

Simulation of the liquid distribution in the wall zone of a packed column: case study

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The maldistribution of the liquid phase in a packed column is essential for the efficiency of the mass transfer processes in it. One of the wide-spread methods to measure the liquid distribution in the packing layer includes liquid collecting device (LCD) mounted under the packed bed. The proper design of the LCD is very important for obtaining correct information about the hydrodynamics in the column. The most popular construction of LCD is composed of fixed number of concentric cylindrical sections, with equal or different cross-sectional surface areas. The number and width of these sections is determined so as to ensure enough resolution of the picture of the liquid flow. In this study an analysis and estimation of several variants for possible fragmentation of LCD are provided, based on a dispersion model simulations and calculation of the maldistribution factor. The simulation results are verified with experimental data for metal Raschig Super-Rings 1.5" (RSRM) with an improvement of the LCD. It is shown also, that model parameters identification depends on the LCD fragmentation, especially in the wall zone of the packed column. The present study defines a quantitative criterion for LCD design assessment, which is the fragmentation effect on the maldistribution factor. This solves the issue with the proper data collecting, necessary for obtaining the actual liquid distribution and for parameter identification of the dispersion model.

Keywords: Liquid Collecting Device, liquid distribution, open-structure random packings, modeling, wall zone

INTRODUCTION

The maldistribution of the liquid phase in packed beds and the measures to overcome or reduce it are essential for the efficiency of the mass transfer processes. Probably that is the reason of increasing interest during last years in the investigation of the liquid phase distribution and wall flow observations in columns with diameter $D_c \geq 0.4m$ [1, 2], as well as in the open structure random packings. An experimental study of liquid maldistribution in a 1.2 m diameter column with random packings (Raflux rings, Hiflow rings, RVT saddle rings, Raschig Super-Ring) [1], is followed by development of TUM-WelChem Cell Model for prediction of the liquid distribution in these packings [2]. Our previous papers [3-5] are concerned with experimental investigation [3] of liquid distribution in a column with a diameter of 0.47m and random packings, metal Raschig Super-Ring. The experimental results are used successfully as a base for refinement of a dispersion model [4, 5]. They are in conformity with the observations for an older type of a random packing, like Pall rings. The performance of Raschig Super-Rings and Pall rings was predicted by CFD modeling in a moving pilot plant, for a wide range of liquid loads with varied constant column tilt and different column motion frequencies [6]. A new

cell model, accounting for different liquid behaviour in the bulk and the wall cells, was created in [7], validated by experimental data of Pall rings.

The above mentioned random packings are characterized by a complex shape (a type of a lattice of curved thin lamellae), low pressure drop, and their liquid spreading capacity in the radial direction is much lower than conventional packings of older generations [8, 9].

The distribution of the liquid phase in the packing layer can be recorded by various experimental techniques - collection devices, tracer methods, non-invasive tomography methods, etc. In [7], for example, a tracer conducting method and a wire-mesh tomographic sensor are combined, which allows a two-dimensional picture of the phases/liquid distribution across the apparatus section and obtains the development of this distribution over time.

The liquid phase distribution is most often studied experimentally by liquid collecting devices (LCD) (see Tab.1). A LCD typically comprises coaxially positioned cylindrical pipes open from top and closed from bottom. They are mounted under the packed bed to measure the distribution of the superficial velocity of the liquid flowing in the packing from the liquid distributor at the top of the apparatus. With a sufficient number of sections of the LCD, a detailed picture is obtained of the distribution and the radial spreading of the liquid

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phase in the apparatus. Often, in countercurrent flow of the gas and liquid phases, the collecting device is combined with the gas inlets [8, 13]. The LCD can also be mobile [12], in order to measure the radial distribution for different heights of the layer or to obtain a two-dimensional (radius and angle) pattern of distribution.

One important aspect in the design of collecting devices is the problem of correctly measuring the wall flow in a column with liquid flow with or without gas flow. The width of the section located next to the column wall should be appropriately selected [16]. Tab.1 shows the part of the cross-section area of the section collecting the wall flow,

accepted in existing investigations. If it is too big, a portion of the liquid coming from the bulk [11, 12, 15, 17] will be collected in addition to the wall flow, thus giving an inaccurate measured value. For example, the authors of [17] used a collecting device of four concentric cylindrical rings with the same area, i.e., the cross-section area of the section collecting the wall flow was 25% of the entire column cross-section area with a diameter $D_c = 0.3m$. In [11, 15] a 15 mm wide section was selected, which corresponded to 11.64% of the entire column diameter $D_c = 0.5m$.

Table 1. Previous studies of liquid distribution in packed beds by LCD

Reference	D_c [m]	δw [mm]	Area ratio [%]	Packing, size [mm]
Baker et al. (1935) [17]	0.3	20	25	Spheres, Saddles
Porter and Templeman (1968) [18]	0.3	3.2	4	ceramic Raschig rings - 12.7 metal Raschig rings - 25.4 ceramic Intalox saddles - 12.7 metal Pall ring- 15.9
Dutkai and Ruckenstein (1968) [10]	0.3	3.2	4	ceramic Raschig rings-10, 15, 20, 25 ceramic Intalox saddles-15, 25 ceramic Berl saddles - 25 plastic Pall ring - 35
Gunn and Al-Saffar (1993)[8]	0.3	25	30.56	Metal Nutter ring - 25 Plastic IMTP - 25 Plastic Pall rings - 25 Metal Super Intalox saddles- 25
Hoek (1983) [12]	0.5	10	16	Glass Raschig rings-10, 20, 30 Ceramic Intalox saddles - 15 polypropylene Intalox saddles - 50 metal Pall rings- 25
Stikkelmann (1989) [13]	0.5	12.7	10	Plastic Torus saddles - 25 Plastic Ralu ring - 25/38 Metal IMTP- 25 Metal Pall ring- 25
Kouri and Sohlo (1996) [11]	0.5	15	11.64	Ceramic Intalox saddles - 38 Plastic Pall rings - 25/ 50
Yin et al. (2000) [19]	0.6	4.7	3.12	Metal Pall ring - 25.4
Zhu (2005) [16]	0.3	12	15.13	Metal Pall ring - 25.4
Dzhonova et al. (2007) [20] Dzhonova et al. (2018) [3, 4] Petrova et al. (2018) [5]	0.47	5	4.21	Metal IMTP - 40/ 50/ 70 Plastic Ralu ring - 25/ 50 Metal Raschig Super rings - 12.5/ 25/ 37.5/ 50/ 75 plastic Raschig Super rings -15 / 50
Hanusch et al. (2017, 2018) [1, 2]	1.2	24	3.96	Metal Raflux ring - 35-5/ 50-5 Metal RVT saddle rings - 50-4/ 70-5 Plastic Hiflow ring - 50-6/ 90-7

A similar technique was used in [13] in a 0.5m diameter column to investigate the liquid distribution in 3rd generation packings of 25-38 mm sizes. The wall-flow collecting section has a

width of $\frac{1}{2}$, or about 10% of the entire cross-section.

The choice of a smaller width, <5 mm, for the wall-adjacent section and a cross-section area about

4% of the entire cross section limits the mixing of the wall flow with the bulk zone liquid, but may also measure a smaller wall flow of the actual, especially in countercurrent gas flow and at higher velocities of the liquid phase [16].

The choice of other researchers [8, 21] of the wall section width was within 1 packing element diameter (for element sizes up to 25 mm), and in columns with diameters of 0.291m and 0.3m, respectively. In [21], it is mentioned that the wall flow can be removed prior to reaching the collector by specially designed auxiliary device.

As can be seen from the literature survey, the number and the cross-section area magnitude of the concentric sections of the LCD are essential to obtain a correct picture of the radial distribution of the liquid, particularly for the measuring wall effects and the development of the wall flow for packings of different generation and in columns of various diameters. The existing models that provide analytical or numerical solutions for radial liquid distribution after a packing layer are based on experimental data obtained for specific conditions for this distribution through different types of LCDs. So far, the effect of "fragmentation" in the LCD on the parameters in model solutions has not been studied.

The present work defines and solves the following tasks:

- Influence of the number and width of the sections in the wall-adjacent area of the LCD on the picture of liquid radial distribution in a packed column;

- Influence of "fragmentation" in the LCD on the identification of parameters in the dispersion model; verification of simulation results and estimation by the maldistribution factor of LCD through real experimental data in a column with a diameter of 0.47m and RSRM 1.5" packing.

The first task was solved by simulating the various options for fragmentation of the LCD in the wall zone using the dispersion model [4, 5]. Eight variants of virtual fragmentation of the original LCD used in [3, 4] were tested calculating for each of them a maldistribution factor, as an integral characteristic of the model radial liquid distribution. The obtained results confirm the observation reported by other authors, that the most important is the width of the section collecting the wall flow. They also confirm the experimental data for the bulk zone liquid distribution from our previous studies [3, 4], as well as those of other authors [1, 14] for columns of a larger diameter.

The second task is consequence of the fact that with the data measured by the primary design of the

LCD used in our previous studies [4, 5], the dual identification of the model parameters turns out impossible, due to automodelity of residual variance in respect to one of the parameters (residual variance independence of the parameter). It is shown that Variant 2 of the LCD enables the dual parameter identification by the global minimum of the residual variance. This is achieved by means of simply dividing the section next to the wall-adjacent section of the primary structure and retaining its width. With the parameter values so identified, the adequacy of the model is proven by the example of a metal Raschig Super-ring (RSRM) 1.5" packing. The comparison between the experimental and model values of the maldistribution factor for the original and the improved LCD design proves the advantages of the latter.

SIMULATION AND ESTIMATION OF RADIAL LIQUID MALDISTRIBUTION IN LCD

It was experimentally found [3] that the liquid irrigation density in the central (bulk) zone of the original LCD (i.e. from 1st to 5th section, all sections are 8) did not change significantly with the liquid load, as well as with the packing redumpings. The same observation was confirmed through dispersion model simulations [5]. Therefore, it was decided to investigate theoretically only the column cross-section zone after the 5th section to the column wall, and to consider different variants of fragmentation of this zone and their effect on the liquid irrigation density distribution and the maldistribution factor. The latter is used as an integral estimation of the liquid distribution.

Eight variants of "fragmentation" of each section in the wall zone (after 5th section) of the original LCD, have been examined. The original LCD with 8 sections is presented by Variant 1. For all variants the first two sections are merged because their areas are too small. For each other variant, the fragmentation of 7th and 8th section is different. Section 6 is divided into three parts (sub-sections) with different areas for Variants 2 to 8. The fragmentation of section 7 starts from 2 sub-sections (Variant 2) to 3 or 4 sub-sections (Variant 3 and 4), with different combinations of areas. The area fragmentation of the last section is kept unchanged for Variants 1 - 4 (4.2 %), and then starts to increase from 6.3% (Variant 5) to 16.3% (Variant 8).

On the scheme (Fig.1), all 8 virtual variants are presented graphically for better visibility. The variant numbers are presented horizontally; the

fragmentation sub- sections areas in percentages for each variant are given vertically. In the authors' software, created for calculation of the theoretical distribution of the radial liquid irrigation density by the dispersion model, the radii of the LCD sections are set as external data.

Tab.2 gives the radii corresponding to the fragmentation after 5th section for each of the variants, as well as the calculated maldistribution factors [2, 4] by the following formula:

$$M_f = \frac{1}{F_0} \sum_{i=1}^{ns} F_i \left| \frac{L_i - L_0}{L_0} \right| \quad (1)$$

In Eq. (1) the ratio F_i/F_0 represents the ratio of the area of the respective section i to the entire area of the LCD (i.e. column cross-section), m^2 , ns is the number of sections of the LCD, L_i/L_0 is the dimensionless theoretical or experimental irrigation density in the section i of LCD, limited between the radii r_{i-1} and r_i ($r_i > r_{i-1}$). Theoretical mean density in i^{th} section of LCD is obtained from dispersion model according to:

$$f_i = \frac{2}{r_i^2 - r_{i-1}^2} \int_{r_{i-1}}^{r_i} f(r, z) r dr \quad (2)$$

The solution of the dispersion model, $f(r, z)$ at uniform initial liquid distribution has the form [5]:

$$f^u(r, z) = A_0 + \sum_{n=1}^{\infty} A_n' J_0(q_n r) \exp(-q_n^2 z), \quad (3)$$

$$A_0 = \frac{C}{1+C}, \quad A_n' = \frac{2(q_n^2/B - 2C)}{[(q_n^2/B - 2C)^2 + q_n^2 + 4C]} J_0(q_n)$$

As can be seen from Eqs. (1) and (3), the theoretical maldistribution factor and the solution depends on r , z and dispersion model parameters B, C and D for the respective packing and current packing layer height $z = DH/R^2$.

Since we are interested in the influence of fragmentation in the wall zone area along the radius, the maldistribution factor in Tab.2 is calculated from the solution in Eq. (3) at preselected values of z , B, C and D , for the corresponding $r = R_m/R$, F_i/F_0 and ns , for each considered variant.

The analysis of the results obtained in Tab.2 leads to the following conclusions:

- The additional fragmentation after 5th section in the wall zone of the LCD does not cause a significant variation of the maldistribution factor, if the cross-section area of the wall-adjacent section, where the wall flow is measured, is not changed;



Fig.1. Scheme of fragmentation variants of original LCD in the wall zone of the column after the 5th section: fraction of section area in % versus number of variants

- When increasing the area of the wall-adjacent section to the technologically reasonable and practically defined limits (between 3 and 16% of the total cross-section area of the column), the theoretical maldistribution factor decreases.

In fact, this decrease is due to the increase in the F_w/F_0 ratio for Variants 5 to 8 from 6 to 16%. According to the dispersion model, the model wall flow is dimensionless and its value does not depend

on r , but only on the height of the layer and the value of parameters B, C and D . If only the area of the last section increases, the wall flow will not change, but the theoretical M_f will be artificially much lower than the actual value. For example, for parameter values close to those in Tab.2 and for LCD Variant 1, the experimental maldistribution factor value for RSRM 1.5" is about 0.28 [3], i.e. close to the theoretical 0.26. While for Variant 8 the

theoretical M_f value is 0.1560 or 44% lower. Therefore, it is appropriate to choose such a variant of section fragmentation in the wall zone, for which the theoretical and experimental maldistribution

factors do not differ by more than 10%. It is envisaged to obtain experimental confirmation of this conclusion in our future work, which will require a reconstruction of the LCD.

Table 2. Sections radii of LCD, corresponding to the fragmentation after 5th section, for each of the 8 variants and calculated respective maldistribution factors

No. Variant	1	2	3	4	5	6	7	8
	R_{in}, m							
No. section								
1+2	0.076	0.076	0.076	0.076	0.076	0.076	0.076	0.076
3	0.105	0.105	0.105	0.105	0.105	0.105	0.105	0.105
4	0.135	0.135	0.135	0.135	0.135	0.135	0.135	0.135
5	0.165	0.165	0.165	0.165	0.165	0.165	0.165	0.165
6	0.195	0.195	0.175	0.175	0.175	0.175	0.175	0.175
7	0.23	0.213	0.185	0.185	0.185	0.185	0.185	0.185
8	0.235	0.23	0.195	0.195	0.195	0.195	0.195	0.195
9		0.235	0.205	0.205	0.205	0.205	0.205	0.205
10			0.22	0.215	0.215	0.215	0.215	0.215
11			0.23	0.225	0.2275	0.225	0.2225	0.235
12			0.235	0.230	0.235	0.235	0.235	
13				0.235				
ns	7	8	11	12	11	11	11	10
M_f^{model} $B=10, C=1.5,$ $D=0.0022m$	0.2615	0.2615	0.2615	0.2615	0.2411	0.2219	0.2037	0.1560

A complementary conclusion of the study is that the value of the maldistribution factor strongly depends on the parameter B and less on the parameter C , which has been already observed in the model solution in our previous work [5]. Since the parameter C is determined exactly by the experimental data measured in the wall zone of the column, it is very important which variant of the LCD fragmentation is selected. Subsequently, this will also affect the identification of the other two parameters in the model.

In the above-mentioned work, it was shown that dual identification of B and D is not possible due to automodelity of residual variance for RSRM 0.7", 1.5" and 3", and a hybrid method for their determination is proposed.

However, it is necessary to investigate and verify for a real example, whether the dividing of the wall zone of a particular LCD is not the cause of the automodelity.

INFLUENCE OF THE WALL ZONE FRAGMENTATION ON THE PARAMETERS' IDENTIFICATION – CASE STUDY

A modification of the LCD wall zone area in the pilot installation described in [3, 4] corresponding to Variant 2 (Tab.2) is made. Section 7 is divided into two parts with the same area, as it is too large compared to the remaining sections of the LCD (Fig.2). In this modification the areas of the

remaining sections have been kept unchanged, especially the outermost one, in which the wall flow is collected. Experiments were carried out to measure the radial distribution with the modified LCD after a layer of a packing RSRM 1.5" at a layer height $H = 0.6m$ with two different types of initial liquid irrigation - uniform and on the wall. The range of initial liquid flow rates, the number of redumpings of the packing layer, and the measurement technique are described in details in [3].

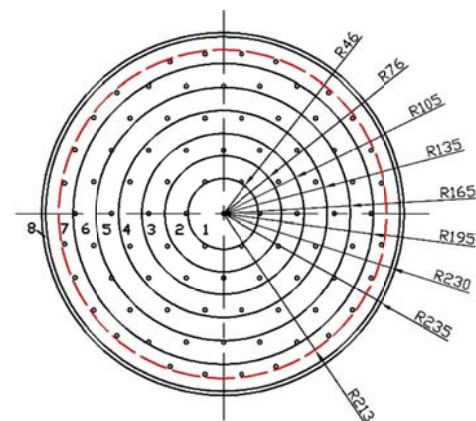


Fig.2. Scheme of LCD radial fragmentation (Variant 1) [5]. (Red dashed line dividing 7th section corresponds to Variant 2.)

With the experimental data obtained, the value of parameter C was recalculated on the base of four sections because of the division of the 7th section.

The newly obtained value $C = 0.993$ for the packing RSRM 1.5” is close to the previous one - 0.981, calculated without division of the 7th section. With the calculated value of $C = 0.993$ a dual identification of the parameters B and D of the dispersion model is performed. The criterion for reaching their optimal values is the minimum of the residual variance between the experimental and model mean density of irrigation, across all sections of the modified LCD.

Fig.3 shows the results of double identification as a contour map. A global minimum of the residual variance of $0.1302e-01$ for the model parameters’ values $B = 9, D = 0.00275m, C = 0.993$ was identified, indicated by arrow.

Adequacy verification of the obtained model parameters was made. The reproducibility variance of the experiments carried out is $S_0^2 = 0.674e-02$ of a sample size $m' = n - ns = 16$ of $n = 24$ and $ns = 8$ sections of the modified LCD with $n_i = 3$ redumpings (parallel experiments) of the packing layer.

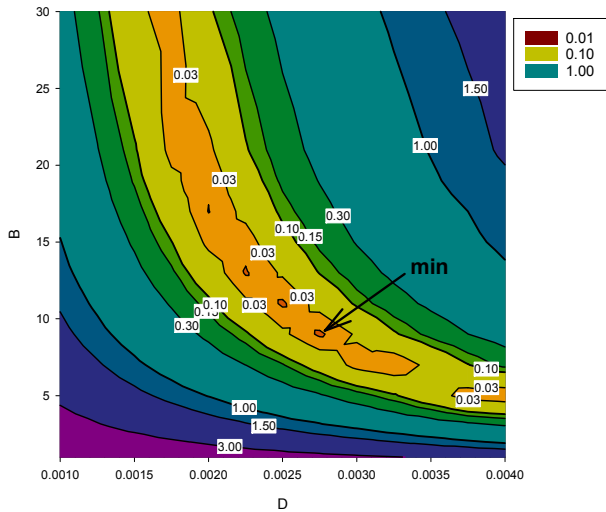


Fig.3. A contour map of residual variance as a function of model parameters B and D

The minimum residual variance between experimental and model mean densities of irrigation in all sections of LCD,

$$S_A^2 = \left(\sum_{i=1}^{ns} n_i (f_{iexp} - f_{imod})^2 \right) / (ns - 1) \text{ is } 0.1302e-01$$

Table 3. Experimental and theoretical values of density of irrigation in the modified LCD and average relative error $\delta\%$ in sections

No. section	I+II	III	IV	V	VI	VII	VIII	IX
f_{ie}	0.908	0.964	0.967	0.985	0.889	0.5709	0.589	4.67
f_{ic}	0.9995	0.9958	0.9815	0.9355	0.8246	0.6762	0.5331	4.667
$\delta, \%$	9.15	3.19	1.48	-5.29	-7.81	15.56	-10.49	-0.06

for volume of the sample $m = ns - 1 = 7$.

At a level of significance $\alpha = 0.05$, Fisher's criterion shows adequacy:

$$F = \frac{\min(S_A^2)}{S_0^2} = 1.931 < F(m, m') = 2.66 \quad (4)$$

The experimental and theoretical values of the irrigation density in the modified LCD along with the average relative error $\delta\%$ by section are given in Tab.3.

The results confirm the assumption that splitting of section 7 of the original LCD is sufficient to ensure that both parameters B and D are identified by a new value of the third parameter C of the dispersion model.

For comparison, the model and experimental maldistribution factors for the original LCD - Variant 1 and three sizes of packings, obtained in our previous work (Fig.4), are calculated too. It can be seen that the relative error between the model and experimental values of the maldistribution factor is highest ($\sim 24\%$) for the smallest packing size, for the data obtained using the LCD of Variant 1.

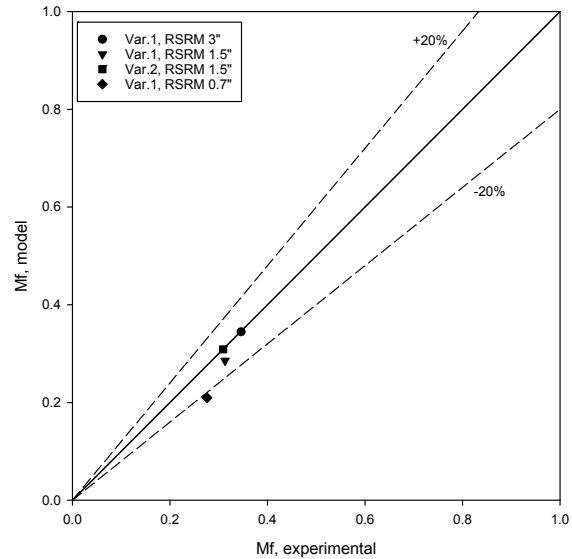


Fig.4. Comparison between experimental and model maldistribution factors for RSRM 0.7, 1.5 and 3”, at optimal values of model parameters for Variant 1 [5] and Variant 2

This deviation is probably due to insufficiently precise determination of the parameter C in the wall zone, its value being much lower (0.630) compared to the C values for the other two sizes - 0.981 and 1.541. It is known that parameter C depends on the diameter of the packing [22], as well as on the coefficient of radial spreading D , but for lattice- type packings, it is difficult to determine which dimension is the characteristic one. According to [20], this size is the width of the lamella of the packing element. This characteristic width increases with the nominal size of the packing. This is connected with the increase in the coefficient of radial spreading D , as well as in the wall flow.

It should be noted that after the modification, the model and experimental maldistribution factor for the examined case study for the packing RSRM 1.5" completely coincided, whereas for one-parameter identification and the experiment of Variant 1, the relative error was 8.7%.

CONCLUSIONS

The present study examines the effect of different fragmentation of the LCD in the column wall zone on the dispersion model's solution and the identification of its parameters, as well as on the experimental data obtained in the LCD. Eight variants of virtual dividing into sub- sections in the wall zone of the original LCD used in [3, 4] were tested. For each of them, the integral characteristic called maldistribution factor [2], of the radial liquid distribution obtained by the model, was computed. The results confirm the observation, reported by other authors, that the width of the section collecting the wall flow is the most important.

It is shown that Variant 2 of the LCD fragmentation (Tab.2) solves the no-minimum issue in two-parameter identification by simply dividing the section next to the last one and retaining the latter's width. With the proposed modification of the LCD, experiments with a RSRM 1.5" packing were performed and the adequacy of the model was proven for the identified parameter values. The comparison between the experimental and model maldistribution factor for the original and the improved LCD design confirms the advantages of the latter.

The presented procedure for evaluation of the effect of the LCD wall zone fragmentation, by calculation of the respective maldistribution factor, suggests a quantitative criterion for proper design of the experimental set-up. The increase of

the wall section width should be accompanied with difference between values of the maldistribution factors (experimental and theoretical) not exceeding 10 % in order to be sure to obtain a correct flow distribution in LCD.

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NOMENCLATURE

A_0, A_n^u - coefficients of dispersion model solution for uniform initial irrigation;

B - dispersion model parameter, a criterion for exchange of liquid between the column wall and the packing;

C - dispersion model parameter, expresses the equilibrium distribution of entire liquid flow between the wall and the packing when equilibrium state is attained $z \rightarrow \infty$;

D - dispersion model parameter, coefficient of radial spreading of liquid, m;

D_c - column diameter, m;

d_p - diameter of a single packing element, m;

H - packing layer height, m;

F_i - area of section i in LCD, m²;

F_0 - column cross-section area or that of LCD, m²;

F_w - area of the section next to the column wall, m²;

$f(r, z)$ - dimensionless dispersion model solution for uniform initial irrigation;

\tilde{f}_i - the mean dimensionless density of irrigation in i -th annular section of the LCD, delimited by the radii r_{i-1} and r_i ($r_i > r_{i-1}$);

L_i/L_0 - ratio of local to mean irrigation densities, in section i of LCD;

M_f - maldistribution factor for radial liquid distribution in packed column cross-section, or in LCD;

m, m' - degree of freedom for reproductive and residual variances, respectively;

n - sample size of experimental data, measured in LCD, packing redumpings are included;

ns - number of sections in LCD;

R - column radius, m;

$r = r'/R$ - dimensionless radial coordinate;

r' - radial coordinate, m;

q_n - the roots of the characteristic equation, following from boundary condition in [5];

S_0^2 - reproductive variance for experimental data, with parallel experiments (packing redumpings);

S_A^2 - residual variance between model and experimental values;

$z = DH/R^2$ - dimensionless axial coordinate;

Greek symbols

α - significance level in Fisher criteria;

δ - mean relative error, in %, between experimental and model densities of irrigation;

δ_w - width of the wall flow collecting section (Tab.1), mm;

Subscripts

ic - calculated values in section *i* of LCD;

ie - experimental values in section *i* of LCD;

in - inner radii of sections in LCD;

w - wall

Superscripts

model - model;

exp - experimental;

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