# ABOUT ONE PARTIAL SIMILARITY CRITERION OF CHEMICAL TECHNOLOGICAL PROCESS

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To date, despite the abundance of works in the field of modeling on similarity criteria, the investigation of the chemical technology processes (CTP) are limited by theory. The practical results are used only in those particular cases when the phenomena of flow continuity, transfer of momentum, mass and energy are of decisive importance [1-6].

Attempts to incorporate the similarity criterion into the number of "physical criteria" for the chemical and physico-chemical transformations are summarized in the investigations of Damkehler [7] and Diakonov [8, 9].

The reason is that the problem of creating a model that satisfies an already large set of similarity criteria for the geometric parameters of the model and the object, the transfer of momentum, mass and energy, becomes practically insoluble when considering more requirements of chemical similarity[1].

Moreover, the problem is complicated by the statement about the principle impossibility of processes similarity with chemical transformations taking place in reactors of different sizes. The following considerations served as the basis for this.

1. The reaction rate $r = k \cdot \Delta C$ exponentially depends on temperature, since the rate constant of the Arrhenius reaction is:

$$k = k_0 \cdot e^{-\frac{E}{RT}}$$

2. Chemical and physico-chemical transformations taking place during CTP are accompanied by the release or absorption of heat (thermal effect).

3. The temperature of the reaction mixture is determined by the ratio heat of the chemical reaction : heat which is exchanged between the reaction volume and external environment.

Hence, the concentration and temperature fields in the reactor volume are determined by this ratio, which should be considered as a similarity criterion for the processes with chemical reactions and physico-chemical transformations taking place in the object and in the model.

Let CHT proceeds in a spherical reactor with the volume $V_0$ and radius $R_0$, which is bounded by a surface with area $S_0$.

Assuming that the reaction occurs simultaneously at all points of the volume $V_0$, it is asserted [4] that the reaction heat $(Q_r)_0$ is proportional to $V_0$.

If we consider the surface of the sphere as the heat exchange surface of the reaction volume with the external environment, then the heat of heat exchange $(Q_h)_0$ is proportional to the area $S_0$.

Following the geometric similarity, we take the reactor model in the form of a sphere with the radius $R_m << R_0$ with the volume $V_m$ and area $S_m$.

Realizing the same reaction in the model reactor, we expect that the heat $(Q_r)_0$ is proportional to $V_m$, and the heat of heat exchange $(Q_h)_0$ is proportional to $S_m$.

[1] It is assumed that a complete similarity of the model and the object may be achieved only if the similarity conditions are simultaneously satisfied by the criteria of geometric, hydrodynamic, mass-exchange, thermal and chemical similarity.

Now, we can take the ratio (1) as a similarity criterion for the CHP occurring in the model and industrial reactors

$$\frac{Q_r}{Q_m} = idem \tag{1}$$

$$\frac{(Q_r)_m}{(Q_m)_m} = \frac{(Q_r)_0}{(Q_m)_0} \tag{2}$$

Then, taking into account the regulations about proportionality of the heats to the reactor volume and surface, the equation (2) can be rewritten as:

$$\frac{V_m}{S_m} = \frac{V_0}{S_0} \tag{3}$$

Since the sphere volume is

$$V = \frac{4}{3} p\ R^3 \tag{3.1}$$

and its surface is

$$S = 4p\ R^2 \tag{3.2}$$

it follows from (3) that

$$R_m = R_0 \tag{4}$$

As can be seen, this equality contradicts the necessary condition that ensures the economy of the model:

$$R_m <<< R_0 \tag{5}$$

On this basis, we conclude that condition (1) leading to equation (4) can not be fulfilled, so for CTP in the model and in the object (reactor) the equation (6) is always valid:

$$\frac{Q_r}{Q_m} \neq idem \tag{6}$$

Despite the obviousness of the statement about proportionality of heats to the reactor volume and surface, during the transformation of (2) into (3) we observe the loss of the similarity criterion main property – its dimensionlessness: in contrast to the dimensionless values in (2), the values in (3) have a length unit.

This is already enough to prove the fallacy of expression (6) and, hence, the assertion about impossibility of “chemical” similarity of the model and the object.

Returning again to (2), let us note that the introduction of volume and area values into this equation must be carried out taking into account dimensional constants $\alpha_r$ and $\alpha_h$ which establish an equivalence between heat and length units:

$$Q_r = a_r \cdot V \tag{7.1}$$

$$Q_r = a_h \cdot V \tag{7.2}$$

where $\alpha_r$ – specific heat (specific thermal effect) of the chemical reaction, J/m$^3$; $\alpha_h$ – specific heat of heat exchange, J/m$^2$.

When substituting (7.1) and (7.2) in (2) we obtain the condition of “chemical” similarity as:

$$\frac{a_r^m \cdot V_m}{a_h^m \cdot S_h} = \frac{a_r^0 \cdot V_0}{a_h^0 \cdot S_0} \tag{8}$$

After substitution of (3.1) and (3.2) in (8) and cancellation of dimensionless units we obtain:

$$\frac{a_r^m}{a_h^m} \cdot R_m = \frac{a_r^0}{a_h^0} \cdot R_0 \tag{9}$$

Thus, the processes with “chemical” thermal effects occurring in the object and in the model can be simulated, and they can be investigated by the methods of similarity theory.

For example, from (9) we can determine the size of a traductive model for investigating the object similar to the processes occurring in it:

$$R_m = \frac{a_r^m}{a_h^m} \cdot \frac{a_r^0}{a_h^0} \cdot R_0 \tag{10}$$

Hereinafter we take into account that

$$Q_h^m = \frac{l^m}{d^m}\left(t_r^m - t_{ex}^m\right) \cdot S_h^m \cdot t_h^m \tag{11}$$

where $l^m$ –coefficient of heat transfer, $\frac{\text{J}}{\text{m} \cdot \text{s} \cdot \text{degree}}$; $d^m$ – wall thickness of the model reactor, m; $t_r^m$ and $t_{ex}^m$ – temperature of the reactor wall from the side of reaction mixture and outside temperature, respectively, degree; $t_h^m$ – time of heat exchange, s.

So, the dimensionality of this equation is $\frac{\text{J}}{\text{m} \cdot \text{s} \cdot \text{degree}} \cdot \frac{1}{\text{m}} \cdot \text{degree} \cdot \text{m}^2 \cdot \text{s} = \text{J}$. Hence, $[a_h^m]$ = J/m$^2$, that corresponds to the equation (7.2).

$$a_h^m = \frac{l^m}{d^m}\left(t_r^m - t_{ex}^m\right) \cdot t_h^m \tag{12}$$

When substituting (12) in (11) we obtain:

$$R_m = \frac{a_r^m}{a_h^m} \cdot \frac{R_0}{a_h^0} \cdot \frac{l^m}{d^m}\left(t_r^m - t_{ex}^m\right) \cdot t_h^m \tag{13}$$

From (13) we find:

$$t_{ex}^m = t_r^m - \frac{a_r^m \cdot a_h^0}{a_r^0} \cdot \frac{d^m}{l^m \cdot t_h^m} \cdot \frac{R_m}{R_0} \tag{14}$$

It can be seen that the similarity of the model to the object by the criterion $Q_r/Q_h$ is achieved by creating the temperature of the external environment, as well as by fitting the thickness of the reactor wall and the construction (multilayer construction) of the model wall.

References


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