EXISTENCE OF A SOLUTION OF THE BALANCE SIMULATION PROBLEM

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The balance simulation problem (BSP) is one of the most frequent problems occurring in the design and intensification of integrated chemical technologies. In contrast to the simulation problem, BSP does not always have a solution. It is therefore important to know such values of the independent variables (some parameters of apparatuses and some balance quantities) for which the solution does not exist. To estimate the intervals of the independent variables for which no solution of the BSP exists, the results of a simulation under uncertainty are used.

The calculation of the material and energy balance of large chemical technologies forms the key part of the design calculations. There are two different methods of the balance calculations, namely balancing[1] and simulation[2]. The former is based on the conservation law of mass and energy, hence the mathematical models of unit operations involved in the technology whose balance is to be made are not considered. On the other hand, the simulation method consists in that the relations forming models of apparatuses are solved together with the balance equations.

The mentioned problem definitions are, however, incomplete. It is necessary not only to set up the equations but also to specify which quantities are independent variables. Only parameters of mathematic models of apparatuses (the heat transfer area of the heat exchanger, the reactor volume, *etc.*) can be considered as independent variables of the simulation problem. The only balance quantities that can be specified as a part of the formulation of the simulation problem are the flow rates of the components and enthalpies in system inputs (*e.g.*, raw materials).

There are several programming systems that can be used both for balancing and simulation[3]. However, many practical problems are formulated neither as balance nor as simulation ones. The reason for this consists in the choice of the set of independent variables. The system of equations forming the mathematical model of the technology remains always the same, but the elements of the set of independent variables change. A great majority of real problems related to the design of chemical processes involves predetermined properties of raw materials (amount, concentration, *etc.*) and at least some properties of products. Some parameters of the apparatuses are often also given beforehand. The problem then consists in the determination of the values of those parameters of the apparatuses which were not predetermined, in order that the technology for the given raw materials might produce products of the desired properties.

Such problem is neither a balance nor a simulation one, but a certain combination of these. We shall call it a balance-simulation problem (BSP) (ref.[4]). Its solution is in comparison with the "pure" balance and simulation cases much more complicated. There is a possibility how to solve BSP by repeated solution of the simulation problem[4], however it is not certain that BSP has a solution.

Therefore, the existence of a solution of BSP is studied from a practical point of view in the present paper. From the mathematical point of view[5], it is possible to obtain some information about the existence of a solution of a system of nonlinear equations, however this is too general and hence practically useless.

Definition of the Problem

For convenience, we shall introduce the following symbols:

F Set of all components, K set of all nodes, S^t_{ij} flow of component t from node i into j, S set of all component flow rates in all streams, Q set of all balance quantities (*e.g.*, concentration, mass flow rates, splitting fractions *etc.*) that can be expressed as simple functions of the elements of the set S, R discrete finite set, R_g subset formed by such elements of the set R whose numerical values are given or chosen, R_c complement of subset R_g, $R_c = R - R_g$, A_i set of equations forming the mathematical model of node i,

$$Y_i = A_i(X_i, P_i) \tag{1}$$

where X_i denotes the set of all such components of the set S for which

$$X_i = \{S^t_{ji} \mid j \in K, t \in F\} \tag{2}$$

Y_i is the set of all flows in all streams which go from the node i, and P_i is the set of all parameters of the node i; M mathematical model of chemical process:

$$M = A \cup B\,, \tag{3}$$

where

$$A = \bigcup_{i \in k} A \tag{4}$$

and B is the set of all balance equations, V set of all independent variables (variables that can be chosen o r that were by somebody specified):

$$V = S_g \cup P_g \cup Q_g , \tag{5}$$

W set of all dependent variables, *i.e.*, variables that are determined by calculation, u exponent denoting the upper limit of the interval in which the values of the elements of the set can change, l superscript denoting the lower limit.

For the study of the existence of the solution of BSP, the results of the solution of the so-called simulation under uncertainty[6] are used. The latter shall be therefore briefly mentioned.

The difference between the simulation under uncertainty (u simulation) and simulation consists in the intervals of uncertainty which are given for some or all parameters:

$$I_p = \{P \mid P^l \leqq P \leqq P^u\} . \tag{6}$$

With the assumption that the parameters change within the limits given by intervals (6), the flow rate of the components in the streams change in the intervals

$$I_s = \{S \mid S^l \leqq S \leqq S^u\} . \tag{7}$$

Algorithms that can solve the u simulation problem are known. They can hence determine the intervals of uncertainty of the flow rate (7) if the intervals of uncertainty of the parameters (6) are given beforehand. It is apparent that the following relation holds:

$$I_s = I_s(I_p) . \tag{8}$$

The Existence of the Solution of BSP

BSP is defined by a mathematical model M and a set of independent variables V. The set of numerical values of the dependent variables, W, represents the solution of BSP (ref.[7]), whose existence is influenced not only by the choice of the independent variables but also by their numerical values. A change of the value of the element(s) may result in that the BSP thus modified will have no solution although the original BSP has one. In contrast to the classical simulation problem, which has always a solution, BSP need not therefore have a solution for all possible values of the elements of the set of independent variables V.

We shall assume that for a given chemical process, *i.e.*, for a certain mathematical model M and a set of independent variables V it is possible to find such values of the independent variables that the BSP under study has a solution. This means that such an interval of independent variables, I_v, must exist in which their values can change without causing the BSP to have no solution.

The determination of such intervals is difficult, since it is difficult to decide whether the BSP under study has a solution. A complete study of its solvability is in general impossible. The only practical way how to decide whether the BSP has a solution is to solve it. If we do not succeed in finding a solution, then we cannot say nothing about its existence since it is possible that the algorithm used failed.

We shall attempt to interpret the results of the U-simulation so that it might be possible to say something about the existence of a solution of the BSP. The latter represents the following functions:

$$(P_c, S_c) = f(P_g, S_g)\,. \qquad (9)$$

The u simulation transforms the intervals of uncertainty of the parameters, I_p, to those of the flow rates, I_s. We shall assume that

$$I_p = I_{p_g} \cup I_{p_c}\,, \qquad (10)$$

where I_{p_g} is an infinitely small interval:

$$P_{p_g} = 0\,. \qquad (11)$$

The requirement that I_{p_g} be infinitely small follows from the fact that the values of the elements of the set P_g are known and their changes need not be considered. Now we shall ask whether such an interval of uncertainty of the parameters, I_{p_c}, exists so that we have

$$S_g \in I_s(I_p)\,. \qquad (12)$$

If such an interval does not exist, then no solution of the BSP exists. The relation (12) can hence be used to find a sufficient condition for the nonexistence of the solution. This condition, however, cannot indicate the existence of the solution: if (12) is not fulfiled then we cannot say that the solution of BSP exists.

Various chemical engineering or construction reasons lead to restrictive conditions for the parameters. From these we can determine the upper and lower limits in which the numerical values of the independent variables can change, hence the interval $I^M_{p_c}$. So we can use the following relation to prove the nonexistence of the solution:

$$S_g \in I^M_{s_c}(I^M_{p_c})\,. \qquad (13)$$

If this relation holds, we can say nothing about the existence of a solution of BSP and a detailed analysis, *e.g.*, by the Monte Carlo method, is necessary. This requires rather much of the computer time.

On the other hand, it is clear that if no such indeterminancy interval of uncertainty of the parameters,

$$P_g \in I_p \tag{14}$$

TABLE I
Variants of Balance Simulation Problem

BSP No	1	2	3	4	5
S_1^2	120 000	120 000	125 000	125 000	125 000
S_7^6	4 500	4 600	4 700	4 800	4 900
A	0·9	0·9	0·9	0·9	0·9

TABLE II
Flow Limits of Components

Stream	Component					
	1	2	3	4	5	6
			Upper limit			
1	52 946	155 180	6 707	116 920	29	11 692
2	44 024	138 290	7 455	129 960	3 309	17 710
3	44 024	138 290	7 455	129 960	33	17 710
4	44 024	138 290	7 455	129 960	33	12 996
5	39 607	124 420	6 707	116 920	29	11 692
6	5 168	16 233	873	15 390	4	1 539
7	0	0	0	0	0	4 822
8	0	0	0	0	3 276	0
			Lower limit			
1	43 258	124 010	5 022	87 497	25	8 749
2	35 087	109 360	5 889	102 610	2 920	14 879
3	35 087	109 360	5 889	102 610	29	14 879
4	35 087	109 360	5 889	102 610	29	10 261
5	29 919	93 252	5 022	87 497	25	8 749
6	4 299	136 660	711	13 039	3	1 304
7	0	0	0	0	0	4 563
8	0	0	0	0	2 891	0

exists for which the condition (*12*) would be fulfilled, then the BSP under study has no solution.

Example: We choose the classical Williams Otto technology (Fig. 1); we have three parameters, namely T, temperature in the chemical reactor, V, reactor volume, and A, splitting fraction for stream No 5. These parameters are in the following indeterminancy intervals of uncertainty:

$$670 \leqq T \leqq 673\,, \quad 32 \leqq V \leqq 32{\cdot}3\,, \quad A = 0{\cdot}9\,. \qquad (15)$$

The splitting fraction, A, is an independent variable with respect to the definition of the BSP. The other two parameters must be found in order to maintain the given flow of the second component through the first stream S_1^2 and the flow of the sixth component through the seventh stream S_7^6. Hence, the set of independent variables V in the test BSP contains the splitting fraction A and the flow rates S_1^2 and S_7^6. All other quantities including both remaining parameters (temperature and volume of the reactor) are dependent variables.

We shall study the existence of a solution of the following five variants of the BSP; they differ only by the values of the independent variables (Table I).

We solved the u simulation for the given intervals of uncertainty of the parameters (*15*) (ref.[7]); the result, *i.e.*, the upper and lower limits for the flows of all six components in all eight streams (Fig. 1) is seen from Table II. It is apparent that the intervals in which the flows S_1^2 and S_7^6 change owing to changes in the temperature T and volume V of the reactor are:

$$124\,010 \leqq S_1^2 \leqq 155\,180\,, \quad 4\,563 \leqq S_7^6 \leqq 4\,822\,.$$

Hence it follows that the problems No 1, 2, and 5 have no solution.

CONCLUSIONS

The application of the program for the solution of simulation under uncertainty for the study of the existence of a solution of BSP is very effective. It enables to determine such combinations of the values of independent variables for which the BSP has no solution, hence it is possible to study a number of BSP's at once. A suitable program for the solution of u-simulation is necessary and can be relatively easily elaborated by modifying the simulation system.

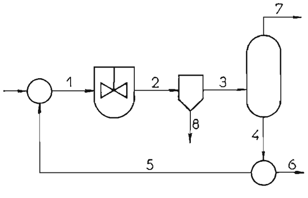

FIG. 1
Williams–Otto Testing Technology
1—8 Streams between nodes.

In practice, simulation problems are usually solved first and then the BSP. It is expected that the accessibility of a simulation programming system is not a hindrance in the exploitation of the proposed algorithm for the study of the existence of a solution of BSP; its drawback consists, however, in that the existence of such a solution cannot be proved.

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