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Modeling of Liquid Distribution in a Packed Column with Open-structure Random Packings

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The scientific interest in the efficiency of packed bed columns is a part of the world-wide pursuit of sustainability of the processes. The maldistribution of the phases in the apparatus reduces the efficiency and makes difficult the prediction of process performance and scaling up. The present work aims at modeling of liquid distribution in a packed column with high performance open-structure random packings - metal Raschig Super-Rings 0.7”, 1.5” and 3” and metal Pall rings 1”. Some new approaches for estimation and calculation of model parameters are proposed and tested, using own experimental data for Raschig Super-Rings and published data for Pall rings. A new procedure for identifying one of the model parameters, called by us “overlapping confidential intervals” solution, is developed and illustrated for Raschig Super-Ring packing in the case of partial radial insensitivity (“plateau”) of the residual variance between the model and experimental data. The obtained results show that using appropriate statistical methods of estimation, the dispersion model parameters can be successfully identified achieving a very good prediction of the experimental data. Several numerical examples and case studies are considered and discussed. For the case of Pall rings, the dispersion model predictions are in very good agreement with both published experimental data and predictions made by Computational Fluid Dynamics(CFD) modeling.

1. Introduction

The recent interest in the modeling of liquid distribution in packed columns is connected withthe efficiency of separation processes like absorption and rectification. One of the first models proposed to predict the liquid distribution in a packed bed is the random walk model of Tour and Lerman (1939) for liquid spreading in unconfined packing with no wall effect. Later, the dispersion model of Cihla and Schmidt (1957) with confined random packings (spheres, Raschig rings, Intalox saddles) was developed by Staněk and Kolář (1968) to account for the wall flow. The Monte-Carlo cell model (Stikkelman, 1989) is capable of simulating small scale maldistribution of the liquid, wall flow and spreading of both phases for random packings Pall and Ralu rings, IMTP, and Torus saddles as well as for structured packingsMellapak, BX, Ralupak, etc. A 3-D geometry- based model is constructed to predict the trickle flow of liquid down a randomly packed bed of metal Pall and Raschig rings (Wen et al., 2001). Meanwhile, the CFD is widely employed (Yin, 1999 and Haddadi et al.2016) for prediction of the liquid distribution by treating the packing bed as a porous media with permeability resistance. The investigated random packings are Pall rings (Yin, 1999) and spheres and cylinders (Haddadi et al., 2016) and the comparison showsgood coincidence between CFD simulations and experimental results.
Without doubt, the experimental data for liquid distribution is highly needed for validating the model predictions. The recently published experimental results for open-structure packings like Raschig Super-Rings (RSR) in Dzhonova-Atanasova et al. (2018a), and for Raflux-Rings, RVT Metal Saddle Rings and Hiflow-Rings in Hanusch et al. (2017), are very welcome to prove in detail the various model hypothesis. The aim of the present work is modeling of liquid distribution in a packed column with the help of experimental data for high performance open-structure random packings - metal Raschig Super-Rings 0.7”, 1.5” and 3” (Dzhonova et al., 2018b) and metal Pall rings 1” (Yin,1999). The 3-parameter model of Staněk and Kolář (1968) is used with newly developed recommendations and methodologies for parameters’ identification. The model predictions are verified at several case studies and show very good correlation with experimental data.

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2. Model description

In this part a brief description of model equations, boundary conditions, and solution is presented (Staněk and Kolář,1968). The process of liquid flow distribution in a packed-bed column is described by the following dimensionless equation:

$$\left(\frac{\partial^2 f(r,z)}{\partial r^2}+\frac{1}{r}\frac{\partial f(r,z)}{\partial r}\right)=\frac{\partial f(r,z)}{\partial z} \tag{1}$$

where $r=r'/R$ is dimensionless radial coordinate; r' is radial coordinate, m; R is column radius, m; $z=Dh/R^2$ is dimensionless axial coordinate; D is the packing liquid spreading (distribution) coefficient, m; h is axial coordinate, m; $f=L/L_0$ is dimensionless superficial velocity; L, L_0 are local and mean liquid superficial velocity, m^3/(m^{2}s).
The boundary conditions are:

$$-\left.\frac{\partial f}{\partial r}\right|_{r=1}=B(f-CW)\ , \qquad \left.\frac{\partial f(r,z)}{\partial r}\right|_{r=0}=0\ , \tag{2}$$

where parameter B is a criterion for exchange of liquid between the column wall and the packing; parameter C expresses the equilibrium distribution of entire liquid flow between the wall and the packing when equilibrium state is attained $z\to\infty$; W is dimensionless wall flow. The equations defining two parameters are:

$$B=\beta R/D\ , \qquad C=\pi R^2\gamma\ , \tag{3}$$

where β and γ are parameters in the boundary conditions. At $z=0$ the uniform initial irrigation is:

$$f(r,z)\big|_{0\le r<1,\, z=0}=1\ . \tag{4}$$

There exists a dimensionless analytical solution f^u (index "u" means uniform initial irrigation) of the above model in the form of infinite series with coefficients A_0 and A_n^u :

$$f^u(r,z)=A_0+\sum_{n=1}^{\infty}A_n^u J_0(q_n r)\exp\left(-q_n^2 z\right),\quad A_0=\frac{C}{1+C},\ A_n^u=\frac{2\left(q_n^2/B-2C\right)}{\left[\left(q_n^2/B-2C\right)^2+q_n^2+4C\right]J_0(q_n)} \tag{5}$$

The dimensionless wall flow W^u is obtained from the material balance:

$$W^u=\frac{1}{1+C}-2\sum_{n=1}^{\infty}A_n^u(q_n)\frac{J_1(q_n)}{q_n}\exp\left(-q_n^2 z\right), \tag{6}$$

where J_0, J_1 are Bessel functions of the first kind, zero and first order; q_n are the roots of the characteristic equation, following from boundary condition (2), i.e, $\left[(2C/q_n)-(q_n/B)\right]J_1(q_n)+J_0(q_n)=0$.

3. Experimental data used for model validation

3.1 Metal random packings Raschig Super-Rings 0.7", 1.5" and 3"

The experimental installation is a steel column of a 0.47 m diameter. The measurements are performed by means of the liquid collecting method with an annular 7-segmentLiquid CollectingDevice (LCD) under a packing layer with a height of*H*=0.6 m,in a single-phase flow of tap water at room temperature, fed at the top of the column (Dzhonova et al., 2018b). Two types of initial irrigation – uniform and on the wall are performed for each packing; for the uniform one the flow rates are in the range $Q_0=1.87\div 7.49$ m^3/h , and for the wall irrigation - $Q_0=0.3; 0.45; 0.6$ m^3/h . At each initial flow rate of irrigation (uniform and on wall),three redumpings of the packing layer weremade. It was clarified that the results didnot depend substantially on the magnitude of initial irrigation, but essentially ontheredumpings. The obtained results are presented briefly in Table 1 for all packings at uniform initial irrigation. All values in segments are averaged first over all initial densities of irrigation, then over the redumpings. The relative areas of LCD segments are given too - F_i/F .In Table 1 the first two segments are summedbecause they have small areas.

Table 1: Experimental mean densities of irrigation in segments of LCD for metal RSR 0.7", 1.5" and 3"

Segments	1 + 2	3	4	5	6	7	8
F_i/F ,%	10.5	9.5	13.0	16.3	19.6	26.9	4.2
$f_{\exp}$,RSR 0.7"	1.06	1.06	1.04	1.09	0.93	0.539	3.51
$f_{\exp}$,RSR 1.5"	1.07	1.07	0.962	0.912	0.898	0.564	4.40
$f_{\exp}$,RSR 3"	0.928	0.948	1.01	0.910	0.914	0.521	5.09

3.2 Metal random Pall rings, 25 mm

Experimental data for the liquid distribution in a column filled with metal Pall rings, 1" used in this paper are taken from the PhD thesis of Yin (1999). They are obtained in a pilot column with a 0.6m diameter, for a packing height of 0.9 m, and liquid and gas loads $L = 4.78\,\text{kg}/\left(\text{m}^2 s\right), G = 0.75\,\text{kg}/\left(\text{m}^2\text{s}\right)$. The LCD consists of 6 segments andthe initial irrigation is uniform.

4. Discussion on the methodologies for identification of dispersion model parameters for random packings

There are three parameters in the coefficients A_0 and A_n^u of dispersion model solution Eq(5) - B, C and D. In Dzhonova et al.(2018a) a few possible formulas to calculate the value of C are presented; usually this parameter is obtained from the experimental data of wall flow or from the flow rate in selected segments of LCD, both at two different initial irrigation (uniformand on the wall). The other way to obtain C is from data for the wall flow at different packing heights and reached equilibrium between the bulk and the wall flow for uniform irrigation only(see Eq(6) at $z \to \infty$).For Pall rings in 3.2 the obtained value of C from Eq(6) is $C = 5.92$,which is very close to the value $C = 5.29$, obtained for ceramic Pall rings 1" in (Semkov et al.,2000). For packings in 3.1 the value of parameter C found for metal RSR 1.5" is $C = 0.981$ (Dzhonova et al., 2018a).If the value of D for the considered packing is also known (Staněk and Kolář, 1968), there is only one model parameter B to be identified, usually by non-linear optimization, minimizing the residual variance S_A^2 between the model and experimental data:

$$S_A^2 = \frac{1}{k-1}\sum_{i=1}^{k} n_i \left(f_{i\exp} - f_{i\,\mathrm{mod}}\right)^2 , \tag{7}$$

where f_i , n_i are the mean dimensionless density of irrigation and the number ofparallel experiments(redumpings) in i^{th} annular section of the LCD ($i = 1 \div k$), respectively. Each section is delimited by the radii r_{i-1} and $r_i\left(r_i > r_{i-1}\right)$, and f_i is determined by the expression:

$$f_i = \frac{2}{r_i^2 - r_{i-1}^2}\int_{r_{i-1}}^{r_i} f(r,z)\,r\,dr \tag{8}$$

If the value of D is not known, atwo-parameter non-linear optimization can be performed, varying simultaneously β and D values in finite intervals (Semkov et al., 2000) and again searching the minimum value of S_A^2 . It isshown there that this technique works for older type of packings like ceramic Intalox saddles and Pall rings, but is not appropriate for Cascade Mini-rings; where an auto-model regime of S_A^2 in respect to parameter D occurs; after some value of D the value of S_A^2 decreases very slow, forms a "plateau" and no global minimum of S_A^2 exists. The same behavior for S_A^2 can be observed for metal RSR 1.5", if two- parameter identification of B and D is performed (Figure 1a). The possible exits of the situation with the S_A^2 "plateau" are to find the value of D for the packing and then apply Eq(7) and identify B only, or to search for other methods to identify both parameters. Unfortunately, in the last two decades only few results for liquid spreading coefficients of modern packings (IMTP, metal and plastic RSR and Ralu Flow) were found (Dzhonova et al., 2007), using two different experimental methods for obtaining of D. The existing literature data of D for metal Pall rings, 1" are somewhat confusing as they differ significantly – the result of Stikkelman (1989) is about 3 times bigger ($D = 0.0025\,\mathrm{m}$) than that of Wen et al. 2001 ($D = 0.0007\,\mathrm{m}$),although both are obtained by the same method.

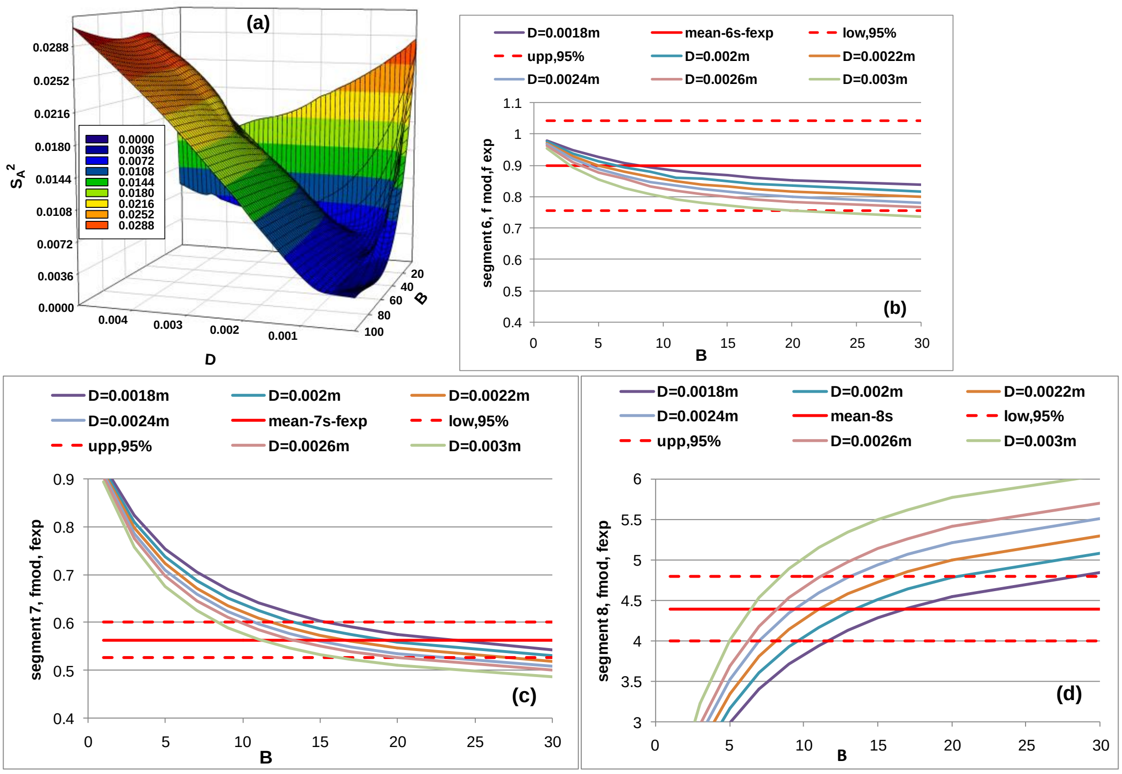

Figure 1: 3D plot for insensitivity ("plateau") of the residual variance S_A^2 between the model and experimental data vs dispersion model parameters B, D - (a), and "overlapping confidential intervals" method for B, D in last three segments 6,7 and 8 of LCD– (b), (c) and (d), respectively (for metal RSR 1.5")

A new method, called here "overlapping confidential intervals" is developed for the case of unknown D and S_A^2 "plateau". Preliminary analysis shows, that in Eq(7) only for segments (6÷8), which are near to the column wall, $f_{i,\mathrm{mod}}$ changes with the value of B and introduces a significant impact in S_A^2. This behavior is in agreement with the boundary condition on the column wall Eq(2). The differences $\left(f_{i\,\mathrm{exp}} - f_{i\,\mathrm{mod}}\right)$ in segments 1÷5 (bulk region) remain practically constants in respect to changes in B. Therefore, the value of S_A^2 will depend mostly on $f_{i,\mathrm{mod}}, i = 6 \div 8$ and from the statistical deviation of data $f_{i,\mathrm{exp}}$ in these segmentswith packing redumpings. A brief algorithm of the new graphical method implementation is:

- From experimental data in 3.1 in segments 6÷8 of LCD, calculate the mean value of $f_{i,\mathrm{exp}}$ from packing redumpings (n_i) and confidential intervals in each segment, using 95 or 98 % confidence level. Draw the mean values and confidence intervals in each segment vs B (in respect to B they are constant lines).
- Calculate $f_{i,\mathrm{mod}}$ at various B for fixed values of D and C, for segments 6÷8. Add like an additional curve to the abovementioned graphics. When $f_{i,\mathrm{mod}}$ intersect the confidential intervals of $f_{i,\mathrm{exp}}$ at each

of the segments 6÷8, and these three intersection intervals have common section (overlap), for chosen values of D and C, that will be the real value (or interval of values) for parameter B.

In the next section the proposed new method is validated and illustrated in the case of metal RSR 1.5”. The other case studies, with one-parameter identification of B at known D and C for metal RSR 0.7” and 3”, as well as for Pall rings 1”, are considered too.

5. Results and discussion

5.1 Case study: application of the new method of “overlapping intervals” for packing metal RSR 1.5”

The application of the new algorithm for “overlapping intervals” is presented in Figure 1b,Figure 1c, and Figure 1d foropen–structure random packing metal RSR 1.5”. At $C = 0.981$ for several fixed values of D it was checked if there existed a narrowest common section for parameter B in all three segments 6÷8 between $f_{i,\mathrm{mod}}, i = 6 \div 8$ and 95% confidential intervals for $f_{i,\exp}, i = 6 \div 8$. It turned out, that the best common graphical solution (section) waspossible only for values of $B \in (9.8 \div 11)$ and $D = 0.0026\ \mathrm{m}$. For values of D smaller or bigger than $D = 0.0026\ \mathrm{m}$, the results gave possible common intersection wider than the found one or intersectiondid not exist.

5.2 Case studies: one-parameter identification with known D and C for packings Pall rings, metal RSR 0.7”, 1.5” and 3”

For metal packings RSR 0.7”, 1.5” and 3” the following values of parameter C are calculated, following the formulas for C in Dzhonova et al. (2018a),for two types of initial irrigation. For RSR 0.7” and RSR 3” the obtained values are $C = 0.630$ and $C = 1.541$, respectively. For values of D for all considered RSR, the results from asingle jet method from Dzhonova et al. (2007) are taken: $D = 0.00146\ \mathrm{m}$ (RSR 0.7’), $D = 0.0022\ \mathrm{m}$ (RSR 1.5”) and $D = 0.00349\ \mathrm{m}$ (RSR 3”). The identified values of B after calculation of S_A^2 in the range of $B = 1 \div 30$ are $B = 10$ for both RSR 0.7” and RSR 3” and $B = 11$ for RSR 1.5”, for the abovementioned obtained and fixed values for D and C. The clearly defined minimums of S_A^2 curve have obtained: $\min(S_A^2) \approx 10^{-2} \div 10^{-3}$ for all three cases. In Figure 2a a comparison between model predictions for identified parameters (lines) and experimental data for packings RSR 0.7”, 1.5” and 3” (points) is presented. In the bulk region – segments 1÷5, the liquid distribution (both experimental and model one) for all packings are practically similar and close to the uniform distribution, but differ in the last 3 segments with strong increasing of the flow to the wall with the packing size increasing. The relative error between model and experiment does not exceed 10% for all packings. For packing RSR 1.5”, comparing the values of identified parameters from new method and one-parameter identification, it is encouraging, that they are very close to each other ($B = 11$ and $B \in (9.8 \div 11)$) for two relatively close values of D.

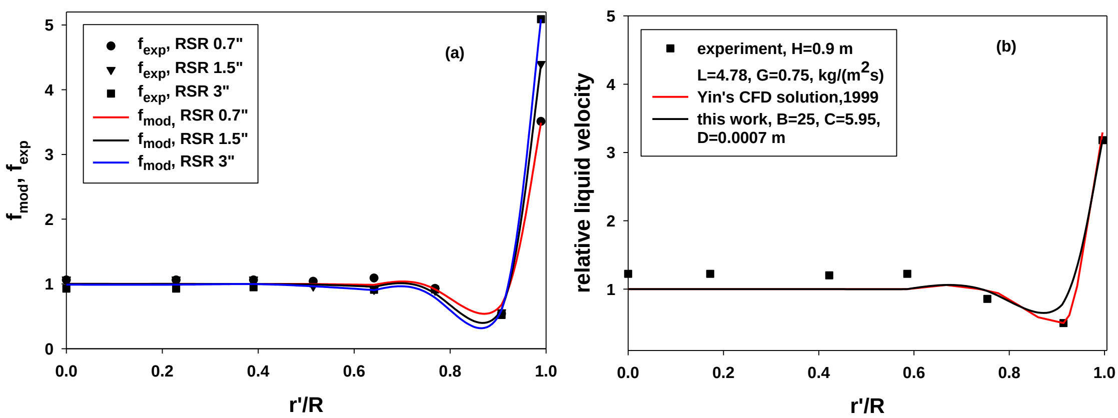

Figure 2: Comparison of dispersion model predictions and experimental data for metal RSR 0.7”, 1.5”and 3”, H=0.6m-(a) and comparison of experimental data for Pall rings, 25 mm and CFD predictions (Yin, 1999) with dispersion model, H=0.9m-(b)

For the case of Pall rings, 1”, the value of $C = 5.29$ is obtained from experimental data of Yin (1999) for wall flow at several packing heights. The value of $D = 0.0007$ m is taken from Wen (2001). The identified value of B after calculation of S_A^2 in the range of $B = 1 \div 50$ is $B = 25$ .As can be seen from Figure 2b, the dispersion model predictions (black line) fit very well with both experimental data (black points) and the Yin’s CFD predictions (red line).

6. Conclusions

In this paper two methods for identification of dispersion model parameters are presented and validated by the authors’ experimental data for liquid distribution in open-structure metal random packings RSR (0.7”, 1.5” and 3”) and experimental data for metal random Pall rings, 1”. Anew method of “overlapping confidential intervals” is proposed and successfully tested in the case of plateau of residual variance S_A^2 between model and experimental data for metal RSR 1.5”. The second method for identification of only one of the dispersion model parameters (B)by minimizing S_A^2 is possible after using both the experimental data (metal RSR and Pall rings) and model predictions to find the rest two model parameters D and C . It is shown that the dispersion model predictions fit very well toall experimental data used, as well as to the CFD predictions. As a future work, the authors plan to test both methods using the recently published data for other open-structure random packings - Raflux-Rings, RVT Metal Saddle Rings and Hiflow-Rings.

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