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SCALE-UP UNDER CALCULATING A WORKING ZONE OF CHEMICAL APPARATUSES WITH ACCOUNTING TO THE DISTRIBUTION OF PHASES

Abstract. In this work, the new approach to modelling the scale factor under the calculation of an efficiency of mass transfer in the reactors has been submitted. The approach is based on the dividing the apparatus work volume into zones with different ratios between interacting phases streams. The expressions obtainedcan be applied to the design of chemicalreactors with allowance for the scaling phenomena.

Keywords: scale-up, chemical apparatus, packing, degree of conversion, mass transfer.

Introduction. Numerous experimental studies and experience of industrial exploitation show that when calculating devices of large unit capacity from experimental data obtained from small-scale experimental installations, it is primarily to ensure the calculated efficiency of their operation. It is established that this efficiency tends to decrease with an increase in the sizes of the apparatus [1, 2]. This phenomenon has been called the scale effect and has recently become the subject of research by many scientists [1-3].

The presence of stagnant zones, recirculation sites and areas with a complex hydrodynamical structure in the apparatus volume creates major problems in the development of mathematical models. However, even a workable model is not always correctly used in the design of an industrial device due to the noted problem of a scale transition, since the structure of the streams can change with a change in the overall sizes of the apparatus and its power [4, 5].

This paper deals with an approach to this problem, based on some ideas proposed in [2], which makes it possible to give a fairly simple technique for estimating the influence of the scale factor on the mass transfer efficiency, suitable for use in engineering calculation methods.

The approach is based on the idea that the entire volume of the apparatus has divided into zones with different ratios of interacting flows. It is assumed that the structure of the streams in the isolated small volume cell of the reactor corresponds to the structure of flows in the laboratory apparatus with the same flux ratio and uniform phase distribution [2].

Mathematical model. In order to take into account the uneven distribution of flows, it is assumed that each volume element can be associated with the local value of the bulk mass transfer coefficient obtained on laboratory installations of small size with a known flow structure [6, 7].

The equations for the interaction of phases in elementary volumes are as follows:

$$\frac{\partial Y}{\partial z} = L(z,r)\frac{\partial X}{\partial z}; \qquad (1)$$

$$\frac{\partial Y}{\partial z} = K_V(z,r)\frac{d\chi}{dV}, \qquad (2)$$

where X, Y are the dimensionless concentrations of the reacting reagents; K_V – volumetric mass transfer coefficient; z – longitudinal coordinate; r – radial coordinate; χ – degree of conversion; V – volume of the reactor; L is the ratio of the fluxes of the interacting phases.

In the linear approximation, we can put:

$$\frac{d\chi}{dV} \approx k_{st}X - Y\,, \tag{3}$$

where k_{st} is the rate constant.

Then system (1), (2) can be reduced to the following

$$\begin{cases} \dfrac{\partial^2 Y}{\partial z^2} - D(z,r)\dfrac{\partial Y}{\partial z} = 0, \\ \dfrac{\partial^2 X}{\partial z^2} - \left[D(z,r) - \dfrac{\partial(\ln L)}{\partial z}\right]\dfrac{\partial X}{\partial z} = 0. \end{cases} \tag{4}$$

The effective diffusion coefficient reads [4]:

$$D(z,r) = \frac{\partial(\ln K_V)}{\partial z} + K_V(\lambda - 1), \tag{5}$$

where λ is the mass transfer factor [2]:

$$\lambda == k_{st}L \tag{6}$$

Since the average value λ does not depend on the distribution of fluxes and the one is constant along the length of the reactor, the average value of the mass transfer coefficients can be calculated from the formula:

$$\overline{K}_V = \frac{1}{f}\iint\limits_f K_V(L)df \tag{7}$$

After some rearrangements, we obtain the equation of the process line of the mass transfer in the apparatus

$$Y = Y_0\frac{1}{\lambda - 1}\left[(1-\lambda\chi)\exp\left(\frac{\lambda-1}{J_Y}f\int_0^z \overline{K}_V ds\right) - \lambda(1-\chi)\right] + X_0\frac{k_{st}}{\lambda-1}\left[1 - \exp\left(\frac{\lambda-1}{J_Y}f\int_0^z \overline{K}_V ds\right)\right] \tag{8}$$

The formula for calculating the degree of conversion of substances in the reactor when there are n successive sections in the apparatus with different phase flow structures can be derived as follows:

$$\chi = \frac{\exp\left(\dfrac{\lambda-1}{J_Y}f\sum\limits_{i=1}^{n}\int_0^{H_i}\overline{K}_{V(i)}ds\right) - 1}{\lambda\exp\left(\dfrac{\lambda-1}{J_Y}f\sum\limits_{i=1}^{n}\int_0^{H_i}\overline{K}_{V(i)}ds\right) - 1}\left(1 - \frac{k_{st}X_0}{Y_0}\right). \tag{9}$$

An analysis of the mathematical model for the distribution of the dispersed liquid phase in the reactor shows [4, 5] that there is a certain characteristic radius R_S at which the average intensity of the liquid flow is stabilized, and this radius is set at a certain distance H_S from the reactor inlet cross-section.

The following estimates are obtained for the indicated radius and average intensity:

$$R_S = \sqrt{\frac{aD}{2}\ln\left(\frac{4D}{\pi a}\right)}\,, \tag{10}$$

$$\bar{j} = J\sqrt{\frac{2h}{H_S}}\exp\left(-\frac{hR_S^2}{2a^2H_S}\right). \tag{11}$$

Thus, in carrying out the estimated calculations, the entire volume of the apparatus can be conditionally divided into two zones: a zone of stabilization in height H_S, within which the region of intensive mass transfer occupies only a certain part of the volume of the working zone of the apparatus, and a zone of steady-state mass transfer in which the local mass-transfer coefficients reach, on average, optimal values in the entire volume of the reactor.

In this case, in the first zone the so-called mass transfer loss coefficient γ, equal to the ratio of the mass-transfer coefficient in this zone to the optimal one according to experimental data [1, 2], can be introduced.

For the minimum local intensity of the flow of the disperse liquid phase, we obtain the estimate based on the stochastic walk model:

$$i_{\min} = \frac{4I\sqrt{\dfrac{a}{\pi d_0}}}{\exp\left(-\dfrac{d_0}{4a}\right)}. \tag{12}$$

Here, the initial distribution of the disperse phase has characterized by some conventional step between point sources of irrigation d_0 and a characteristic longitudinal size a of the reactor's elementary volume (for example, the size of the packing element) has been introduced.

The graph of the dependence on the ratio d_0/a of the minimum local flux density to the total initial irrigation density $i_{\min}/I$ is shown in figure 1.

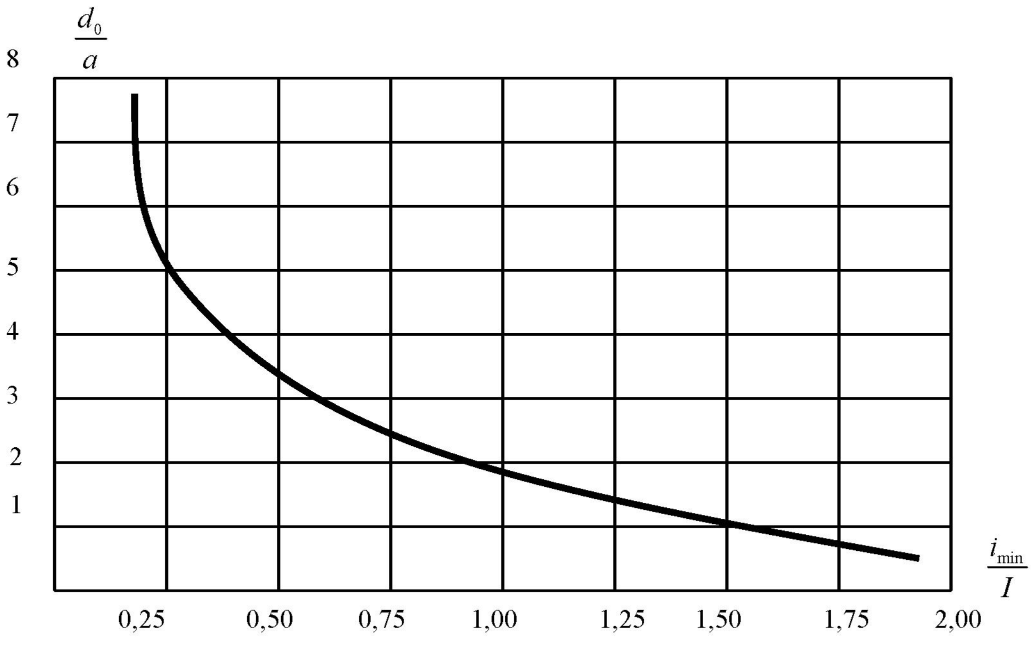

Figure 1 – Graph of solutions of equation (12)

Methods of calculation and discussion of the results. Based on the above models, the calculated ratios for the degree of conversion of substances in the reactor, taking into account the presence of zones in the reactor with a different distribution of phase flows in the zones have been obtained: for $\lambda \neq 1$:

$$\chi = \frac{\exp\left(\frac{\lambda - 1}{G} F\overline{K}\left[H - (1-\gamma)\right]H_S\right) - 1}{\lambda \exp\left(\frac{\lambda - 1}{G} F\overline{K}\left[H - (1-\gamma)\right]H_S\right) - 1}. \tag{13}$$

For $\lambda = 1$:

$$\chi = \frac{\frac{F}{G}\overline{K}\left[H - (1-\gamma)\right]H_S}{\frac{F}{G}\overline{K}\left[H - (1-\gamma)\right]H_S + 1}. \tag{14}$$

In ratios (13), (14), F isthe total cross-section of the apparatus, G is the intensity of the flux of the continuous phase (gas).

If the idea of the height of the unit of mass transfer will be used to estimate the efficiency of the apparatus with accounting to the uneven distribution of flows in the volume [8, 9], then the calculation of the corresponding characteristic can be performed using the formulas

$$h = h^* + \Delta h, \tag{15}$$

$$\Delta h = \frac{(1-\gamma)H_S}{N}, \tag{16}$$

$$N = \frac{1}{\lambda - 1}\ln\left(\frac{1-\chi}{1-\lambda\chi}\right), \tag{17}$$

where h^* is the height of the unit of transfer for a uniform distribution of fluxes (according to experimental studies on a laboratory bench).

Then it is possible to introduce the integral factor of the scale effect in the form:

$$\Phi = \frac{\lambda - 1}{Q_g} F \sum_{i=1}^{n} \overline{K}_{g(i)} H_i \tag{18}$$

Factor (18) links the following physicochemical characteristics: (λ), mass-transfer indicators of intensity ($K_{g(i)}$), as well as scale indicators of the process, namely: geometric characteristics (F and H_i) and load value (Q_g).

Then the expression for calculating the total degree of absorption in the countercurrent of the contacting phases acquires a compact form:

$$\eta_{\uparrow\downarrow} = \frac{\exp(\Phi) - 1}{\lambda\exp(\Phi) - 1} - \frac{\beta C_l^{(0)}}{C_g^{(0)}} \frac{\exp(\Phi) - 1}{\lambda\exp(\Phi) - 1} \tag{19}$$

And for concurrent flows the conversion degree reads:

$$\eta_{\uparrow\uparrow} = -\frac{\exp(\Phi) - 1}{\lambda\exp(\Phi) - 1} + \frac{\beta C_l^{(0)}}{C_g^{(0)}} \frac{\exp(\Phi) - 1}{\lambda\exp(\Phi) - 1} \tag{20}$$

Figures 2 and 3 show some results of numerical experiments.

In accordance with the method described above and with the numerical experiment, the height of the calculated section in the packed column is related to the main geometric parameters of the packed column, namely: with the diameter of the column and the characteristic dimensions of the packing bodies, and also with the conventional number of irrigation points by the ratio [4]:

$$H_i / h = \frac{D^2}{a^2\psi(k)}, \tag{21}$$

where

$$\psi(k) = \frac{4.64 + 1.76k}{(k+1)^2} \tag{22}$$

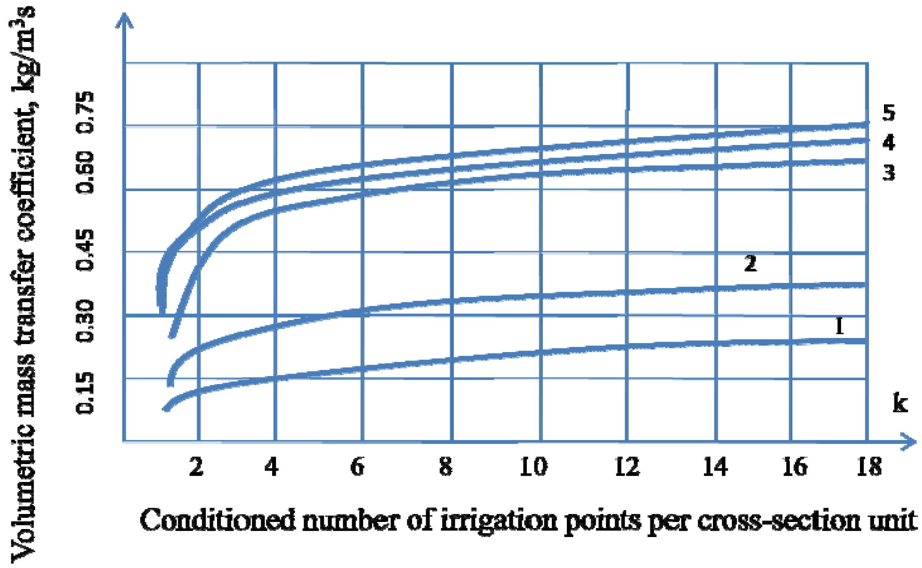

Figure 2 – The degree of extraction at three conditional parts of the column
with changing along the height an average mass transfer coefficient. Countercurrent case.
Countercurrent case. Irrigation densities, m/s: 1 – $0.5{\cdot}10^{-3}$; 2 – $1.25{\cdot}10^{-3}$; 3 – $2.0{\cdot}10^{-3}$; 4 – $2.75{\cdot}10^{-3}$; 5 – $3.5{\cdot}10^{-3}$

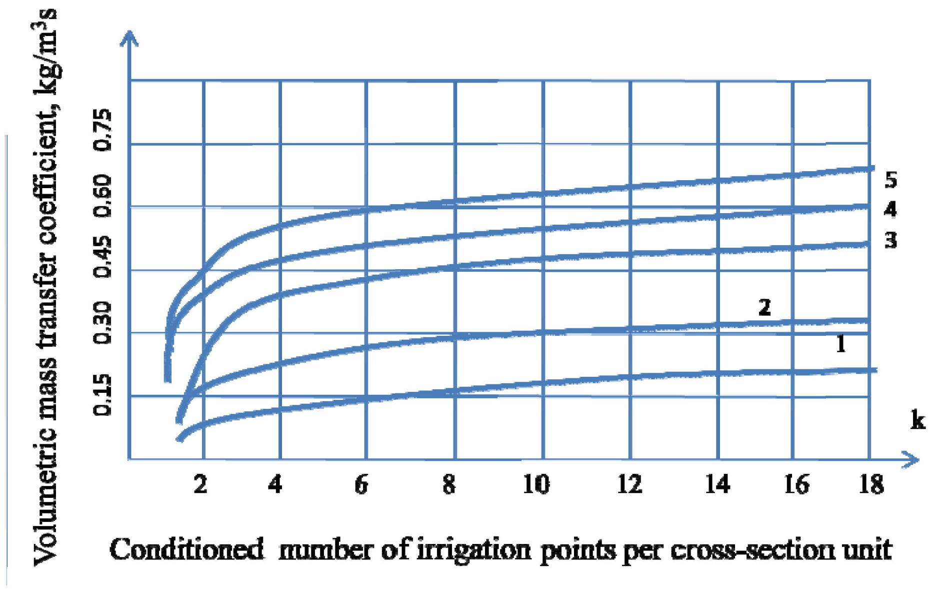

Figure 3 – The degree of extraction at three conditional parts of the column
with changing along the height an average mass transfer coefficient.
Concurrent case, m/s: 1 – $0.5{\cdot}10^{-3}$; 2 – $1.25{\cdot}10^{-3}$; 3 – $2.0{\cdot}10^{-3}$; 4 – $2.75{\cdot}10^{-3}$; 5 – $3.5{\cdot}10^{-3}$

From here, the inverse problem was solved, from which an expression for calculating the conditional number of irrigation points necessary for achieving uniform irrigation at a given height has been obtained:

$$k = \left(\frac{0.88}{\Gamma} - 1\right) + \sqrt{\left(\frac{0.88}{\Gamma} - 1\right)^2 + \frac{4.64}{\Gamma}}, \tag{23}$$

where Γ is the dimensionless complex geometric parameter of the packed column:

$$\Gamma = \frac{H_i a^2}{hD^2} \tag{24}$$

Further, according to the described method and dividing the height of the column into three conventional sections described, the change in the total conversion rate was calculated as a function of the integral factor (18). At the same time, the dependence of the degree of extraction on the regime parameter, namely, on the volume density of irrigation per unit cross-section of the apparatus (figures 2 and 3) was studied.

Figure 4 compares the results of the application of the developed scaling methodology to the calculation of the efficiency of the capture of ammonia and carbon dioxide (i.e., the important impurity biogas components) and experimental data obtained earlier in columns with chordal packing [4].

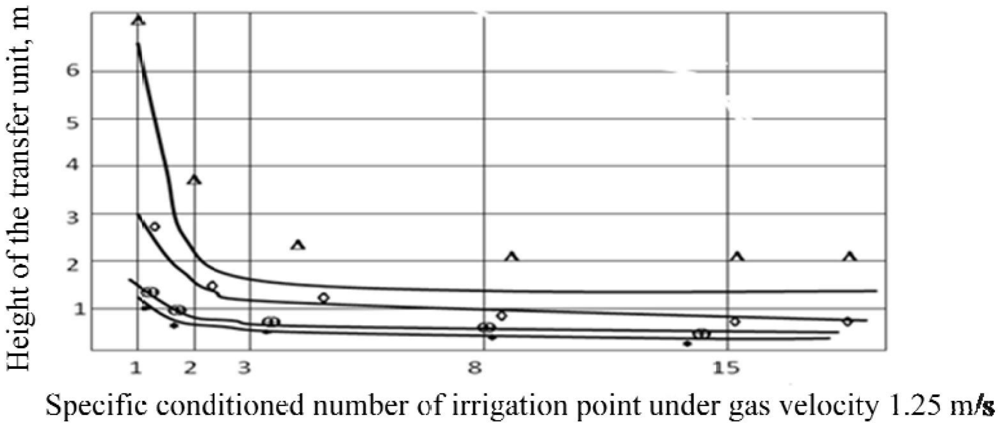

Figure 4 – Comparison of calculations for the model and generalized experimental data
for the processes of ammonia capture by water and carbon dioxide capture by $NaOH$-H_2O system [4].
The average density of irrigation: Δ – 0.25 m^2/h; – 0.75m^2/h; –1.25 m^2/h. Solid lines – calculated values

The known experimental results [4] show that the effect of the uneven distribution of the liquid phase on the efficiency of the absorption process is very strong. This is especially true for higher irrigation densities and in the case of concurrent liquid and gas phases.

At the same time, at lower irrigation densities, an increase in the conditional number of irrigation points leads to decrease in irrigation densities in many areas of the column packed section. This phenomenon and the increase in the degree of uniformity of irrigation are two competing factors.

A numerical experiment shows that improving the uniformity of irrigation leads to an increase in the degree of conversion. This effect will be most pronounced in the case of highly soluble gases [9, 10]. In this case the contact surface of the phases plays a decisive role, and the influence of the integral factor of the scale effect manifests itself more sharply [2, 11, 12].

Conclusion. The main aspects of the problem of large-scale transition in the design of flowing chemical apparatus have been scientifically substantiated. It is shown that the nature of the scale effect in this case is of a complex nature, having both regime technological aspects and hydrodynamic causes.

The developed approach makes it possible to use the results of laboratory studies on small-sized installations and the relationships obtained by mathematical modeling of the distribution of phases in the volume of the apparatus and on their basis to calculate the industrial apparatus.

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ФАЗАНЫҢ КӨЛЕМДІ БӨЛІНУІН ЕСКЕРЕ ОТЫРЫП АҒЫНДЫ ХИМИЯЛЫҚ ҚҰРЫЛҒЫЛАРДЫҢ ЖҰМЫС АЙМАҒЫН ЕСЕПТЕУ КЕЗІНДЕГІ АУҚЫМДЫ АУЫСУ

Аннотация. Мақалада реакторларда масса тасымалдаудың тиімділігін есептеуде ауқымды әсерді модельдеуге жаңа әдіс сипатталған. Бұл әдіс құрылғының барлық жұмыс көлемін өзара әрекеттесетін фазалар ағындарының әр түрлі қатынастары бар аймақтарға бөлуіне негізделген. Алынған өрнектерді химиялық құрылғыларды есептеу практикасында қолдануға болады.

Түйін сөздер: ауқымды әсер, химиялық құрылғы, саптама, шығару дәрежесі, масса тасымалдау.

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МАСШТАБНЫЙ ПЕРЕХОД ПРИ РАСЧЕТЕ РАБОЧЕЙ ЗОНЫ ПРОТОЧНЫХ ХИМИЧЕСКИХ АППАРАТОВ С УЧЕТОМ ОБЪЕМНОГО РАСПРЕДЕЛЕНИЯ ФАЗ

Аннотация. В работе описан новый подход к моделированию масштабного эффекта при расчете эффективности массоопереноса в реакторах. Этот подход основан на делении всего рабочего объема аппарата на зоны с различными соотношениями потоков взаимодействующих фаз. Полученные выражения могут найти применение в практике расчета химических аппаратов.

Ключевые слова: масштабный эффект, химический аппарат, насадка, степень извлечения, массоперенос.

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