FUNDAMENTAL STUDIES IN ENGINEERING 4

CHEMICAL PROCESS DYNAMICS

REZSÖ MOHILLA
and
BÉLA FERENCZ

ELSEVIER

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BY

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INTRODUCTION

Mankind, over a period of many decades, has brought about the mechanization of production. It can now be said that most processes requiring great physical strength are carried out by machines, or at least, that this is technically feasible. It is only a matter of investment and economics whether or not this possibility is actually realized. This means that the process of mechanization has, essentially, been completed. Naturally, this process was backed by the necessary theoretical prerequisites. The theoretical background to the processes concerned had to be known and the physical relationships had to be formulated mathematically. Mechanization in chemical industries gave birth to modern large-scale technologies. At the same time, there was a strong movement towards continuous operation. Correspondingly, the relationships mentioned above dealt primarily with steady-state processes. These relationships are the results of cooperative efforts by the experts in the interrelated fields: technology, unit operations, mechanics and mathematics. However, due to the inherent nature of the chemical industry, these relationships have never reached the depth achieved in mechanics or electronics. Refinement of the existing mathematical treatment of chemical industries is an intense, continuous activity.

Since human physical strength no longer places a limit on technological innovations, man has been able to harness far more powerful forces. Vast stores of energy were released, while plant sizes and capacities were increased causing their value to soar as well. However, the risks associated with these processes increased enormously, and temporary carelessness could cause huge losses. The burden of responsibility placed on human control increased beyond reasonable limits. This – inevitably – led to the point when man had to hand over control to more alert systems and this transfer was, to a great extent, in his best interest.

When even control functions were assigned to machines, a new age, of automatic control and the automation of equipment began. In the chemical industries this trend has a history of some thirty years, in other industries, perhaps, rather

longer. Obviously, this activity called for the clarification of theoretical relationships as well, and since the main point here was the reinstitution of the steady-state operation of a disturbed process, the mathematical descriptions of non-steady-state phenomena had to be examined. Unfortunately, very little has been done in the field of mathematical analysis of non-steady-state operation units, i.e. process dynamics has a very short history. Few publications deal with this topic and even these lack a common systematic theoretical foundation. Furthermore, most of them, in their present form, are unsuitable for automation design purposes. This results in the undesirable, but nevertheless existing, situation that control systems are designed – at best – according to qualitative considerations and it is left to the operating personnel, to experience (or suffer) the performance of their system. On the other hand, if one looks at, for example, the mechanical engineering industries, extremely accurate control systems closely following predetermined patterns are to be seen. The explanation is fairly simple, the mathematical analysis of these processes can be carried out very precisely.

Before analysing the causes of the present situation in chemical industry, let us quote – as our motto – D.P.Campbell, the "father" of chemical process dynamics: "As long as the designers of industrial process control systems concentrate upon instruments and controllers and fail to recognize the plant as the central and most fundamental issue, we cannot hope for much progress. In process control, knowledge of process behaviour comes first" [1].

In our view, the present situation can be traced back to the following causes.

At the beginning chemical engineers did not consider process automation "their business". Automation was thought to be the field of specialists trained as electrical or mechanical engineers.

There is no denying that this isolation of the subject, at least at the beginning, was also to be found in mechanical engineering industries. However it should not be forgotten that here process behaviours had to be described by analysing essentially mechanical and electrical relationships. This, electrical and mechanical engineers (based solely on their basic training) were generally able to do. Thus the necessary process dynamical knowledge was available after all. However, such specialists could not have been expected to know chemical engineering to the same depth. In fact, it would be hard to find a field more alien to them. Therefore, close cooperation between chemical engineers and process dynamics experts is essential, and meaningful results can only be expected when this is present.

Once this cooperation started, the signs of development did appear. However, we have found that several obstacles remained unchanged. One of them is the fact that chemical process dynamics experts are not really concerned to give their studies a common basis. Therefore, different authors describe the very same

operation unit by means of totally dissimilar equations, both in character and structure. Then again, operation units are frequently discussed on the basis of the particular technological process, not recognizing the fact that quite often even completely different operation units can be described by rather similar equations. The other fact is that, figuratively speaking, chemical engineers and process control experts speak different languages. This, in itself, is quite evident, but the problem is, that the gulf between them is so great, that they do not even understand each other any more. Process control theory has developed its vast armoury of detailed mathematical treatments. Using these devices – if the dynamic mathematical model of the process is known – process control theory can solve quite advanced design problems. However, only those mathematical relationships which can be accommodated by the existing mathematical arsenal can be used. This means that in describing a particular process, the chemical engineer has to use the mathematical tools of process dynamics, i.e. he is compelled to learn their language. We are convinced that most control systems installed up to now would not have been necessary if the operation unit in question had been designed with process dynamics in mind.

It would be a gross immodesty to state that a panacea is presented in this book for all the problems enumerated above and that engineers concerned with process control will find here a ready-made answer for all their grievances. More fittingly, this book represents one of the first steps towards bringing together experts of the two respective fields.

This book was written with a double purpose in mind: on the one hand, an attempt was made to create a common technical language and introduce terms well understood in both fields, and on the other hand, to structure and order process dynamics itself. The latter goal can be achieved by explaining the fundamentals of process control to the chemical engineers concerned. Also, the fundamental equation set used to describe chemical operation units is briefly shown far the sake of non-chemist readers.

As far as possible, relationships are presented as transfer or frequency-functions. In our view, this is the form most readily compatible with the mathematical devices of process control. No special emphasis was placed on transient (time-dependent) behaviour. Although they are quite easily visualized, in our view they are not worth the time and effort required to obtain them, at least compared with their effective use in process control. At the same time, unlike several other authors, we tried to exercise some restraint and attempted not to overburden the reader with flowsheets and electrical analogy circuits. As far as a single operation unit and not a system composed thereof is concerned, we do not think that very much more information could be extracted from a flowsheet than from an appropriately formulated equation.

As for electric analogies, they are only used occasionally and even then only to demonstrate certain principles. We are ready to go a long way to defend our view that any formula is of value only as long as the engineer can substitute the appropriate quantities into it. From this viewpoint an analogy using coefficients which cannot be determined leads nowhere.

Unfortunately, this attitude does occasionally necessitate certain compromises relating to both the content and the mode of presentation, namely:

1. Relationships are necessarily attempted to be obtained in the form of linear equations. This is because Laplace transformation, the mathematical device used to obtain transfer functions, can only be applied in the case of constant coefficient linear differential equations. This limitation is not as severe as it would appear at first glance, for in practice one is generally concerned with small changes, small periodic deviations from a steady-state value. These changes, moreover, can adequately be described by linear equations. Further, process control theory, by definition, obtains the transfer function from the Laplace transform of the differential equation under zero initial conditions. This means that the initial condition, i.e. the steady-state value of the characteristic variable in question, is arbitrarily put equal to zero. In the final analysis, chemical engineering is expected to determine its value. In the present treatment this value occurs, at most, as a constant coefficient.

2. Neither the mathematical description of multivariable, multiparameter systems, nor operation unit behaviour under stochastic signals are dealt with here. We are fully aware of the fact that computerized process control and dynamical optimization problems will soon raise these issues as well. There is only a relatively loose connection between these problems and the true internal relationships of operation units, so there is no real organic unity between these two fields and the rest of the present book.

Throughout this book we will attempt to put forth only such equations characterizing operation unit behaviour which can really be used in practice. To make the relationships work, all physical quantities are given in the SI system. Occasional numerical coefficients are taken care of in the final form of the equations.

SYMBOLS

a dB	attenuation
a	coefficient
$a=\frac{\lambda}{\varrho c_p}$ m^2s^{-1}	coefficient of thermal diffusivity
a_t m^2s^{-1}	coefficient of turbulent thermal diffusivity
A m^2	area
$A_á$ m^2	area of transfer
b	coefficient
B $m^3\,s^{-1}$	volume current
c $kg\,m^{-3}$	concentration
c_p $kJ\,kg^{-1}\,K^{-1}$	specific heat at constant pressure
C $m\,s^2$	capacity
d m	diameter
d_p m	characteristic length of column filling
D $m^2\,s^{-1}$	coefficient of axial turbulent diffusion (dispersion)
$\mathscr{D}$ $m^2\,s^{-1}$	coefficient of diffusion
$\|\mathbf{D}\|$	determinant
e	base of natural logarithm
E	coefficient
E	symbol of function
f s^{-1}	frequency
f	function
F	transfer function
g	weight function (pulse response)
g $m\,s^{-2}$	gravitation constant
G $kg\,m^{-2}\,s^{-1}$	specific gas loading
G $kmole\,s^{-1}$	molar current of vapour
G $kJ\,m^{-3}\,s^{-1}$	intensity of heat source

$h=\frac{H}{\mathbf{Bo}}$	characteristic lengtht of dispersion
h m	level
H m	length of chemical process unit
ΔH kJ kg^{-1}	enthalpy of evaporation, enthalpy of reaction
$i=1, 2, \ldots$	constant
I kJ s^{-1}	heat current
$j=\sqrt{-1}$	
$\mathbf{j}$	current density (in general)
k	constant
k	constant of partition
k	reaction constant
k_v m^2	equivalent cross section of valve
K	constant
K	transfer coefficient
L kg m^{-2} s^{-1}	specific liquid loading
L kmole s^{-1}	molar current of liquid
$\mathscr{L}$	Laplace-operator
m	Henry constant (dimensionless)
m kg	mass
$\dot{m}$ kg s^{-1}	mass current
M kg kmole^{-1}	molar mass
n	number of process units
N kmole	number of moles
p	coefficient
P N m^{-2}=Pa	pressure
q	coefficient
$q=\frac{P_1}{\Delta P}$	parameter of the characteristic function of valve
r kg m^{-3} s^{-1}	intensity of component source
r	reflexion coefficient
R kJkmole^{-1}K^{-1}	gas constant
R	reflux coefficient
s s^{-1}	Laplace variable
t s	time
$\bar{t}$ s	residence time
T s	time constant
U	step function
v m s^{-1}	velocity of convective current