# STOP CRITERION AND SIMULATION ALGORITHM

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Mathematical model of a simulated process describes an actual equipment only with some accuracy. Thus, there is no reason to require that the numerical method should solve the simulation problem with a greater accuracy than with which the mathematical model approximates the behaviour of an actual existing equipment. The problem is thus in designing a suitable stop criterion of the simulation problem under uncertainty. The vector standards are used for this purpose. One of the most suitable is the elliptic norm for its simple algorithm and suitable description of the region of uncertainty of solution.

Application of programming systems for solution of simulation problems is at present quite usual. The attention is now paid to the study of individual special questions which should decrease the computer time if the chemical engineering and design aspects of these problems are neglected. Here a suitable selection of the stop criterion of iteration methods for solution of simulation problems is studied.

From the mathematical point of view is the problem of simulation algorithm identical with the solution of a complex system of strongly-nonlinear equations. The numerical mathematics supplies only the iteration algorithm and from the point of view of the stop criterion it gives only few information. This problem, however, cannot be solved even in the frame of numerical mathematics as only the user *i.e.* the project engineer or the plant manager can decide on the adequate accuracy of computation.

But it is not possible to expect that the user will consider the question of selection of the stop criterion too carefully. It is possible to assume that he will prefer the strict stop criterion which guarantees a higher accuracy than he requires at the cost of greater computer time consumption. But this approach does not require any addition work so that he may devote his attention to the purely engineering part of the problem.

This fact has forced us to prepare an algorithm which alone selects the adequate value of the stop criterion on basis of information which can be easily supplied. The basical consideration on which is based the next analysis is very simple. It is based in comparison of two accuracies, the first one with which the system of equations approximates the simulated process and the second one of the used numerical method. It is obvious that it is not appropriate to increase the accuracy of the method above the accuracy of approximation.

From the point of view of system engineering there appears another aspect here. In complicated simulation and especially optimisation computations there appear very frequently such problems which must be solved iteratively on several levels of given structures of the programming system.

In Fig. 1 is *e.g.* proposed a hierarchy of iterative computation of the heat transfer process with the phase change. The used method for computation of the phase equilibrium requires numerical solution of the system of non-linear algebraic equations (iterative base *1*). In iterative computations of heat exchangers in which a partial condensation takes place the procedure for calculation of phase equilibrium is used (iterative base *2*). The simulated chemical process is formed by several condensers or other units whose interconnection forms one or several loops. It is thus necessary to solve the simulation problem by the iterative procedure (iterative base *3*). There might appear also problems with multibase iterations. It suffices to realize that the iteration problem in Fig. 1 will be four level if the chemical technology is optimized. The simulation computation will thus many times repeat.

The block structure of the process thus forces us to determine the stop criteria on several levels. Already the own qualitative consideration suggests that it is not advantageous to let the stop criterion to be constant for the first iteration level. In this case we should let it to be equal to such value which guaranties the required accuracy of the final result. But such an accuracy has a significance only in the last iteration of the highest level (in our case the level *3* in Fig. 1).

Here we consider the selection of the stop criterion on one level. But it is possible to extend the proposed procedure also to several level stop criteria.

As has already been mentioned, the mathematical model describes the actual equipment only with some accuracy. The reasons of inaccuracies rest in the next facts: the constants used in the mathematical model are not known accurately (mostly the physico-chemical), it is not possible to keep some values on the required value, *e.g.* it is not possible to keep the temperatures of input streams at the required value, the own mathematical model is inaccurate which rests in the insufficient understanding of the process or in the negligence of some relations because of simplicity of the mathematical description.

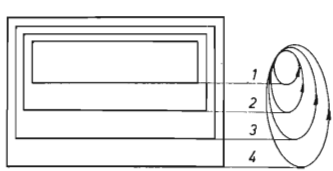


FIG. 1

Structure of Computation Process of Heat Transfer

Individual iteration levels represent: *1* computation of physical properties, *2* mathematical model of the node, *3* simulation, *4* optimization.

The until now used methods are applying for the criteria of convergence the test of absolute or relative error *i.e.*

$$\|z_{i+1} - z_i\| < \varepsilon$$

or

$$\|z_{i+1} - z_i\| / \|z_i\| < \varepsilon ,$$

where $z_i$, $z_{i+1}$ are vectors of variables in two succeeding iterations, $\varepsilon$ is the tolerance prescribed by the user. But none of these criteria tests is completely satisfactory as has already been pointed out by several authors[1,2].

The user usually knows which accuracy he needs for engineering purposes but he cannot determine from it the value $\varepsilon$, as the value $z_{i+1} - z_i$ is not only a function of the actual error but also of convergence of the iteration method. The user is thus exposed to the risk of obtaining an inaccurate result or to the excessive computer time consumption as has been already pointed out.

*Analysis of the Problem*

The mathematical model of chemical technology is the system of non-linear equations

$$F(X, K, P) = 0 \qquad (1)$$

in which there appears the set of all flow rates through all streams (vector $X$), vector of constants $K$ and parameters $P$. The solution of the system of Eqs (*1*) is thus dependent on the numerical values of constants and parameters

$$X_r = f(K, P) .$$

But in solutions of practical problems are the values of constants and parameters not known exactly but become the values from some known regions

$$K \in \mathscr{K}(X_r) , \quad P \in \mathscr{P}(X_r) .$$

The problem formulated in this way is the problem under uncertainty. Its solution is not a single value $X_r$ but a whole region $R$ which can be described in the following way

$$R = \{X_r \mid f(X_r, K, P) = 0 , \quad K \in \mathscr{K}(X_r) , \quad P \in \mathscr{P}(X_r)\} .$$

The first problem which must be solved is finding of the region $R$. But this is very combersome as the relations forming the mathematical model are in general non-linear. Thus let us assume that the region of uncertainty is sufficiently small so that on it we can approximate the non-linear relations (*1*) by the linear ones.

For this purpose was the studied problem slightly transformed into the known form of Nagiev balance[3] Eqs (3). The system (1) then has the form

$$S_i^t + \sum_j \alpha_{ji}^t \lambda_j^t = \lambda_i^t \qquad (2)$$

$$i = 1, \ldots, K \; ; \quad t = 1, \ldots, F \, ,$$

where $K$ is the number of nodes of the balanced system, $F$ number of components, $S_i^t$ is the input into the i-th node, $\alpha_{ji}^t$ is the splitting ratio, $\lambda_j^t$ is the flowrate through the j-th node.

To the looked for flowrates $\lambda_j^t$ correspond the variables $X_r$ of the system (1).

The effect of errors of constants and parameters is in the system (2) manifested in the next way

$$S_i^t + \delta S_i^t + \sum_j \lambda_j^t (\alpha_{ji}^t + \delta \alpha_{ji}^t) = \lambda_i^t \, , \qquad (3)$$

where

$$\delta S_i^t \in \langle -\Delta S_i^t, \; \Delta S_i^t \rangle \, , \qquad (4)$$

$$\delta \alpha_{ji}^t \in \langle -\Delta \alpha_{ji}^t, \; \Delta \alpha_{ji}^t \rangle \, .$$

For the estimate of the region of solution a number of methods 4 has been studied. As the most suitable one can be considered the estimate in the elliptic norm[4] (see Appendix) for the following reasons: – suitable mathematical description of the set which includes the region of solution, – simple algorithm.

*Proposal of the Stop Criterion*

The linearized mathematical model of the chemical process under uncertainty can be now easily solved. As the result we obtain the set (let us denote it as $R_E$) in which the flow rates of all components $\lambda_i^t$ can change if the coefficients are varying in the range of the uncertainty interval (4). If we use the elliptic norm the $R_E$ has the form of the multidimensional ellipsoide.

Solution of the simulation problem can be obtained by the algorithm for the simultaneous simulation (if the algorithm for sequence simulation is used the results could be interpreted as at the simultaneous simulation). From the mathematical point of view the simultaneous simulation is based on solution of the sequence of the system of linear equations. At each iteration the coefficients of linear equations must be calculated by use of the non-linear models of nodes and results from the foregoing iteration. The difference between the corresponding values of coefficients in two succeeding iterations gives certain interval of uncertainty on coefficients.

If the elliptic norm is used as for the estimate of $R_E$ the set is obtained (let us denote it as $R_1^i$) in which the flowrates can change if the coefficients vary in the range of the uncertainty interval due to the i-th iteration.

If the next inclusion is satisfied on the i-th iteration

$$R_E \supset R_1^i \tag{5}$$

there is no reason why to continue in the computation of the (i + 1)st iteration. Another improvement of solution *i.e.* decrease of the estimate $R_1^i$ is depreciated by the inaccuracy of statement of the problem *i.e.* by the estimate of solution by the set $R_E$ (Fig. 2).

The condition (5) can be thus considered to be the stop-criterion of the simulation computation. The practical check of satisfaction of the inclusion (5) is very simple because of the used elliptic norm. In individual iteration steps two ellipsoides are compared which have the same dimensions, common centre and axes.

*Example.* For illustration of the described stop criterion was used the fictive chemical process according to the authors Otto and Williams. The simplified block diagram is in Fig. 3.

For simplicity the calculation is not based on uncertainty on constants $K$ and parameters $P$ but directly on splitting ratios $\alpha$. Let us assume that errors of splitting ratios of all 6 components are independent of flowrates, thus they are constant and equal to the next values

$$\Delta\alpha = 0{\cdot}01, \quad \Delta\alpha_2 = \Delta\alpha_4 = 0, \quad \Delta\alpha_3 = \Delta\alpha_1/2 .$$

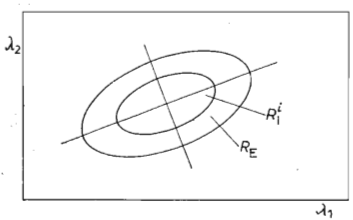


FIG. 2

Estimate of the Region of Solution in Elliptic Norm on the i-th Iteration

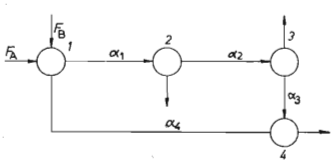


FIG. 3

Simplified Diagram of the Otto–Williams Process

*1* Reactor, *2* decanter, *3* distillation column, *4* splitter.

The check of convergence is performed in the recycle stream No 4 for all components.

For comparison the results of the simulation computation are given with the "classical" stop criteria to test the absolute and relative error as well as with the one newly proposed. In Table I the absolute and relative errors are given in dependence on iterations for the most disadvantageous component according to which is the computation stopped.

According to the new stop criterion is the computation terminated after 7 iterations. The number of iterations for individual components at which is the condition (*5*) satisfied is given in Table II.

TABLE I

Absolute and Relative Errors in Dependence on the Iteration

| Number of iteration | Absolute error 2nd component | Relative error 3rd component |
|---|---|---|
| 2 | 6 420 | 0·2798 |
| 3 | 3 780 | 0·1462 |
| 4 | 2 250 | 0·0794 |
| 5 | 1 370 | 0·0473 |
| 6 | 840 | 0·0267 |
| 7 | 510 | 0·0158 |
| 8 | 330 | 0·0095 |
| 9 | 200 | 0·0058 |
| 10 | 120 | 0·0035 |
| 11 | 90 | 0·0023 |
| 12 | 50 | 0·0012 |
| 13 | 30 | 0·0010 |
| 14 | 20 | 0·0004 |
| 15 | 10 | 0·0004 |
| 16 | 10 | 0·0002 |
| 17 | 10 | 0·0002 |
| 18 | 0 | 0 |

TABLE II

Numbers of Iterations of Satisfaction of Condition (*5*)

| Number of component | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| Number of iterations | 6 | 7 | 7 | 6 | 3 | 5 |

## CONCLUSION

There is no sense to perform the simulation computation very accurately as the accuracy of mathematical models is low. For this reason an algorithm enabling an objective evaluation of the stop criterion was developed.

From practical point of view it would be useful to operate with the problems under risk as the description of errors of the distribution function corresponds to the actual state better than the estimate of errors in some interval as in the approach under uncertainty.

To be able to test the stop criterion in a wider range it would be suitable to modify the commerially available simulation program by this stop criterion.

Considerable reduction in computer time can be expected provided that the given problem will be considered as a part of optimization task which we would like to study in the future.

## APPENDIX

Let us have the set of linear equations $A\lambda = S$, whose solution is $\lambda_r^0$. The elements of the matrix of the system A and of the vector $S$ are not known accuratelly but they are determined as the upper limit of errors $\Delta A$ and $\Delta S$. Thus we need to find the set of permissible solutions $\lambda_A$ which satisfy the following system of equations

$$(A + \delta A)\,\lambda = S + \delta S\,,$$

where

$$\delta A \in \langle -\Delta A,\ \Delta A \rangle$$

$$\delta S \in \langle -\Delta S,\ \Delta S \rangle\,.$$

If the errors of coefficients are expressed in the spherical norm *i.e.*

$$\|\Delta A\| < \varepsilon_1\,, \quad \|\Delta S\| < \varepsilon_2$$

then the matrix

$$K = 2(\varepsilon_1^2 \|\lambda_r^0\|^2 + \varepsilon_2^2)\,(A^T A)^{-1}$$

determines the ellipsoide whose centre is situated in the point $\lambda_r^0$, second powers of half axes are equal to the eigen values and the axes are situated in the directions of eigen vectors of the matrix $K$. So determined ellipsoide represents the set of permissible solutions $\lambda_A$.

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