

Predicting Liquid Flow Profile in Randomly Packed Beds from Computer Simulation

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Our previous work on the simulation of packing processes was extended to study the liquid trickle flow down randomly packed beds. An algorithmic procedure with detailed geometrical description of packing elements was developed for tracking the liquid flow and holdup distributions in packed beds. Unlike the conventional continuum-based models such as the diffusion model, it goes into the subparticle scale to capture the geometrical characteristics of the packed bed. Three mechanisms of the trickle flow—film flow, dripping flow, and splash—were observed in packed beds, and the first two were captured in the model. At each point within a packed bed, liquid flow is simplified to two possible directions: vertically down and horizontally in the direction of the negative gradient of the packing surface. The 3-D geometric model constructed with the packing process simulation was used to determine the direction of the horizontal flow and fraction of the flow rate in each direction. By assuming that the liquid flow is uniform free surface flow, the Manning formula was used to predict the liquid holdup with the width of the liquid rivulet on a packing surface calculated by the Shi and Mersmann correlation. Metal Pall rings and metal Raschig rings were simulated with water as the fluid. Results of liquid flow distributions and average liquid holdup were validated against experimental data and semiempirical correlation from Billet et al.

Introduction

Liquid-flow-distribution in packed beds is an important parameter that crucially affects the transport mechanisms, such as mass/heat-transfer efficiency and the pressure drop. As much as 50–75% decrease in mass-transfer efficiency, caused by a poor liquid distribution, has been reported in randomly packed distillation columns (Nutter et al., 1992). It is essential to reliably predict the liquid-flow-profiles and the liquid-holdup-distribution for the design and analysis of packed distillation and absorption columns, trickle bed reactors, and so on.

Models have been proposed in literature to predict the liquid-flow-distribution in randomly packed beds. From the point of the scale on which a model captures the flow patterns, the existing models can be classified into three categories: equipment scale, packing element scale, and the scale between them. Representative of the first type is the widely used *diffusion model* (Cihla and Schmidt, 1957, 1958). The

diffusion model balances axial convection with radial dispersion by using a partial differential equation. The flow characteristics of a packed bed are accounted for by an overall empirical parameter called a *spreading* or *dispersion* coefficient. The natural flow models (Albright, 1984; Hoek et al., 1986; Song et al., 1998a), so named by some authors (Zuiderweg et al., 1993; Song et al., 1998a), fall into the particle scale category. These kinds of models intend to describe the tendency of the liquid flowing down a packed bed to redistribute in a natural fashion (nature flow), based on the concept that liquid continuously splits and recombines on the scale of the packing elements. They simulate the liquid flow by determining the directions and the fractions of the liquid splitting in certain *random* manner. The computational fluid dynamics (CFD) based methods that take the packed beds as porous medias and solve the volume averaged Navier-Stokes equations (Song et al., 1998b; Sun et al., 2000) also fall into this category. This kind of CFD method can consider the spatial variations of the characteristics of a packed bed, such as

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porosity, dispersion coefficient, interphase drag force, resistance force, and so on, on the scale of the packing element. The zone/stage model (Zuideweg et al., 1993) is between the scales of the equipment and the packing element. Based on the same principle as the natural flow models, the zone/stage model splits liquid into the adjacent zones after each stage height. The zones, which are concentric rings of equal width, are larger in scale than the particle size.

Since the scales are on the order of particle size or larger, the conventional models are not able to capture the structural characteristics of the packing. To simulate liquid flow successfully, the model parameters, such as the dispersion coefficient, the splitting fraction, the interphase drag coefficient and so on, must be specified or need to be determined from experiments for each type of packing. By going into the subparticle scale to capture the geometrical characteristics of the packing, it is possible to develop more predictable and more general models for liquid trickle flow in randomly packed beds. It is possible to develop such a model for the first time since the packing process could be simulated as outlined in our previous work (Nandakumar et al., 1999) that yields detailed geometrical information.

From the point of fluid dynamics, liquid trickle flow in packed beds is a kind of free surface flow. The limitations of numerical techniques and computing power make the rigorous approach to solve the Navier-Stokes equations with free boundaries and contact lines infeasible, except for simple cases such as a few droplets or bubbles at low Reynolds or Weber numbers (Scardovelli and Zaleski, 1999). The complicated geometry of the packing and the large number of packing elements in a bed make the problem in randomly packed beds much more complicated. Therefore, in a series of articles, a somewhat more macroscopic method than the rigorous CFD is proposed to model the geometrical, hydrodynamic, and mass-transfer characteristics of randomly packed beds on the subparticle scale.

In Part I of this series (Nandakumar et al., 1999), we developed a computer simulation of the packing process of arbitrarily complex 3-D packing objects, such as Pall rings, Raschig rings and so on, into a cylindrical container using collision detection algorithms. A 3-D model of each packing element is constructed by triangulating the complex surface and used as input to the simulation program. The program then determines the position and orientation of each packing element within a large bed so that any two packing elements are merely touching each other. The result from such a simulation is a detailed 3-D model for the geometry of the packed bed, that is, the shape, size, location, and orientation of each triangular piece of the packing surfaces, which is used to extract useful geometrical properties such as *spatial variation of porosity* and *specific surface area*. In the present work we build on this idea to develop a geometry-based model to predict the trickle flow of liquid down a randomly packed bed.

Model and Algorithm

Mechanisms of the liquid flow

We consider the liquid trickle flow in a packed bed, that is, liquid is introduced to the top of the bed through a distributor and it flows down the bed in a not fully filled manner

(that is, the bed is not saturated). Observations show that three mechanisms exist for liquid trickle flow in a packed bed.

- In *film flow*, the liquid flows along the surfaces of the packing or the wall of the bed as thin film.
- In *dripping flow*, liquid drops from the edges of the packing and goes down through the void spaces until it reaches another piece of the packing surfaces.
- In *splash flow*, the liquid that drops onto a packing surface may splash into the neighborhood, a process which is quite difficult to model.

The predominant mechanisms are the film flow and dripping flow. Splash only happens where the local kinetic energy of the liquid is high, such as immediately under the drip points of some liquid distributors. Therefore, only film flow and dripping flow are considered in the model.

Liquid flow distribution

To quantitatively model liquid flow distributions in a packed bed, we need to figure out the velocity vector, that is, the flow direction and the flow rate, at every point in the bed. Due to the action of gravity, the direction of the dripping flow is straight down, and, for the film flow, liquid flows down along a packing surface following the negative gradient of the surface at that point. Through the simulation of the packing process, the geometry of the packed bed is constructed in great detail. The coordinates of each triangulated piece of the packing surfaces are obtained, therefore, the gradients of the packing surfaces are easy to determine.

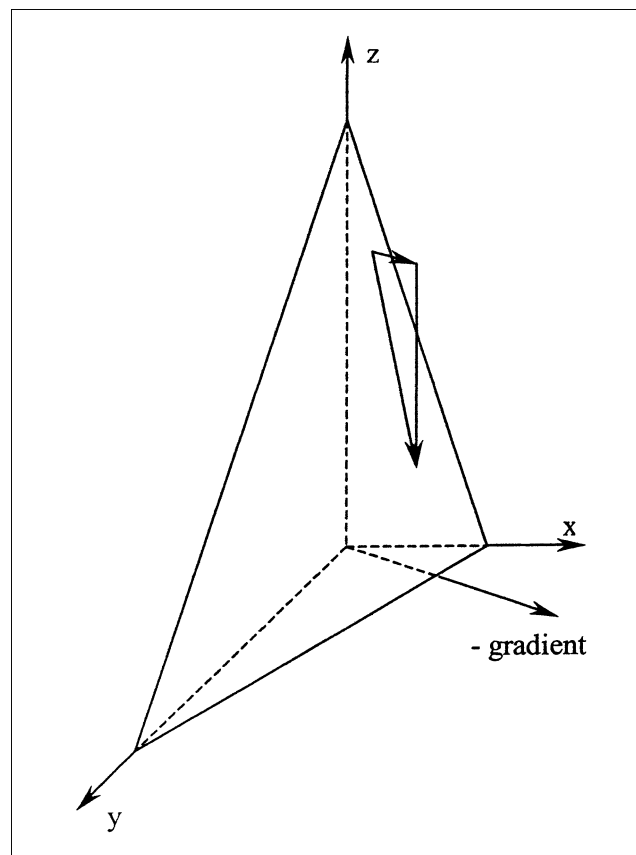


Figure 1. Decomposition of the film flow.

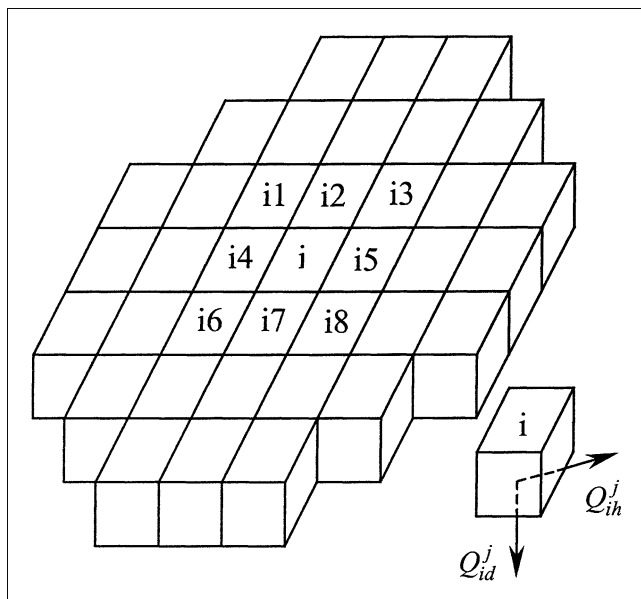


Figure 2. Layer of cells and the outward flow of a cell.

To simplify the calculation of the film flow, we decompose the flow into two elements: horizontal flow along the negative gradient of the packing surface and vertical downward flow, as shown in Figure 1. After the decomposition, only two possible directions of the liquid flow need to be considered at each point: the negative gradient of the packing surface and vertically down. By determining the fraction of the flow in each direction, the liquid flow rates can be calculated.

To keep the liquid flow model tractable, further assumptions are necessary. The detailed assumptions and description of the model are as follows:

To carry out numerical simulation, the computational domain is discretized first. This is done by dividing a packed bed into layers in the vertical direction; then each layer is divided into a mesh of cuboid cells. Figure 2 shows one layer of the mesh. To catch the geometrical characteristics of the packing, the cell size should be much less than the size of a packing element.

Triangulated packing surfaces in the packed bed are constructed from the 3-D model available with the packing process simulation. For each cell, the triangles of the packing surfaces that intersect with the cell are searched and then clipped such that they are contained entirely within the cell. The Sutherland-Hodgman polygon clipping algorithm (see Plastock and Kalley, 1986), which is also used in the simulation of the packing process (Nandakumar et al., 1999), is employed for the clipping operation. The result of the clipping operation between a triangular piece and the 3-D cell is a general polygon. The resulting polygons are triangulated again to yield a group of subtriangles that are used to build up the geometrical properties within each cell.

For each cell, the surface properties are assumed to be characterized by an average planar surface with the area equal to the total area of all the subtriangles within the cell and a gradient equal to the mean value of the gradients of all the subtriangles weighted with their surface areas.

For each cell, liquid may flow *into* the cell from the cell above it and the eight neighboring cells (determined by their local gradients) in the same layer, as shown in Figure 2. The total volumetric flow rate in cell i of layer j is calculated by

$$Q_i^j = Q_{id}^{j-1} + \sum_{l=i1}^{i8} \delta_{li}^j Q_{lh}^j \quad (1)$$

$$\delta_{li}^j = \begin{cases} 1 & (\text{flow from } l \text{ to } i) \\ 0 & (\text{no flow from } l \text{ to } i) \end{cases} \quad (1a)$$

For each cell, the outward liquid flows into either one of the adjacent cells in the same layer along the direction of the negative gradient of the cell and/or the cell under it in the next layer. The fraction of the downward flow f_d is assumed to equal the fraction of the free area (uncovered area by the packing surfaces) in the horizontal section of the cell. The downward and horizontal flow rates out of a cell are calculated by

$$Q_{id}^j = f_d Q_i^j \quad (2)$$

$$Q_{ih}^j = (1 - f_d) Q_i^j \quad (3)$$

As a boundary condition, the liquid that reaches the column wall is reflected back into the nearest cell inside the bed. At the top of the bed, the liquid distributor design determines the location of the drip points and the operating conditions determine the liquid flow rates from each drip point.

Liquid holdup

In a packed bed, liquid holdup is defined as the volume occupied by liquid inside a certain sample 3-D space divided by the volume of the sample space. When the sample space is taken as the entire volume of a packed bed, the average liquid holdup is obtained. It is the average liquid holdup that is usually reported and modeled for packed beds in literature, although computed tomography techniques make detailed distribution of holdup measurements possible (Toye et al., 1998).

After the liquid flow distributions are determined, liquid holdup can be calculated for each cell based on hydrodynamic models for free-surface-flow on an inclined plate. By assuming that the liquid flow is free-surface-flow of uniform depth, the widely used Manning formula (Manning, 1891) can be deduced (Peerless, 1967)

$$Q = \frac{1}{n} A \left(\frac{A}{b} \right)^{2/3} (\sin \alpha)^{1/2} \quad (4)$$

The liquid holdup in the cell is then calculated by

$$h_L = \frac{A \cdot l}{V} \quad (5)$$

In Eq. 4, b is the width of the liquid rivulet on the average planar packing surface in each cell, which needs to be deter-

In Cartesian coordinates, divide the bed into layers of cells
For each layer, from top down
For each cell
Find all the triangular pieces intersecting with the cell
Clip all the intersecting pieces so that they are entirely within the cell
Triangulate all the clipped pieces into sub-triangles
Find the surface area and gradient of each sub-triangles
Calculate the properties of the average planar surface
Calculate the fraction of the downward flow
For each cell which has liquid coming from above (source cell)
Trace the liquid horizontal flow until all the liquid flows down
For each cell in the track
Add the liquid flow rate from the source cell to its total flow rate
For each cell
Calculate the downward and horizontal liquid flow rates
Calculate the liquid holdup
Calculate the velocity profile along the radial direction
Calculate the average liquid holdup for all the layers above

Figure 3. Solution algorithm.

mined. Shi and Mersmann (1985) proposed a correlation for the width of liquid rivulet on an inclined plate based on an experimental study, which is used in this work

$$b = BV_L^{0.4} v_L^{0.2} \left(\frac{\rho_L}{\sigma_L g} \right)^{0.15} (1 - \cos \theta)^{-1} \quad (6)$$

Solution algorithm

Given the liquid flow pattern at the top of a packed bed (that is, the pattern introduced with the liquid distributor), the calculation of the liquid flow and holdup proceeds from the top down, as outlined in Figure 3.

The solution algorithm is programmed with C++ and is portable to both Unix and Windows platforms. Simulations have been carried out on a SGI Origin 2000 computer. The simulation results produce the liquid flow and holdup in each cell. Such data can then be used to obtain liquid velocity profiles along the radial direction at any height by averaging the liquid velocities in the circumferential direction. Similarly, averaging the liquid holdup data over the entire packed column, we can obtain the mean holdup in the packed bed under various flow conditions. The computing time varies with the size of the packed bed, the structure and size of the packing, and the size of the cells used. For a 0.6 m diameter and 3.0 m height packed bed, dumped with 0.0254 m metal Pall rings, when the cell size is $0.00254 \times 0.00254 \times 0.00254 \text{ m}^3$, the required CPU time on a SGI Origin 2000 computer with 195 MHz CPU is 95 h.

Simulation Results

Liquid flow distribution

Liquid distribution experiments were carried out in our laboratory by using a 0.6 m diameter column dumped with 0.0254 m (1 in.) stainless steel Pall rings (Yin, 1999). To investigate the effect of the initial liquid distribution on liquid flow patterns, two liquid distributors were employed in the experiments. The first distributor, with 31 uniformly distributed irrigation points over the cross section of the column (or equivalently 110 irrigation points per square meter), is representative of industrial distributors. The second one is obtained by blocking the outermost ring of the drip holes of the first distributor, which results in 16 irrigation points in the central region of the tower. This liquid distributor covers only 43% of the total cross section of the column. Those two initial distributions of liquid flow will be referred to as the 100% inlet distribution and the 43% inlet distribution, respectively, later in this article. Liquid velocity profiles were measured with a collector at different packed depths (the packed height from the top down). The collector consists of six annular spaces to collect liquid at different radial positions. The widths (δr) of the six rings are 0.1, 0.05, 0.05, 0.05, 0.0447, and 0.0038 m respectively, from the center to the wall.

Simulations of the experiments have been carried out for water flow at different liquid loads. In the simulations, the initial liquid flow patterns were defined according to the geometrical size and locations of the drip points that define the two variations of the liquid distributors used in experiments. To represent the resolution of the liquid collector in the experiments, each layer of the bed is divided into 235×235 cells, and the height of each layer is 0.00254 m. The resulting cell size is $0.00254 \times 0.00254 \times 0.00254 \text{ m}^3$, which corresponds to a resolution of $1/10^{\text{th}}$ of the packing object size.

Figure 4 and Figure 5 show the comparison between predicted relative liquid velocity profiles and the experimental data for the 100% inlet distribution, at three different packed bed depths of 0.9 m, 1.8 m, and 3.0 m. The results for two typical liquid loads of $0.00291 \text{ m}^3/\text{m}^2/\text{s}$ and $0.00666 \text{ m}^3/\text{m}^2/\text{s}$ are shown in these figures. The simulation results are in satisfactory agreement with the experimental data. Good agreement between the predictions and the experiments is also found for the 43% inlet distribution, except at the packed depth of 0.9 m. At short depths such as 0.9 m, the effect of splashing is believed to be important, and one way of accounting for it is presented later in this article. Figure 6 shows the comparisons at a liquid load of $0.00478 \text{ m}^3/\text{m}^2/\text{s}$.

Figure 7 shows 3-D profiles of the liquid distribution for the 100% inlet distribution, at four different packed bed depths of 0.01 m, 0.35 m, 0.57 m, and 0.90 m, which shows the development of the liquid flow patterns at various heights. First, the liquid from the drip points of the distributor merges and covers the whole cross section of the column within 0.35 m of the packed depth. Then, the wall flow builds up, which can be seen from Figure 7c and 7d. Circumferentially averaged values are shown in Figure 4 and Figure 5.

By averaging the liquid flow rates obtained from the simulation at the level of one packing element, the local liquid maldistribution on the particle-size scale can be investigated with the present approach. Some types of maldistribution factors have been proposed to characterize the small-scale

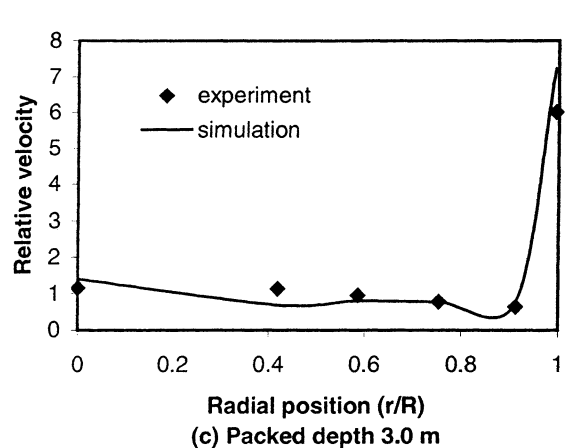
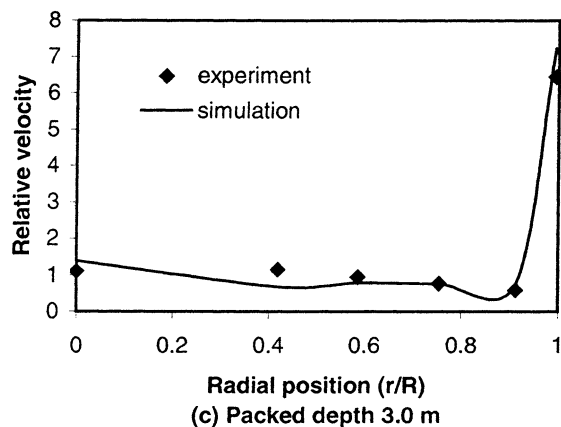
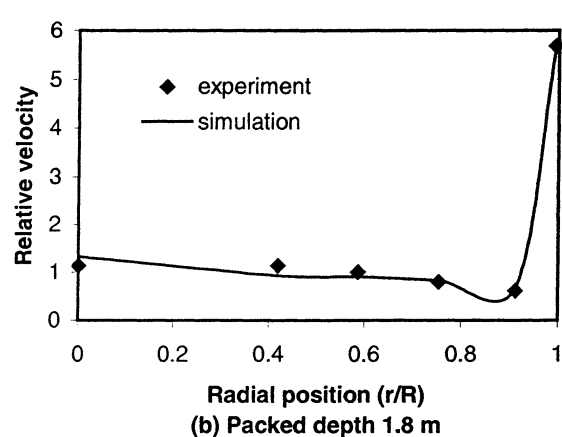
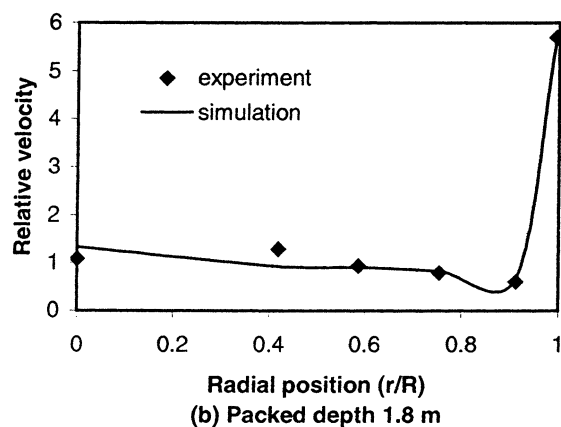
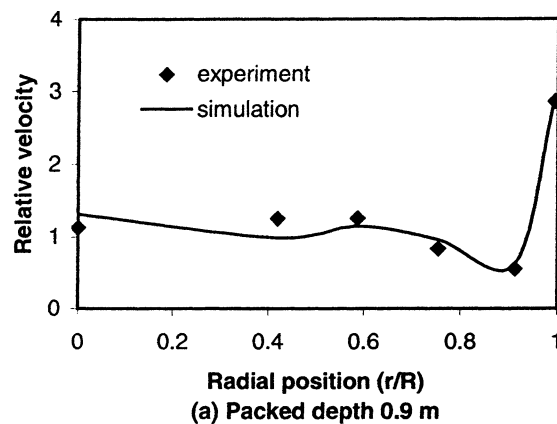
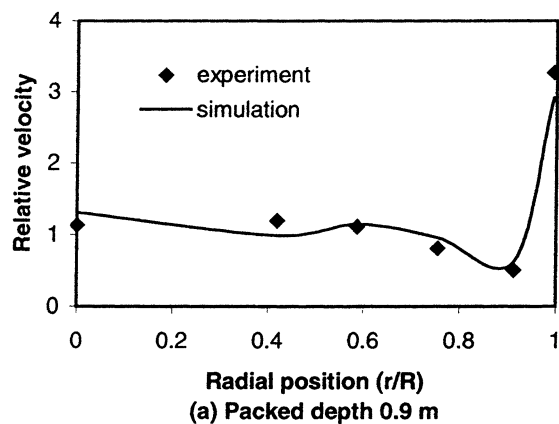


Figure 4. Liquid flow distribution for 100% inlet distribution at liquid load of 0.00291 m³/m²/s.

Figure 5. Liquid flow distribution for 100% inlet distribution at liquid load of 0.00666 m³/m²/s.

liquid maldistribution. The definition (Eq. 7) from Hoek et al. (1986) is employed in this article.

$$Mf = \frac{1}{m} \sum_{i=1}^m \left(\frac{Q_i - \bar{Q}}{\bar{Q}} \right)^2 \quad (7)$$

Figure 8 shows the calculated maldistribution factors for the 100% inlet distribution and the 43% inlet distribution

with the combined cell number $m = 472$. The maldistribution factors for the 100% inlet distribution correspond to the liquid distributions shown in Figure 7. When the liquid covers the whole cross section of the column, the most uniform liquid distribution is obtained. Therefore, the maldistribution factor reaches the lowest value. Then, the Mf increases with the development of the liquid wall flow and tends to reach an equilibrium value. The trend of the maldistribution factors

for the 43% inlet distribution is similar to the ones of 100% inlet distribution, but the Mf have higher value at the top of the column and develop more slowly due to the nonuniform initial distribution.

Liquid holdup

The liquid holdup distributions have also been computed in the prior simulations. In addition, simulations for columns randomly packed with 0.035 m metal Pall rings and 0.015 m metal Raschig rings have also been carried out for water systems. Because of the shortage of liquid holdup data, a semi-empirical correlation from Billet and Schultes (Billet, 1995; Billet and Schultes, 1999) has been used as a reference for comparison. In the simulations, the values of the constants $n = 0.046$ in Eq. 4 and $B = 12$ in Eq. 6 were determined by minimizing the deviation between the average holdup predicted by this work and the Billet correlation for 0.0254 mm metal Pall rings, and were adopted in all other simulations.

The Billet correlation is based on numerous experiments on varieties of packing, systems and column setups. The correlation is as follows

$$h_L = \left(12 \frac{1}{g} \frac{\mu_L}{\rho_L} u_L a^2 \right)^{1/3} \left(\frac{a_h}{a} \right)^{2/3} \quad (8)$$

$$\text{Re}_L = \frac{u_L \rho_L}{a \mu_L} < 5: \quad \frac{a_h}{a} = C_h \left(\frac{u_L \rho_L}{a \mu_L} \right)^{0.15} \left(\frac{u_L^2 a}{g} \right)^{0.1} \quad (8a)$$

$$\text{Re}_L = \frac{u_L \rho_L}{a \mu_L} \geq 5: \quad \frac{a_h}{a} = 0.85 C_h \left(\frac{u_L \rho_L}{a \mu_L} \right)^{0.25} \left(\frac{u_L^2 a}{g} \right)^{0.1} \quad (8b)$$

Figures 9 and 10 show the comparisons of the average liquid holdup between the model proposed in this article and the Billet correlation for metal Pall rings and metal Raschig rings, respectively. It can be seen from the figures that the results predicted by this work are in good agreement with the Billet correlation. Figure 11 shows a sample distribution of liquid holdup over a cross section of the bed for 0.0254 m metal Pall rings.

Discussion

The comparisons show that the liquid flow distribution and average holdup predicted by this model are in good agreement with the experimental data and the semiempirical holdup correlation from Billet et al. for water systems, except for the liquid velocity profiles at the packed depth of 0.9 m for the 43% inlet distribution.

The discrepancy for the 43% inlet distribution at 0.9 m is caused by the fact that the model doesn't consider the splash of liquid as a mechanism for increased spreading. For central or other heterogeneous initial distributions, like the 43% inlet distribution, the splash of liquid will cause a greater effective coverage of liquid than the actual size of the distributor, which will lead to faster development of the liquid distribution. The effect of the liquid splash at the top layer of the packing on the liquid distribution has been reported for the initial liquid distributions of a single jet (Hoek et al., 1986),

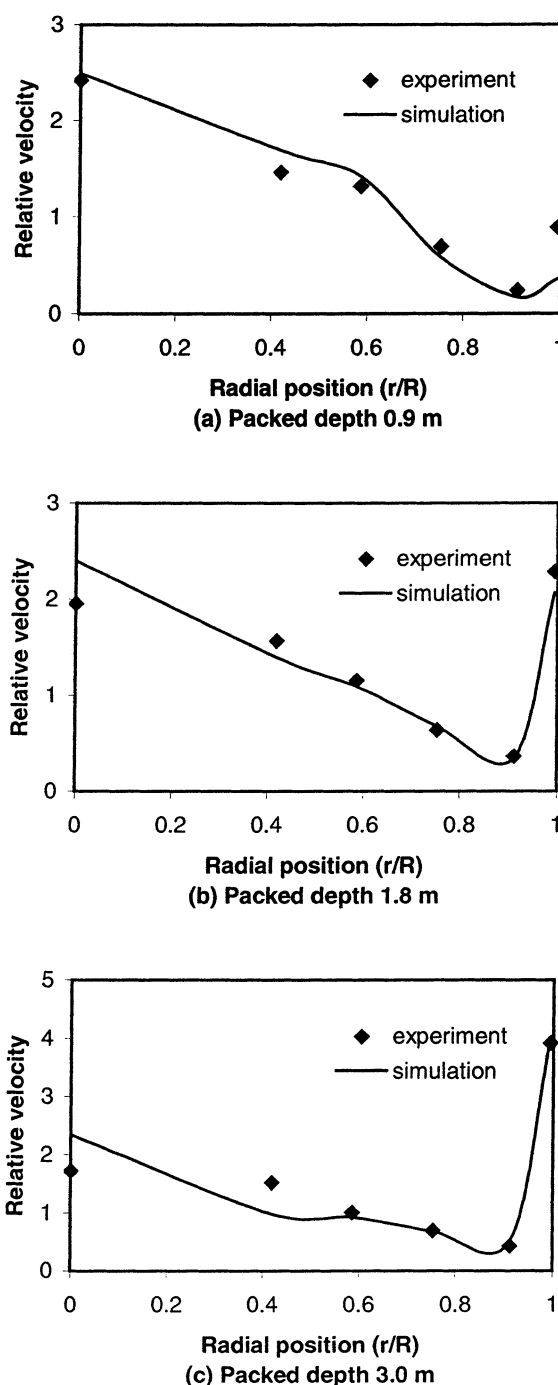


Figure 6. Liquid flow distribution for 43% inlet distribution at liquid load of $0.00478 \text{ m}^3/\text{m}^2/\text{s}$.

line source (Porter et al., 1968), and 64% of the column cross section (Kouri and Sohlo, 1996). This is believed to be the cause of the larger discrepancy between the model prediction and the experimental data in Figure 6(a). For the uniform initial distributions like the 100% inlet distribution, the liquid covers the total cross section of the bed at the top (or through a very short depth of the packing). Although splashing might still be present for the uniform inlet (as it depends only on

the liquid velocity from the drip points), its effect is felt uniformly over the entire cross section at the top, resulting in very little net effect on the liquid distribution at the top. For the case of nonuniform inlet distribution, the splashing between the wet and dry boundary would result in faster spreading of the liquid into the dry part of the bed. Hoek et al. (1986), when discussing the diffusion model, found a need to add a fictitious height to the bed to account for the liquid splash. By increasing the height of the packing by 0.36 m at the top of the bed, a simulation was repeated for the 43% inlet distribution. The simulation results are shown in Figure 12. After adding the fictitious height, the agreement between the simulation results and the experimental data is very good. This provides an effective way to account for the liquid splash flow in packed beds, an idea that was used already by Hoek et al. (1986) for the diffusion model. Hoek et al. (1986) find

the need to use different heights for each case in their experiments, and correlating the effective height needed to the degree of splashing requires still further investigation.

In this model, the prediction of liquid flow distributions is based on first principles and the 3-D model for the geometry of the packed bed. No model parameters have been adjusted to fit the experimental data in the simulations. For the prediction of liquid holdup, only one set of model parameters, n in Eq. 4 and B in Eq. 6, is used for all three kinds of packing, while in the Billet correlation, the model parameter C_h needs to be set for each size of packing even within the same type. These features demonstrate the capability of the model to capture the geometrical characteristics of both randomly packed beds and packing for liquid flow prediction. It can also be concluded that the two main mechanisms, film flow and dropping flow, govern the liquid flow in packed beds,

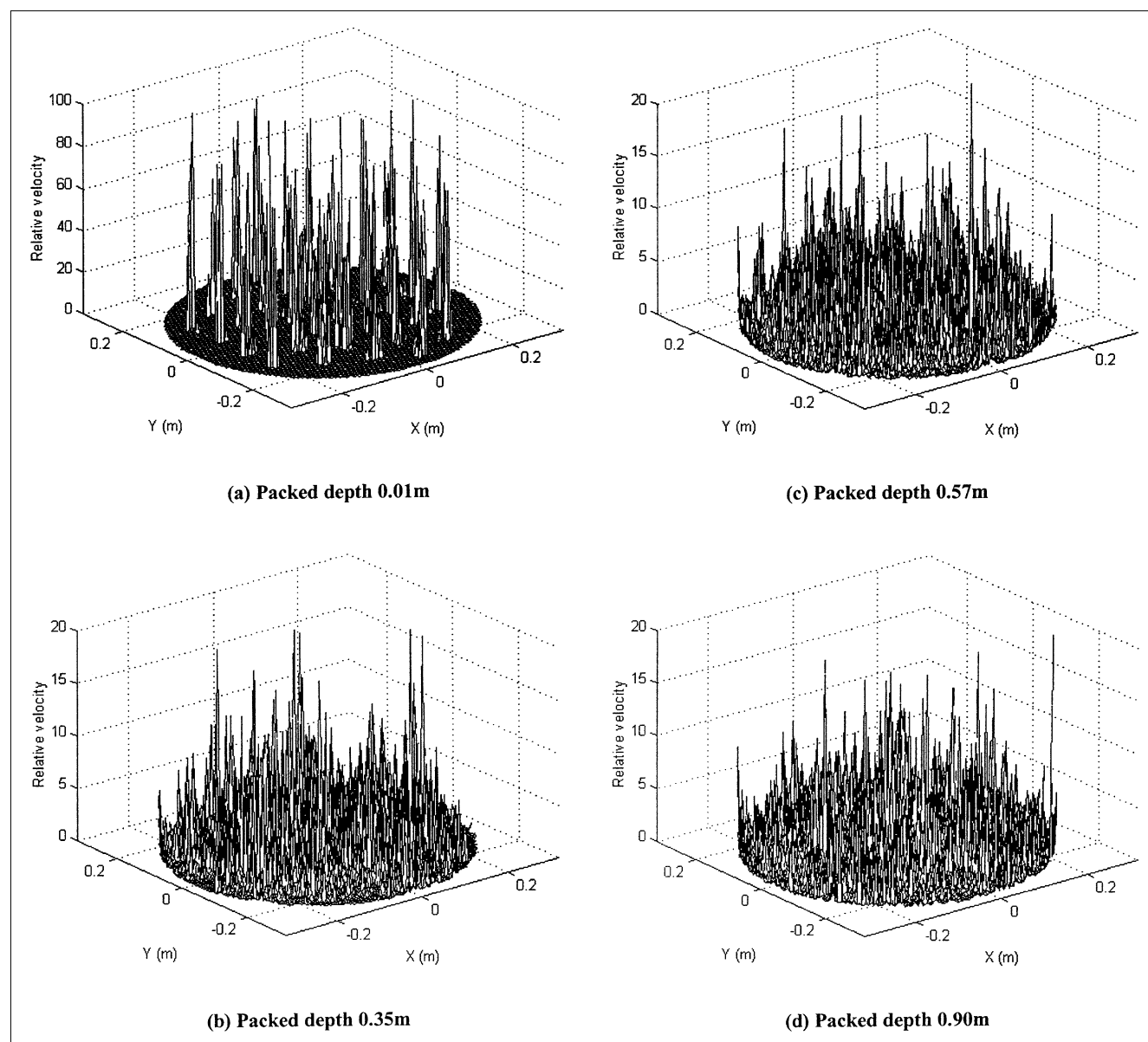


Figure 7. Liquid flow distribution for 100% inlet distribution at liquid load of $0.00478 \text{ m}^3/\text{m}^2/\text{s}$.

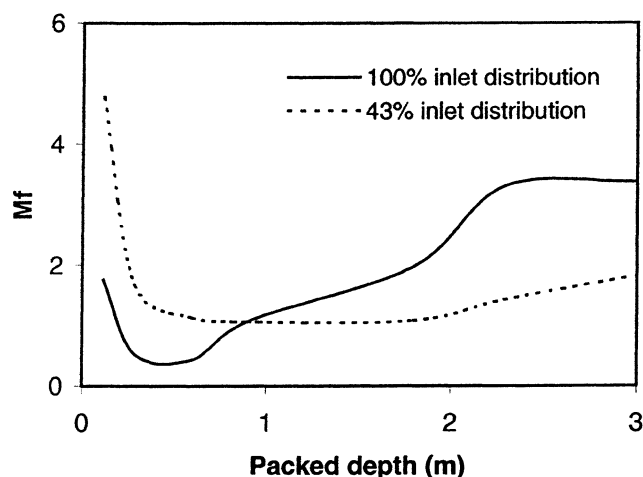


Figure 8. Liquid maldistribution factors.

except in regions with large nonuniform liquid distribution, such as the initial section under a liquid distributor with a small number of drip points.

It should be noted that system properties have not been included in the model for the simulation of liquid flow distributions, and the model has only been tested with the water system. Liquid properties, such as viscosity and surface tension, may have effects on liquid distributions in packed beds. The description of the effects of system properties needs to be studied further.

It can be seen that, in the development of the model, no assumptions have been made on the specifics of randomly packed beds. It only requires detailed geometrical data on the packings. Hence, a similar approach may also apply to structured packings when its geometry is constructed in sufficient detail. Further validation of this idea for structured packing must be carried out.

It should also be noted that the solution of the present model is time-consuming. Therefore, the most favorite utility of this simulation approach is in developing a conceptual design of new packing structures according to certain hydraulic

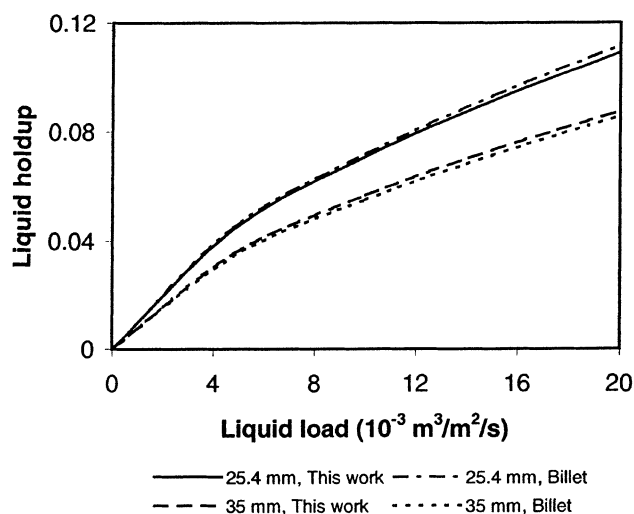


Figure 9. Average liquid holdup of metal Pall rings.

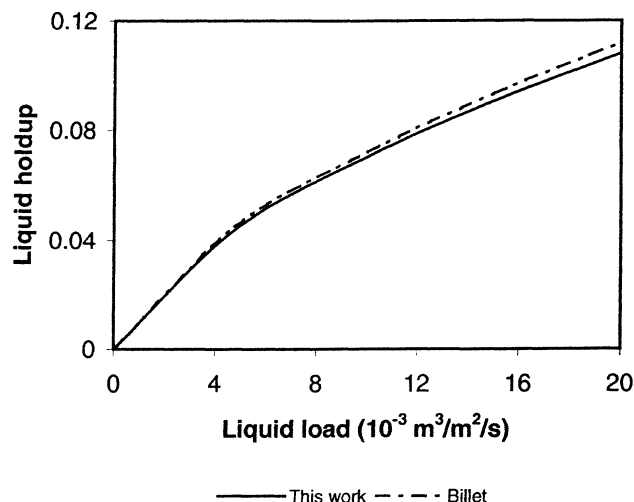


Figure 10. Average liquid holdup of metal Raschig rings.

requirements, and comparing the hydraulic properties of such packing with existing packing. If connections can be built up between this model and the conventional ones, such as the diffusion model, it is also helpful for the development of a regular design approach for new types of packed columns. From this viewpoint, a preliminary investigation has been made to get the dispersion coefficient of the diffusion model using the present approach, which provides a useful link between the two approaches. In the diffusion model, governed by Eq. 9, D is the dispersion coefficient, which can be evaluated with an analytical solution (Eq. 11) (Soukup et al., 1973; Bemer and Zuiderweg, 1978) of the model for the boundary conditions shown in Eq. 10.

$$\frac{\partial u(r, z)}{\partial z} = D \left(\frac{1}{r} \frac{\partial u(r, z)}{\partial r} + \frac{\partial^2 u(r, z)}{\partial r^2} \right) \quad (9)$$

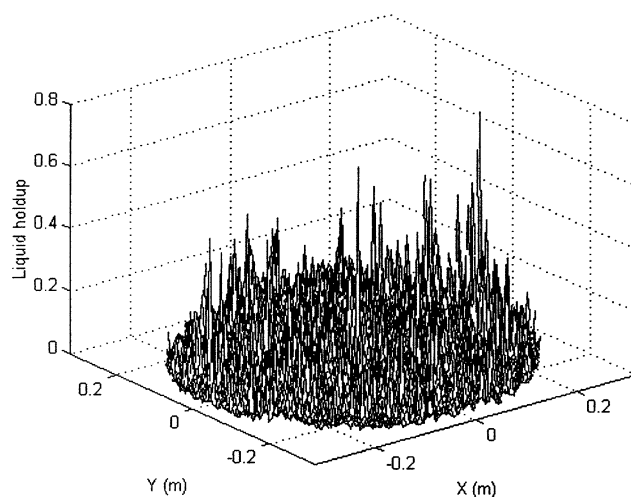


Figure 11. Sample liquid holdup distribution of 0.0254 m metal Pall rings.

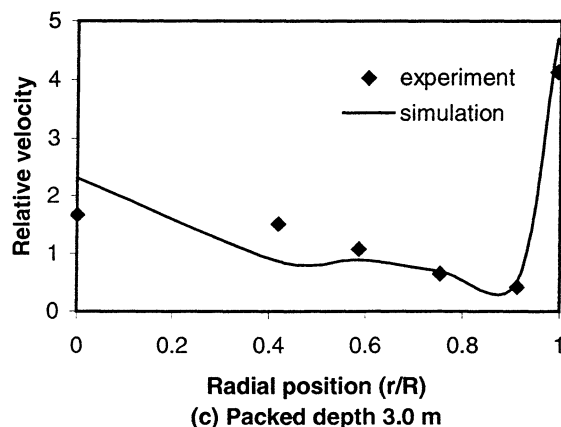
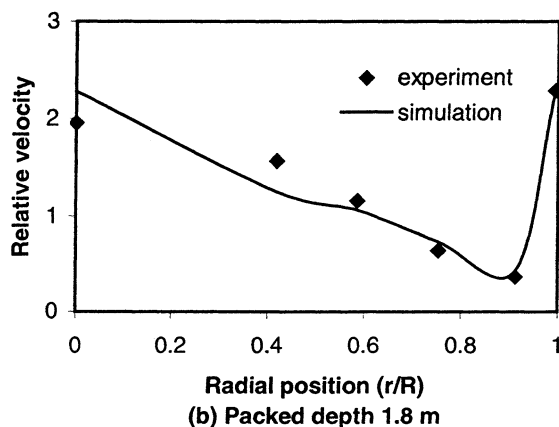
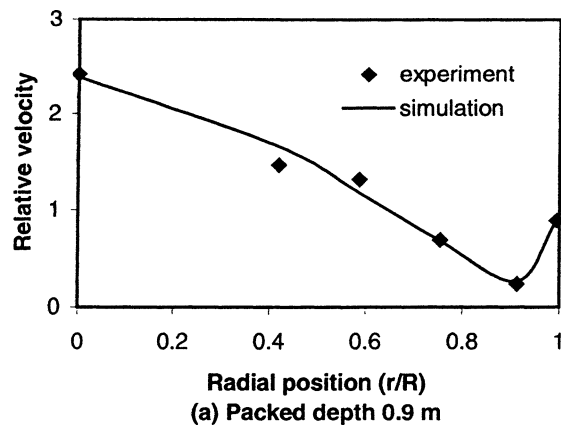


Figure 12. Comparison of liquid flow distribution.

Simulation with the fictitious height of 0.36 m and experiment for 43% inlet distribution at liquid load of $0.00478 \text{ m}^3/\text{m}^2/\text{s}$.

$$\begin{aligned} u(0,0) &= u_0 \\ u(r,0) &= 0 \quad \text{for } r \neq 0 \\ u(\infty,z) &= 0 \end{aligned} \quad (10)$$

$$u(r,z) = \frac{Q_0}{4\pi Dz} \exp\left(-\frac{r^2}{4Dz}\right) \quad (11)$$

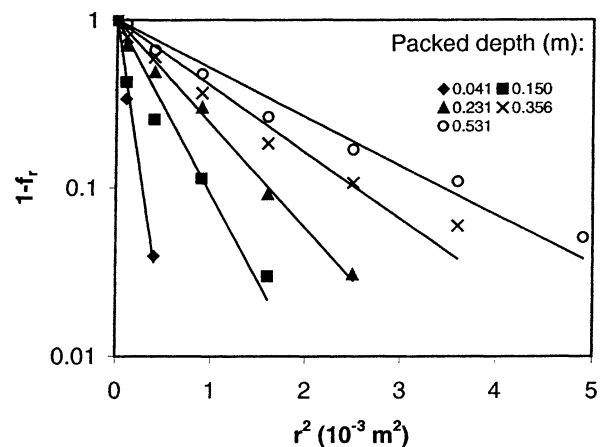


Figure 13. Determination of the liquid dispersion coefficient.

The boundary conditions are valid for the top section of a bed with a central point source before the liquid reaches the column wall. By integration, it can be derived from Eq. 11 that (Hoek et al., 1986)

$$r^2 = -4Dz \ln(1 - f_r) \quad (12)$$

where f_r is the fraction of the total injected liquid flowing within a circle of radius r at a packed depth of z , which can be obtained with the present approach for a central point source. Then, the values for the dispersion coefficient D can be determined by linear regression from relation 12. This has been outlined in Figure 13 as an example for a 0.6 m diameter column packed with 0.0254 m metal Pall rings and the water system. It can be seen from Figure 13 that $\ln(1 - f_r)$ and r^2 are in reasonable linear relations. The dispersion coefficients for different packed bed depths (see Table 1) remain a constant which demonstrates the possibility to make connections between the present model and the diffusion model. This also demonstrates the similitude between the two models. The similitude is not surprising. In this model, the directions and rates of liquid flow are predicted based on the geometrical properties of the bed in each cell. Generally speaking, because the bed is packed randomly, this model falls into a broad family of random walk models and, therefore, the overall flow development obeys the law of diffusion (Eq. 9). While compared to the existing models with a random walk character, including the diffusion model and the natural flow models, the present approach is more predictable as previously discussed, due to the capture of the geometrical characteristics of packed beds and the liquid flow mechanism of film flow and dropping flow within the beds.

Table 1. Liquid Dispersion Coefficients

Packed Depth (m)	Dispersion Coeff. (m)
0.041	0.00074
0.150	0.00070
0.231	0.00076
0.356	0.00077
0.531	0.00071

Conclusions

A geometry-based model and a solution algorithm have been developed to track the liquid-trickle-flow down randomly packed beds. Based on the mechanisms of the trickle flow and the 3-D model for the geometry of a packed bed constructed with the packing process simulation, liquid flow profiles along a packed bed can be predicted by the model. Liquid holdup distributions can then also be computed.

The model has been validated by making comparisons between the predicted liquid flow distributions and experimental data obtained in a 0.6 m diameter column dumped with 0.0254 m stainless steel Pall rings. Comparisons of the average liquid holdup between this model and the Billet correlation for 0.0254 m metal Pall rings, 0.035 m metal Pall rings, and 0.015 m metal Raschig rings also indicate validation of the holdup model. These results show that the geometry-based model is able to capture the geometrical characteristics of packed beds, and can describe the liquid film flow and dropping flow within the beds.

Notation

- a = total surface area per unit packed volume, m^2/m^3
- a_h = hydraulic area of packing per unit packed volume, m^2/m^3
- A = cross-sectional area of a liquid rivulet, m^2
- b = width of a liquid rivulet, m
- B = coefficient of Eq. 6
- C_h = coefficient of Eq. 8
- D = liquid dispersion coefficient, m
- f_d = fraction of liquid flows down
- f_r = liquid fraction within a circle of radius r of the total flow rate
- g = gravitational acceleration, m/s^2
- h_L = liquid holdup
- l = length of an average planar packing surface in a cell, m
- n = Manning's roughness coefficient
- Q = liquid flow rate in a cell, m^3/s
- \bar{Q} = average liquid flow rate, m^3/s
- Q_0 = total liquid flow rate at inlet, m^3/s
- r = radial coordinate, m
- R = radius of a packed bed, m
- u = local liquid flow rate per unit area, $\text{m}^3/\text{m}^2/\text{s}$
- u_0 = liquid flow rate per unit area at the inlet, $\text{m}^3/\text{m}^2/\text{s}$
- u_L = liquid load with reference to the bed cross section, $\text{m}^3/\text{m}^2/\text{s}$
- V = volume of a cell, m^3
- V_L = liquid flow rate in a rivulet, m^3/s
- z = axial coordinate, m

Greek letters

- α = angle of inclination for an average planar packing surface to the horizontal, $^\circ$
- θ = contact angle, $^\circ$
- μ_L = dynamic viscosity of liquid, $\text{kg}/\text{m}/\text{s}$
- ν_L = kinematic viscosity of liquid, m^2/s
- ρ_L = density of liquid, kg/m^3
- σ_L = surface tension of liquid, N/s

Indices

- i = cell index
- j = layer index, from top down
- l = cell index
- d = vertically downward flow
- h = horizontal flow

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