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ALGEBRAIC DESCRIPTION OF TECHNICAL CHEMICAL SYSTEMS I.

THE SIGNIFICANCE OF MODERN ALGEBRAIC METHODS IN CHEMICAL SYSTEMS ENGINEERING

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The series of papers entitled algebraic description of technical chemical systems has the following chapters:

material systems and transformations,
combination and projection of material systems,
technical chemical operators,
compositions of technical chemical operators,
generalization of the set of technical information.

The possible applications of systems theory, systems engineering and modern algebra in technical chemistry are discussed in the introductory paper, and the position, assignments and expected results of the algebraic treatment are defined. The following tasks are encountered in the study and optimalization of technical chemical systems:

1. Qualitative description and study of technical chemical systems.
2. Study of the functions interpreted on technical chemical systems and of the connections of these functions with one another.
3. Optimalization of static systems.
4. Description, control and optimalization of dynamic systems.

Modern algebraic methods of treatment are adequate for the solution of the first task, a fact that will be confirmed by later papers to be published in this series.

INTRODUCTION

The task of every technical science, and also of technical chemistry is the study of material (or energetical) systems, which - directly or indirectly - serve to satisfy some sort of demand. Accordingly, the task of technical chemistry is the study of systems, which permit the production of a product or final product of the desired properties from the raw material.

Prior to their design, the systems have to be vigorously studied. The claims defining the final product and the transformations producing it must be defined and a theoretical model must be constructed in this manner. The elements of the theoretical model must be scrutinized with regard to the conditions of their realization. When, during the analysis of the theoretical model, the "building bricks" of the system are reached, the physical entities corresponding to these must be found,i.e. the system that is found to be adequate from a theoretical point of view, must be "questioned", bearing in mind the problems of practical realization. The next step is the task of synthetizing, building up the complex physical system and its study while in operation.

In the study of both the theoretical model and the actual operating system as a whole, the treatment based on systems theory is of considerable assistance.

General systems theory was introduced by the justified endeavour towards uniform science. There is no intention here to describe the individual trends, but a few basic concepts taken from the introduction to the selected essays on systems theory,published in 1971 are quoted [1]:

"... Operation research deals with the operation of existing systems, whereas systems engineering is the totality of methods used for designing systems. The two approaches cannot be sharply separated in practice, and from a theoretical point of view they converge to the general systems theory.

- The first step of systems engineering is: specification of what is demanded, and the definition of the claims.

- This is followed by modelling and identification of the given parts of the system. The variables should be chosen and the equations describing their connections should be established.
- The next step after analysis of the equations is the synthesis, i.e. a description of the model of the whole system in accordance with the previously established specification. Systems synthesis mainly consists of the theory of optimalization.
- Finally, the last step of systems engineering is the designing, i.e. the decomposition of the model obtained during synthesis to its physical components".

It is apparent from the foregoing that the formulation of the problems in accordance with systems engineering and the level of demands, which at the present time is a necessity in the study of technical chemistry, have to conform to each other.

The idea of applying the results of systems theory and systems engineering in technical chemistry seemed self-evident, because the results obtained in this way are of general validity and can be utilized in other fields of science.

In order to be able to characterize the technical chemical systems and their characteristics, their mathematical models must be established.

The totality of physically or mentally encompassed elements, in which the elements are in a direct or indirect relation to any of the others, may be defined as a system.

It is an unequivocal fact that technical chemistry deals with materials. These materials in themselves can be regarded as systems. They represent the manifestation of a number of material properties, there are certain relations between these properties and accordingly they can be regarded as elements of the material systems. The totality of these material systems - including also raw materials and final products - comprises the <u>set of material systems</u>.

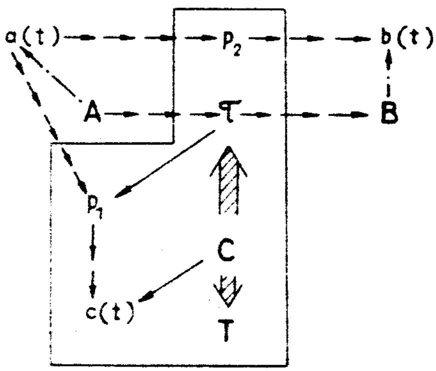
Chemical technology produces different materials (products) from the given elements of a set of material systems, i.e. it projects the set of material systems upon itself. In mathematics such a system is termed an operator, and accordingly, in the following a system producing a final product from a raw material is termed a chemical technological operator. A system of operators possesses a definite internal structure. In a similar manner to that applied in the case of material systems, a <u>set of technical chemical operator systems</u> can be defined.

During the realization of a concrete technological process, a connection is established between the individual elements of the sets described in the foregoing. The system produced in this manner is termed a <u>technical chemical system</u>, which includes

raw material systems,
operator systems and
final product systems.

The <u>set of these technical chemical systems</u>, together with all the information they contain, represent <u>technical chemistry</u>.

The structure of the systems is demonstrated in the following Figure:



The C technological operator system produces a material system B from material system A. System C comprises (τ) functional and

T existential parts. (τ) is the totality of the elements of the system which are necessary for the operator function, whereas T represents those necessary for the existence of the system. (τ) can be resolved to two operators: p_1 and p_2. The systems are regarded as function systems, so that A corresponds to a(t), B to b(t) and C to c(t). Any changes in a(t) act upon c(t) through operator p_1, and upon b(t) through operator p_2 (where t is time). In general, when studying a system, it was only the function systems and their connections which were studied, and very rarely the structure of the system. However, in our opinion, the latter is the first step. It must be known first, what sort of an operator is adequate to transform system A into system B; knowledge of the concrete function connections comes only after this.

With regard to the foregoing, the main points of view and characteristics of technical chemical systems theory can be summarized in the following.

1. Algebraic description

The process of the satisfaction of the demand can be regarded in the following manner: a system of Γ_o initial state (state of unsatisfied demand), upon the action of the final product A_v - as an operator - becomes state Γ_v (state of satisfied demand):

$$A_v [\Gamma_o] = \Gamma_v \tag{1}$$

A demand can be e.g. the depression of the temperature of a patient in a feverish state. In this case

Γ_o - is the feverish state,

Γ_v - is the normal state,

operator A_v - is a pharmaceutical product,an antifebrile medicine.

A quantitative and economic description of the satisfaction of the demand can be expressed by the expenses of the satisfaction of the specific demand:

$$N\Gamma = G(A_v) \cdot N\tau(A_v) \qquad (2)$$

where

$N\Gamma$ - is the expense of satisfaction of the specific demand,

$G(A_v)$ - is the amount of product needed for satisfaction of the specific demand,

$N\tau(A_v)$ - is the expense of the final product.

Accordingly, the task is to design an A_v material system which is capable of bringing the passive system from the state Γ_o to state Γ_v with a minimum expense.

The final product A_v, which satisfies the demand, is produced from the raw material A_o by the action of the technical chemical operator T:

$$T\left[A_o\right] = A_v \qquad (3)$$

Consequently, the process in which a demand is satisfied can also be regarded in the following manner: the passive system in state Γ_o is brought to state Γ_v by the joint action of the raw material A_o and the technological operator T. Accordingly, the following is gained by uniting Equations (1) and (3):

$$T\left[A_o\right]\left[\Gamma_o\right] = \Gamma_v \qquad (4)$$

It is apparent that the expenses of the satisfaction of the demand depend on the raw material and on the technological process used. If the A_o raw material is given - and this is the most frequent case - the technological process involving a minimum of expense can be found.

Technological processes are built up of technological stages and accordingly the technological (technical chemical) operator can be resolved into part-operators.

The operator $\mathbf{R}_1$, which carries out the first technological stage, transforms the raw material A_o into an intermediate product A_1:

$$R_1[A_o] = A_1 \tag{5}$$

In the second technological stage, material A_1 is transformed to material A_2 by the action of operator R_2:

$$R_2[A_1] = A_2 \tag{6}$$

and in the n^{th} stage:

$$R_n[A_{n-1}] = A_v \tag{7}$$

Accordingly, the total technological process can be described by:

$$\prod_{i=1}^{n} R_i[A_o] = A_v \tag{8}$$

It follows from the foregoing that the technological process is defined by the following facts: operators that realize the technological stages to be employed and in what order they are employed.

Technical chemical operators - as opposed to mathematical operators - possess a unique structure, which can be characterized by the following formula:

$$R\ [V,\ A,\ R]$$

where

V - is the transformation realized by the operator,
A - is the material supply of the operator,
R - is the totality of the operator elements necessary for the operator to exist, i.e. existential structure (e.g. apparatus).

This form of representation differs from the usual methematical representation, but it seems reasonable to immediately write after the operator its structure in brackets, rather than the material system upon which it acts. This form of representation will be used in the following. The transformation of the material system upon the action of the operator will be designated in the following manner:

$$A_o + T = A_v \qquad (9)$$

or

$$A_o + R_1 = A_1 \qquad (10)$$

These equations express the same facts as equations (3) and (5), written in the conventional form.

The transformation of the material system may proceed in time:

$$A_{to} + R_1 = A_{tv} \qquad (11)$$

where

A_{to} - is the material system introduced at the beginning,
A_{tv} - is the material system taken away after the transformation,

or it may proceed according to place:

$$A_{yo} + R_1 = A_{yv} \qquad (12)$$

where

A_{yo} - is the input material flow,
A_{yv} - is the output material flow.

If changes occur with respect to both time and place (unstationary system), the following can be written:

$$A_{to} + A_{yo} + R = A_{tv} + A_{yv} \qquad (13)$$

By studying their structure, the operators that realize the technological stages can be resolved to further components.

Operators which bring about one single elementary change - upon whose action only one property of the material system is changed - are termed elementary operators.

Technological stages that include more than one elementary change can be realized by a composition of elementary operators. Operator systems constructed in this manner can be classified into two main groups:

1. The two or more operators which form the operator system - and whose existential structure is identical - act jointly in space and time.

$$R_a\left[V_a, A_a, R_{\underline{a}}\right] \wedge R_b\left[V_b, A_b, R_{\underline{a}}\right] = R\left[V_a \wedge V_b, A_a \wedge A_b, R_{\underline{a}}\right] \qquad (14)$$

This group comprises:

operators of total change,
composite operators.

1.a) Operators of total change are encountered if an elementary operator - due to the permitted single change - would lead to production of a non-existent, fictive material system and consequently the action of further elementary operators is necessary to obtain a real, existent material system. The operator of total change is the combination of the minimum number of elementary operators which permit production of a non-fictive material system as a final product.

For example, the preparation of solid crystalline material from a solution may be regarded as the result of four elementary changes:

separation of material from the solution,
attainment of the crystalline structure,
attainment of form,
attainment of dimensions.

The first operator, which makes the material to be separated from the solution, leads to a fictive system, since there is no solid matter without form and dimensions. Accordingly, in this case the operator of total change comprises four elementary operators.

1.b) If there is no fictive material system among the products of the elementary operators acting together, a composite operator is encountered.

2. The existential structure of the elementary operators is different, the action of the operators is separated in space or time, and any connection between the operators can be realized only through the material system. Depending on the fact, whether the material system ensuring the connection is variable in time or space, we can speak of an

operator block and,
an operator series.

The continually more sophisticated systems, ranging from the elementary operator to the operator series, can be resolved to elementary operators.

Such a resolution of the technological stages and the defining of the possible types of operator structure represents the qualitative description of technical chemical operators.

2. Analytical description and optimalization

The quantitative description is obtained if the $x_1, x_2, \ldots x_n$ functions - their total number being n_F - are interpreted in connection with the elements of the operator structure, and the z function in connection with the change V. The number of the connections between the functions is n_k.

The number of free functions is:

$$n = n_F - n_K \tag{15}$$

The solution of the n_K functions for a system of elementary change is

$$f_i \left[z, x_1, x_2, \ldots x_n, A'', A''', R\right] \tag{16}$$

where

A'' - is the auxiliary material,

A''' - is the packing material.

In the case of any type of systems of composite change the following is gained:

$$RF_i\left[Rf_1,\ R\ f_2,\ \ldots\ z,\ A_r,\ A_t\right] \qquad (17).$$

where

A_r - is the recirculated material,

A_t - is the block auxiliary material.

The expense function will now be considered in connection with the system of elementary change:

$$Nf_i\left[z_o,\ z_v,\ x_1,\ x_2,\ \ldots\ x_n,\ A'',\ A''',\ R\right] \qquad (18)$$

by defining the auxiliary materials $\mathring{A}''$, $\mathring{A}'''$ and the structure $\mathring{R}$, the optimal values of the free functions can be obtained:

$$Nf_i\left[z_o,\ z_v,\ \hat{x}_1,\ \hat{x}_2,\ \ldots\ \hat{x}_n,\ \mathring{A}'',\ \mathring{A}''',\ \mathring{R}\right] \qquad (19)$$

If the most preferable auxiliary materials and structures are chosen, the optimum function of the system of elementary change will be

$$\hat{N}f_i(z_o,\ z_v) \qquad (20)$$

The expense function, considered for a system of composite change, is

$$\hat{N}F_i(\hat{N}\ f_1,\ \hat{N}f_2,\ \ldots\ z_o,\ z_v,\ A_v,\ A_t) \qquad (21)$$

When the preferable values for A_v and A_t are chosen:

$$\hat{N}F_i(z_o,\ z_v) \qquad (22)$$

The permutations of the isomorphous operator systems are the following:

$$N_{e,i} = \hat{N}F_1(z_o, z_1) + \hat{N}F_2(z_1, z_2) + \dots \hat{N}F_{j+1}(z_j, z_v) \qquad (23)$$

When the most preferable permutation and optimal z_1-z_j values are chosen:

$$\hat{N}_{e,i}(z_o, z_v) \qquad (24)$$

The permutation of the operators of different changes gives the expense of the technological system:

$$\sum_i \hat{N}_{e,i} = N\tau\ (P_M, A_o, A_v) \qquad (25)$$

where P_M represents the permutations, the various permutations being the technological procedures. When the most preferable are chosen from among these:

$$\hat{N}\tau(A_o, A_v) \qquad (26)$$

and an adequate starting material is chosen:

$$\hat{\hat{N}}\tau(A_v) \qquad (27)$$

Returning to equation (2) and taking (27) into consideration, the expense of satisfying the specific demand is obtained:

$$N\Gamma = G(A_v) \cdot \hat{\hat{N}}\tau\ (A_v) \qquad (28)$$

To find the A_v pertaining to the minimal $N\Gamma$; this is

$$\hat{N}\Gamma$$

which was the original task.

So far it was not mentioned that part of the functions interpreted in connection with qualitative elements does change or fluctuate in time, even in the case of systems of continuous operation (e.g. the temperature of input cooling water).

The task of process control is to change a second input signal, in the case of variations in a first input signal, in such a way as to have an unchanged output signal.

If there are fluctuations in the input signal - to keep these fluctuations between given limits is the controlling task - the optimum defined in the foregoing, together with the expense pertaining to the optimum, will also be changed. The smaller the fluctuation, the lower the original expense of the system; at the same time, the controlling operation, intended to decrease the fluctuations in the input signal, acts as an expense-increasing factor.

Accordingly, the preferable control degree must be found by means of a further optimalization calculation.

The controlling operation applied may be regarded as optimal, if the input signals are controlled so as to attain minimal total expenses.

On the basis of the foregoing, the most important questions, which must be dealt with during the application of systems theory in technical chemistry, can be summarized.

1. Qualitative description and study of technical chemical systems.

2. Study of the functions interpreted in connection with technical chemical systems and of the connections of these functions with one another.

3. Optimalization of static systems.

4. Description, control and optimalization of dynamic systems.

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РЕЗЮМЕ

В серии сообщений под заглавием"Алгебраическое описание систем технической химии" предположено автором заниматься следующими разделами:

материальные системы и превращения,
объедимение материальных систем и их проекция,
операторы технической химии,
композиция операторов технической химии,
генерирование множеств информаций технической химии.

В вводной публикации показаны возможности применения теоремы систем, системотехники и современной алгебры в технической химии, и определены место, задачи и ожидаемые результаты алгебраического способа подхода. При изучении и оптимизации систем технической химии предстоят следующие задания:

1. Качественное описание систем технической химии и их испытание.
2. Изучение функций, действующих в данной системе технической химии, а также и их взаимных связей.
3. Оптимизация статических систем.
4. Описание динамических систем, их управление и оптимизация.

Для решения первой из указанных задач исключительно пригодным является алгебраический способ подхода, как это будет представлено в следующих сообщениях серии.