METHODS FOR INVESTIGATING THE STABILITY OF EQUIP-MENTS USED IN CHEMICAL ENGINEERING*

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Knowledge of the properties of the equipment subject to controlling is the precondition of adequately designed simple control circuits as well as complex systems of control. This means that the quantitative relationships of the process characteristics must primarily be known, for only then can the structure of the controlling equipment required for attaining a given goal of controlling be determined.

Mostly, our knowledge of chemical processes is incomplete in this respect (only a fraction of the necessary data are to be found to figure in relevant literature), the designing of the controlling equipment must, therefore, usually be preceded by an investigation with the object of establishing the quantitative relationships mentioned above.

It is expedient to make use of the technological flow diagram of the process in question as an aid in the investigation. First, the controlled process must be delimited on the basis of the flow diagram. This delimitation is necessary both for reasons of engineering and of economy.

After a study of the delimited process (to be denoted shortly as process in the following), its detailed block diagram must be established. The block diagram incorporates all of the variables of the process that are essential from the aspect of control, together with their causative relations.

The process is subdivided into adequately chosen operational units in order to build up the block diagram.

The block diagram outlined above does not supply information on the relationship of the input and output variables of the operational units inasmuch as it does not specify which input variable acts essentially upon which output variable. A supplement is, therefore, required for every block (except, of course, those which possess only a single output and input variable) to unequivocally illustrate the relationships of the variables. Expedient for this purpose are tables whose columns constitute the output variables and whose rows denote the input variables of the same operational unit, the signs inscribed in the

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squares of the table referring to the relationship of the given input and output variables.

The relationships of the input and output variables of the operational units can be determined in various ways. One way is to determine the action of certain input variables on certain output variables on the basis of preliminarily known (flow, heat-transfer, reaction, etc.) equations or empirical relations by means of theoretical considerations, and then to establish the magnitude of these actions. It must be noted, however, that this procedure is feasible and will result in satisfactory results only if the individual operational units are not overly complicated and do not involve an excessive number of state variables determining the course of the operations.

The other way, which, however, can be applied only to processes that have already been realized, consists of the observation of the process and of subsequent analysis [11].

Investigation of the controlled process consists, in both cases, of determining the static variables, investigations on stability and determination of the dynamic behaviour.

Determination of the static variables will not be given separate consideration since they form a part of the dynamic investigations. However, the question of whether the steady state condition [3] alone determines the behaviour of the system from the viewpoint of control engineering must, necessarily, be dealt with.

When subjecting systems of chemical engineering to investigations, most authors find it sufficient to investigate the steady state condition, justifying this as follows:

(a) The system cannot be subjected to dynamic investigation on account of its complexity.

(b) If all of the input variables determining the output variables of the operational unit are kept at constant value, the system remains in the state of equilibrium.

The first statement is true on account of insufficient knowledge of the processes and equipments in chemical engineering. Consequently, the thorough study of every system in chemical engineering demands intensive theoretical and practical work. (For instance, the preparation of a programme for the control by computer of certain distillation towers requires several hundreds of engineer-years.)

The second statement is wrong. The causes are the following:

(a) The constancy of all of the input variables can never be ensured in practice since the output signals of systems in chemical engineering are affected not only by modifiable variables but also by external variables (e.g. by catalyst activity, by ambient temperature, etc.) which cannot be maintained at constant values. This is on the one hand. On the other hand, every closed-loop

control possesses an inherent fault due to which not even the modifiable variables — whose constancy we wish to ensure by means of some closed-loop control — can be maintained at the required constant level when the system is subjected to disturbances.

(b) Even if all of the input variables can be successfully maintained at a constant level, the system may still be subjected to the phenomenon of self oscillations.

It is evident from the preceding that a dynamic investigation is a necessary condition of the appropriate operation of systems in chemical engineering. Systems of various types have, therefore, been recently subjected to numerous attempts to investigate their stability. They will be discussed in the following.

The dynamic behaviour of a system can frequently be specified by means of the methods determining the stability of systems in the chemical industry as well. Consequently, these two investigations will not be conducted separately.

1. Investigations on linear systems

The methods described in this paragraph assume the system subject to investigation to be linear. This implies that the relationship between the output and input signals of the system subject to investigation is described by a linear differential equation.

The methods of investigation considerably differ for one and for several input signals, for concentration and dispersion in space, and for simple or multiple feedback (the latter will not be dealt with).

1.1. Investigation by typical input signals

The essentials of the described method are the following: Any delay time is eliminated by the coordinate transformation of the transfer function, then the values of the dependent variable are substituted into the n-fold integral of the function at as many points of the curve as many constants of the equation describing the curve must be determined.

One of the conditions of applying the method is that the shape of the transfer function of the system must be known. Therefore, the object is to determine the constants of the transfer function.

The values of the determined constants are mostly informative only and are acceptable solely for establishing the order of magnitude of these values.

The method can be used only if the system can be given a relatively large input step. This, however, cannot be done without greatly disturbing the system to a considerable extent; the method is, therefore, impractical.

1.2. Investigation by sinusoidal input signals

Output signals pertaining to sinusoidal constant frequency input signals are measured. The value of the constant frequency must include the entire range of frequencies ($0 < \omega < \infty$). The quotient of the complex numbers formed by means of the amplitudes and phases of the input and output signals gives the transfer function.

In equipments in chemical engineering, the high-frequency range can only but seldom be attained as the amplitude of the output signals is small — on account of the great inertia of the systems — and phase lag is very great. That is why the measurement of the output signal is entirely unfeasible or else meets with difficulties. The method, as a consequence, can be used only infrequently.

VOLJTER's article [15] on the automation of reactors used in the synthesis of ammonia constitutes a good example for the joint application of this method and of the one described in the preceding paragraph.

1.3. Investigation by stochastic input signals

The input signal of the system is the sum of the original input signal and of a constrained white noise [4].

The power density spectrum formed from the cross-correlation function of the noise and output signal yields the transfer function

$$\Phi_{bk}(s) = Y(s)\,\Phi_{bb}(s),$$

where

$\Phi_{bk}(s)$ is the power density spectrum of the cross-correlation function of the input and output signals,

$\Phi_{bb}(s)$ being the power density spectrum of the autocorrelation spectrum of the input signal [4].

The method can be used in that instance when the limit frequency of the noise generator is higher than that of the system subject to investigation and when the noise and the original input signal are not correlated.

The advantage of the method is that it can be used in the case of several input and output signals (which, however, must be in linear relationship) as well.

A broader use of this method was hitherto restricted by the expensiveness and complicated design of the correlator figuring in the block diagram, and by having to convert the signals transmitted by the system into electric signals used by the correlator previous to introducing them into the latter.

1.4. Linear systems with several variables

If the system possesses an m number of input signals and an n number of output signals, then the relationship of the output signals and input signals is

$$Y = \bar{X} \; \bar{G},$$

where

$$\bar{X} = [X_1; \; X_2 \; \dots \; X_m],$$
$$\bar{Y} = [Y_1; \; Y_2 \; \dots \; Y_n],$$

the row matrix of the Laplace transforms of the input and output signals,

$$\bar{G} = \begin{bmatrix} G_{11} \dots G_{1n} \\ \vdots \quad\quad \vdots \\ G_{ml} \dots G_{mn} \end{bmatrix}$$

the so-called transfer matrix.

The relations between the individual input and output signals (i.e. the individual elements of the transfer matrix) can be determined by the stochastic method described in the preceding paragraph.

The method was employed for the investigation of a rectifying column by AMUNDSON [5].

1.5. Distributed parameter systems

The differential equations characterizing the system are partial differential equations since the output signal (or output signals) of the system is a function (or functions) of time as well as of the location parameter.

The investigation of such systems that are describable with partial differential equations can be simplified by the analysis of the transformed differential equation obtained by the Laplace transformation of the equation. If, besides time, we have only a single independent variable, then the transformed equation is an ordinary differential equation. The method is applicable if the partial differential equation describing the system is linear and its Laplace transform exists. This method has been used at our Institute for investigating the stability of isothermal tubular reactors [13].

2. Investigation of nonlinear systems

General methods are available for the discussion of linear systems, yet no general procedure is known as usable with nonlinear systems. This is due among others to the diversity of the various nonlinear functions.

The properties of nonlinear systems considerably differ from those of linear systems. Thus, for instance,

(1) The characteristics (not only the magnitude) of the output signal of a system are functions of the magnitude of the input signal (e.g. diverse products may appertain to various temperatures in catalytic reactions).

(2) The stability of a system is a function of the properties of the input signal also (e.g. the system may develop self oscillation within a given range of temperatures and feeding speeds in certain polymerization reactions).

(3) The amplitude and phase of a system depend also on the direction of the change of frequency. (It may be assumed on the base of certain results of measurements that in industrial reactors, the rate of reaction of the synthesis of ammonia is a function of the direction of the change of temperature as well.)

On account of the diverseness of nonlinearities, the methods of our investigation are each applicable to a group of nonlinear systems. The most important methods for investigating the stability of nonlinear systems will be described in the following.[1]

2.1. Linearization

The essentials of the method are the following. In the vicinity of some working point, the time function of the system is substituted by the approximation of the first order of its Taylor's series.

The method is applicable if
(a) the function is
    (A) continuous,
    (B) analytical,
    (C) monovalent
    in the range subject to investigation;
(b) small changes are being investigated;
(c) the Taylor's series converges rapidly.

From among the above conditions, (C) is frequently not fulfilled (e.g. two temperatures may appertain to a given conversion, etc.). If the system is affected by excessive disturbance, (b) neither will be fulfilled (this occurs rather frequently at breakdowns).

Condition (c) is frequently unfulfilled as well (with functions possessing extreme values or with exponential functions describing the dependence of a chemical reaction on temperature in the practically important range of temperatures).

The method and its errors can be studied on the lectures by HOFTYZER and ZWITERING [12].

The lecturers investigated the high-pressure polymerization reaction of ethylene as functions of oxygen concentration, pressure and temperature.

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[1] Methods founded on the solution of differential equations will not be dealt with in spite of their importance increasing with the spread of computers.

Writing down the equations of the conservation of mass and energy (having neglected the dependence on location of diffusion, concentration (C) and temperature (T), complete permixture having been assumed), then by expanding the equations into Taylor's series according to C, T, and by applying approximation of the first order, they obtained a linear system of differential equations in the close vicinity of the working point.

The stability of the obtained linear system of differential equations was investigated by means of Ljapunov's first criterion of stability. It was found that industrial reactors do not always operate at a stable range. Its cause (i.e. that the system was self oscillating) could not, however, be established due to the limitations of the method.

The conditions of the applicability of the method can be determined only by investigating the original nonlinear system which frequently causes difficulties or is unfeasible.

2.2. Phase plane methods

The use of the so-called phase plane methods for investigations on various systems in chemical engineering is being dealt with increasing frequency in the literature in recent years. We shall not discuss the individual methods on account of their great number and because of the difficulty of offering short descriptions [1], we only wish to point out that AMUNDSON et al. have written numerous articles on this subject (e.g. [7]).

Use of the phase plane methods involves the advantage of being able to investigate the original differential equation (all other methods incorporate certain neglections); the results obtained with these methods are therefore true.

Phase plane methods, at present, lend themselves only to the investigation of autonomous systems that can be described, at best, with differential equations of the second order.*

Differential equations of the third, or of higher, order can be investigated by means of phase space methods or with phase space methods with more than three dimensions. In contradiction to the phase plane method their common disadvantage is the lack of descriptiveness.

2.4. Method of Ljapunov's functions

The basis of the so-called Ljapunov's method is all follows. If some V function of the solutions of the differential equation of a system of n-th order is a definite Ljapunov function and if the first differential quotient according

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* Some attempts have recently been made to investigate nonautonomous systems as well [10].

to time (W) of V is also definite (or semidefinite), furthermore, if the signs of V and W differ, then, according to Ljapunov, the system is considered stable [4].

One of the first attempts to investigate the stability of chemical reactors by Ljapunov's second method is constituted in an article by BERGER and PERLMUTTER [9] who subjected the stability of adiabatic reactors to investigation for the following cases:

1. When the constants figuring in mass and energy equations (density, specific heat, velocity, heat transfer coefficient) are real constants.

2. The effect of diffusion is negligible.

3. Concentration and temperature are not functions of the location coordinate.

2.5. Numerical methods

The simplest (and frequently the only) method for investigating real systems is graphical integration. (Pains are taken, however, to use analytical methods whenever possible on account of the cumbrousness of the method.) Figuring among these is the method of isoclines, furthermore the method suggested by LIENARD [2] and RUNGE [1].

The first two methods are related to phase plane methods, the third being serviceable for any method and is illustrated by AMUNDSON's article [6] describing the investigation on the dynamics of a certain polymerization process.

2.6. Analysis by regression

The method is the following: we endeavour to find an empirical relationship — on the basis of data obtained by measurements — between the individual parameters characterizing the system. Two cases may occur:

(a) All of the variables are known. The obtained functional relationship is a constant relationship in this case.

(b) Not all of the variables are known. Then the functional relationship will also vary according to the effect of the unknown variable.

The principle of the method is as follows:

Let the multitude of points of measurement be considered the image of a given functional relationship. The constants figuring in the functional relationship of given shape are determined by means of the minimum square error method. The problems arising during application are the following.

(1) If the functional relationship cannot be defined with a linear equation, then there is no general method to indicate the nonlinear function with which an attempt can be made to approximate the system. The search for an adequate functional relationship entails tedious trial and error as well as voluminous numerical work.

(2) The method being founded on the analysis of data of measurement, a correct result will be obtained only when data are available of the entirety of the surface of the function in sufficient density. Usually, this condition is not fulfilled — indeed, only a small portion of the surface is known on account of the limitations of the technological method — the procedure, therefore incorporates an extrapolation of very uncertain quality.

This method cannot satisfy scientific requirements on account of the above, nor can it be recommended for practical use without taking certain limitations into account.

In fields to which the method can be applied is process control by computer, e.g. in the manufacture of soda [14].

2.7. Method for solving differential equations

As the use of computers becomes widely popular, the method, based on solving the equations has greater importance in analysing systems that can be defined by functions not analytically treatable.

The common advantages of the methods are:

a) They can be used both for stability checking and for solving as well as the dynamic characteristics.

b) They can be used in wider range than the analytical ones.

Their common disadvantages are:

a) In case of non-counted initial conditions the behaviours of the systems can be only estimated (and this estimation often leads to defective results).

b) The results which are derived, cannot be generalized. Therefore quite amount of data of the analysed function surface (dynamic characteristics) must be known, and this needs a high computer capacity and quick computers.

The example, which was discussed is the following [16]:

Stability checking of exotermic chemical reactions in case of homogeneous non-adiabatic systems.

The discussed systems are the following:

The first one is an ideal mixing reactor.

The second system is a solid catalyst surface, with reacting gas flowing continuously beside it.

The third system is a solid fuel surface (e.g. coal), placed in the way of flowing gas (e.g. air).

2.8. Other methods

Some other methods are discussed in this chapter, that cannot be put into any of the before mentioned groups. There are those, with which the authors used methods differing from the before mentioned ones and those, at which

the description of the examining method is missing, e.g.: the stability of the oxo-synthesis process is discussed by KRINKIN and RUDKOVSKIJ [17].

Summary

A general method for investigations on the dynamics of processes and equipments in chemical engineering. Inferences drawn from the analysis of the steady state condition. Investigations on systems of various types in the chemical industry, such as concentrated and distributed parameter systems, single and multiple parameter systems, linear and non-linear systems. The evaluated methods are the following: classical, stochastic and matrix methods, linearization, phase plane methods, Ljapunov's direct method, numerical methods, regression analysis, method for solving differential equations, and other methods.

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