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Methods for Evaluating the Influence of Large-Scale effect on Heat and Mass Efficiency of Chemical Apparatuses

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The known results in the theory of chemical apparatuses scaling are devoted mainly to apparatuses with non-regular packings. How the phases distribution over the regular packings in chemical columns effects the heat and mass efficiency is studied lesser. This paper deals with the methods for simulating the scaling effects regarding to the chemical towers with regular packings of various types. The models for describing the influence of initial liquid and gas distribution in chemical columns with regular packing on the mass transfer efficiency have been submitted. The sufficiently simple methods for evaluating the influence of large-scale factor on the efficiency of mass transfer have been obtained. These methods can be suitable for use in engineering calculation techniques.

1. Introduction

Increase in unit power of chemical apparatuses allows reducing a specific quantity of materials and energy provided maintaining even distribution of the phases in an apparatus. At the same time the maintenance of the even phase distribution on entire apparatus volume is a complex technical problem. It is especially true for large-scale apparatuses. And for uneven distribution of phases the flows ratios which are optimum from the point of view of maximum conversion, turn out to be violated in different areas of an apparatus. As a result, the average conversion decreases. This phenomenon is known as large-scale effect (Rozen and Kostanyan, 2002). The well-known results in the theory of the large-scale effect are devoted to apparatuses with non-regular packings mainly (Dil'man et al., 2012). And how the phases distribution over the regular packings of chemical columns effects the heat and mass efficiency is studied lesser.

It is obvious that both liquid phase and gas phase distributions have significant influence on the efficiency of mass transfer in the chemical apparatuses. As a rule one of the interaction phases is dispersed. So, on our opinion, the dispersed phase distribution deserves of more intent consideration. Indeed, it is rather difficult to reach the even distribution of disperse phase on entire apparatus volume. Besides, simulation of the structure of disperse phase flow is more complex problem than the one for a continuous phase (Timashev, 2000).

Our study was intended to the situation when the disperse phase is liquid. This situation is characteristic for packed towers under the regimes of a moderate liquid load.

The character of liquid distribution on a packed tower depends both on the liquid distribution at the initial cross section of an apparatus, i.e. at the zone of spraying devices, and on the design of packing (Synoradzki, 2003).

As the distance from the initial irrigated cross section increases, the evenness of liquid distribution in the apparatus cross section as a result of exposure to the packing can be improved or, conversely, can become worse.

Our paper deals with the problem of evaluating the influence of large-scale effect on mass transfer efficiency of chemical apparatuses.

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2. The concept of random walk methods for describing the liquid phase distribution on regular packings

Most studies on the distribution of dispersed liquid phase over the packings have been performed for the film regime of liquid flow over the packing units, i.e. when the gas stream has a little effect on the liquid flow. The general theory of liquid distribution over various packings that would adequately describe the influence of all constructive and regime parameters, however, is absent. This can be explained by the extreme complexity of hydrodynamic situation that is formed in the apparatus when the dispersed liquid flows through the packed bed in counter-current with the gas stream (Bertei et al., 2013).

The random walk methods were successfully used for describing the liquid distribution over the regular shelf packings (Brener, 2002). At the same time there is no apparent cause why these methods cannot be adapted for describing liquid distribution over regular packings of various types (Lapkin and Plucinski, 2010).

The appropriate approach (Brener, 2002) is founded on two main assumptions.

The first assumption is that probability for the system to change its state from the one state to other depends on these pairs of states only, i.e. the system states form the Markov chain. The main assumption lies on that the intensity of liquid stream on the packing unit depends on local space orientation of this unit, and on orientations of certain neighbouring units, but the structure of local liquid flow is supposed to be independent on local stream intensity. It may be correct to some extent (Kulov and Slin'ko, 2003).

The second assumption is that increase of distance between two packing units leads to rapid decrease of the probability of the liquid direct overflowing from one of the mentioned packing units to another. For many types of packings this assumption will be practically fulfilled provided sizable non-uniformity of the packing is absent (Zlokarnik, 2006).

Whether the packing design is that allows formation of more complex structure of liquid flow over the packing units then we can formulate the uniformity condition as the probability of liquid overflowing depends only on the difference $\left|x_i - x_j\right|$. Thus, it is possible to give the adequate mathematical description of the distribution of the disperse phase on volume of the packing tower, even with complicated internal devices, with the help of stochastic methods, in particular, the random walk methods. Therefore we can talk about the prospects of the development of such methods for describing the structure of the flow phases in chemical apparatus.

In the works (Brener, 2002) the random walk methods were used for the mathematical description of liquid distribution over the regular packing. The results of computer simulation that was carried out for regular chord and shelf packings, have a good agreement with the experimental data in the case when packing is watered from a system of point sources of irrigation.

Thus, the local specific liquid flow intensity i_{rz} while packing into the column of diameter D which is watered from one axis-symmetric spray is determined by the following formula

$$i_{rz} \approx I \frac{2h}{\pi z} \left\{ \exp\left(-\frac{h}{2a^2 z} r^2 \right) + \exp\left(-\frac{h}{2a^2 z} (D-r)^2 \right) + \exp\left(-\frac{h}{2a^2 z} (D+r)^2 \right) \right\} \tag{1}$$

Here I is intensity of the liquid source, a is a characteristic longitudinal size of a packing unit, h is a characteristic vertical size of a packing unit, D is an apparatus diameter, r is a current axial coordinate, z is a current vertical coordinate.

In the presence of a set of point sources of irrigation the local flow intensities can be evaluated with the help of the methods of local sources superposition (Herbert Vogel, 2005).

In normal case, under the even distribution of liquid over the regular packing, the liquid flows down from each packing unit to the certain number of downstream units. This number depends on the design both of the packing units and of the packing as whole. Studies show that under the certain gas velocities and under the liquid flow intensity that are optimum for the given design of packing there exist conditions for establishing the uniform liquid distribution over the cross section of an apparatus at some distance from the initial section where the liquid sprayers have set.

The size of the spreading zone H_s can be defined as the distance from the cross-section irrigated to the cross-section, wherein the unevenness distribution coefficient, i.e. the ratio of the maximum of the local liquid flow intensity to the minimum of the local intensity reaches a predetermined optimum value. As it is shown by calculations and confirmed by experimental data (Brener, 2002), the irrigation intensity maxima are observed under the liquid sources up to the certain distance from initial cross-section. The size of this spreading zone is determined by the peculiarities of packing design at the upper site of the chemical

apparatus, where the liquid stream does not reach wall of the apparatus and by the part of a layer of packing which are located below, and where the wall of apparatus influences the liquid distribution.
As the distance from the irrigated section increases, the maximum of the local liquid intensity is formed on the axis of the apparatus, in the absence of bypass in the peripheral zone. In the presence of draining nearby the walls the maximum of intensity may be formed at the walls of the apparatus on some distance from the initial section. Such hydrodynamic regime leads to a significant reduction in process efficiency (Lavric and Woehl, 2009).
Thus, the full height of the apparatus can be divided into two zones. In the first zone, which can be designated as zone of liquid spreading, the liquid distribution over the cross section of the column may differ significantly from even distribution. In the second zone the distribution is close to uniform in the absence of obvious defects of the packing units or the packing assembly. In order to determine the characteristics of absorption with account of the liquid distribution it is necessary to know the dependence of the specific mass transfer coefficients on the local intensity of irrigation. Such approach allows simplifying the mathematical model and to propose also a simplified technique for engineering calculations.
Let us define the coefficient of the distribution unevenness k_u at the end of the spreading zone as

$$k_u = \frac{i_{0,H_s}}{i_{R,H_s}} \tag{2}$$

Geometric properties of the irrigation device can be characterized with the help of the parameter *n* - a number of point sources of irrigation per unit of cross-section.
Figure 1 depicts some results of the numerical experiment that have been carried out according to random walk model (Rozen and Kostanyan, 2002).
On the results of numerical experiment the following approximation was derived (under k_u=1.15)

$$\frac{H_s}{h} = \frac{(D/a)^2}{4.64+1.76n} \tag{3}$$

Analysis of the results of numerical experiments shows that increasing of the number of sources of irrigation can save or decrease the height of spreading zone only under increasing *n*, what will be fulfilled when step between sources at the irrigating cross-section decreases.

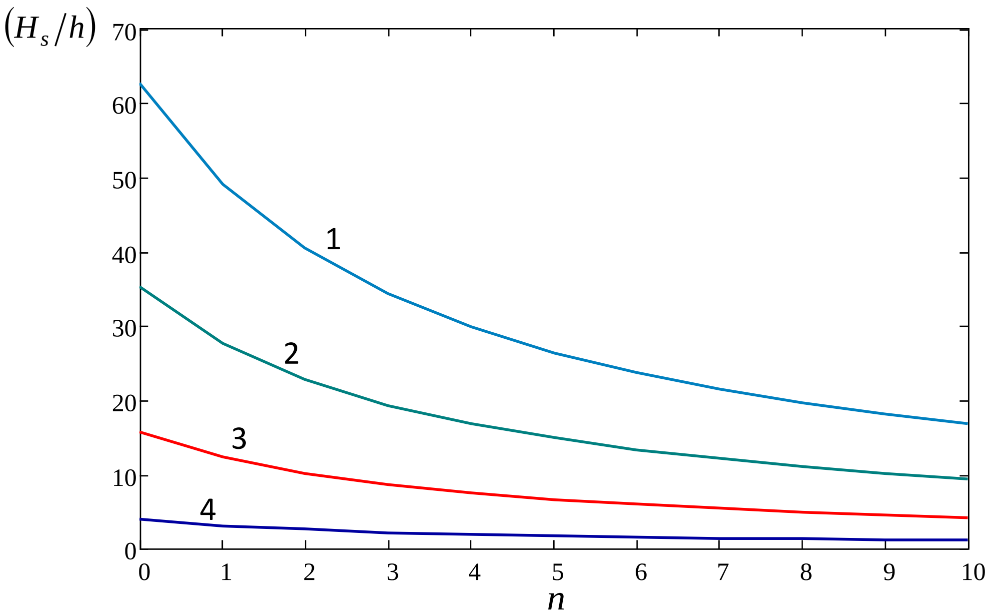

Figure 1: Dimensionless height of the spreading zone (H_s/h) as function of the number n of point sources of irrigation per unit of cross-section for chord packing. D/a *= 20(1); 15(2); 10(3); 5(4),* $k_u = 1.15$

Another principal result of the analysis of liquid distribution model is that there exists characteristic radius R_a for which the local intensity of liquid flow is equal to average value calculated for complete cross-section. Moreover, this characteristic radius becomes constant at certain distance H_a from the initial cross-section, i.e. R_a does not change further over the apparatus height.

The following estimations for the radius R_a and corresponding to it average intensity of the liquid flow was obtained

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

$$\bar{j} = J\sqrt{\frac{2h}{H_S}}\exp\left(-\frac{hR_S^2}{2a^2H_S}\right) \tag{5}$$

3. Evaluation of large-scale effect from the point of liquid distribution

The influence of uneven liquid distribution on the efficiency of absorption in the spreading zone is determined by three main reasons. They are: decrease of the specific surface of liquid dispersion due to low intensity of irrigation at the part of packing units, dependence of the local mass transfer coefficients on the local liquid flow intensity and, finally, a varying absorption factor (Gianni et al., 1997) over the apparatus cross-section. Of course, these reasons are interconnected, and by acting in common they lead to decrease of the average mass transfer coefficient into the spreading zone as compared with beyond of the spreading zone where more or less uniform liquid distribution can be established. In the works (Rozen and Kostanyan, 2002) the reduction of the mass transfer coefficient due to uneven liquid distribution has been described with the help of so called “coefficient of worsening”.

In our work we offer a semi-empirical approach according to which the coefficient of worsening is a ratio

$$\gamma = \frac{k_{ms}}{k_m} \tag{6}$$

where k_{ms} is the average mass transfer coefficient into the spreading zone; k_m is the empirical mass transfer coefficient corresponding to the average absorption factor outside the spreading zone.

Thus two cases should be distinguished. In the first case, the average intensity of irrigation is sufficient to achieve the optimal regime of intensive mass transfer. In the second case, the average intensity of irrigation may not be sufficient to achieve the optimum performance for mass transfer.

Let us further assume that the first case is realized. If the main resistance to mass transfer is concentrated in the gas phase that of all influencing factors the reduction of the specific surface of contact between the phases is brought to the fore front.

The influence of liquid distribution on the mass transfer intensity and efficiency of absorption process in the column with regular shelf packing was investigated on the pilot plan (Dil’man et al., 2012). Known experimental results confirm this thesis (Figure 2).

While analysing the experimental results some conclusions can be made. First, growth of the average irrigation intensity leads to increase in the coefficient of worsening, and it becomes stable at a certain level depending on the number of point sources of irrigation. Such behaviour of the coefficient of worsening completely corresponds to the theoretical conceptions described above.

Second, the local values of the mass transfer coefficients can be got from empirical data (Timashev, 2000). It means that for accounting the uneven liquid flow distribution it is assumed that each point of the apparatus volume element can be conventionally associated with the local value of the mass transfer coefficient obtained in the laboratory facilities of small size with a known structure of interacting flows (Preisig, 2013).

Thus, under the rather high specific intensity of irrigation the coefficient of worsening can be calculated from mere geometrical considerations, namely – as a ratio between a volume of a watered part of the spreading zone and its complete volume (Puschke and Preisig, 2011). For a local minimum of liquid flow rate on the basis of stochastic random walk model we obtain:

$$i_{\min} = \frac{4I\sqrt{\frac{a}{\pi d_0}}}{\exp\left(-\frac{d_0}{4a}\right)} \tag{7}$$

Here, the geometrical parameter of the initial liquid distribution is characterized by some conditional step d_0 between point sources of irrigation.

On the base of the distribution model the expressions for calculating a degree χ of substances conversion at the outlet of apparatus with allowing for the presence of two zones marked above have been obtained

$$\chi = \frac{\exp\left(\frac{\lambda-1}{G}F\overline{K}\left[H-(1-\gamma)\right]H_S\right)-1}{\lambda\exp\left(\frac{\lambda-1}{G}F\overline{K}\left[H-(1-\gamma)\right]H_S\right)-1} \tag{8}$$

In Eq(8) F is the total cross section surface, G is the flow rate of the continuous phase.

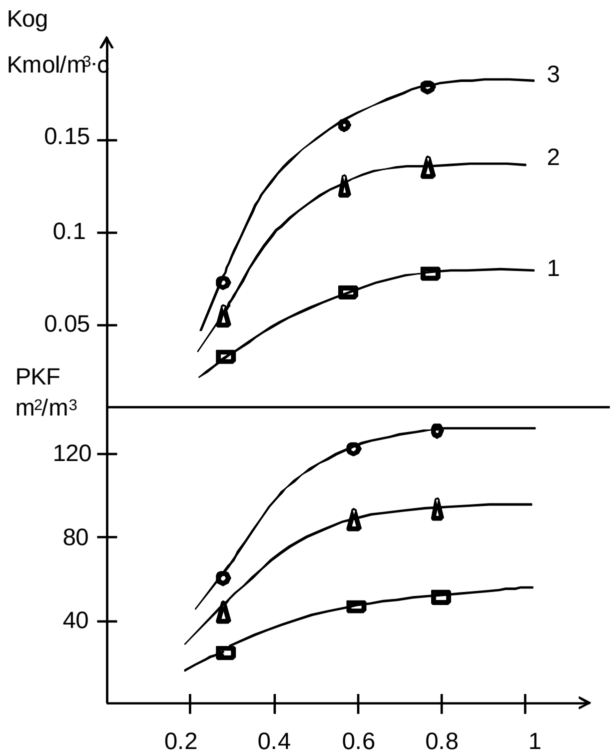

Figure 2: Dependence of the specific interphase surface s and volume mass-transfer coefficient in the gas phase Kog on the average intensity of irrigation i: 1-w_g=1 m/s, 2-w_g=1.25 m/s, 3-w_g=1.5 m/s

When evaluating the effectiveness of the device due to the uneven flow distribution in the amount of using the representation of the height of the transfer unit $\tilde{h}$, the calculation of the relevant characteristics can be produced by the formulas:

$$\tilde{h} = \tilde{h}^* + \Delta\tilde{h} \tag{10}$$

$$\Delta\tilde{h} = \frac{(1-\gamma)H_S}{N} \tag{11}$$

$$N = \frac{1}{\lambda - 1} \ln\left(\frac{1-\chi}{1-\lambda\chi}\right) \quad (12)$$

where $\tilde{h}^*$ is the height of the transfer unit for the uniform distribution of flows (according to experimental studies on laboratory bench), λ is the absorption factor.

4. Conclusions

The new approach for describing the scaling effect in chemical towers with regular packings has been submitted. This approach is founded on the concepts of random walk along mathematical grids which are adopted to the disperse phase distribution over packing with allowing for the peculiarities of phases distribution on the initial site at the vicinity of the spraying device. It is established that there exists some fixed characteristic radius, on which the flow rate of the disperse phase (liquid) is equal to the average value over the cross section of the apparatus independent on the distance from sprayer. This radius is stabilized at a certain distance from the inlet cross section. This approach allows us to decompose the apparatus work volume onto zones with different heat and mass transfer efficiency. So the sufficiently simple methods for evaluating the influence of large-scale factor on the efficiency of mass transfer have been obtained. These methods can be suitable for the engineering calculation techniques.

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