# Simulation of chemical and hydrometallurgical processes

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## 1. INTRODUCTION

The use of computer simulation, is now a basic tool for process design and optimization, as evidenced by its increasing use of practicing engineers through commercially available simulator software products. Engineers, in charge of designing equipment for the hydrometallurgical plants have to be able to select the most suitable equipment for each application and to predict the performances under different process conditions. With the increasing capacity of microcomputers, the software companies would like to provide computer tools for plant operators to obtain the best results from the equipment and process. In order to allow the process engineers to concentrate on their task, the simulation software has to offer a user-friendly interface combined with quick and accurate calculations.

Most of the available software tools in this field were developed in the eighties offering a reliable calculation package with the overhead of a text-based user interface. Creating customized unit models was rather difficult or even impossible. The database management system usually was integrated with the simulator, making difficult to update and extend the database files. Data sharing between a group of users was not possible.

In order to overcome these problems a new simulator is under development, which offers a fully graphical user-interface, open database connectivity and application oriented unit model library. The purpose of the developed software is to integrate the already existent calculation algorithms, database files and process unit models into a completely new user-friendly and open-architecture system. The above mentioned knowledge exists in universities and companies under different representation forms. In the field of hydrometallurgy the simulation facilities offered by the available commercial software products are very limited and the unit models usually are fixed. Our aim is to implement specific unit models and to adapt them to the research and/or industrial application in study. However, the simulator has to contain a set of basic unit models and convergent overall calculation routines as well.

## 2. MAIN MODULES OF THE SIMULATOR

The process engineer has to be able to represent the material flow including chemical and physical properties and operation units with their important parameters as well. The most important feature of this software is to gather all the following proprieties:

- graphical user interface
- specific unit models for hydrometallurgical applications
- chemical database with open connectivity
- dynamic simulation
- steady-state material-balance calculations
- model development possibilities

The software is written in C++, using the object-oriented methodology proposed by Rumbaugh (1991). It is divided into five modules: graphical flowsheet editor, unit library, chemical database, simulation and help modules, as presented in Figure 1.

The *graphical flowsheet editor* module is supplying all the graphical functionality. Generic classes are created for operational units, connection streams and text labels in order to provide the graphical functionality. Specific unit models are derived from the generic ones. The representation of the circulating mass is implemented using *streams*.

The *unit library* is a collection of unit models, which incorporates data structures, parameter dialog boxes and calculation routines. For steady state material balance calculation the sequential modular flowsheet solving strategy is used, thus for every unit all the natural specifications has to be given, as suggested by Reklaitis (1983). The operation units are described by I/O models, one for dynamic simulation and the second for steady-state material and energy balancing. The measure of progress for undergoing chemical reactions can be given by the means of steady state reactant conversion, key component specifications or exponential rate functions.

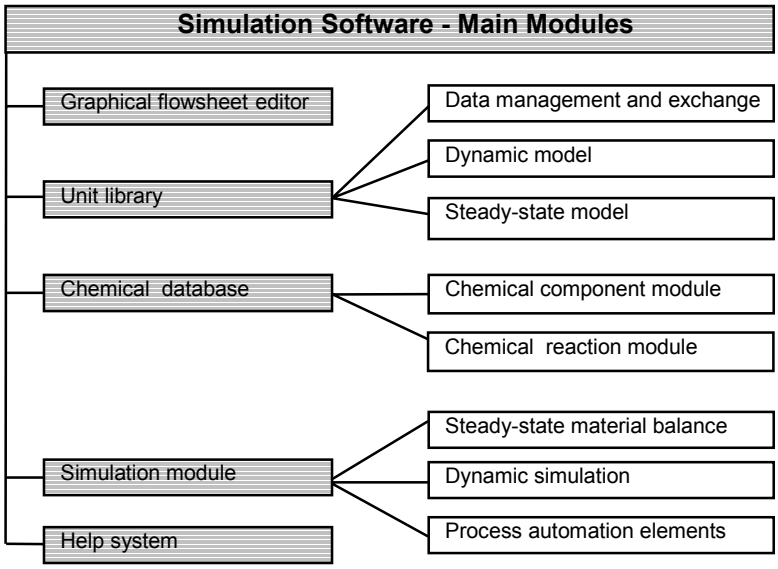


*Figure 1*. Main modules of the simulator

The *database* can be implemented using any relational database management system with a proper 32-bit ODBC driver, which is used to connect it with the simulator. The database file can be shared among several users in the same LAN (Local Area Network), and managed also from a database management system independent from the simulation software. At run-time, the chemical properties are retrieved directly from the database. An important additional feature is that reaction stoichiometry can be saved in the database. In this way the user will have available a large collection of chemical reactions, with the possibility to add new items or modify the existing ones.

The *simulation module* takes care of the material and information flow through the whole flowsheet. In steady state the sequential modular strategy is used. Applying the mixer-labeling algorithm presented by Reklaitis (1983) and the bounded Wegstein convergence promotion method described by Westerberg (1979) the computation time is reduced considerably. The calculation routine is implemented as an independent thread, running in parallel with the user interface thread. The dynamic simulation routine is updating the outflow of all the units within the flowsheet based on the content of their input streams, current time and integration step size. The content of the streams can be represented versus time or replication number. The final content can be displayed in separate lists for steady state and dynamic calculation modes. Measurement and initialization compositions can be specified as well.

The *help system* provides the user with information and assists among the simulation work.

## 3. CASE STUDIES

The structure of the software will be presented and evaluated among two examples. The steady state material balance calculation capabilities will be illustrated on a textbook example, while the dynamic simulation will be presented through a copper heap leaching case study.

### 3.1. Nitric acid production

This nitric acid production process is reported by Reklaitis (1983) as a basic example for material balance calculations in process flowsheets. The flowsheet contains four reactors, one with multiple reactions, recycle streams, multiple inflow and outflow streams. The calculated values are compared with the results obtained by using a commercial available simulation software product with good reputation, namely PRO II (trademark of SIMSCI). The steady state reaction handling is based on the conversion percentage for selected reactants, a value that has to be specified for every chemical reaction. This algorithm is sensible to the sequence in which the reactions are defined.

Oxidizing ammonia with air and absorbing HNO3 in water can produce nitric acid. The simplified simulation flowsheet incorporates also the ammonia production part, which consists of three basic units: synthesis gas production, gas clean up and the ammonia synthesis, as presented in Figure 2. The resulting ammonia becomes the feed to the oxidation unit (Reactor 1) and then to the absorber (Reactor 1). The residual gases from the absorber are split and part is purged while the remainder is sent to the reformer (Reactor 2). The final product is obtained at the output stream 1.

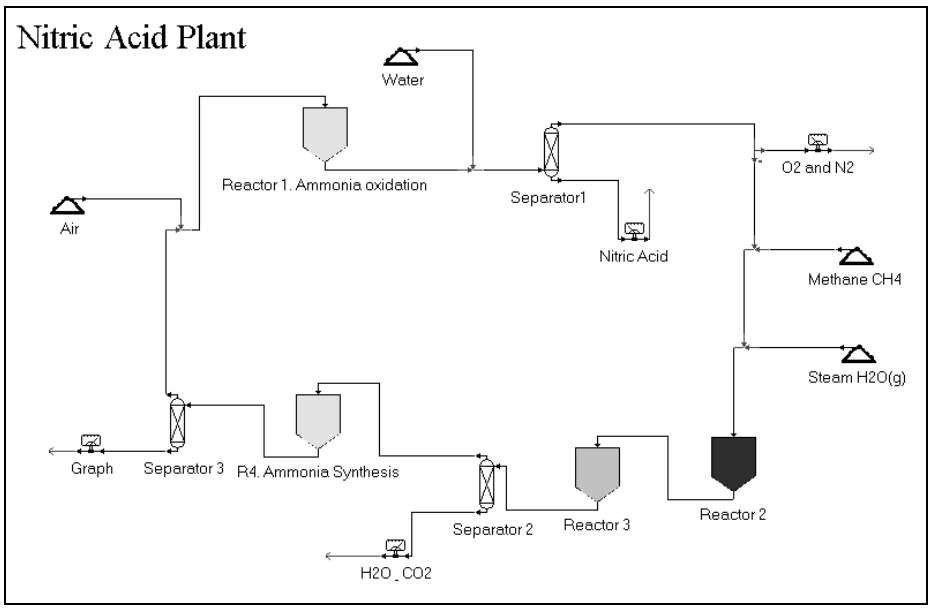


*Figure 2*. Flowsheet of the nitric acid production process

Steady state material balance is calculated with the developed software and compared with the results obtained by simulating the same flowsheet using a commercial software package, as listed in appendix 1. The undergoing chemical reactions and important unit parameters are listed in tables 1 and 2 while the process specifications are given in table 3. The convergence of the calculations is illustrated in Figure 3, where the calculated HNO3 flowrate is represented in function of the replication steps. The computation time was under 3 seconds using a normal desktop personal computer.

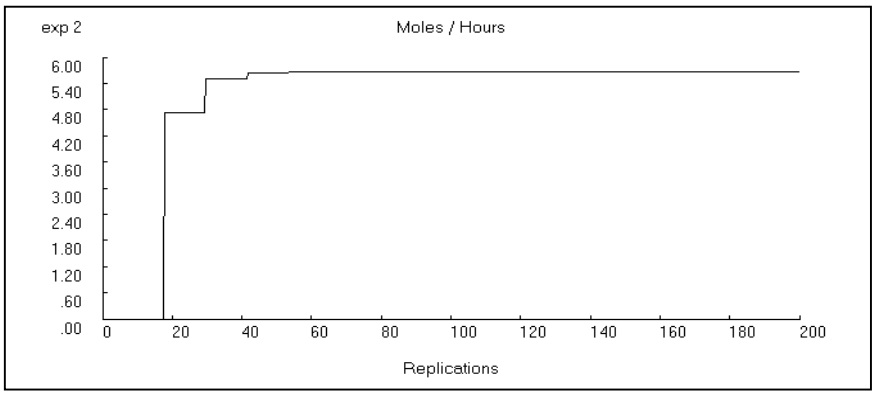


*Figure 3*. HNO3 content of Output 1 [kg moles/hour]

*Table 1.* Considered chemical reactions and conversion percentages

| Reactor | | Chemical reactions | Base reactant | Conversion % |
|---|---|---|---|---|
| 1 | 1 | NH3(g) + 2O2(g) -> HNO3(g) + H2O(g) | NH3(g) | 100 |
| 2 | 1 | CH4(g) + 0.5O2(g) -> CO(g) + 2H2(g) | O2(g) | 70 |
| | 2 | CH4(g)+O2(g) -> CO2(g) + 2H2(g) | O2(g) | 100 |
| | 3 | CH4(g) + H2O(g) -> CO(g) + 3H2(g) | CH4(g) | 100 |
| 3 | 1 | CO(g) + H2O(g) -> CO2(g) + H2(g) | CO(g) | 100 |
| 4 | 1 | N2(g) + 3H2(g) -> 2NH3(g) | H2(g) | 90 |

*Table 2.* Separators

| Separator 1 (top stream) | | Separator 2 (top stream) | | Separator 3 (top stream) | |
|---|---|---|---|---|---|
| H2O(g) + (aq) | 100 % | H2O(g) + (aq) | 100 % | H2(g) | 100 % |
| HNO3(g) | 100 % | CO2(g) | 100 % | N2(g) | 100 % |

*Table 3.* Process specifications

| Stream | Compound | Mole fraction % |
|---|---|---|
| Nitric Acid | HNO3(aq) | 30 |
| | H2O(aq) | 70 |
| Reactor 4 inlet | N2(g) | 25 |
| | H2(g) | 75 |
| Purge | N2(g) | 99 |
| | O2(g) | 1 |

## 3.2. Copper production based on heap leaching

The dynamic simulation capabilities are illustrated on a copper heap leaching process, where the most essential part of the research work is connected with the process dynamics.

Leaching is a process conducted with a solution in which there is a solubility of the dissolving minerals or compounds in the material being leached sufficient to obtain an acceptable concentration of valuable metals in solution. In case of heap leaching, the crushed and prepared ore is placed in form of heaps on gently sloping flat ground covered with an impervious pad. The heap is sprinkled with an aqueous acidic solution. The contact of the leaching lixiviant with the surface of solid ore particles leads to selective metal dissolution. Naturally the dissolution process is very slow or it does not

happen as reported by Peters (1991). Therefore, bacterial populations are used to catalyze the reactions. In this way, the leaching time is reduced to some month up to two years, depending on the ore composition as written by Acevedo (1995). Air is necessary for biological activity, in this sense the heaps should be enough porous to provide the reactions with oxygen. The network of pipes and channels collect the liquid solution into the storage pond. The PLS (Pregnant Leach Solution) is a solution with the metal content, usually 5-10 gram/liter. From the gathered solution the solvent extraction unit extracts the copper bearing component. At this step the acid from the PLS is recovered and recycled to the raffinate pond, as presented in Figure 4.

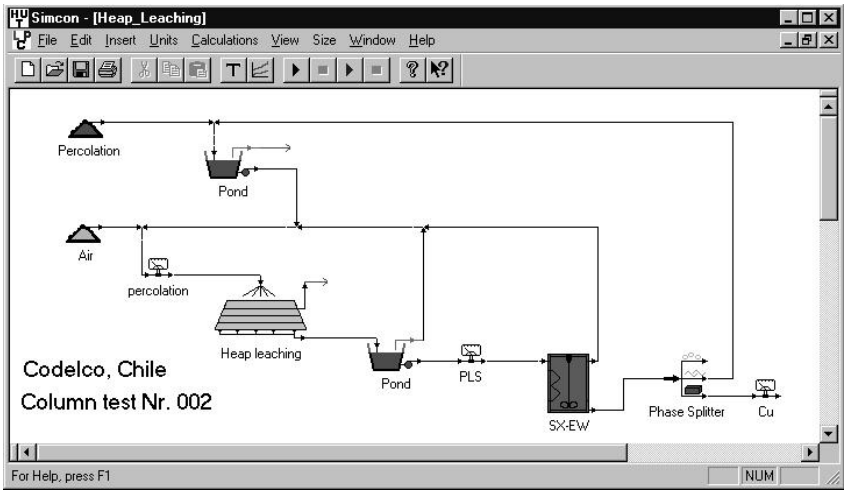


*Figure 4.* Flowchart of copper production based on heap leaching

From the metal bearing component, the desired metal is extracted through electrolysis. At the electrowinning stage the final product is achieved, in form of high purity (98-99,8%) copper cathodes and considerable amount of acid is regenerated and recycled to the raffinate pond. The leaching time usually is three to six months for oxide ores, and ten to twenty months for sulfides. The most important is to predict the expected metal extraction versus time.

*Table 4.* Configuration parameters of the heap-leaching unit

| Configuration values | | | Estimated coefficients | | |
|---|---|---|---|---|---|
| Parameter | Value | Unit | Coefficient | Value | Unit |
| Area | .27 | [$m^2$] | Fast reacting copper (1) | 69.46 | % [mass] |
| Height | 5.28 | [m] | Slowly reacting copper (2) | 30.54% | % [mass] |
| Total mineral | 950 | [kg] | Reaction rate constant 1 | 0.1581 | |
| Copper content | 1.02 | % [mass] | Reaction rate constant 2 | 0.03406 | |
| Acid cure | 13 | [kg/ton] | | | |
| Leaching time | 60 | [days] | | | |
| Temperature | 18 | [Celsius] | | | |
| Channeling | 1 | % [vol] | | | |
| Moisture content | 4 | % [mass] | | | |

The configuration values are based on real experimental data from Codelco, Chile. The column test configuration parameters for this simulation example are listed in the table 4. The ore is a mixture of two types, one fast and one slow reacting component. In the first step, the simulator calculates the amounts of fast and slow reacting copper with their reaction rates based on the column-test extraction

curve. The kinetics of the undergoing main chemical reactions are described by reaction rate laws with the estimated kinetic parameters. The solvent-extraction and electrowinning (SX-EW) are substituted with a simple reactor followed by a phase-splitter unit. Their dynamic modeling is subject of future research projects. This block has assigned as outputs the produced copper cathodes, gaseous Oxygen and the recycled lixiviant.

The composition of the percolation solution and the CuSO4 content of the obtained PLS are presented in Figure 5. The computed total copper extraction curve is very close to the experimental one as compared in Figure 6.

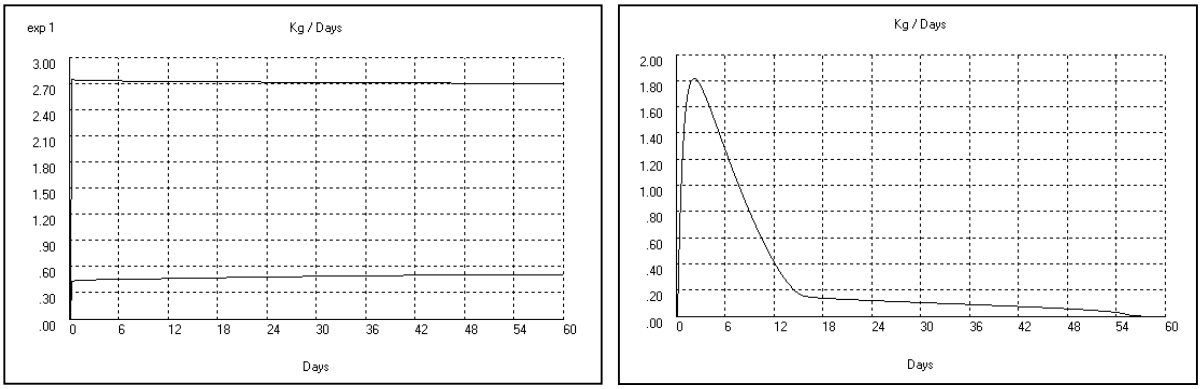


*Figure 5.* Simulated percolation rate and CuSO4 content of the PLS

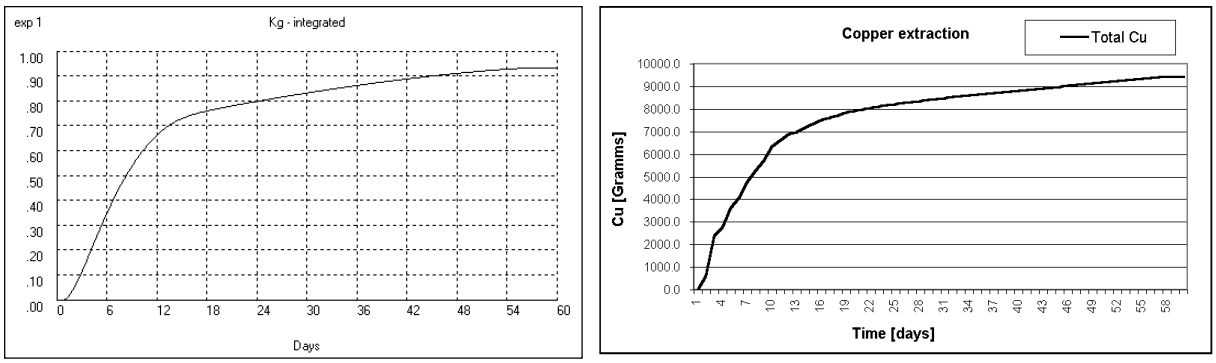


*Figure 6.* Simulated (left) and experimental copper extraction curves

## 4. CONCLUSIONS

The steady state material balance calculation results are very close to the values obtained using a commercial software package with good reputation. Calculation time is minimized considerably, the handling of the chemical reactions is made more easy and the flowsheet building quicker. The reaction stoichiometry can be saved in the database for later use in other flowsheet calculations.

The heap leaching simulation results are very close to the reference data, which let us to conclude that simulation can be used as an efficient tool in hydrometallurgical applications.

Although the incorporated models are relatively simple, the software offers a frame for further development. New models easily can be added to the unit library. Additional process control elements will be added to the simulator in the near future.

## 5. REFERENCES

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*Appendix 1.* Input/output stream compositions

| NITRIC ACID PLANT | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ***Stream*** **Name** ***Description*** | | **Inputs process resume** | | **Reactor 4 inlet stream** | | **Nitric acid output stream** | | **Purge** | | **Reactor 2 outllet stream** | |
| | | **Pro/II** | **Simcon** | **Pro/II** | **Simcon** | **Pro/II** | **Simcon** | **Pro/II** | **Simcon** | **Pro/II** | **Simcon** |
| **Component Molar Rates** | **KG-MOL/HR** | | | | | | | | | | |
| NITROGEN | N2 | 4439.000 | 4439.000 | 310.730 | 310.730 | 0.000 | 0.000 | 4128.270 | 4128.270 | 310.730 | 310.730 |
| HYDROGEN | H2 | 0.000 | 0.000 | 950.481 | 950.481 | 0.000 | 0.000 | 0.000 | 0.000 | 712.308 | 712.309 |
| WATER | H2O | 1417.000 | 1417.000 | 0.000 | 0.000 | 1320.288 | 1320.288 | 0.000 | 0.000 | 482.692 | 482.691 |
| NITRIC ACID | HNO3 | 0.000 | 0.000 | 0.000 | 0.000 | 570.288 | 570.288 | 0.000 | 0.000 | 0.000 | 0.000 |
| AMMONIA | NH3 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| OXYGEN | O2 | 1180.000 | 1180.000 | 0.000 | 0.000 | 0.000 | 0.000 | 36.665 | 36.663 | 0.000 | 0.000 |
| METHANE | METHANE | 239.000 | 239.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| CARBON DIOXIDE | CO2 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.828 | 0.828 |
| CARBON MONOXIDE | CO | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 238.172 | 238.172 |
| **Total** | **KG-MOL/HR** | **7275.000** | **7275.000** | **1261.211** | **1261.211** | **1890.575** | **1890.576** | **4164.935** | **4164.933** | **1744.730** | **1744.730** |
| **Component Mole Fractions** | | | | | | | | | | | |
| NITROGEN | N2 | 61.02% | 61.02% | 24.64% | 24.64% | 0.00% | 0.00% | 99.12% | 99.12% | 17.81% | 17.81% |
| HYDROGEN | H2 | 0.00% | 0.00% | 75.36% | 75.36% | 0.00% | 0.00% | 0.00% | 0.00% | 40.83% | 40.83% |
| WATER | H2O | 19.48% | 19.48% | 0.00% | 0.00% | 69.84% | 69.84% | 0.00% | 0.00% | 27.67% | 27.67% |
| NITRIC ACID | HNO3 | 0.00% | 0.00% | 0.00% | 0.00% | 30.16% | 30.16% | 0.00% | 0.00% | 0.00% | 0.00% |
| AMMONIA | NH3 | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% |
| OXYGEN | O2 | 16.22% | 16.22% | 0.00% | 0.00% | 0.00% | 0.00% | 0.88% | 0.88% | 0.00% | 0.00% |
| METHANE | METHANE | 3.29% | 3.29% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% |
| CARBON DIOXIDE | CO2 | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.05% | 0.05% |
| CARBON MONOXIDE | CO | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 13.65% | 13.65% |