간단한 물질수지식 계산을 위한 모사기 개발

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Development of Simple Simulator for Mass Balance Calculation

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Introduction

Process simulator is performed mainly for two different purposes - design of a new process and assessment of an existing process. For the design purpose, it is crucial to rigorously simulate the unit processes since few is known for them. But for the assessment purpose, a lot of operating condition and data are given, validation of these data becomes an important issue.

Since most of commercial process simulators cover the two cases simultaneously, they are neither cost-effective nor suitable to deal with given data if the user is only interested in assessing material and / or energy balance of existing processes.

Present research aims at developing a simple process simulator which is capable to calculate the steady-state mass balance as well as to reconcile the noisy operating data.

Problem Formulation

In order to evaluate the process conceptually, we need to consider the detailed and time-consuming task of the heat and mass balances. This precedes the later tasks of plants equipment sizing and economic evaluation. Development of simple relations among process variables allows us to gain some insight into the candidate design and calculate a complete mass and energy balance simply and quickly for further evaluations.

There are two methods for process simulation based on flowsheet, the modular and the equation-oriented mode. In the equation-oriented mode, all process equations can be expressed as a large, sparse equation set. This set is then solved simultaneously, after first partitioning the equation system to determine independent subsets. The advantage of this approach is that more efficient solution strategies are employed than the other method.

In this research, we think only about mass balance, as the evaluation of mass balance is more important industrially than those of energy balance. And the unit calculations are structured so that the process flowsheet can be represented as a linear system of component equations. This linear system leads to a rapid calculation procedure for the mass balance. It is possible to develop a linear set of equations for each process unit and solve the entire process flowsheet with these equations.

There are solution strategies for the mass balance calculation. When there is no recycle stream in the process, equations can be solved sequentially from feed to product. However, if the process has recycle streams, equations should be solved simultaneously. It leads the system to be large and sparse.

Tearing is required to solve the equation efficiently. It makes the recycle simple. The number of unknown variables is reduced through tearing. Then, the model becomes small dense system. For that reason, it is very important to find the recycle system. When the streams is changed into the proper form involving recycle streams, the number of variables is reduced and it results in the small problem. Next, small problem can be solved easily. In the present study, MS Excel is used as a program solver. However, there is a problem that it is difficult to identify the recycle stream property.

To remove this problem, following procedures are adopted : first, we select a process which has the feed stream as its input stream. If the process has other stream besides feed, it is considered as a recycle stream. If recycle streams are known, the other stream are obtained sequentially from the former stream and the overall mass balance is solved. So, recycle streams are decision variables, problem can be solved using solver.

Case study

In this research, a chemical process network is considered. The system is shown in Figure 1. It contains two components, five units and nine streams. Two streams are recycled among the process streams. Also, there are one reaction and overhead split fractions in the system. The equations for reaction and split fraction is written as:

Reactor

$A \rightarrow B$ Conversion: η

Separator

Top $f_{out} = \xi f_{in}$

Bottom $f_{out} = (1-\xi) f_{in}$

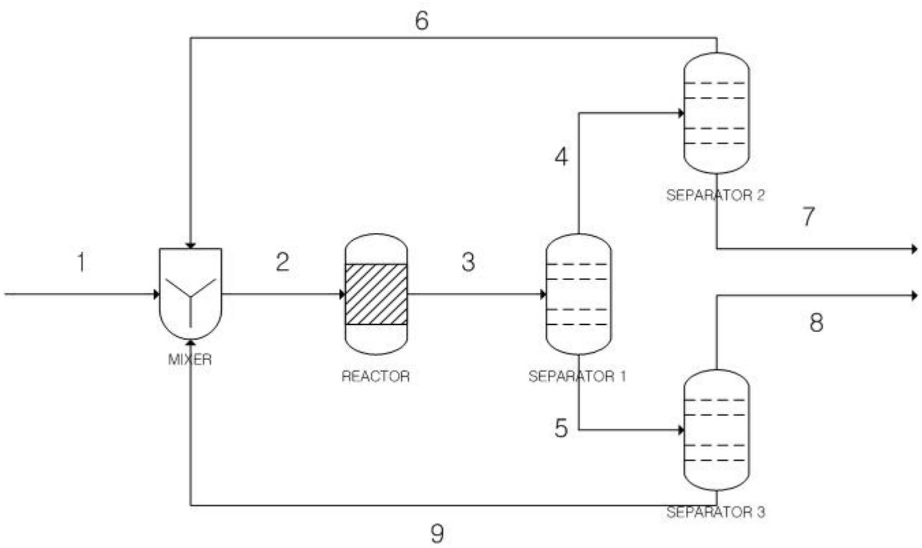

Figure 1. A chemical process network

When split fractions and input informations are known, the number of variable is 16 which is derived from the multiplication of unknown stream and component (8×2).

First, the mixer which has the feed stream as input stream is selected. There are other input streams, so stream 6 and 9 are considered as recycle streams. Then the number of variables are 4 (two recycle stream 2×component 2). If stream 6 and 9 are known, the other streams can be calculated sequentially. Stream 2 is known from stream 1, 6 and 9. Stream 3 is obtained from stream 2. Stream 4 and 5 is estimated from stream 3. The value of stream 6 and 7 comes out from stream 4. We can get stream 8, 9 from stream 5. All streams are calculated. And stream 6 and 9 are compared with initial values. These tearing procedure makes the problem solved efficiently.

The first solving step is to make a numerical expression in each cell. Next, find streams which are considered as recycle streams. Then, they become decision variables. The flow and composition of all streams is obtained through "solversolve function" in MS Excel.

Convergence criterion is the difference between the calculated value and the initial guess. The solver leads to minimize the accumulation of mixer. The variable is the flow and composition of guessed stream. The constraints are zero accumulation of each unit.

Result and Discussion

Process informations and program results can be represented as follows.

Input

Stream 1	
Component 1	70
Component 2	0

Reaction Coefficient

0.7

Split factor

	Separator 1	Separator 2	Separator 3
Component 1	0.8	0.9	0.3
Component 2	0.7	0.2	0.8

Output

	Component 1	Component 2
Stream 1	70.0	0.0
Stream 2	94.3	16.5
Stream 3	28.3	82.5
Stream 4	22.6	57.8
Stream 5	5.7	24.8
Stream 6	20.4	11.6
Stream 7	2.3	46.2
Stream 8	1.7	19.8
Stream 9	4.0	5.0

In order to reduce the size and to enhance the user-affinity of the simulator package, it is developed based on the Microsoft Excel with Visual Basic Applications.

And the noisy operating data can be also reconciled using solver. The objective of reconciliation problem is to minimize the sum of squared differences between each actual data value, or observation, and the corresponding predicted value. This sum has a minimum value of zero, which occurs only when the actual and predicted values are all identical. The solving routine of reconciliation will be added to the mass balance solver.

Conclusions

The flow and composition of each stream can be calculated using a few information through this simulator. It has the advantage that mass balance is evaluated excellently in the assessment of existing processes. This simulator has opened program structure. And it is accessed easily. And it is confirmed that the steady-state mass balance is calculated in a short time. Reconciliation can be added in the mass balance solver. It can be applied to wide industrial ranges.

Acknowledgement

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References

Biegler L.T., Grossman E.I., & Westerberg A.W. (1997). *Systematic Methods of Chemical Process Design*, Carnegie Mellon University