DOI: УДК 662.74:669.162.16 V.D. Barsky, Doctor of Engineering Sciences, full professor A.V. Kravchenko, Doctor of Engineering Sciences, senior researcher Ukrainian State University of Chemical Technology, Dnipro, V.M. Gulyaev, Doctor of Engineering Sciences, full professor D.V. Jakovlev-Barsky, portgraduate student Dniprovsk State Technical University, Kamianske

# ABOUT LIMITATIONS ON SIMILARITY MODELLING OF CHEMICAL-TECHNOLOGICAL PROCESSES

Despite the abundance of research in the field of similarity modeling, when studying the processes in chemical technology researchers are usually limited to theory and, in particular, to those cases where the phenomena of continuity of flow, transfer of momentum, matter and energy are of decisive importance.

This is due to the fact that the task of creating a model that satisfies an already large set of similarity criteria for the geometric parameters of the model and the object, the processes of transferring by them the amount of motion, mass, and energy was extremely difficult to solve, given the chemical similarity requirements.

Moreover, this problem is especially challenging given the statement about fundamental impossibility of similarity in processes with chemical transformations taking place in reactors of different sizes.

Presented paper shows the inconsistency of assumptions about fundamental impossibility of similarity modelling of processes with chemical and physico-chemical transformations relying on solutions to both the first and second situations, which gained wide popularity at the time.

*Key words*: similarity criteria, modelling, substance transfer, energy transfer, chemical reaction.

Незважаючи на велику кількість робіт в області моделювання за подобою, при вивченні процесів хімічної технології обмежуються теорією і, особливо, практикою тільки тих випадків, коли вирішальне значення мають явища нерозривності потоку, перенесення кількості руху, речовини і енергії.

Це пояснюється тим, що виняткову складність завдання створення моделі, що задовольняє і без того великого набору критеріїв подібності геометричних параметрів моделі і об'єкта, процесів переносу в них кількості руху, маси і енергії, представлялася практично нерозв'язною при обліку ще і вимог хімічного подоби.

Більш того, особливу гостроту цієї ситуації додає твердження про принципову неможливість подібності процесів з хімічними перетвореннями, що відбуваються в реакторах різного розміру.

У даній роботі на прикладі вирішення завдань, що відносяться як до першої, так і другої ситуацій і отримали в свій час широку популярність, показана неспроможність висновків про принципову неможливість моделювання за подобою процесів з хімічними та фізикохімічними перетвореннями.

*Ключові слова*: критерії подібності, моделювання, перенесення речовини, перенесення енергії, хімічна реакція.

Despite the abundance of work in the field of similarity modeling, in studying the processes of chemical technology the researchers are limited to theory and, in particular, to the individual cases when the phenomena of flow continuity, transfer of momentum, matter and energy are crucial [1—6].

Attempts to introduce the criteria of similarity for chemical and physico-chemical transformations into the category of "physical criteria" are reduced to the work of Damkehler [7; 8, p. 462] and G.K. D'yakonova [9, p.49—64; 10]. This is explained by the fact that an extremely challenging task of creating a model that satisfies an already large set of similarity criteria for the geometric parameters of model and object, the processes of motion, mass, and energy transfer was extremely difficult to solve, given the chemical similarity requirements<sup>\*</sup>.

Moreover, this situation is given specific sharpness by the statement about principle impossibility of similarity in processes with chemical transformations taking place in reactors of different sizes.

In the present paper, when considering both the first and second situations, the following provisions are essential.

1. The speed of reaction

$$r = k \cdot \Delta C \tag{1}$$

depends on the temperature exponentially, since the Arrhenius reaction rate constant is:

$$k = k_0 \cdot e^{-\frac{E}{RT}}, \qquad (2)$$

and it also depends on the driving force  $\Delta C$ , which is the product of multiplying power functions of the concentrations of interacting substances (reagents):

$$\Delta C = C_A^{\nu_A} \cdot C_B^{\nu_B} \cdot \dots \tag{3}$$

2. Chemical and physicochemical transformations occurring during the processes of chemical technology are accompanied by the radiation or absorption of heat (thermal effect).

3. The temperature of the reaction mixture depends on the ratio between the heat of the chemical reaction and the heat which the reaction volume radiates to the external environment.

The most vivid example, "justifying" the need for partial similarity, we have found in [3, p. 46], where they try to combine criteria of geometric  $\begin{pmatrix} \Gamma & D_o \\ D_M \end{pmatrix}$ , hydrodynamic (Re), chemical

(Da I) and thermochemical similarity (Da III), limiting the inputs of the task to the use " of a substance with the same properties in the apparatus and model (density, viscosity, heat capacity, thermal conductivity, etc.)."

Apparently, temperature must be considered one of the "other" properties of the stream substances, all the other above-listed properties always depend on it, and, as follows from the Arrhenius equation, the rate constant of the reaction also does.

Moreover, replacing the rate of the reaction r by the rate constant of the reaction k in the expressions for the criteria Da I  $\mu$  Da III, the authors viewed the composition of the reaction mixture among "others" terms.

In this situation criteria Da I and Da III degenerate, growing identical:

$$\frac{D_o}{\omega_o} = \frac{D_M}{\omega_M}$$

and at the same time losing their chemical and thermochemical value.

Thus, the formula's form as follows

$$k_o = \left(\frac{D_o}{D_M}\right)^{-2} \cdot k_M$$

arrived at with the use of mathematical expressions

$$\frac{k_o \cdot D_o}{\omega_o} = \frac{k_M \cdot D_M}{\omega_M} \quad \text{and} \quad \frac{k_o \cdot D_o}{\omega_o \cdot \Delta t_o} = \frac{k_M \cdot D_M}{\omega_M \cdot \Delta t_M}$$

can not be considered.

<sup>\*</sup> It is assumed that the complete similarity of the model and the object can be achieved only if the similarity conditions are fulfilled simultaneously for them according to the criteria of geometric, hydrodynamic, mass transfer, thermal and chemical similarity. In other cases [11 p. 37-38], we can talk only about partial (incomplete) similarity, which, of course, reduces the level of the model's inductance.

In this regard, the conclusion of authors that "... the speed of reaction in the model should be  $\left(\frac{D_o}{D_u}\right)^2$  times more than in the industrial apparatus" can not be attributed to the processes considered

in this case: here, to establish their similarity, it is sufficient to have the similarity of Reynolds criterion in similar points of the model and the object (given all properties of the flows are assumed to be the equal, all other similarity criteria will have the same values).

Let us consider the same problem, but without restrictions on the differences in properties of substances and the characteristics of processes occurring in the industrial reactor (object) and model.

By the condition for geometric similarity we shall imply the proportionality of the characteristic dimensions of the object ("o") and model ("M"):

$$L_o = \Gamma \cdot L_M, \tag{4}$$

which can be represented by diameter, radius etc.

The hydrodynamic similarity will be determined based on Reynolds criterion:

$$\frac{\rho_0 \cdot \omega_0 \cdot L_0}{\mu_0} = \frac{\rho_{\rm M} \cdot \omega_{\rm M} \cdot L_{\rm M}}{\mu_{\rm M}},\tag{5}$$

where  $\rho$  and  $\mu$  — density  $\left(\frac{kg}{m^3}\right)$  and dynamic viscosity of the reaction mixture is  $\left(\frac{kg}{m \cdot \sec}\right)$ , respectively.

The chemical similarity corresponds to the condition of equality of the values in Damkehler criterion Da I in the model and the object

$$\frac{r_o \cdot L_o}{\rho_o \cdot \omega_o} = \frac{r_M \cdot L_M}{\rho_M \cdot \omega_M} \tag{6}$$

where  $r_o$  and  $r_m$  — are speeds of reaction, running in the object and the model,  $\frac{kg}{m^3 \cdot \sec}$ .

The thermochemical similarity is confirmed when we observe equality of values of the Damkehler criterion for the object and the model:

$$\frac{q_o \cdot r_o \cdot L_o}{\rho_o \cdot C_p^o \cdot \omega_o \cdot T_o} = \frac{q_M \cdot r_M \cdot L_M}{\rho_M \cdot C_p^M \cdot \omega_M \cdot T_M},\tag{7}$$

where  $q_o$  and  $q_M$  — specific thermal effects of chemical reactions occurring in the object and in the model,  $\frac{J}{kg}$ ;  $C_p^o$  and  $C_p^M$  — specific heat capacity of flow substances,  $\frac{J}{kg \cdot \deg}$ ;  $T_o$  and  $T_M$  — temperature in the object and in the model, deg.

The accumution of the comparison of the comparis

The assumption of the geometric and dynamic similarity of the object and the model allows via substitution of (4) into (5) to represent a relation of their sizes ( $L_o$  and  $L_M$ ) with the characteristics of the flow substances ( $\rho_o, \mu_o, \rho_M, \mu_M$ ) and the linear velocities of the latter ( $\omega_0, \omega_M$ ):

$$\omega_o = \frac{L_{\rm M}}{L_o} \cdot \frac{\rho_{\rm M}}{\rho_o} \cdot \frac{\mu_o}{\mu_{\rm M}} \cdot \omega_{\rm M} \,. \tag{8}$$

It leads to the fact that for geometric and hydrodynamic similarity, the characteristic size of the model must be related to the compatible size of the industrial reactor (object) by the relation:

$$L_{\mathcal{M}} = \frac{\rho_{o} \cdot \mu_{\mathcal{M}} \cdot \omega_{o}}{\rho_{\mathcal{M}} \cdot \mu_{o} \cdot \omega_{\mathcal{M}}} \cdot L_{o} \,. \tag{9}$$

Since it follows from the requirement of profitability of the model that it should be much less than the object ( $L_M \ll L_0$ ), we define via (9) that for similarity both in geometry and in hydrodynamics it is necessary to reduce  $L_M$  by increasing the flow density ( $\rho_M > \rho_0$ ), reducing its viscosity ( $\mu_M < \mu_0$ ), increasing linear velocity  $\omega_M > \omega_0$  in accessible value intervals.

To make the model similar to the object geometrically, hydrodynamically and chemically, we need to include the Damkehler criterion in the similarity estimate, for which we add (8) into (6):

$$\frac{r_o \cdot L_o}{\rho_o \cdot F \cdot \omega_M} = \frac{r_M \cdot L_M}{\rho_M \cdot \omega_M},\tag{10}$$

where

$$F = \frac{L_o}{L_M} \cdot \frac{\mu_M}{\rho_o} \cdot \frac{\mu_o}{\mu_M}.$$
 (11)

By transforming (10) and taking into account (11) and (1), we arrive to:

$$L_{M} = L_{o} \cdot \sqrt{\frac{\mu_{M}}{\mathbf{k}_{M} \cdot \Delta C_{M}}} \cdot \frac{k_{o} \cdot \Delta C_{o}}{\mu_{o}} \,. \tag{12}$$

It can be seen that the reduction in size of the model similar to the object, in criteria of geometric, hydrodynamic and chemical similarity, is possible by reducing the viscosity of the flow material in the model ( $\mu_M \ll \mu_0$ ) and also by speeding up the reaction via increasing the temperature and using the catalyst ( $k_M \gg k_0$ ) (see equation (2)), as well as by increasing the driving force of the reaction ( $\Delta C_M \gg \Delta C_0$ ) (see expression (3)).

We note that the recommended changes in the viscosity, participating in (9) and (12) are forwarded in one direction.

And finally, in order to introduce the thermal effect of the chemical reaction to the characteristics of the model and the object, we use the criterion of thermochemical similarity from Damkehler Da III. To do this, taking (11) into account, we introduce (8) into (7) and obtain:

$$\frac{q_o \cdot r_o \cdot L_o}{\rho_o \cdot C_p^o \cdot F \cdot \omega_M \cdot T_o} = \frac{q_M \cdot r_M \cdot L_M}{\rho_M \cdot C_p^M \cdot \omega_M \cdot T_M}.$$
(13)

We introduce (11) into (13), and after reductions we obtain:

$$L_{\mathcal{M}} = L_{o} \cdot \sqrt{\frac{\mu_{\mathcal{M}} \cdot C_{p}^{\mathcal{M}} \cdot T_{\mathcal{M}}}{k_{\mathcal{M}} \cdot \varDelta C_{\mathcal{M}} \cdot q_{\mathcal{M}}}} \cdot \frac{k_{o} \cdot \varDelta C_{o} \cdot q_{o}}{\mu_{o} \cdot C_{p}^{o} \cdot T_{o}} .$$
(14)

It can be seen from (14) that it is possible to reduce the size of the model, keeping its thermochemical similarity by reducing the value of viscosity  $\mu_M \ll \mu_0$ , heat capacity  $C_p^M \ll C_p^o$ , and increasing the specific thermal effect  $q_M \gg q_o$ .

As for temperature  $T_{\mathcal{M}}$ , in this case, its increase directly influences the characteristic size of the model, and indirectly via heat capacity, viscosity, and, most importantly, via the rate constant of the chemical reaction, decreasing  $L_{\mathcal{M}}$  exponentially. In connection with the latter, the temperature should be increased.

It can be seen from (12) and (14) that, under the conditions adopted in [3, p.46] (... provided that the apparatus and model use a substance with the same properties ...), such processes can be realized in chemical and thermochemical terms only in reactors of the same size ( $L_M = L_0$ ). It follows from (9) that  $\omega_M = \omega_0$ , so here we are not talking about similarity modelling, but about the exact reproduction of the object in the "model".

At the same time, equations (9), (12) and (14) indicate that similarity modelling with the maximum, complete coverage of essential characteristics of the object and model, has no fundamental limitations: the problem is reduced to overcoming the technical difficulties of constructing a material model on which it is possible to simulate processes of chemical technology with definite properties of substances, the speed and the thermal effect of the reaction, and under conditions that ensure the fulfilment of in equation:

$$L_{\mathcal{M}} \ll L_{o} \,. \tag{15}$$

In this connection, the equality that follows from the comparison of (12) and (14) turns meaningful:

$$\frac{q_o}{C_p^o \cdot T_o} = \frac{C_p^M \cdot T_M}{q_M} \,. \tag{16}$$

Returning to the assumption that the temperature of the reaction mixture is determined by the ratio of the heat of chemical reaction and that of heat exchange with the surrounding environment, we assume that as long as the main characteristics of the processes in the model and object depend on this temperature, the abovementioned ratio of heats should be considered as a similarity criterion of processes with chemical reactions and physico-chemical transformations occurring in the object and in the model.

Let the chemical technological process be carried out in a spherical reactor of  $V_o$  volume, bounded by a surface  $S_o$ , with the radius of the sphere being  $R_o$ .

Assuming that the reaction occurs simultaneously in all points of the volume  $V_o$ , it is asserted [4] that the magnitude of the thermal effect of this reaction  $(Q_{x,p})_o$  is proportional to  $V_o$ .

If we consider the surface of the sphere to be the heat exchange surface of the reaction volume with the surrounding (external) environment, then for the same reasons we arrive at a conclusion that the heat exchange temperature  $(Q_{m.o.})_o$  is proportional to the square  $S_o$ .

Observing geometric similarity, we take the sphere-shaped reactor model with radius  $R_{M} \ll R_{o}$ , the volume  $V_{M}$  and area of the confining surface  $S_{M}$ .

Running the same reaction in the model reactor, we expect that the thermal effect  $(Q_{x.p.})_{M}$  is proportional to  $V_{M}$ , and the heat of heat exchange  $(Q_{m.o.})_{M}$  is proportional to  $S_{M}$ .

Now, as a similarity criterion for chemical technological processes, occurring in the model and industrial reactors, we can take the ratio

$$\frac{Q_{x.p}}{Q_{m.o.}} = \text{idem}, \qquad (17)$$

$$\frac{Q_{x.p.}}{Q_{m,0}}_{\mu} = \frac{(Q_{x.p.})_{o}}{(Q_{m,0})_{o}}.$$
(18)

Or

Further, taking into account the assumption on the proportionality of the heats to the volume and surface of the sphere, expression (18) is rewritten in the form:

$$\frac{V_M}{S_M} = \frac{V_O}{S_O} \,. \tag{19}$$

As long as the volume of the sphere is

$$V = \frac{4}{3} \pi \pi^{3}$$
(19.1)

and the surface is

$$S = 4 \pi \pi^2$$
 (19.2)

(19) results in

$$R_{\mathcal{M}} = R_o \,. \tag{20}$$

As can be seen, this equality contradicts the necessary condition, ensuring the cost-efficiency of the model:

$$R_{M} \ll R_{0}. \tag{21}$$

On this basis, it is concluded that the condition (17) leading to equation (20) can not be fulfilled, thus the following is always true for chemical technological processes occurring in the model and in the object (reactor):

$$\frac{Q_{x.p.}}{Q_{m.o.}} \neq \text{idem} \,. \tag{22}$$

Here, however, it is worthwhile to return to the assumption about proportionality of the heat of the chemical reaction to the volume of the reactor and the amount of heat exchange — its surface area, which served as the justification for the transition from expression (18) to expression (19).

Despite the evidence of this statement, we find that during the mentioned transition the main property of the similarity criterion is lost - namely its dimension lessness: in contrast to the dimensionless relations in (18), the relations in (19) have a unit of length measurement.

This is already enough to prove the erroneousness of the expression (22) and, besides, the assumption about impossibility of chemical similarity between the "model" and the object.

Returning again to (18), let us note that the introduction of volume and square into this equation must be carried out taking into account the dimensional constants  $\alpha_{x.p.}$  and  $\alpha_{m.o.}$ , which establish the equivalence between the units of measurement of heat and length:

$$Q_{x.p.} = \alpha_{x.p.} \cdot V \tag{23.1}$$

 $Q_{m.o.} = \alpha_{m.o.} \cdot S_{m.o.}$ where, judging from the units of measurement,  $\alpha_{x,p}$  — specific heat (specific heat effect) of chemi-

cal reaction, 
$$\frac{J}{m^3}$$
;  $\alpha_{m.o.}$  — specific amount of heat exchange,  $\frac{J}{m^2}$ 

By introducing (23.1) and (23.2) into (18), we obtain the condition of «chemical» similarity as follows:

$$\frac{\alpha_{x.p.}^{M} \cdot \mathbf{V}_{M}}{\alpha_{m.o.}^{M} \cdot \mathbf{S}_{M}} = \frac{\alpha_{x.p.}^{O} \cdot V_{O}}{\alpha_{m.o.}^{O} \cdot S_{O}}.$$
(24)

After introducing (19.1) and (19.2) into (24) and reducing measureless values we obtain an expression:

$$\frac{\alpha_{x.p.}^{M}}{\alpha_{m.o.}^{M}} \cdot R_{M} = \frac{\alpha_{x.p.}^{O}}{\alpha_{m.o.}^{O}} \cdot R_{O} .$$

$$\tag{25}$$

Thus, processes with "chemical" thermal effects occurring in the object and in the model can be modelled and, on this basis, investigated by methods of similarity theory.

For example, with (25) it is possible to determine the size of a transductive model to study an object in terms of the processes occurring in them:

$$R_{\mathcal{M}} = \frac{\alpha_{x.p.}^{o}}{\alpha_{m.o.}^{o}} \cdot \frac{\alpha_{m.o.}^{\mathcal{M}}}{\alpha_{x.p.}^{\mathcal{M}}} \cdot R_{o} .$$

$$\tag{26}$$

For later we shall bear in mind

$$Q_{m.o.}^{M} = \frac{\lambda^{M}}{\delta^{M}} \cdot \left( t_{p.c.}^{M} - t_{6.c.}^{M} \right) \cdot S_{m.o.}^{M} \cdot \tau_{m.o.}^{M}$$
(27)

where  $\lambda^{M}$  and  $\delta^{M}$  — coefficient of heat conductivity  $\left(\frac{J}{m \cdot \sec \cdot \deg}\right)$  and the wall thickness (m) of

the model reactor;  $t_{p.c.}^{M}$  and  $t_{e.c.}^{M}$  — the temperature of the model wall from the side of the reaction mixture and from external side, deg;  $\tau_{m.o.}^{M}$  — duration of heat exchange, sec.

Dimensional form of this equation:

$$\frac{J}{m \cdot \sec \cdot \deg} \cdot \frac{1}{m} \cdot \deg \cdot m^2 \cdot \sec = J$$

Hence:

$$\left[\alpha_{m.o.}^{M}\right] = \frac{J}{m^{2}}$$
, which corresponds fully to the expression (23.2):

(23.2)

$$\alpha_{m.o.}^{\mathcal{M}} = \frac{\lambda^{\mathcal{M}}}{\delta^{\mathcal{M}}} \cdot \left( t_{p.c.}^{\mathcal{M}} - t_{6.c.}^{\mathcal{M}} \right) \cdot \tau_{m.o.}^{\mathcal{M}} .$$
(28)

By introducing (28) into (27), we obtain:

$$R_{\rm M} = \frac{\alpha_{\rm x.p.}^{\rm O} \cdot R_{\rm O}}{\alpha_{\rm x.p.}^{\rm M} \cdot \alpha_{m.o.}^{\rm O}} \cdot \frac{\lambda^{\rm M}}{\delta^{\rm M}} \cdot \left(t_{p.c.}^{\rm M} - t_{{\rm e.c.}}^{\rm M}\right) \cdot \tau_{m.o.}^{\rm M} \,. \tag{29}$$

With (29) we define:

$$t_{g.c.}^{M} = t_{p.c.}^{M} - \frac{\alpha_{x.p.}^{M} \cdot \alpha_{m.o.}^{O}}{\alpha_{x.p.}^{O}} \cdot \frac{\delta^{M}}{\lambda^{M} \cdot \tau_{m.o.}^{M}} \cdot \frac{R_{M}}{R_{o}}$$
(30)

Dimensional form of the equation (30):

$$\deg = \deg - \frac{\frac{J}{m^3} \cdot \frac{J}{m^2}}{\frac{J}{m^3}} \cdot \frac{m}{m \cdot \sec \cdot \deg} \cdot \frac{m}{m} = \deg ,$$

confirms the correctness of the abovementioned.

Relying upon

$$\alpha_{x.p.} = q_{x.p.} \cdot r_{x.p.} \cdot \tau_{x.p.} . \tag{31}$$

where  $q_{x.p.}$  — is specific heat effect of chemical reaction,  $\frac{J}{kg}$ ;  $r_{x.p.}$  — speed of chemical reaction,

 $\frac{kg}{m^3 \cdot \sec}$ ;  $\tau_{x.p.}$  — duration of chemical reaction, sec, let us assume that

$$q_{x.p.}^{\mathcal{M}} = q_{x.p.}^{o}, \tag{31.1}$$

$$r_{x.p.}^{M} = r_{x.p.}^{o}, \qquad (31.2)$$

$$\tau_{x.p.}^{M} = \tau_{x.p.}^{o}. \tag{31.3}$$

This permits to suppose that

$$\alpha_{x.p.}^{\scriptscriptstyle M} = \alpha_{x.p.}^{\scriptscriptstyle O}$$

and reduce (30):

$$t_{p.c.}^{\mathcal{M}} - t_{g.c.}^{\mathcal{M}} = \frac{\alpha_{m.o.}^{\mathcal{O}} \cdot \delta^{\mathcal{M}}}{\lambda^{\mathcal{M}} \cdot \tau_{m.o.}^{\mathcal{M}}} \cdot \frac{R_{\mathcal{M}}}{R_{o}} \,. \tag{32}$$

It is seen from (32) that with increasing differences in the dimensions of the object and the model  $\frac{R_M}{R_o} \rightarrow 0$  and, as a consequence, the temperatures from different sides of the wall grow similar,

which displays a decrease in the amount of heat exchange in the model.

Another boundary for the driving force of heat exchange in the model corresponds to the equality of model and object dimensions, where  $\frac{R_M}{R_o} = 1$ , so that the left side (32) is determined only by the thermophysical characteristics of the model and object walls.

It follows that in the interval

$$0 \le \frac{R_{_{\mathcal{M}}}}{R_{_{O}}} \le 1 \quad \text{with} \quad \frac{\alpha_{m.o.}^{o} \cdot \delta^{^{_{\mathcal{M}}}}}{\lambda^{^{_{\mathcal{M}}}} \cdot \tau_{m.o.}} = \text{const},$$

the similarity of the model to the object with the criterion  $\frac{Q_{x.p.}}{Q_{m.o.}}$  is attained by creating the tempera-

ture of the external medium, the value of which is determined from (32).

Additional possibilities here are also related to the selection of the material, thickness and design (multilayer structure) of the model wall.

### List of reference links

- Kasatkin A. G. Osnovny'e proczessy' i apparaty' himicheskoj tehnologii. M.: Himiya, 1973. 754 s.
- [2] Guhman A. A. Vvedenie v teoriyu podobiya. M.: Vy'sshaya shkola, 1973. 295 s.
- [3] Romankov P.G., Kurochkina M.I. Gidromehanicheskie proczessy' himicheskoj tehnologii. M.: Himiya, 1974. – 288 s.
- [4] Zakgejm A.Yu. Vvedeniya v modelirovanie himiko-tehnologicheskih proczessov. M.: Himiya, 1982. – 288 s.
- Planovskij A.N., Nikolaev P.I. Proczessy' i apparaty' himicheskoj i neftehimicheskoj tehnologii. M.: Himiya, 1987. – 496 s.
- [6] Kogan V.B. Teoreticheskie osnovy' tipovy'h proczessov himicheskoj tehnologii. L.: Himiya, 1977. – 592 s.
- [7] Damkohler, G. Chem. Fabrik. 1939. Bd. 43, 44.
- [8] Obshhie osnovy' himicheskoj tehnologii / S. Bretshnajder, V. Kaveczkij, YA. Leko, R. Marczinkovskij. – L.: Himiya, 1977. – 504 s.
- [9] D'yakonov G.K. Modelirovanie proczessov fiziko-himicheskih prevrashhenij. M.: izd. ANSSSR, 1951. – 285 s.
- [10] D'yakonov G.K. Voprosy' teorii podobiya v oblasti fiziko-himicheskih proczessov. M.–L.: izd. ANSSSR, 1956. – 206 s.
- [11] Venikov V.A. O modelirovanii. M.: Znanie, 1974. 64 s.

# ПРО ОБМЕЖЕННЯ НА МОДЕЛЮВАННЯ ПО ПОДІБНОСТІ ХІМІКО-ТЕХНОЛОГІЧНИХ ПРОЦЕСІВ Барський В.Д., Кравченко О.В., Гуляєв В.М., Яковлєв-Барський Д.В.

### Реферат

Не зважаючи на велику кількість робіт в галузі моделювання по подібності, при вивченні процесів хімічної технології обмежуються теорією і, особливо, практикою тільки тих випадків, коли вирішальне значення мають явища безперервності потоку, переносу кількості руху, речовини та енергії.

Це пояснюється тим, що виключно складна задача створення моделі, що задовольняє і без того великому набору критеріїв подібності геометричних параметрів моделі та об'єкта, процесів переносу в них кількості руху, маси та енергії, ставала практично не вирішуваною при врахуванні ще й вимог хімічної подібності.

Більш того, особливу гостроту цієї ситуації придає твердження про принципову неможливість подібності процесів з хімічними перетвореннями, що протікають в реакторах різної величини.

В цій роботі на прикладі вирішення задач, що відносяться як до першої, так і до другої ситуації, та які отримали в свій час широку відомість, показана неспроможність висновків про принципову неможливість моделювання по подібності процесів з хімічними та фізикохімічними перетвореннями. Показано, що при відміні обмежень, що складаються з використання «в апараті і моделі речовини з однаковими властивостями (щільністю, в'язкістю, теплоємністю, теплопровідністю та інше)», геометрична, гідродинамічна, хімічна та термохімічна подібність можлива, якщо виконуються наступні співвідношення між розмірами об'єкту та моделі:

$$\begin{split} L_{\scriptscriptstyle M} &= \frac{\rho_o \cdot \mu_{\scriptscriptstyle M} \cdot \omega_o}{\rho_{\scriptscriptstyle M} \cdot \mu_o \cdot \omega_{\scriptscriptstyle M}} \cdot L_o \,, \ L_{\scriptscriptstyle M} = L_o \cdot \sqrt{\frac{\mu_{\scriptscriptstyle M}}{k_{\scriptscriptstyle M} \cdot \Delta C_{\scriptscriptstyle M}}} \cdot \frac{k_o \cdot \Delta C_o}{\mu_o} \,, \\ L_{\scriptscriptstyle M} &= L_o \cdot \sqrt{\frac{\mu_{\scriptscriptstyle M} \cdot C_p^{\scriptscriptstyle M} \cdot T_{\scriptscriptstyle M}}{k_{\scriptscriptstyle M} \cdot \Delta C_{\scriptscriptstyle M} \cdot q_{\scriptscriptstyle M}}} \cdot \frac{k_o \cdot \Delta C_o \cdot q_o}{\mu_o \cdot C_p^{\scriptscriptstyle O} \cdot T_o} \,. \end{split}$$

Ці рівняння вказують на те, що моделювання по подібності з максимальним, з повним охопленням існуючих характеристик об'єкта і моделі, не має ніяких принципових обмежень: задача зводиться до подолання технічних труднощів побудови матеріальної моделі, на якій можливо реалізувати ХТП з властивостями речовин, швидкістю та тепловим ефектом реакції та в умовах, що забезпечують виконання нерівності  $L_{M} \ll L_{o}$ .

В роботі також, виходячи із положення про те, що температура реакційної суміші визначається співвідношенням теплоти хімічної реакції і теплообміну з навколишнім середовищем, показано, що через незалежність основних характеристик процесів, що протікають в моделі і об'єкті, від цієї температури, згадане співвідношення теплоти слід розглядати як критерій подібності процесів з хімічними реакціями і фізико-хімічними перетвореннями, що протікають в об'єкті і в моделі.

Отримано вираз:  $\frac{\alpha_{x.p.}^{M}}{\alpha_{m.o.}^{M}} \cdot R_{M} = \frac{\alpha_{x.p.}^{o}}{\alpha_{m.o.}^{o}} \cdot R_{o}$ , що встановлює співвідношення між розмірами

об'єкта і моделі в залежності від величин питомої теплоти хімічної реакції і теплообміну з навколишнім середовищем.

Зроблено висновок: процеси з «хімічними» тепловими ефектами, що протікають в об'єкті і в моделі, можуть моделюватися і, на цій основі, досліджуватися методами теорії подібності.

### Література

- 1. Касаткин А.Г. Основные процессы и аппараты химической технологии. М.: Химия, 1973. 754 с.
- 2. Гухман А.А. Введение в теорию подобия. М.: Высшая школа, 1973. 295 с.
- 3. Романков П.Г., Курочкина М.И. Гидромеханические процессы химической технологии. М.: Химия, 1974. – 288 с.
- 4. Закгейм А.Ю. Введения в моделирование химико-технологических процессов. М.: Химия, 1982. 288 с.
- 5. Плановский А.Н., Николаев П.И. Процессы и аппараты химической и нефтехимической технологии. – М.: Химия, 1987. – 496 с.
- 6. Коган В.Б. Теоретические основы типовых процессов химической технологии. Л.: Химия, 1977. 592 с.
- 7. Damkohler, G. Chem. Fabrik. 1939. Bd. 43, 44.
- 8. Общие основы химической технологии / С. Бретшнайдер, В. Кавецкий, Я. Леко, Р. Марцинковский. Л.: Химия, 1977. 504 с.
- 9. Дьяконов Г.К. Моделирование процессов физико-химических превращений. М.: изд. АНСССР, 1951. – 285 с.
- 10. Дьяконов Г.К. Вопросы теории подобия в области физико-химических процессов. М.–Л.: изд. АНСССР, 1956. 206 с.
- 11. Веников В.А. О моделировании. М.: Знание, 1974. 64 с.