-CBA) refinery. Optimisation studies were conducted in the desilication, digestion and precipitation areas, as well as for future project opportunities such as the conversion of dual stream to single stream digestion.

Keywords: Process simulation; process modelling; numerical modelling; computational programming.

1. Introduction

Companhia Brasileira de Alumínio (CBA), of the Votorantim Group, is located in Alumínio, 74 km from São Paulo city. It is the largest integrated aluminium plant in the world. CBA started to operate in 1955 and today produces 0.475 Mt of primary aluminium.

The Bayer process can be divided into two parts, commonly referred to as the red side and white side. To briefly summarize, on the red side alumina minerals such as boehmite, diaspore ($Al_2O_3.H_20$) or gibbsite (alumina trihydrate $Al_2O_3.3H_2O$), are dissolved in a caustic solution at temperatures between 100 and 300 °C, and bauxite residue is separated from pregnant liquor. On the white side, alumina trihydrate is precipitated from pregnant liquor and afterwards the removal of structural water from this hydrate is effected in the next major process step of the Bayer Process, calcination, generating the product we call alumina (Al_2O_3).

To assist process control and the optimization and the predictability of process variables, tools and procedures were developed to monitor all areas of the plant, many of them using spreadsheets, often of great complexity. This existent modeling presents the plant operation and shows how distant from ideality it is. On the other hand, it is rarely reliably predictive.

Aiming for better predictability and flexibility, CBA teams are now utilizing Kenwalt's software SysCAD, to develop improved process simulations.

2. Developments

2.1. Pre-desilication and digestion

Pre-desilication and Digestion are both areas in an alumina refinery where significant reactions and complex energy exchanges take place. Firstly, the bauxite slurry from grinding is heated in contact heaters with flashed steam from the flash tanks of digestion area. This heated slurry then flows to a desilication tank (14C) and then to the paste heater batteries, which are heated with reflashed live steam from digestion area. Afterwards, the slurry goes to other desilication tanks (14A and 14B) with the some recycle flow to tank 14C. Then, the slurry flow follows to 3 digestion units.

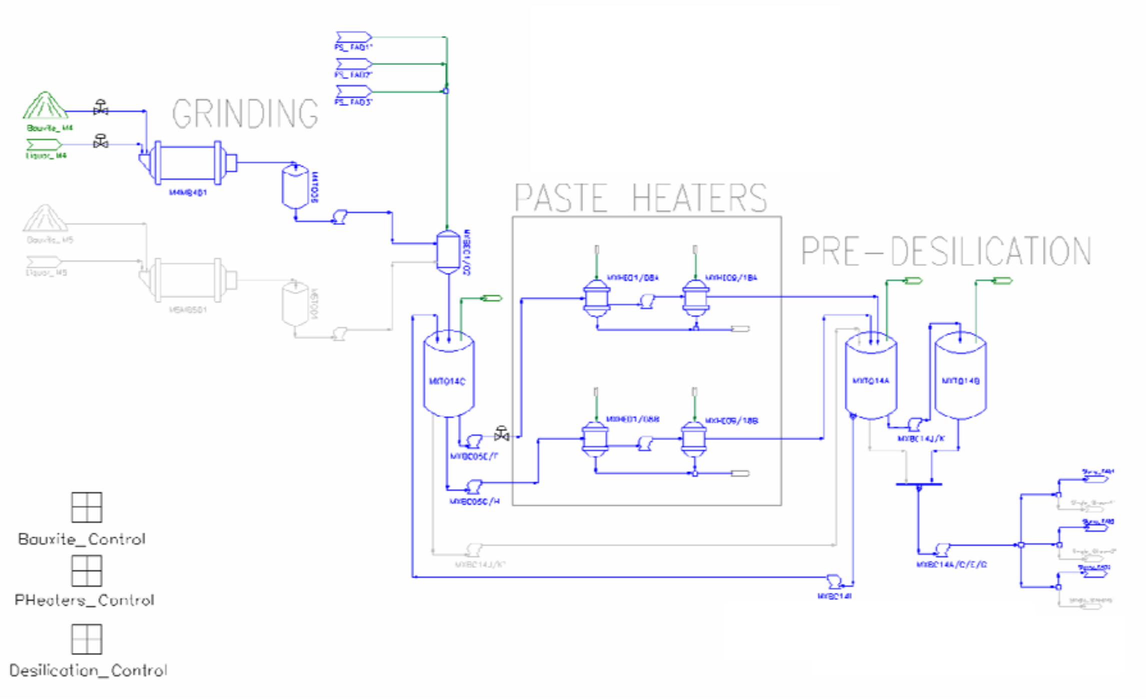
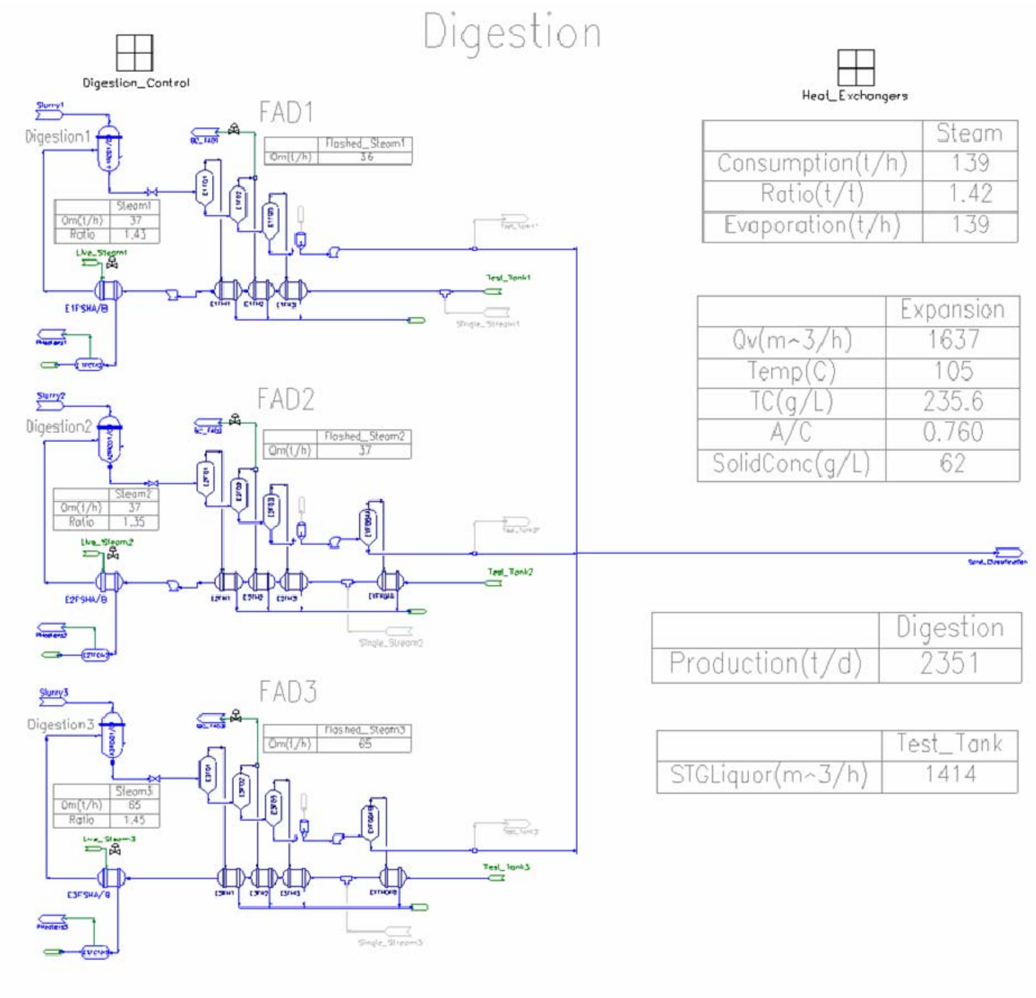


Figure 1. CBA’s grinding, paste heaters and pre-deslication systems on SysCAD interface.

Digestion units include autoclaves that receive the bauxite slurry and the heated caustic liquor. This equipment setup promotes the ore’s alumina trihydrate ($Al_2O_3.3H_2O$) dissolution under elevated pressure and temperature. The digested slurry from the autoclaves then flows to flash tanks in which the temperature is reduced to avoid boiling in the atmospheric decanters, the next step of process. The flashed steam is sent to recuperative heaters, where the strong liquor from the test tanks is heated. After recuperative heating, the strong liquor flows to live steam heaters and soon after to the autoclaves. The live steam flow to the live steam heaters is controlled according to the autoclaves’ set point temperature (close to 144 °C). The live steam condensate is reflashed in pot tanks and its steam is sent to the desilication contact heaters. The excess steam from second flash tank in each digestion unit is sent to the paste heaters, forming a complex energy exchange system.



	Flashed_Steam1
Qm(t/h)	36

	Steam1
Qm(t/h)	37
Ratio	1.43

	Flashed_Steam2
Qm(t/h)	37

	Steam2
Qm(t/h)	37
Ratio	1.35

	Flashed_Steam3
Qm(t/h)	65

	Steam3
Qm(t/h)	65
Ratio	1.45

	Steam
Consumption(t/h)	139
Ratio(t/t)	1.42
Evaporation(t/h)	139

	Expansion
Qv(m~3/h)	1637
Temp(C)	105
TC(g/L)	235.6
A/C	0.760
SolidConc(g/L)	62

	Digestion
Production(t/d)	2351

	Test_Tank
STGLiquor(m~3/h)	1414

Figure 2. CBA's Digestion system on SysCAD interface.

Simulation of this area provides important information and insights to process, operation and maintenance teams:

1. Heaters energy transfer performance and cleaning cycle residual life
2. Reaction performances and energy loss in desilication tanks and autoclaves
3. Evaluation of digestion productivity and production

2.2. Precipitation

The cooled pregnant liquor from the Heat Interchange Departments (HIDs, the stage responsible for cooling the liquor from the red side), flows to the first precipitation tanks, where agglomeration occurs after adding fine seed. After this stage, the liquor and its agglomerated solids flow to the precipitation growth stage, via the Interstage Coolers (ISC). These coolers consist of flash tanks, barometric columns and cooling towers. The growth tanks receive coarse seed from the classification area. The resulting suspension flows through the precipitation chain to the last growth tanks and later to the hydrocyclone classification system.

The first hydrocyclone batteries separate the final product from seed which, in turn, are separated between fine and coarse seed by new hydrocyclone batteries. Both product and seed are filtrated to recover liquor; the product is then sent to calcination, the fine seed to the agglomeration tanks and the coarse seed to the growth tanks.

2.2.1. Agglomeration

a. Principles

The product size (% -45 µm), product strength and product occluded soda are largely controlled during agglomeration. In this stage, it is very important that the fine particles are gathered in bigger clusters, and that these clusters are cemented into strong agglomerates. Moreover, the generation of fine particles by nucleation is not desirable.

b. Control philosophy

In the hydrate precipitation circuit, due to the dynamics of process conditions, the product particle size varies and consequently, so do the fine and coarse seed introduced in the process. As a consequence, the precipitation process cycles with fining or coarsening of the hydrate particles.

When the precipitation circuit has a tendency towards fining, the following decision is taken, either separately or altogether:

1. Reducing the fine seed charge.
2. Increasing the temperature in agglomeration.
3. Increasing residence time.
4. Increasing A/C ratio in the beginning of agglomeration.

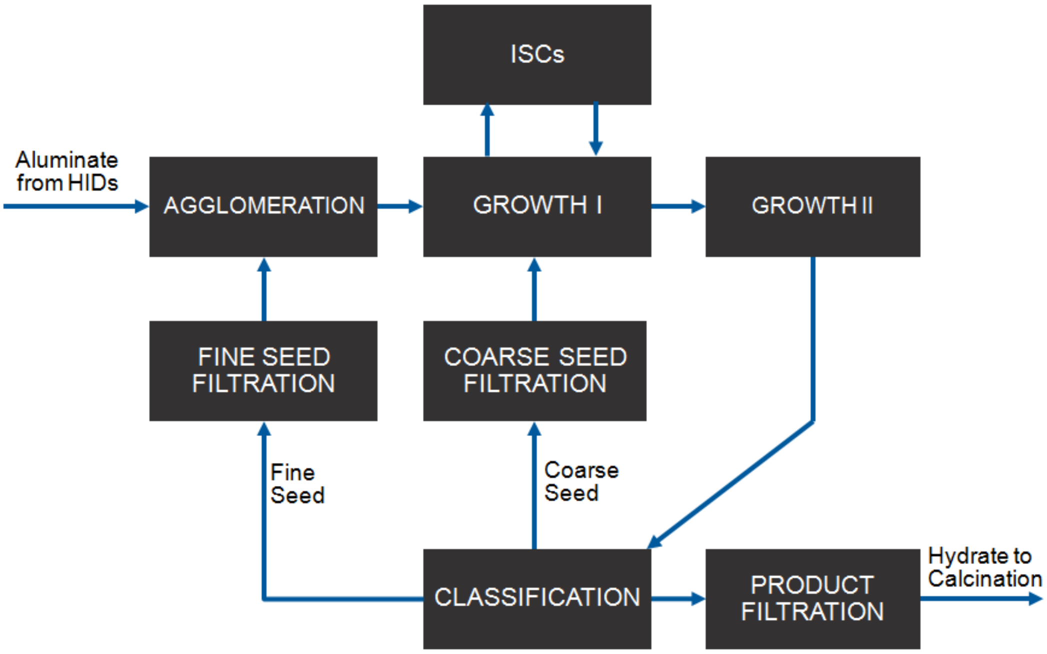


Figure 3. Block diagram for CBA’s precipitation and classification system.

The first option is more immediate and the others may require longer planning. The coarsening control is done by the exact opposite measures.

CBA's classification system has three by-passes which allow the transfer of precipitation product straight to seed classification (1); to the seed cyclones overflow tank (2); or to the seed cyclones underflow tank (3), as seen in the figure below:

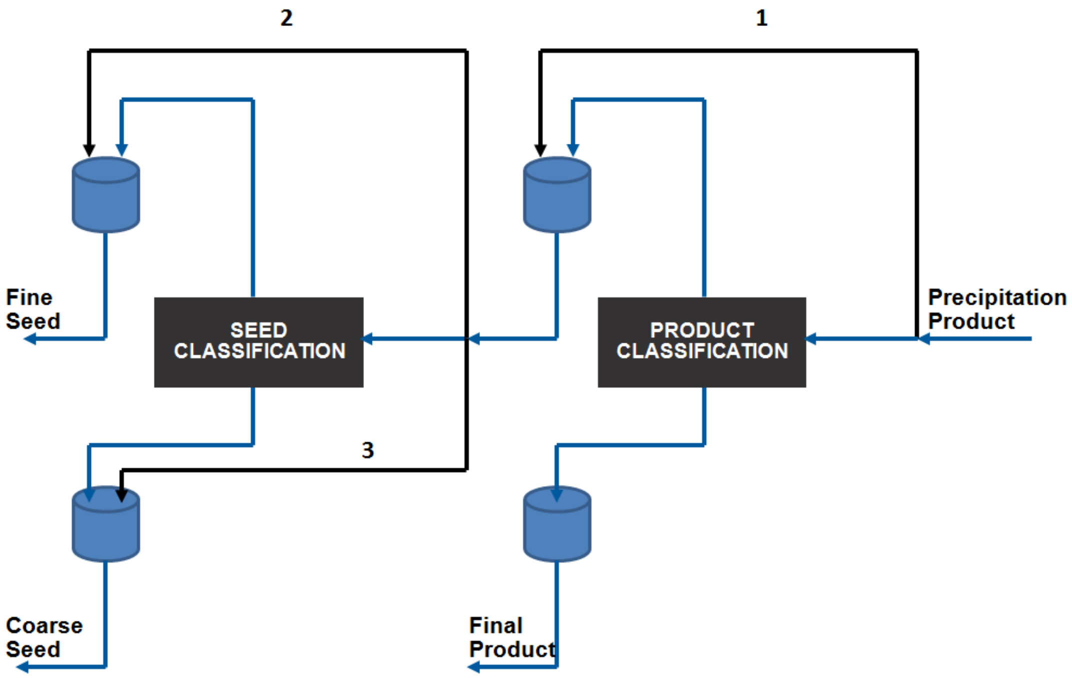


Figure 4. CBA's hydrate classification schematic diagram.

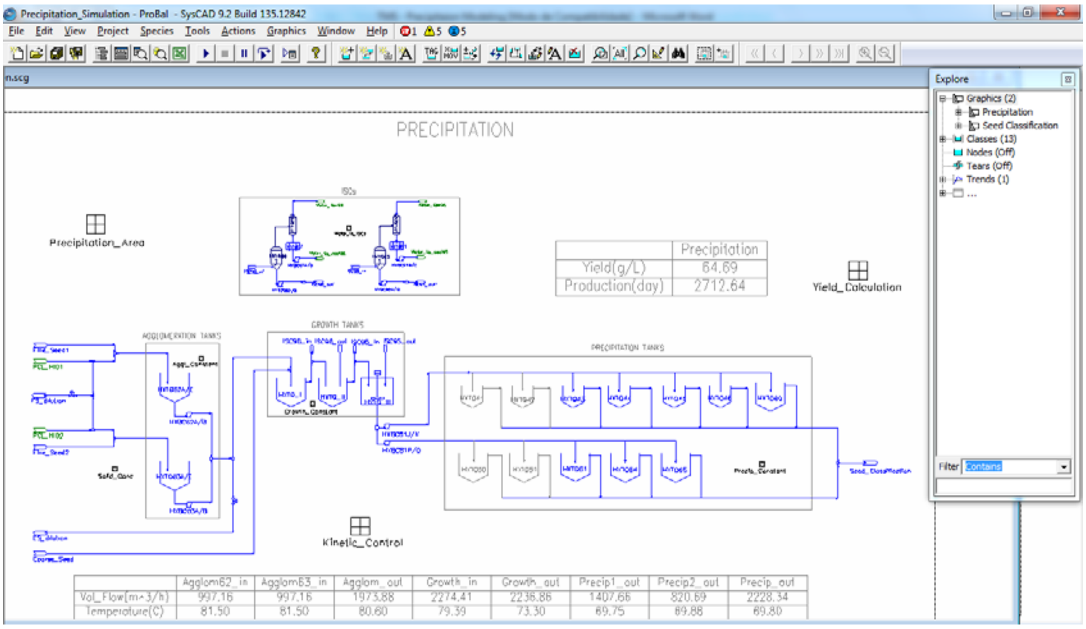
2.2.2. Growth

a. Principles

During Growth, the main objective is to maximize yield. The linear growth of crystal by means of hydrate deposition occurs, favored by relatively lower temperatures in comparison with agglomeration.

b. Control philosophy

At CBA's refinery, the temperature decrease is assisted by ISCs, which generate new fine crystals by nucleation.



	Precipitation
Yield(g/L)	64.69
Production(day)	2712.64

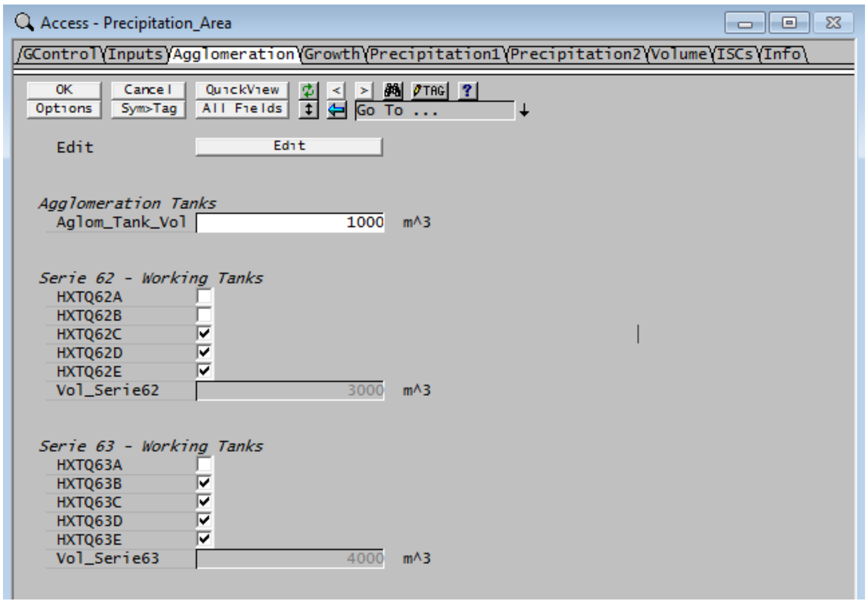
	Agglom62_in	Agglom63_in	Agglom_out	Growth_in	Growth_out	Precip1_out	Precip2_out	Precip_out
Vol_Flow(m^3/h)	997.16	997.16	1973.88	2274.41	2236.86	1407.66	820.69	2228.34
Temperature(C)	81.50	81.50	80.60	79.39	73.30	69.75	69.88	69.80

Figure 5. CBA’s precipitation system on SysCAD interface.

2.2.3. Input data system

CBA’s precipitation chain is divided into an agglomeration tank series of 1000 m^3, a growth series with tanks of 3300 and 4400 m^3, and growth series tanks at the end of chain of 470 and 1000 m^3, totaling 75 tanks. It also includes the cooling system for the growth tanks, the ISCs (Interstage Cooling).

The model was created as simple as possible, considering the dynamic plant routine of inserting and removing tanks and changing ISCs position between growth tanks. A system was programmed that inserts or removes tanks by selecting checkboxes and choosing ISC positions.



Edit

Agglomeration Tanks
Aglom_Tank_Vol 1000 m^3

Serie 62 - Working Tanks
HXTQ62A ☐
HXTQ62B ☐
HXTQ62C ☑
HXTQ62D ☑
HXTQ62E ☑
Vol_Serie62 3000 m^3

Serie 63 - Working Tanks
HXTQ63A ☐
HXTQ63B ☑
HXTQ63C ☑
HXTQ63D ☑
HXTQ63E ☑
Vol_Serie63 4000 m^3

Figure 6. Insert/remove tank system on SysCAD interface.

The data input to calibrate the modeling is done by transferring historical plant data from a spreadsheet. Selected pregnant liquor, fine and coarse seed and spent liquor process variables are sent to software instantaneously.

2.2.4. Kinetic reaction calibration system

The alumina tri-hydrate precipitation reaction, as well as other reactions, is influenced by countless factors. It is presented as follows:

$$2NaAlO_2\,(aq) + 4H_2O\,(l) \rightarrow Al_2O_3.3H_2O\,(s) + 2NaOH\,(aq)$$

The hydrate precipitation driving force (supersaturation), chemically represented by the difference between the alumina concentration in the liquor (a) and alumina concentration at equilibrium (a*), is strongly influenced by the liquor caustic concentration. Precipitation kinetics can be expressed by linear growth rate (G) of hydrate crystals:

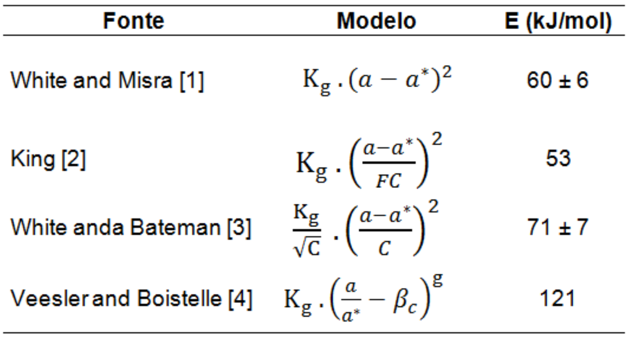
$$G = dL/dt = K_{g\,.}\, f(S) \qquad (1)$$

Where, L is the characteristic crystal length, K_g is the growth constant and S is the supersaturation. The growth constant is influenced by temperature (T) according with Arrhenius equation:

$$K_g = k.\exp(-E/RT) \qquad (2)$$

Where, E is the activation reaction energy of precipitation. Numerous modeling correlations were already published:

Table 1. Kinetic models of hydrate precipitation.



Fonte	Modelo	E (kJ/mol)
White and Misra [1]	$\mathrm{K_g} \,.\, (a - a^*)^2$	60 ± 6
King [2]	$\mathrm{K_g} \,.\, \left(\frac{a-a^*}{FC}\right)^2$	53
White anda Bateman [3]	$\frac{\mathrm{K_g}}{\sqrt{\mathrm{C}}} \,.\, \left(\frac{a-a^*}{C}\right)^2$	71 ± 7
Veesler and Boistelle [4]	$\mathrm{K_g} \,.\, \left(\frac{a}{a^*} - \beta_c\right)^{\mathrm{g}}$	121

SysCAD has precipitation kinetic models available for precipitation unit simulation.

2.2.4.1. Calibration principle

A value of activation energy (E) has to be adopted, then controllers find values for the growth constant and for the ambient losses, respecting in the final tank conditions, A/C ratio and temperatures presented in plant data. To calibrate the model developed, real plant data taken in stable periods of operation is utilized.

2.2.4. Results

The mathematical simulation achieves great results in relation to calibration with plant data in stable periods. It is possible to compare precipitation production and yield in these two situations:

Table 2. Comparison between calibration and simulation.

	Production (t/day)			Yield (g/L)		
Period	**Calibration**	**Simulation**	**Difference**	**Calibration**	**Simulation**	**Difference**
1	2713	2690	-1 %	64,7	64,2	-1 %
2	2035	2135	5 %	60,1	62,8	4 %
3	2494	2596	4 %	69,5	72,1	4 %
4	2297	2412	5 %	66,3	69,4	5 %
5	2529	2702	7 %	68,0	72,4	6 %
6	2398	2384	-1 %	65,8	65,4	-1 %
7	2129	2255	6 %	59,3	62,6	5 %
8	2657	2822	6 %	67,6	71,7	6 %

The observed difference between simulation and calibration, both for production and yield, is fairly low, with values of 5 % on average.

3. Conclusions and Perspectives

Process simulation is a tool of great importance for refinery operation, being useful to perform mass and energy balances, predict process behavior, calculate equipment sizing and train control room operators. It is also essential in projects for increasing plant capacity or to implement new technologies, supporting the estimation of the benefits to the company.

Some examples of project simulation in VM-CBA:

1. Single Stream Digestion: estimate the steam savings and predict digestion heater performance due to the addition of bauxite slurry prior to the recuperative heaters.

2. Filter Press: estimate caustic liquor recovery, energy and mass balances after adding press filters for the de-liquoring of bauxite residue.

3. Decanter Centrifuge: estimate the alumina recovery by adding a decanter centrifuge receiving the thickener underflow and sending it to the first washer.

The development of modelling for process simulation at CBA has been extremely satisfactory, with differences between simulation and model calibration data of 5 % on average. It is expected that process simulation will become an increasingly effective tool in the refinery.

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