Application of Process Simulation Software METSIM in Metallurgy

Zhao Qiuyue*, Zhang Tingan, Lv Guozhi, Zhu Xiaofeng, Liuyan
Key Laboratory of Ecological Utilization of Multi-metal Intergrown Ores of Ministry of Education, School of Materials and Metallurgy, Northeastern University
3-11 Wenhua Rd, Heping District
Shenyang, 110004, China, T: 86-24-83686283, F: 86-24-23906316
*corresponding author, e-mail: zhaoqy@smm.neu.edu.cn*, zhangta@smm.neu.edu.cn, lvgz@smm.neu.edu.cn, zhuxiaofeng@163.com

Abstract

Now the using of process simulation software is more and more widely in many fields especially in chemistry and metallurgy plant designing. The process simulation software provides great convenience for experts and engineers, they can analysis the new process and calculate the heating/material balance by process simulation software, and calculate complex process that the traditional tool EXCEL can not do. The paper introduced the current major process simulation software, includes mainly introducing the application of METSIM and SYSCAD software in metallurgical process, and summary the computational process of them by a few examples, at the same time the application status of the process simulation software was pointed out.

Keywords: process, simulation, software, metallurgy

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1. Introduction

Chemical and metallurgical plants design, process design, such as metal and mass balance calculations are both the basis of the entire design work, but also indeed keys to accurate and secure design. Metallurgical calculation is often separated from process design work, and are done under help of excel manual calculations. It is a heavy workload and the work efficiency is very low, at the same time this calculation is not sufficiently sophisticated, especially in face of more complex processes, the demand for raw materials, "three wastes " volume of output are difficult for estimating [1-4].

Process simulation technology computes with the help of the establishment of a mathematical model calculated by unit operations, thermodynamic methods. Process simulation technology can calculate material balance, heat balance, estimate equipment size and energy analysis, and make environmental and economic evaluation. It is the combination of chemical engineering, thermodynamics, systems engineering, computational methods and computer application technology. It is a new technology developed in recent decades. Process simulation technology can achieve device tuning, process analysis and process synthesis, so as to realize production optimization, resource conservation, friendly environment and improving economic efficiency, thus helps process development, engineering design and optimizing operations to provide theoretical guidance [5, 6].

Currently, the wider application of process simulation software is show as below: Aspen Plus [7], Chem CAD [8], Hysys, etc. Most of the software is applied in the petrochemical field. There are some process simulation software application in the field of hydrometallurgy, such as SYSCAD and METSIM. This software can be divided into three categories:
(1) Thermo chemical properties of calculation software, such as HSC, OLI, STABCAL, FACTSAGE;
(2) Mineral process simulation and optimization software, such as JKSimMet, JKSimfloat, USIMPAC, etc;
(3) Process simulation software, such as METSIM, SYSCAD, IDEAS, etc;

The process simulation software METSIM is highlighted in this paper.
The basis for analysis of all chemical and metallurgical processes is the mass and energy balance. Plant design, capital costs, and technical evaluations are all dependent on such calculations. METSIM is a general-purpose process simulation system designed to assist the engineer in performing mass and energy balances of complex processes. METSIM uses an assortment of computational methods to effect an optimum combination of complexity, user time, and computer resources usage. METSIM originated as a metallurgical process simulation program, written to perform mass balances around the major unit operations of complex process flow sheets. Application of the program proved so successful that it was expanded to include detailed heat balances, chemistry, process controls, equipment sizing, cost estimation, and process analysis. The unique nature of the programming language, APL, allows modification and expansion of the system with minimum effort and permits the incorporation of continuing technological innovations in process simulation. Some have described the application of METSIM to an electrolytic zinc plant circuit[9] and a copper flash smelting plant[10].

2. Research Method

The basic calculation philosophy used in METSIM is that the feed streams is taken to a unit operation module and then a mechanical device handled the inputing materials according to a module program and outputs the calculation results. Most unit operation modules mix the feed streams first and then the mechanism is applied to deal with it. The mechanism can be preceded by chemical reactions or a phase change and if the result required is not achieved then the mechanism or chemical reaction can be changed or a control is applied as a feed forward or feedback loop. Because of the structure of the program, it is possible to add chemistry to any unit operation and then add controls to simulate any type of reactor without having a specific reactor model. METSIM performs mass and energy balances for chemical processes using the sequential modular approach. This method is used because of its elegance and to simplify divers and complex flow sheets. METSIM can easily be expanded to encompass new processes and techniques. A major advantage of this approach is that intermediate results may be obtained from any stage of the process in an intelligible form. This attribute of METSIM is invaluable when attempting to detect possible modeling or specification errors. If an output stream parameter is to be controlled, a feedback controller must be added to sample the output and adjust an input stream, a reaction extent or another unit operation parameter to achieve the desired results.

In conformance with the sequential modular approach, METSIM comprises modules containing subsets of equations describing the design specifications and performance characteristics for each process step. The system solves the equation subset for each module, allowing for an individual analysis of each unit operation in the flow-sheet. Given data on design variables and input stream composition, each module calculates all of the output stream variables, which can then be used as input stream values for the next process step. The modules access data on all independent stream variables from the data arrays contained within the APL global workspace. Additional input data required to solve the equations in each module are requested by the program and are stored as global variables. The user may supply actual data obtained from operating or pilot plants, from similar processes, or from estimates supplied by the engineer.

Creating METSIM model must have a plan and the entire modeling process can be divided into eight main steps:

1. Enter the basic information of the project and select parameters such as quality and time units;
2. Select the elements and draw up system phase table that lists each of the elements and compounds system contains, and select phase of each compound;
3. Draw process flow sheet including all operations units and logistics;
4. Input the name, flow and composition of the inflow stream;
5. Enter chemical reaction of each operating unit and set the necessary parameters;
6. Add the process controller, input function command in order to achieve the expected results;
7. Check the results, check input values and process mechanism, debugging model until the display shows no error;
8. Display the results.
3. Results and Analysis

3.1. Practical procedures of METSIM in alumina production process

According to above eight steps the basic information of the project and parameters will be input and the dialog box is shown as below:

The new alumina production process was simulated by METSIM as below. The process involves compounds as Table 1.

The related reactions are shown as below:

\[
\text{AlO(OH)}(s) + \text{NaOH}(a) \rightarrow \text{NaAl(OH)}_4(a)
\]
\[
\text{Al}_2\text{O}_3\cdot2\text{SiO}_2\cdot2\text{H}_2\text{O}(s) + \text{AlO(OH)}(s) + \text{Ca(OH)}_2(a) + \text{H}_2\text{O}(a) \rightarrow 3\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot 0.64\text{SiO}_2 \cdot 4.72\text{H}_2\text{O}(s)
\]
\[
3\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot 0.64\text{SiO}_2 \cdot 4.72\text{H}_2\text{O}(s) + \text{CO}_2(g) \rightarrow \text{CaCO}_3(s) + \text{Ca}_2\text{SiO}_4(s) + \text{Al(OH)}_3(s) + \text{H}_2\text{O}(a)
\]
\[
\text{Al(OH)}_3(s) + \text{NaOH}(a) \rightarrow \text{NaAl(OH)}_4(a)
\]
\[
\text{NaAl(OH)}_4(a) \rightarrow \text{Al(OH)}_3(s) + \text{NaOH}(a)
\]

So the next is establishing elements and compounds database based on reactions. The table list as Figure 2.

![Figure 1 Input dialog box of the project and parameters](image1)

Table 1 Compounds

<table>
<thead>
<tr>
<th>Solid</th>
<th>Aqueous</th>
<th>Gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlO(OH)</td>
<td>NaOH</td>
<td>CO2</td>
</tr>
<tr>
<td>Al2O3-2SiO2-2H2O</td>
<td>NaAl(OH)4</td>
<td>H2O</td>
</tr>
<tr>
<td>3CaO-Al2O3-0.64SiO2-4.72H2O</td>
<td>Ca(OH)2</td>
<td>Steam</td>
</tr>
<tr>
<td>CaCO3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ca2SiO4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fe2O3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CaO</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

![Figure 2 Elements and compounds database](image2)
After proper elements and compounds are selected the process flow sheet is drawn as Figure 3-5.

Figure 3 Process flow sheet of section 1

Figure 4 Process flow sheet of section 2

Figure 5 Process flow sheet of section 3
METSIM was originally developed to calculate mass and energy balances around any type of flow sheet in a timely manner. To facilitate this task several generic unit operation modules were used. Chemistry and heat balance data may be added to any of these units. The general unit operations are adopted in this alumina production process. This operation concludes all we needs, what shows as Table 2.

Table 2 General unit operation

<table>
<thead>
<tr>
<th>Section Pump, Sump</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream Pump, Vacuum</td>
</tr>
<tr>
<td>Recycle Stream Links Pipe</td>
</tr>
<tr>
<td>Stream Mixer Pipe Connection</td>
</tr>
<tr>
<td>Solid/ Liquid Separator Stream Distributor</td>
</tr>
<tr>
<td>Tank - agitated tank with internal coils for heating or cooling</td>
</tr>
<tr>
<td>Component Splitter Tank - agitated tank with external jackets for heating or cooling</td>
</tr>
<tr>
<td>Phase Splitter Tank - agitated storage tank</td>
</tr>
<tr>
<td>Stream Splitter Tank - with internal coils for heating or cooling</td>
</tr>
<tr>
<td>Sump Tank - with external jackets for heating or cooling</td>
</tr>
<tr>
<td>Launder Tank - simulates a storage tank</td>
</tr>
<tr>
<td>Pump, Centrifugal Tank - decant tank for separating organic from aqueous</td>
</tr>
<tr>
<td>Pump, Positive Displacement Tank - electrolyte or compartmented tank</td>
</tr>
<tr>
<td>Pump, Vertical Tank - process tank with agitation</td>
</tr>
<tr>
<td>Pump, Metering Tank - storage tank without agitation or heating</td>
</tr>
</tbody>
</table>

When above works have been done the information about streams and operations should be input and FBC control should be set up. The content of compounds in raw materials is shown as Table 3.

Table 3. Content of compounds

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Boehmite (%)</th>
<th>Lime (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al₂O₃</td>
<td>54.41</td>
<td>1.17</td>
</tr>
<tr>
<td>SiO₂</td>
<td>16.55</td>
<td>2.38</td>
</tr>
<tr>
<td>Fe₂O₃</td>
<td>7.16</td>
<td>0.58</td>
</tr>
<tr>
<td>TiO₂</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>Na₂O</td>
<td>0.15</td>
<td>0</td>
</tr>
<tr>
<td>CaO</td>
<td>0.5</td>
<td>86.5</td>
</tr>
<tr>
<td>crystal water</td>
<td>12.89</td>
<td>0</td>
</tr>
<tr>
<td>other</td>
<td>5.85</td>
<td>2.58</td>
</tr>
</tbody>
</table>

So we can draw conclusion from calculations the flow rate of washing water needed is about 6000 kg and flash water is about 1373 kg for producing one ton alumina. For the same process we can set different forms of flow sheet. Figure 6 is other form for alumina producing process.

Figure 6 Process flowsheet in one section
All of the operations are arranged in one section in figure 6, it is more directly and easy for reading but when the process is more complex it can not be achieved. The results are similar for the two schemes and we should study furthermore to get the best scheme.

There are other applications for METSIM. Ming. Wang [12] calculated metal/material balance of separation of ionic rare earth. The annual equivalent processing capacity of REO is 1500t (5000 kg/d) rare earth raw materials, 25% is the rare earth oxide containing 92% REO, 75% is rare earth carbonate with 40% REO, the process is acid dissolution- extraction - precipitation - burning for preparation of single rare earth oxide. Only acid-soluble process is selected as example using METSIM. Total of rare earth elements are 17 species and all of the 15 kinds of elements are need to be addressed except Sc and Pm, because these elements exist with the form of oxygen compounds, carbonates and chlorides, the corresponding compounds of primary metal are as many as 45 kinds. If using existing method of Excel to calculate Metal / material balance, it will be difficult to achieve balance of the main metal material. METSIM is reliable for these calculations no matter how many kinds of elements and compounds. Acid-soluble process and towards of streams using METSIM software are shown as figure 7. The figure shows that the acid dissolution process is mainly including acid-soluble oxidation rare earth raw (operating unit), acid-soluble rare earth carbonate raw (operation unit 3), aging (operation unit 4), and Plate-frame Pressure of supernatant (operation unit 5), the viscous liquid natural filtering (operation unit 6). The Component of oxygen rare earth and rare earth carbonate are input to steam 1 and stream 4. The industrial hydrochloric acid (stream 2 and stream 5) is added for decomposition reaction. (For convenience, the rare earth ions are carried as trivalent).

\[
\begin{align*}
\text{RE}_2\text{O}_3 + 6\text{HCl} & = 2\text{RECl}_3 + 3\text{H}_2 \text{O} \\
\text{RE}_2(\text{CO}_3)_3 + 6\text{HCl} & = 2\text{RECl}_3 + 3\text{H}_2\text{O} + 3\text{CO}_2
\end{align*}
\]

Figure 7 Process flow sheet of acid dissolution in rare earth separation [11]

The amount of hydrochloric acid was controlled by the controller 1001 and the controller 1002, which ensure that the pH value is 1 after acid-soluble. The acid soluble slurry (stream 3 and stream 6) flow into the aging tank, after aging for 24 h supernatant (stream 8) flow into the plate-frame pressure filtration, viscous liquid (stream 13) flow into the natural filtration tank for filter and is washed by water (stream 9 and stream 14), the amount of washing water is controlled by the controller 1003 and the controller 1004, so that the metal content of the residue reached a certain low value. Filtered feed solution (stream 12 and stream 17) enter the...
next step of extraction process, the lotion (stream 11 and stream 16) return to the main flow, filter residue (stream 10 and stream 15) are sent to the residue field storage.

The whole process needs oxidized rare earth materials 1 359 kg/d, rare earth carbonate raw materials 9 375 kg/d, acid consumption 31 745 kg/d, filtrate Output 40 507.7 kg/d, the containing main metal equivalent REO 4 903.7 kg/d, 98% yield; the output of wet residue to 378.8 kg/d, producing slag was 3.5%. The total input streams and total output streams are both 42 831.9 kg/d, the material balance is achieved.

4. Conclusion
Chemistry and metallurgy process simulation software is convenient for calculate heat/balance of material. The soft ware METSIM and SYSCAD are better software among numerous process soft wares. The calculations examples for alumina production process, acid dissolution in rare earth separation process, the desilverising of lead by the reagent zinc and Nickel laterite acid leaching process are all successful by using the simulation software. Study on the process simulation software in China is later and is not widespread, more and more people can to master the process simulation software and be able to develop our own software.

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