IDEAL MODELS OF REACTORS

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Summary

The range of application of chemical reactors is extremely broad not only in the chemical industry but also in the petrochemical industry and in refineries. Recently these apparatuses have also been more often used in the dynamically developing field of biotechnology as well as in the processes connected with environmental protection.

The main goal of the discipline named chemical reaction engineering is to elaborate quantitative fundamentals for reactor design and for a proper operation of these apparatuses in real industrial conditions. The tool applied in these investigations is modeling, whose task is to establish relationships which could quantitatively describe the course of the process in reactors of various types and scales. These relationships constitute the mathematical model. The mathematical model is usually much simpler than the real physical object but should comprise all these features and parameters whose influence on the process is crucial.

The rational basis for developing these models is provided by the principles of conservation of mass, momentum and energy.

The models presented in this article are therefore named “Ideal Reactor Models” as they introduce the minimum amount of complexity. Nevertheless, they have been widely accepted as very useful and effective in reactor design. It has to be stressed that the application of these models enables the development of straightforward methods for choosing the optimal type of reactor.

1. Introduction

One of the basic apparatuses of the chemical industry, constituting the "heart" of the majority of industrial plants, is the chemical reactor. The range of applications of this apparatus is extremely broad not only in the chemical industry but also in the petrochemical industry and in refineries. These apparatuses are also widespread in the dynamically developing field of biotechnology as well as in the processes connected with environmental protection.

In this apparatus a qualitative transformation of the matter is performed characteristic of the chemical and biochemical processes, and its goal is to obtain semi – final and final products indispensable for the economy. Analysis of the phenomena taking place in the chemical reactor is the subject of research of the discipline named chemical reaction engineering - an intensively developing branch of chemical engineering. The main goal of the investigations carried out within this discipline is to elaborate a basis for the quantitative description of the phenomena taking place in chemical reactors over a possibly broad range of parameters characterizing the process. These generalized quantitative formulations create the fundamentals for modeling and design, scale – up and optimization of the reactors as well as for their proper operation in real industrial conditions.

The simplified scheme of a typical chemical process is shown in Figure 1.

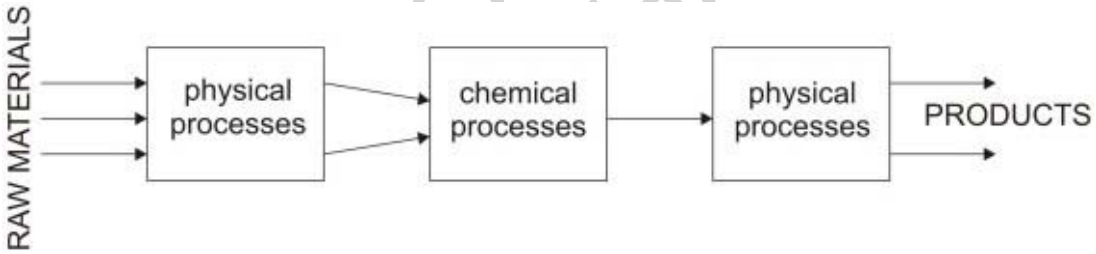

Figure 1. Simplified scheme of a typical chemical process

The raw materials are processed by means of particular physical operations in order to make them suitable for the application in the chemical reactions considered. The reaction mixture leaving the reactor has to be separated and purified also using physical operations to obtain the desired products in proper amount and quality.

The physical operations usually applied are the so called unit operations like absorption, distillation or extraction.

The chemical reactor constitutes a complicated system characterized by physical, physico–chemical and design parameters. Therefore, the method of designing of the reactors and providing a control of their proper operation in industrial conditions is performed by means of the synthesis of information collected from various fields of science. The goal of this synthesis is an accurate quantitative interpretation of the phenomena occurring in the reactor. An especially important feature of the chemical

reaction engineering is that the range of problems of this discipline stretches form the microscale of the molecular level to the macroscale of the complete industrial systems. Thus, chemical kinetics, catalysis, transport phenomena, applied mathematics, modeling and design connected with optimization form the core and the intellectual fundamentals of chemical reaction engineering.

The main tool applied in chemical reaction engineering for the quantitative description of the processes mentioned above is modeling. Modeling is widespread as a method of research in various disciplines like hydrodynamics, heat and mass transfer and the like. Generally speaking modeling consists in investigating the processes using models, in order to establish relationships which could show the course of the process in reactors of various types and scales. In chemical reaction engineering modeling forms the theoretical basis and simultaneously the method of designing the reactors and estimating the optimal conditions of their operation. The model is usually much simpler than the real physical object investigated but should retain all these features and parameters whose influence on the process (according to our assumptions) is crucial and should be determined.

Models are usually divided into two groups: real or physical models and mathematical models.

The physical model has identical physical characteristics as the object investigated. It differs mainly in the scale and some idealized conditions of carrying out the process, which, as has been mentioned before, should not change substantially the most important features of the object.

Examples of the physical models are pilot plants of various scales extending from laboratory installations to demonstration installations. The basis for the physical modeling is formed by the similarity theory, which determines the conditions of similarity for the model and the real object providing the right connection between theory and experiments. The method of investigations by means of physical models is tedious, time – consuming and expensive, because the experiments have to be performed in pilot plants of various scales. Therefore the main method of research in chemical reaction engineering consists in developing mathematical models of processes taking place in chemical reactors.

The mathematical model is in principle a mathematical description of the process investigated which should as exactly as possible foresee the course of the process in the reactor over a relatively broad or practically important range of parameters.

This model is formulated as a result of deriving the balances of mass, momentum and energy. The rational basis for the derivation of these balances is provided by the principles of conservation of mass, momentum and energy. As the dominating phenomena taking place in the reactor are transformation of the matter caused by the chemical reactions as well as the transport of mass, momentum and energy, a very important problem is to define exact constitutive relationships unequivocally determining the intensity of these phenomena as functions of the state variables (composition, temperature and pressure).

The introduction of the constitutive relationships defining the kinetics of chemical reactions and the fluxes of mass, momentum and energy into the balances allows us to follow the changes of composition, temperature and pressure of the reacting mixture as a function of the position in the reactor and time (unsteady – state process).

The balances to be derived are:
n mass balance equations for n components
momentum balance equation
energy balance equation
equation of state defining the relation between temperature, pressure and density

By solving these balance equations the following state variables can be determined:
u_i $(i = 1,2...n)$ – concentrations of components determining the composition of the reacting mixture

T – temperature of the reacting mixture
P – pressure in the reactor
w – velocity vector of the flow of the reacting mixture.

The equations have to be supplemented by adequate boundary and initial conditions. The model thus developed is usually very general and forms a system of complex equations (algebraic and ordinary or partial differential equations). In order to derive a model corresponding with a special type of reactor one has to introduce into the balance equations the assumptions and approximations characteristic of this type of reactor. Strictly speaking the choice of an adequate model is an optimization procedure taking into account the complexity of the model, mathematical methods suitable for the solution of the model equations, number of model parameters and the desired accuracy of the results.

At this point it is worth citing Einstein's definition of an ideal model: "An ideal model should introduce the minimum amount of complexity while capturing the essence of relevant physics".

A detailed classification of chemical reactors encounters considerable difficulties because of the diversity of the types of reactors and their various applications. It cannot be concluded that there exist strict correlations between the kind of reaction (oxidation, reduction) or the complexity of a reaction system (i.e. parallel or consecutive reactions) and the type and form of the reactor. Sometimes the decisive element about the form of the reactor can be very high heat effects connected with the reaction system, which demands a large surface area of heat transfer. It has also to be stressed that many branches of chemical industry based on their long-time experience, developed specific reactor types considered as optimal.

It seems that a very useful and practical (though general) classification of the chemical processes and reactors can be given as follows:

- The reaction system is homogeneous (one – phase system) or heterogeneous (multiphase system)
- The process is continuous or periodic (without inflow of reactants and outflow of products)
- The process is conducted isothermally, adiabatically or by means of heat exchange with the surroundings.

The periodic chemical processes (batch reactors) are usually conducted in tanks equipped with especially chosen mixing devices (mechanical or pneumatic mixing), which ensure the homogenity of the reaction mixture in the whole volume of the reactor (Figure 2).

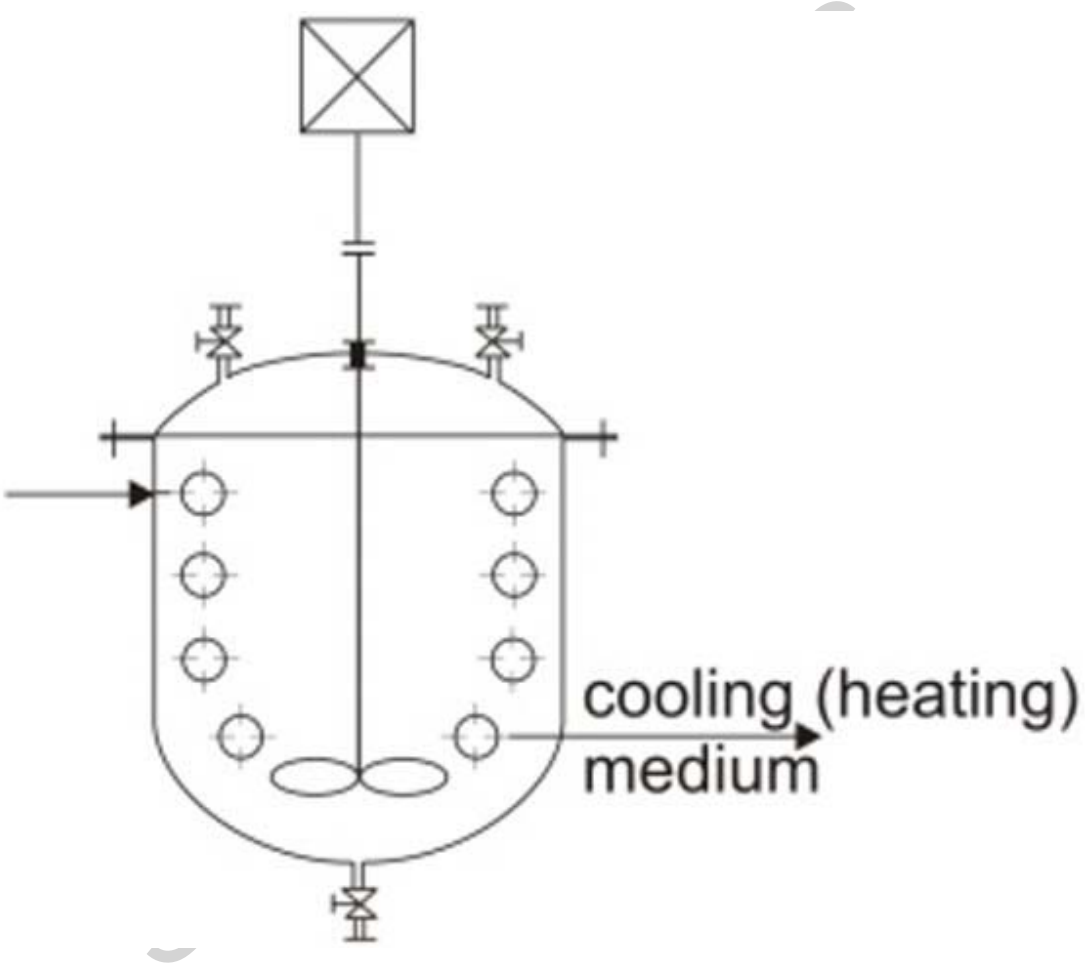

Figure 2. Batch chemical reactor

Among the continuously operating reactors these generally used include tubular reactors and tank reactors equipped with mixing devices (Figure 3 and 4).

The continuously operating tubular or tank reactors resemble in form the majority of real reactors and constitute two basic types of these apparatuses used in the industry.

The terms tubular reactor or tank reactor are sometimes used in an abstract sense, as often the reactor type considered does not conform strictly to a tube or a tank. However,

its physico–chemical characteristics can be formulated based on the model of one of the two types of reactors.

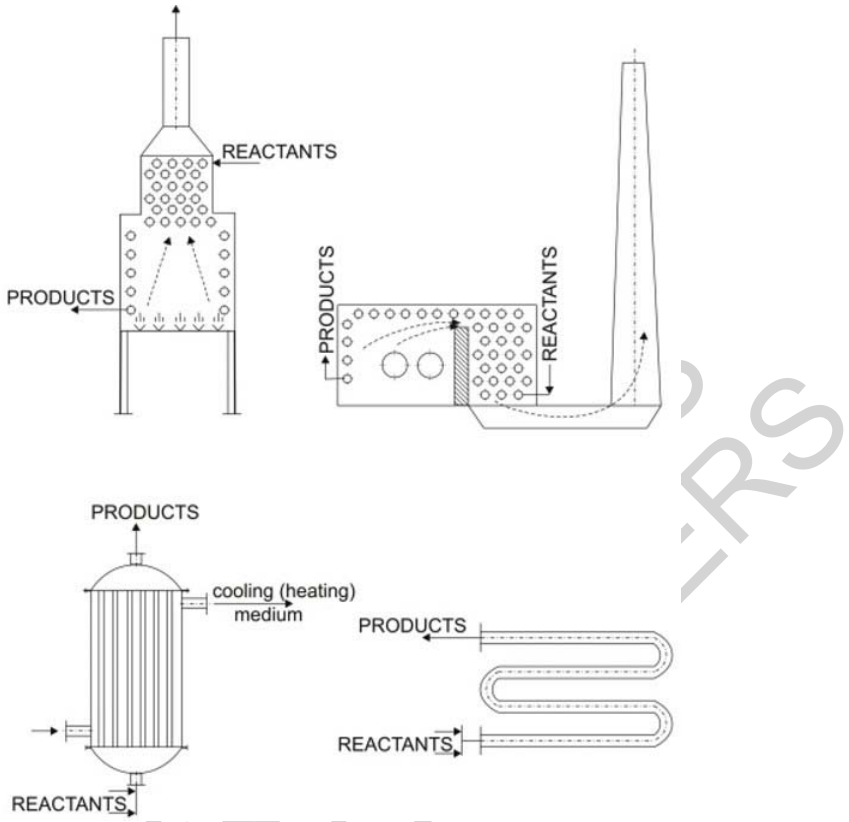

Figure 3. Examples of continuously operating tubular reactors

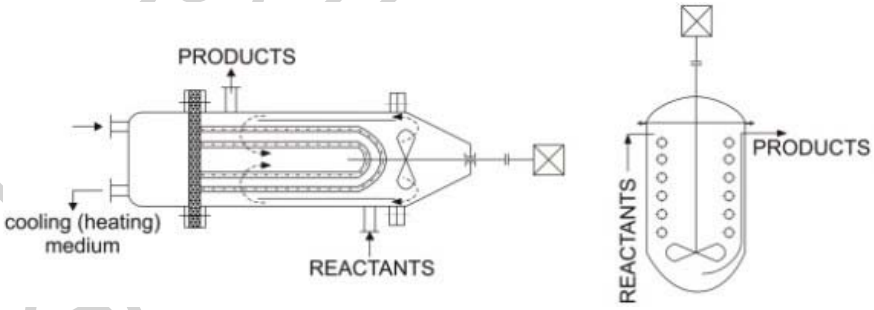

Figure 4. Examples of continuously operating tank reactors

The following qualitative schemes are very helpful in deriving the balances of mass and enthalpy:

$$\begin{bmatrix}\text{Rate of}\\ \text{accumulation}\\ \text{of mass of}\\ \text{component } i\\ \text{in the volume}\\ \text{element}\end{bmatrix} = \begin{bmatrix}\text{Rate of flow}\\ \text{of mass of}\\ \text{component } i\\ \text{into the volume}\\ \text{element}\end{bmatrix} - \begin{bmatrix}\text{Rate of flow}\\ \text{of mass of}\\ \text{component } i\\ \text{out of the}\\ \text{volume element}\end{bmatrix} + \begin{bmatrix}\text{Rate of}\\ \text{production}\\ \text{of mass of}\\ \text{component } i \text{ by}\\ \text{chemical reactions}\end{bmatrix}$$

$$\begin{bmatrix}\text{Rate of}\\ \text{accumulation}\\ \text{of enthalpy}\\ \text{in the volume}\\ \text{element}\end{bmatrix} = \begin{bmatrix}\text{Rate of flow}\\ \text{of enthalpy}\\ \text{into the volume}\\ \text{element}\end{bmatrix} - \begin{bmatrix}\text{Rate of flow}\\ \text{of enthalpy}\\ \text{out of the volume}\\ \text{element}\end{bmatrix} + \begin{bmatrix}\text{Rate of enthalpy}\\ \text{generation by}\\ \text{chemical reactions}\end{bmatrix}$$

$$+ \begin{bmatrix}\text{Rate of}\\ \text{heat exchange}\\ \text{with the}\\ \text{surroundings}\end{bmatrix}$$

The volume element can be a differential volume of the reactor or the whole reactor, depending on the model applied.

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Biographical Sketch

Andrzej Burghardt was born in 1928 in Warsaw, Poland. He received his B.Sc. in 1952 and finally graduated in Chemical Engineering from the Silesian Technical University, Gliwice, Poland obtaining M.Sc. degree. In 1962 he received his Ph.D. while in 1965 the degree Doctor in Technical Sciences from the same university. In 1971 he was awarded a title of Professor in Technical Sciences by the President of the Republic of Poland while some years later, in 1983, he was elected as a member of the Polish Academy of Sciences. In the years 1987-2003 he was a chairman of the Committee of Chemical Engineering at the Polish Academy of Sciences.

Currently he is a member of the Presidium of the Polish Academy of Sciences and of the Scientific Council at the Ministry of Science and Informatics. He is also an active member of the Working Party on Chemical Reaction Engineering of the European Federation of Chemical Engineering.

In the years 1954-1966 he was engaged at the Silesian Technical University, Gliwice, Poland as an Assistant Professor lecturing in Distillation, Mass Transfer and Chemical Reaction Engineering. Then, in 1966, he moved to the Institute of Chemical Engineering of the Polish Academy of Sciences where he was designated to the post of director holding this post until 2002. His field of research focuses mainly on the theory of mass transfer in multicomponent and multiphase systems as well as on chemical reaction engineering with special interest in dynamics of chemical reactors. He is author and co-author of nearly 200 scientific publications in refereed journals and of following books and chapters in collective editions: *Chemical Reactors' Engineering Vol. I and II, Examples of Reactor Design, Dynamics of Processes in a Porous Catalyst Pellet, Mass Transfer in Multicomponent Systems, Condensation of Multicomponent Mixtures in VDI-Wärmeatlas (Three Ed. in German one in English)*. He is also a member of Editorial Boards in several journals.