Constructing models of flow chemicals technology systems by realization theory

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In this paper we present a method and a corresponding computer program for the construction of state-space models of flow systems by realization theory and we report on the results obtained by its application to real measurements. Also, we discuss the problem of the physical interpretation of the constructed models.

Приводится метод соответствующей вычислительной программы для конструкции моделей проточных систем в пространстве состояний при помощи теории реализации и его применение к реальным измерениям. Обсуждается также проблема физической интерпретации созданных моделей.

Since the pioneering work of Danckwerts on residence time distribution a vast number of papers has appeared on the problem of construction of models of the flow in reactors from measurements of input-output data. Almost all of the papers have been concerned with the problem of identifying one or several parameters of a model of a fixed structure which had been chosen in advance.

A continuous reactor can be considered a system, the input (output) of which is the concentration of a given component of the inlet flow (outlet flow, respectively). This system has the remarkable property (which is almost unique among real systems) that it is naturally linear. Therefore, it is logical to use realization theory and techniques for the construction of models of flow systems from input-output data. Nevertheless, there are only few reports on the realization approach in the chemical engineering literature [1—3]. The first two of these references are of expository character; the third paper is to our knowledge the only one reporting on experiences with the realization method based on results of processing a larger amount of input-output data.

In this paper we present a somewhat different approach to the realization problem. Further we report on its program realization and on the results obtained by its application to real measurements. Also, we draw some conclusions from the results which may have a more general scope. Finally we discuss the problem of constructing realizations the coefficients of which would have a physical meaning.

Realization theory and algorithms

In this section we summarize the most important concepts of realization theory of finite dimensional systems which are necessary for the understanding of the paper. For more detailed information the reader may consult [1—3].

By a state-space (dynamic) description (**A**, **B**, **C**) of a finite-dimensional linear continuous system we understand the system of equations

$$\begin{aligned} \dot{\boldsymbol{x}} &= \mathbf{A}\boldsymbol{x} + \mathbf{B}\boldsymbol{u} \\ \boldsymbol{y} &= \mathbf{C}\boldsymbol{x} \end{aligned} \tag{1}$$

where $\boldsymbol{u}$, $\boldsymbol{x}$, $\boldsymbol{y}$ are m-, n-, p-dimensional vectors representing the input, state, and output of the system, respectively.

It is well known from the theory of linear differential equations that given an input function $\boldsymbol{u}(t)$ and an initial state $\boldsymbol{x}(0)$ of the system, its response $\boldsymbol{y}(t)$ can be expressed by the variation of constants formula

$$\boldsymbol{y}(t) = \Phi(t)\boldsymbol{x}(0) + \int_0^t \Phi(t-s)\,\boldsymbol{u}(s)\,\mathrm{d}s \tag{2}$$

where

$$\Phi(t) = \mathbf{C}\exp(\mathbf{A}t)\,\mathbf{B} \tag{3}$$

and

$$\exp(\mathbf{A}t) = \mathbf{I} + \mathbf{A}t + \frac{\mathbf{A}^2}{2}t^2 + \ldots \tag{4}$$

The function $\Phi(t)$ may be considered the impulse response of the system and, as seen from eqn (*2*), it defines completely the input-output map of the system.

It follows from eqns (*3*) and (*4*) that

$$\Phi(t) = \mathbf{C}\exp(\mathbf{A}t)\;\mathbf{B} = \sum_{k=0}^{\infty} \frac{\mathbf{Y}_k}{k!}\,t^k \tag{5}$$

$\Phi(t)$ and, thus, also the impulse response are uniquely determined by the $m \times p$ matrix quantities $\mathbf{Y}_k$, called the Markov parameters. Also, it follows from eqn (*5*) that

$$\mathbf{Y}_k = \frac{\mathrm{d}^k \Phi(0)}{\mathrm{d}t^k} \tag{6}$$

Given a linear input-output map (or, equivalently, its impulse response $\Phi(t)$), the system (*1*) is called the realization of this map (or Φ), if $\Phi(t) = \mathbf{C} \exp(\mathbf{A}t)\,\mathbf{B}$.

A necessary and sufficient condition for a linear input-output map to have a finite dimensional realization can be most concisely formulated in terms of the Markov parameters *via* the infinite Hankel matrix

$$\mathbf{H}_{rs} = \begin{bmatrix} Y_0 & Y_1 & Y_2 & \dots \\ Y_1 & Y_2 & Y_3 & \dots \\ Y_2 & Y_3 & Y_4 & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \tag{7}$$

If we denote by $\mathbf{H}_{rs}$ the submatrix of $\mathbf{H}$ consisting of its first r block rows and s block columns, *i.e.*

$$\mathbf{H}_{rs} = \begin{bmatrix} Y_0 & Y_1 & \dots & Y_{s-1} \\ Y_1 & Y_2 & \dots & Y_s \\ \dots & \dots & \dots & \dots \\ Y_{r-1} & Y_r & \dots & Y_{r+s-2} \end{bmatrix} \tag{8}$$

then this condition can be formulated as follows:

There exists an $n \geq 0$ such that rank $\mathbf{H}_{rs}$ = rank $\mathbf{H}_{nn}$ for all $r, s \geq n$. It is obvious that this condition is satisfied if and only if

$$\text{rank } \mathbf{H}_{n+1,\sigma} = \text{rank } \mathbf{H}_{n+1,\sigma+1} \quad \text{for} \quad \sigma \geq n$$

Also, it can be verified readily that if (**A**, **B**, **C**) is a realization of the impulse response $\Phi(t)$ then we have

$$\mathbf{H}_{rs} = \mathbf{P}_r \mathbf{Q}_s \tag{9}$$

where $\mathbf{P}_r = \text{col}\,(\mathbf{C}, \mathbf{CA}, \dots, \mathbf{CA}^{r-1})$ is the (r-th order) observability matrix and $\mathbf{Q}_s = (\mathbf{B}, \mathbf{AB}, \dots, \mathbf{A}^{s-1}\mathbf{B})$ is the (s-th order) controllability matrix.

If Φ has a finite dimensional realization then it has many such realizations. Among those the most important realizations are the realizations with minimal dimension of the state space or, as we say, minimal realizations. A realization is minimal if and only if it is controllable and observable, *i.e.* if rank $\mathbf{P}_n$ = rank $\mathbf{Q}_n$, where n is its dimension. All minimal realizations are linearly isomorphic, *i.e.* there exists a linear transformation $\boldsymbol{x} = \mathbf{T}\tilde{\boldsymbol{x}}$ in the state space which brings one realization into the other. If (**A**, **B**, **C**) and ($\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$) are these realizations, then

$$\tilde{\mathbf{A}} = \mathbf{T}^{-1}\mathbf{A}\mathbf{T}, \quad \tilde{\mathbf{B}} = \mathbf{T}^{-1}\mathbf{B}, \quad \tilde{\mathbf{C}} = \mathbf{C}\mathbf{T} \tag{10}$$

If the dimensions of both the input and output are equal to one, then the matrix $\mathbf{T} = \mathbf{S}\mathbf{R}$, where

$$\mathbf{R} = (\mathbf{A}^{n-1}\mathbf{B}, \ \mathbf{A}^{n-2}\mathbf{B}, \ \ldots, \mathbf{A}\mathbf{B}, \mathbf{A})$$

$$\mathbf{S} = \begin{bmatrix} 1 & 0 & 0 & \ldots & 0 \\ a_{n-1} & 1 & 0 & \ldots & 0 \\ a_{n-2} & a_{n-1} & 1 & \ldots & 0 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \\ a_1 & a_2 & \ldots & a_{n-1} & 1 \end{bmatrix} \tag{11}$$

brings any minimal realization ($\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$) *via* expression (*10*) to the canonical form ($\mathbf{A}_0$, $\mathbf{B}_0$, $\mathbf{C}_0$), with

$$\mathbf{A}_0 = \begin{bmatrix} 0 & 1 & 0\ 0\ldots 0 \\ 0 & 0 & 1\ 0\ldots 0 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots \\ 0 & 0 & \ldots\ldots 1 \\ -a_0 & -a_1 & \ldots\ldots -a_{n-1} \end{bmatrix} \quad \mathbf{B}_0 = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}$$

$$\mathbf{C}_0 = (b_0, b_1, \ldots, b_{n-1}) \tag{12}$$

where $\lambda^n + a_{n-1}\lambda^{n-1} + \ldots + a_0$ is the characteristic polynomial of $\mathbf{A}$.

Note that the system

$$\dot{\boldsymbol{x}} = \mathbf{A}_0\boldsymbol{x} + \mathbf{B}_0\boldsymbol{u}$$
$$\boldsymbol{y} = \mathbf{C}_0\boldsymbol{x} \tag{13}$$

can be described by the equations

$$x_1^{(n)} + a_{n-1}x_1^{(n-1)} + \ldots + a_0x_1 = u$$
$$y = b_0x_1 + \ldots + b_{n-1}x_1^{(n-1)} \tag{14}$$

the transfer function of which is

$$Y(s) = \frac{b_{n-1}s^{n-1} + b_{n-2}s^{n-2} + \ldots + b_0}{s^n + a_{n-1}s^{n-1} + \ldots + a_0} \tag{15}$$

We can see that the parameters of the canonical form are the coefficients of the transfer function of the system.

Several algorithms for the computation of a minimal realization of a given sequence of Markov parameters have been proposed [2]. However, if the Markov

parameters are obtained from measurements on a real system, they practically never satisfy the rank realizability condition. Therefore, one is interested in finding minimal partial realizations. A system is called a partial realization of order n of a given impulse response if its first n Markov parameters coincide with those of the impulse response. Since there is no a priori test for the order of a good partial realization one usually computes several partial realizations of increasing order and looks for the one most suitable. Rissanen has developed a recursive realization algorithm in which the realizations of higher order are obtained by augmenting those of lower order (*i.e.* the matrices of higher order partial realizations contain those of the previously computed lower order ones as their submatrices). Rissanen's algorithm makes use of the decomposition (*9*) of the Hankel matrix. In the case $m = p = 1$, the first column of **Q** becomes **B**, while $\mathbf{C} = (1, 0, \ldots, 0)$; the matrix **A** is obtained from **P**. The matrix **Q** can be used to estimate the quality of the realization of the corresponding order. If the matrix **Q** is computed from the Markov parameters of a system of dimension n, then the entries in the $n+1$th row of **Q** are zero (or, because of round-off errors, are very small).

Realization of flow systems from experimentally obtained input-output data

Henceforth we shall assume that both the input and the output is scalar ($m = p = 1$) which is frequently the case for flow systems. The input-output relation from which one has to construct the realization is usually given by the response to a particular input function or directly as the impulse response of the system.

Let us assume the latter. The information one has about the impulse response usually consists of its values in a finite number of points. By eqn (*6*), the Markov parameters are derivatives of the impulse response at 0. Therefore, to obtain them one has either to differentiate numerically or to approximate the impulse response by some analytically given function and then differentiate analytically. This latter approach is followed in [3] where the approximation by Chebyshev polynomials is used. The authors formulate conditions under which this procedure is successful.

Our approach is based on Bruni's observation that if **A** is a stable matrix (*i.e.* the eigenvalues of **A** have negative real parts) then the quantities M_k defined by

$$M_0 = \Phi(0) = \mathbf{CB}$$
$$M_k = \frac{(-1)^k}{(k-1)} \int_0^\infty t^{k-1} \Phi(t)\, \mathrm{d}t = \mathbf{CA}^{-k}\mathbf{B}, \quad k = 1, 2, \ldots \tag{16}$$

are the Markov parameters of the system ($\mathbf{A}^{-1}$, **B**, **C**) [2]. The integral in the formula for M_k represents the $k-1$th noncentral moment of $\Phi(t)$. Knowing the

values of M_k one can consider them to be Markov parameters and compute their realization (or partial realization) ($\tilde{\mathbf{A}}$, **B**, **C**) from which **A** is obtained by inversion, $\mathbf{A} = \tilde{\mathbf{A}}^{-1}$

The advantage of this approach lies in the fact that it is easier to compute numerically the moments of an impulse response than its derivatives. On the other hand, as pointed out in [3], the neglection of the "tail" of the response (*i.e.* the approximation of the integrals in eqn (*16*) by integrals over a finite interval) leads to prohibitive errors in the values of higher moments. The reason lies apparently in the fact that multiplication by higher powers of t gives a great weight to the tail. In particular, it happens frequently that the matrix **A** of the realization is obtained unstable (it has an eigenvalue with positive real part).

As our results show this difficulty can be remedied by approximating $\Phi(t)$ for large values of t by an exponential

$$\Phi(t) = a\, e^{-bt} \tag{17}$$

$a > 0$, $b > 0$. Note that if $\Phi(t) = \mathbf{C}\, e^{t\mathbf{A}}\mathbf{B}$ is the response of a finite dimensional system with **A** having distinct eigenvalues with negative real parts and $\Phi(t) > 0$ for all $t > 0$ (as is the case for flow systems) then the eigenvalue λ_1 with largest real part has to be real, so we may write

$$\Phi(t) = \sum_{i=1}^{n} c_i\, e^{\lambda_i t} = c_1\, e^{\lambda_1 t}(1 + \omega(t)) \tag{18}$$

where the remainder $\omega(t)$ decays exponentially. This explains why for large t, $\Phi(t)$ can be approximated by eqn (*17*) fairly accurately.

The realization procedure using the moments includes the inversion of the matrix $\tilde{\mathbf{A}}$. This may be a problem if $\tilde{\mathbf{A}}$ is obtained singular or of small determinant. Nevertheless, this never happened for about 50 impulse responses of both ideal and real systems we have processed.

Of course, even if the tail of the impulse response is taken into account by eqn (*17*), there is no guarantee that the matrix **A** which one obtains would be stable. Indeed, it happened that some of the lower order partial realizations we had computed were unstable. Again, however, the best one has always been obtained stable.

Program MIPAR

For the recursive computation of minimal partial realizations of flow systems with scalar inputs and outputs we have designed a computer program MIPAR. Of course, the program can be used also for other than flow systems.

The data for the program consist of the values of the impulse response $\tilde{\Phi}(t)$ in up to 50 points, not necessarily equidistant. The program computes the normalized

response $\Phi(t)$ from $\tilde{\Phi}(t)$ by the formula

$$\Phi(t) = \frac{\tilde{\Phi}(t)}{\int_0^T \tilde{\Phi}(t)\,\mathrm{d}t} \tag{19}$$

where T is such that $\tilde{\Phi}(t) < \varepsilon$ for $t > T$ and ε is the measurement error. From the last 5—10 values of the response the program computes the values of a, b for the approximations (*18*) of the tail of $\Phi(t)$ by least-square estimation. The integral in the formulae (*16*) for the moments is computed numerically for $t < T$ and by the formula

$$\int_T^\infty t^{k-1}\Phi(t)\,\mathrm{d}t = \int_T^\infty t^{k-1} a\, e^{-bt}\,\mathrm{d}t =$$

$$= a\, e^{-bT} \sum_{i=0}^{k-1} \frac{T^i (k-1)!}{b^{k-i} i!} \quad \text{for} \quad t \geqslant T$$

The maximum of the number of Markov parameters the program can process is 19, the maximum for the dimension of the realization it can compute is 8. The program computes successively the matrices $(\tilde{\mathbf{A}}_n, \mathbf{B}_n, \mathbf{C}_n)$ of partial realizations of dimension n of the Markov parameters $Y_k = M_k$ obtained by eqn (*16*) by Rissanen's algorithm and then obtains the partial realizations $(\mathbf{A}_n, \mathbf{B}_n, \mathbf{C}_n)$, $\mathbf{A}_n = \tilde{\mathbf{A}}_n^{-1}$ of the response $\Phi(t)$ by the inversion of $\tilde{\mathbf{A}}_n$. It computes the eigenvalues of $\mathbf{A}$ and tests the controllability and observability of the realization. If $\mathbf{A}$ is stable and the realization is controllable and observable (and, thus, minimal), then the program transforms the realization to the canonical form (*12*) and computes the values of the impulse response by eqn (*5*). The computation is terminated as soon as either the computed response $\Phi_n(t)$ fits the data sufficiently accurately or the maximal dimension is reached. The quality of the realization is estimated by the integral

$$\gamma = \frac{1}{2}\int_0^T |\Phi_n(t) - \Phi(t)|\,\mathrm{d}t \tag{20}$$

Results obtained by MIPAR

We have tested the program on impulse responses of several ideal finite dimensional systems. We have found that as in the case of the controllability matrix of $\mathbf{A}$, $\mathbf{B}$, the controllability matrix of $\mathbf{A}^{-1}$, $\mathbf{B}$ showed an abrupt decrease of the entries in the $(n+1)$th row compared to the entries of the first n rows when n was the dimension of the minimal realization of the system. This can be illustrated on the following example:

For the input data obtained from the ideal impulse response

$$\tilde{\Phi}(t) = 10e^{-10t} + 0.75e^{-1.5t} - 1.5e^{-3t} \qquad (21)$$

the dimension of the minimal realization of which is 3 the first four rows of the controllability matrix are

9.24	−1	0.261	−0.176	0.13
0	0.158	−0.147	0.111	−0.075
0	0	−0.152	0.016	−0.013
0	0	0	0.00008	0.00011

(it is a property of Rissanen's algorithm that each row of the controllability matrix **Q** has at least one zero more than the preceding one).

We have used the MIPAR program to compute realizations of impulse responses of real systems. In particular, we have processed data from over 20 measurements of a rotational disc column (RDC) and a continuous stirred tank reactor, where mixing was provided by a jet and a diffusor. In both cases the impulse response has been obtained as follows:

The δ impulse has been simulated by a very short injection of 0.5—1.5 ml of saturated solution of KCl into the inlet flow. In order to determine the concentration of KCl in the outlet flow its conductivity has been continuously measured by a conductivity cell. The entire system has been temperated at 24°C. The relation between the conductivity and the concentration has been found to be linear under the conditions of the experiment. Therefore, the continuous measurements of conductivity could be directly used as the impulse response of the real system. For numerical processing of the data the values of the impulse response in 20—50 points have been used.

The impulse response of a particular RDC as well as the impulses of its partial realizations of dimension 1—7 can be seen in Fig. 1. The matrix **Q** is as follows

0	−1	2.09	−2.76	3.01	−2.95	2.7	2.33	1.93	−1.52
−1	0	1.61	−2.77	3.34	−3.47	3.32	−2.96	2.51	−2.02
0	0	0.61	−1.12	1.39	−1.45	1.40	−1.27	1.09	−0.89
0	0	0	−0.02	0.03	−0.03	0.03	−0.02	0.01	−0.01
0	0	0	0	0.005	−0.01	0.02	−0.02	0.025	−0.02
0	0	0	0	0	-8×10^{-4}	2×10^{-3}	-3×10^{-3}	4×10^{-3}	-5×10^{-3}
0	0	0	0	0	-6×10^{-6}	0	-1.3×10^{-5}	2×10^{-5}	-2×10^{-5}

Comparing this matrix with the response in Fig. 1 one can see the connection of the decrease of the entries in the $(n+1)$th row to the quality of the description of the system by its realization of dimension n. So, the significant decrease of the entries in the 4th row indicates a fair realization of dimension 3, while the increase of some of the entries in the 5th row indicates that the realization of dimension 4 will be worse. A decrease in the 6th row and a large decrease in the 7th row indicate that

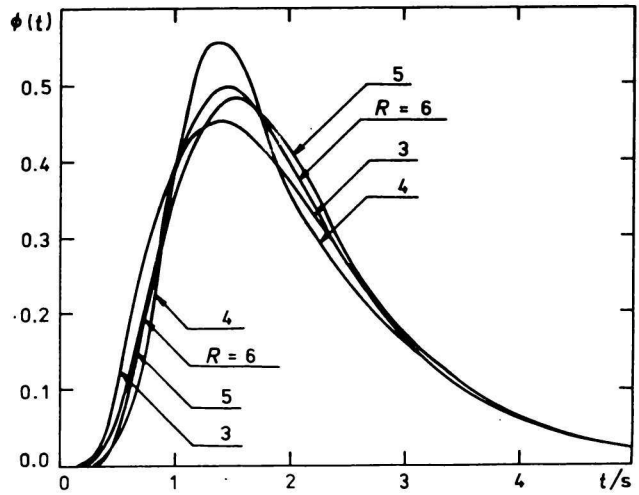

Fig. 1. Experimental and model impulse responses of a RDC (model of dimension 2 is unstable). n — Impulse response of the model of dimension n; R — experimental impulse response.

the natural dimension of the system is 6. These indications are confirmed by Fig. 1: the impulse response of the realization of dimension 6 is practically indistinguishable from that of the real system.

Let us note that most of the measurements of RDC have been processed also by the programs for modelling of flow systems by systems of coupled ideally stirred vessels with predetermined structures. Practically in all cases the dimension of the model was very close to the dimension of the best realization (in the case of Fig. 1 it was 5).

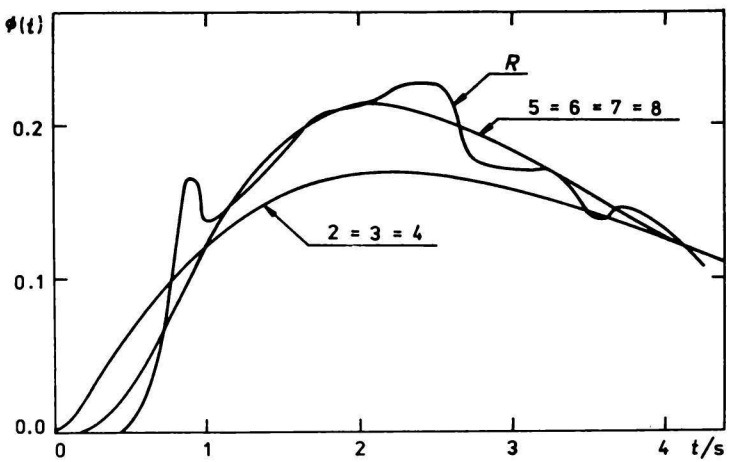

Fig. 2. Experimental and model impulse responses of a RDC.

Fig. 2 demonstrates the results of the realization of the impulse response of RDC under another flow rate. Again, we can see a good fit of the data and a tendency to smooth fast modes of the response.

Figs. 3 and 4 show the realizations of a continuous reactor. They demonstrate increasing accuracy with increasing dimension. Also, Fig. 4 indicates that the natural dimension of the system is 3.

Let us note that in some cases the accuracy of high dimensional realizations may be worse than that of lower dimensional ones. This may be caused by round-off errors as well as by the weight which is put on the tail of the impulse response by higher order moments.

When using the controllability matrix **Q** for the identification of the dimension of the system by the computer one has to build into the program an automatic test for the sufficiency of the decrease of the entries of the matrix. This may be a problem since for system of high dimension the decrease may be gradual. We have used the test

$$|q_{ij}| \leqslant \frac{d}{i-1}\left(\sum_{k=1}^{i-1} q_{kj}^2\right)^{1/2}, \quad 0<d<1 \tag{22}$$

$$|q_{ij}| \leqslant e, \quad e \ll 1$$

to be satisfied by the entries of the i-th row of **Q** in order that the dimension of the system is $i-1$, where the constants e, d had to be chosen for each type of systems separately. For RDC we have chosen the values $d = e = 0.001$, for the continuous reactor $d = 0.001$, $e = 0.005$.

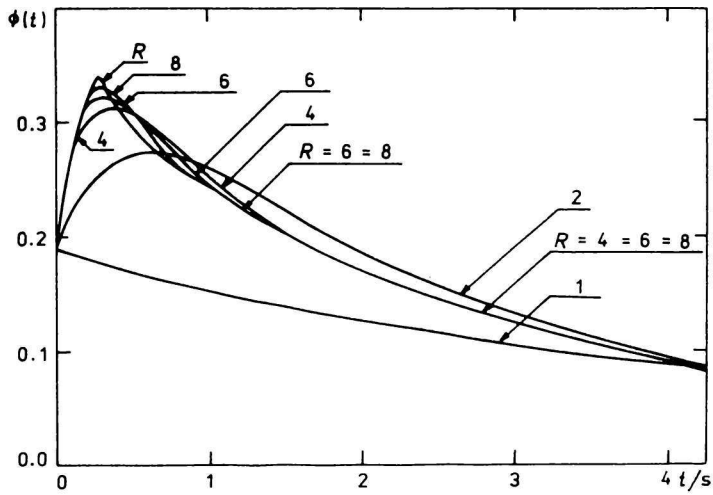

Fig. 3. Experimental and model impulse responses of a CSTR (models of dimension 2, 5, 7 are unstable).

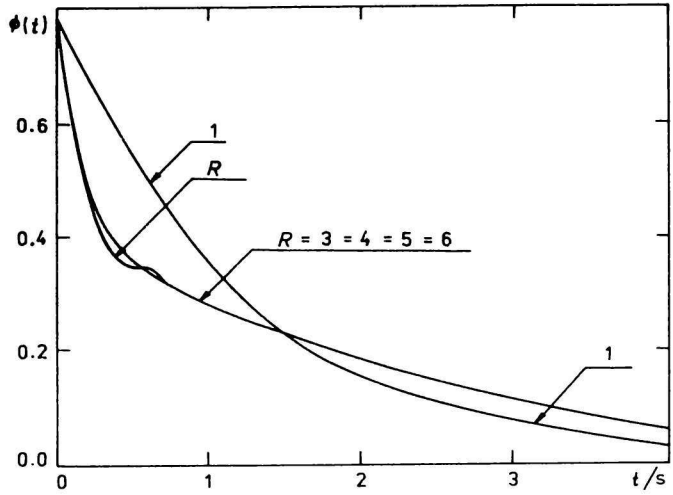

Fig. 4. Experimental and model impulse responses of a CSTR (model of dimension 2 is unstable).

By our experience we may say that the higher the dimension of the system, the larger can be d. The value of e increases with the value of

$$\bar{t} = \int_0^T t\Phi(t)\,\mathrm{d}t \tag{23}$$

This is connected with the choice of time scale and, thus, the slope of the impulse response.

Problem of physically meaningful realizations

As an advantage of model construction by realization techniques one may regard the fact that it is not necessary to predetermine the structure of the model. This, however, has a drawback: the coefficients of the model have no physical meaning in general. Since the possibility to change coordinates in the space gives some freedom for the construction of the model one may ask whether there exists a transformation that would bring the model into a form in which one could give the coefficients a physical meaning. One could for instance try to interprete the model as a system of interconnected ideally stirred vessels, the components x_i of the state space standing for the outlet concentrations of the particular vessel.

It is easy to see that in order that the system may be interpreted in this way it is necessary and sufficient that the following conditions be satisfied

$$a_{ii} < 0,\ a_{ij} \geq 0 \text{ for } j \neq i,\ b_i \geq 0,\ c_i \geq 0,$$
$$\sum_{k=1}^{n} a_{ik} + b_i = 1,\quad \sum_{k=1}^{n} c_k = 1 \tag{24}$$

where $i, j = 1, \ldots n$, $\mathbf{A} = (a_{ij})$, $\mathbf{B} = \text{col}\,(b_1, \ldots b_n)$, $\mathbf{C} = (c_1, \ldots c_n)$. Note that the last two conditions of eqn (*24*) can be rewritten as

$$\mathbf{A}\boldsymbol{i} + \mathbf{B} = 0,\quad \mathbf{C}\boldsymbol{i} = 1 \tag{25}$$

where $\boldsymbol{i} = \text{col}\,(1, \ldots 1)$. Fig. 5 shows the structure of such a system for $n = 2$.

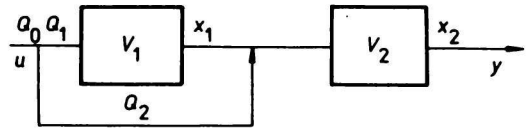

Fig. 5. System consisting of two ideally stirred vessels and the matrices of its mathematical description.

$$\mathbf{A} = \begin{bmatrix} \frac{Q_1}{V_1} & 0 \\ \frac{Q_1}{V_2} & -\frac{Q_0}{V_2} \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} \frac{Q_1}{V_1} \\ \frac{Q_2}{V_2} \end{bmatrix} \quad \mathbf{C} = (0, 1)$$

The structure of the system is reflected in the zeros of the matrices **A**, **B**, **C** — they correspond to missing connections. If one could prove that each state space model of a flow system could be transformed into a form satisfying conditions (*24*) with a uniquely defined structure (by this we mean the placement of zeros in **A**, **B**, **C**), then this structure could give some information about the hydrodynamics of the system.

We have not been able to settle the question whether and under what conditions a transformation bringing the system into a form satisfying conditions (*24*) exists. As for the question of uniqueness of structure, it has, unfortunately, a negative answer, as the following example demonstrates.

Consider a system of the structure given in Fig. 5 with $Q_0 = 2$, $Q_1 = Q_2 = 1$, $V_1 = 1$, $V_2 = 1$ which has the state-space representation

$$\dot{x}_1 = -x_1 + u$$
$$\dot{x}_2 = -2x_2 + x_1 + u \tag{26}$$
$$y = x_2$$

where x_1, x_2 stand for the outlet concentrations of the first and second reactor, respectively and u, y stand for the inlet and outlet concentrations of the system, respectively. This system can be rewritten into the standard vector-matrix form (*1*) with

$$\mathbf{A}=\begin{bmatrix}-1 & 0\\ 1 & -2\end{bmatrix}\quad \mathbf{B}=\begin{bmatrix}1\\ 1\end{bmatrix}\quad \mathbf{C}=(0,1) \tag{27}$$

Note that the second entry in the first row of **A** is zero which reflects the fact that there is no flow from the second to the first reactor.

The state-space transformation $\boldsymbol{x}=\mathbf{T}\tilde{\boldsymbol{x}}$ with

$$\mathbf{T}=\begin{bmatrix}1-\delta_1 & \delta_1\\ \delta_2 & 1-\delta_2\end{bmatrix} \tag{28}$$

brings the system into the form

$$\begin{aligned}\dot{\tilde{\boldsymbol{x}}}&=\tilde{\mathbf{A}}\tilde{\boldsymbol{x}}+\tilde{\mathbf{B}}\boldsymbol{u}\\ \boldsymbol{y}&=\tilde{\mathbf{C}}\tilde{\boldsymbol{x}}\end{aligned} \tag{29}$$

with $\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$ related to **A**, **B**, **C** by expression (*10*). By chosing δ_1, δ_2 sufficiently close to 0 the matrices **T**, $\mathbf{T}^{-1}$ can be made arbitrarily close to the unit matrix, so $\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$ can be made arbitrarily close to **A**, **B**, **C**, respectively. In particular, since a_{11}, $a_{22}<0$, $a_{21}>0$, they can be chosen so small that

$$\tilde{a}_{11},\tilde{a}_{22}<0,\ \tilde{a}_{21}>0 \tag{30}$$

Since $\mathbf{T}\boldsymbol{I}=\boldsymbol{I}$, we have by expression (*10*)

$$\mathbf{A}\boldsymbol{I}+\mathbf{B}=\mathbf{T}^{-1}(\mathbf{A}\mathbf{T}\boldsymbol{I}+\mathbf{B})=\mathbf{T}^{-1}\mathbf{0}=\mathbf{0} \tag{31}$$

$$\mathbf{C}\boldsymbol{I}=\mathbf{C}\mathbf{T}\boldsymbol{I}=\mathbf{C}\boldsymbol{I}=\boldsymbol{I} \tag{32}$$

Finally, for $0<\delta_1,\ \delta_2<1/2$ we have

$$\tilde{a}_{12}=\delta_1>0 \tag{33}$$

Comparing expressions (*30—33*) to expressions (*24*) we can see that for δ_1, δ_2 sufficiently small the system ($\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$) can be interpreted as an interconnected system of two ideally stirred reactors. Since $a_{12}>0$ this system includes a flow from the second to the first reactor, which means that its structure is different from that of (**A**, **B**, **C**).

Conclusion

By modifying the computation of the moments of the impulse response the realization algorithms based on moments can be made effective and satisfactorily precise. The program realization MIPAR of this method is fast and convenient to use. As its results one obtains partial realizations of several dimensions from which one can choose the most suitable one. Also, the program allows to compute the canonical form of the realization (and, thus, its transfer function) as well as the eigenvalues of the matrix **A**, which can be used for checking the stability of the model as well as for the computation of the responses of the system.

As compared to classical methods of constructing models of flow system from input-output data the realization algorithm has the advantage that it contains no iterative numerical procedure. Also, it does not require a preliminary choice of the structure of the model. On the other hand, it gives no information about the hydrodynamics of the flow inside the real system.

Symbols

t time
$\boldsymbol{u}$ vector of input variables
$\boldsymbol{x}$ vector of state variables
$\boldsymbol{y}$ vector of output variables
$\Phi(t)$ impulse response (normalized)
$\bar{\Phi}(t)$ impulse response (not normalized)
Y_k the k-th Markov parameter
$\mathbf{H}$ Hankel matrix of Markov parameters
$\mathbf{P}$ observability matrix
$\mathbf{Q}$ controllability matrix
s complex variable
$Y(s)$ transfer function

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