SOME QUESTIONS OF THE MODELLING OF COMPLEX CHEMICAL SYSTEMS

G.M.Ostrovskij, Yu.M.Volin
Karpov Institute of Physical Chemistry
ul. Obukha 10, 107120, Moscow, B-120/U.S.S.R.

The problem of complex chemical system (CCS) optimization is considered.

Mathematically the CCS optimization problem in many cases may be defined as follows:

$$y_i^{(k)} = f_i^{(k)}(x_j^{(k)}, u_r^{(k)}), \qquad (1)$$

$$k = 1, \ldots, N; \quad i = 1, \ldots, n_k; \quad j = 1, \ldots, m_k; \quad r = 1, \ldots, r_k$$

$$x_i^{(k)} - y_p^{(q)} = 0, \qquad (2)$$

$$F = \sum_{k=1}^{N} F^{(k)}(x_j^{(k)}, y_i^{(k)}, u_r^{(k)}), \qquad (3)$$

$$g_l^{(k)}(u_r^{(k)}) \le 0 \qquad l = 1, \ldots, p_k, \qquad (4)$$

$$y_i^{(k)} = b_i^{(k)} \quad i = 1, \ldots, \bar{g}_k \le g_k, \qquad (5)$$

where $x_j^{(k)}$, $y_i^{(k)}$ are input and output state variables and $u_r^{(k)}$ are decision variables of the k-th block. Equations (1), (2) represent block models and a table of connections between input and output variables. It is assumed that in the k-th block the first s_k (g_k) input (output) variables are CCS input (output) variables: $\bar{x}_j^{(k)}(\bar{y}_i^{(k)})$. The block decision variables $u_r^{(k)}$ and CCS input variables $\bar{x}_j^{(k)}$ are CCS decision variables. These variables must be determined to give F the maximum value.

In this paper we shall consider the direct optimization approach using first derivatives of the criterion F. The solution algorithm in this case consists of three parts: the computation of criterion, the

computation of criterion derivatives and a searching strategy. The last part has been examined in many papers (see, for example, /1/), therefore the attention will be concentrated on the first two ones.

Optimization Criterion Computation

There exist two different criterion computation approaches. At first the fulfilment of conditions (5) is realized through the searching strategy algorithm and all CCS output variables are considered as free at the criterion computation stage. The search of the optimum solution is carried out in the CCS decision variable space:

$$u_r^{(k)},\ \bar{x}_j^{(k)} \qquad r = 1,\dots,r_k;\ j = 1,\dots,s_k;\ k = 1,\dots,N. \tag{6}$$

The criterion computation is the CCS steady-state regime calculation, the values of variables (6) being fixed /2/.

Let us introduce now the function $F^*(u_r^{(k)},\ \bar{x}_j^{(k)})$ which is obtained from F with the help of substitution $x_j^{(k)}$, $y_i^{(k)}$ as functions of CCS decision variables, and consider the second approach. In this case the fulfilment of conditions (5) is realized at the criterion computation stage, so there exist $\bar{q} = \sum_{k=1}^{N} \bar{q}_k$ additional equations. On such a value the number of variables must be increased to fulfil CCS steady-state regime equations. Let us assume that in each block the first $\bar{s}_k$ input variables are used to satisfy conditions (6) and designate $\bar{s} = \sum_{k=1}^{N} \bar{s}_k$. Then

$$\bar{s} = \bar{q}\ . \tag{7}$$

The search of the optimal solution is carried out in the space of variables

$$u_r^{(k)},\ \bar{x}_j^{(k)} \qquad k = 1,\dots,N;\ r = 1,\dots,r_k;\ j = \bar{s}_k + 1,\dots,s_k. \tag{8}$$

The criterion computation is the calculation of the CCS steady-state regime with additional conditions (5), the values of variables (8) being fixed.

Criterion Derivatives Computation

The usual method of criterion derivatives computation (with

the help of differences) has two defects: it is inaccurate and requires lengthy calculations, the number of decision variables is large. First let us consider the case when fulfilment of conditions (5) is realized through the searching strategy algorithm.

The criterion derivatives with respect to decision variables may be expressed in the following form /2/:

$$\frac{\partial F^*}{\partial u_r^{(k)}} = \sum_{i=1}^{n_k} \lambda_i^{(k)} \frac{\partial f_i^{(k)}}{\partial u_r^{(k)}} + \frac{\partial F}{\partial u_r^{(k)}}, \qquad (9)$$

$$k = 1, \ldots, N; \quad r = 1, \ldots, r_k; \quad j = 1, \ldots, s_k$$

$$\frac{\partial F^*}{\partial \bar{x}_j^{(k)}} = \bar{\mu}_j^{(k)} \qquad (10)$$

where $\lambda_i^{(k)}$, $\mu_j^{(k)}$ satisfy the adjoint process equations:

$$\mu_j^{(k)} = \sum_{i=1}^{n_k} \lambda_i^{(k)} \frac{\partial f_i^{(k)}}{\partial x_j^{(k)}} + \frac{\partial F^{(k)}}{\partial x_j^{(k)}} \quad j = 1, \ldots, m_k, \qquad (11)$$

$$\mu_i^{(k)} = \lambda_p^{(q)} - \frac{\partial F^{(q)}}{\partial y_p^{(q)}}, \qquad (12)$$

$$\lambda_i^{(k)} = \frac{\partial F^{(k)}}{\partial \bar{y}_i^{(k)}} \qquad i = 1, \ldots, g_k \quad \text{(boundary conditions)}. \qquad (13)$$

The number of equations (11)-(13) is equal to that of the unknown variables $\lambda_i^{(k)}$, $\mu_j^{(k)}$.

Let us consider now the case when the fulfilment of conditions (5) is realized at the criterion computation stage. It may be shown that the expression of the criterion derivatives has now the form of equations (9), (10) with $j = \bar{s}_k + 1, \ldots, s_k$ (in (10)), and the adjoint process is represented with the equations (11), (12),

$$\bar{\mu}_j^{(k)} = 0 \qquad j = 1, \ldots, \bar{s}_k, \qquad (14)$$

$$\bar{\lambda}_i^{(k)} = \frac{\partial F^{(k)}}{\partial \bar{y}_i^{(k)}} \qquad i = \bar{g}_k + 1, \ldots, g_k. \qquad (15)$$

It may be easily shown that the number of boundary conditions (14),(15) is equal to that of (13) of the first case. So there exists again the equality between the number of unknown variables and that of equations. But the solution of the adjoint process equations in this case is a more difficult problem as the boundary conditions are connected both with the input and output adjoint process variables.

In order to use the adjoint process method it is necessary to have formulae for matrices of partial derivatives

$$\left\| \frac{\partial f_i^{(k)}}{\partial x_j^{(k)}} \quad \frac{\partial f_i^{(k)}}{\partial u_r^{(k)}} \right\|. \tag{16}$$

The programmer must obtain these formulae and the corresponding programs beforehand. In the case of complex block models this may require a lot of preparatory work. Of course the matrix (16) may be computed with the help of differences. The analysis has shown that this modification of the adjoint process method has a definite advantage compared to the method of decision variables differences. But some defects of the last method still remain.

In this connection the following algorithm has been proposed /3/. Let us assume that a sufficiently large set of simple computation operations is available: addition, subtraction, multiplication, sin(x), exp(x) etc (so-called conditionally elementary operations- CEO). Then an arbitrary nonlinear system of equations may be considered as a complex computational system with CEO as blocks of such a system:

$$y^{(k\ell)} = f^{(k\ell)}\left(x^{(k\ell)}, u^{(k\ell)}\right) \tag{17}$$

$$x_i^{(k\ell)} = y_p^{(k\ell)} \tag{18}$$

where k is the number of CCS block and ℓ is that of subblock corresponding to some CEO. The computation of the matrix (16) is equivalent to that of partial derivatives output variables with respect to input variables for the system (17), (18). So the adjoint process method may be used:

$$\mu_j^{(k\ell)} = \sum_{\ell=1}^{n_{k\ell}} \lambda_i^{(k\ell)} \frac{\partial f_i^{(k\ell)}}{\partial x_j^{(k\ell)}}, \tag{19}$$

$$\mu_i^{(k\ell)} = \lambda_p^{(k\ell)}\ i = 1, \ldots, m_{k\ell};\ \ell = 1, \ldots, L_k.$$

In order to compute the matrix (16) it is necessary n times to compute the adjoint process (19), elements of the i-th column of the unit matrix being taken as input adjoint variables at the i-th computation. So in the proposed algorithm the system of equations (1) is replaced by the system of blocks described with simple equations. The CEO and partial derivatives $\partial f_i^{(k\ell)}/\partial x_j^{(k\ell)}$ programs and the organization program (which make it possible on the basis of the structure of the equations (17), (18) to create the program both for the computation of complex CEO system (17), (18) and for that of corresponding adjoint process system (19) for each block of the original CCS) may be made beforehand. In this case the programmer must only describe the structure of the equations (17), (18). Some defect of the method consists in necessity to compute n times the adjoint process system (19) for calculation of partial derivatives (16). It is possible however to avoid this defect. Let the computation system (17), (18) be written for each block of the system (1), (2). Each system (1) being replaced by the corresponding system (17), (18), one gets a new two-level system, CEO being the elements of the first level, and blocks of the original system-those of the second. The adjoint process for the new system includes N adjoint systems (19). Mathematically the new two-level system and its adjoint process are equivalent to the original ones. So in this case it is necessary to compute only once (as before) the two-level adjoint process. That means that the adjoint process corresponding to each block of the CCS must be computed only once.

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