Modelling liquid redistribution in a packed bed

Pawel Niegodajew, Dariusz Asendrych, Maciej Marek and Stanislaw Drobniak
Częstochowa University of Technology,
al. Armii Krajowej 21, 42-200 Częstochowa, PL
E-mail: imc@imc.pcz.czest.pl

Abstract. The paper is devoted to the computational fluid dynamics (CFD) simulation of liquid spreading process in a packed bed. The volume of fluid (VOF) approach was applied to simulate the flow in a realistic porous region composed of 6mm Raschig rings. Modelling results were used to determine the probability density function (PDF) distribution of liquid velocity vector orientation angle which was then implemented into 2-fluid Euler-Euler multiphase model of packing column. The simulation showed that the model is capable to simulate adequately the liquid redistribution in a porous region being, however, much more efficient computationally than the VOF method.

1. Introduction
Packing columns are commonly used in chemical and process engineering industry, just to mention absorption, rectification or extraction processes. Thanks to the enlarged contact area packed beds ensure the liquid holdup at the level needed for the efficient column operation [1]. The porous material also guarantees a uniform liquid distribution along the packing section, what is related to effective liquid transport in column transverse directions [2] commonly called as liquid spreading. Variety of parameters, i.e. packing element type, its size, fluid properties, their rates and others influencing the flow structure, makes the design of packed beds a challenge. That is why the research efforts are needed, both experiments and modelling, to make the progress in the field.

The opaque character of most packed bed structures and their 3D geometries make them difficult for penetration. That is why the liquid spreading process has been of interest of very few experimental research works. These are usually done with the use of visualization techniques as recording the liquid pore-flow through the transparent wall with the use of camera [3] or with the use of X-ray tomography methods [2,4].

The review paper of Wang et al. [5] shows various approaches to the modelling of trickle-bed reactors being the simplest case of the packed beds. The most commonly applied methods are the volume of fluid (VOF) and Euler-Euler approach used both for laminar and turbulent flow regimes. With the VOF mostly the flow through structured packing types is simulated. In particular it concerns the limited portion of packing section (e.g.: [6,7,8,9,10]). With this approach the porous region geometry has to be reconstructed and the inter-phase surface shape can be tracked (see [11,12]) allowing for an insight into the details of flow structure. For certain flow conditions the liquid behaviour may lead to the formation of rivulets and droplets and in turn to flow maldistribution, channelling or partial wetting [5,12]. The drawback of the VOF method is its practical inability to model the large-scale installations filled in with random packings. Moreover, the simulation of complex physio-chemical systems, e.g. carbon dioxide capture by chemical absorption [13], requires
more efficient numerical tools allowing to replace the realistic packed bed geometry and the flow field with their statistical descriptions and in turn reduce computational costs. For such cases the Eulerian approach can be employed as the method not requiring the details of geometry, just replacing it with its statistical description. For instance Sun et al. [14] modelled the hydrodynamics of the packed bed composed of the Pall rings obtaining good correspondence with experimental data. It should be pointed, however, that the Eulerian methodology, needs some assumptions as the input, making it partly artificial and packing column configuration dependent.

2. Numerical model

In the present paper the liquid flow in a cylindrical vertical column filled in with packed bed composed of Raschig rings is approached by the Eulerian two-fluid model simulating the liquid spreading with the use of its statistical description, i.e. probability density function (PDF) of velocity vector orientation in 3D system. As the PDF distribution depends on the number of factors, in particular on the packed bed filling element shape and size, it was necessary to perform an independent simulation with the use of VOF method applied to the liquid flow through the realistic geometry.

2.1. Volume of fluid simulation

In order to obtain reliable PDF of liquid spreading angle, necessary for the stochastic model, a CFD simulation of liquid flow within realistic bed geometry has been performed. The bed geometry composed of 6mm Raschig rings was generated using the in-house code based on simplified mechanics. The algorithm described in [15] allows to construct a packed bed in a realistic way with all elements oriented in a random way, satisfying, however the mechanical equilibrium. The view of a sample packed bed is presented in figure 1a.

The flow equations were solved with classical finite volume Navier-Stokes equation solver on regular structured computational grid and the gas-liquid interface was tracked with VOF [16]. The complex bed geometry was handled by a variant of immersed boundary method [17]. The liquid was supplied at the top of the bed and when the steady state was reached (see figure 1b presenting liquid free surface shape) the flow structure was examined with respect to spreading in lateral direction. The analysis of the velocity field allowed to determine the PDFs of angles describing the deflections of velocity vectors from particular axes of coordinating system. It turned out, that the distribution describing the orientation (described by angle $\theta$) of horizontal vector component (i.e. lying in $z$-$y$ plane, see figure 1b for definition of Cartesian coordination system) is uniform. Therefore, it was decided to represent velocity vector orientation with the single angle $\varphi_u$ being actually velocity vector deflection from vertical axis $x$ (see figure 1b). For a given computational cell that angle was calculated as follows:

$$\varphi_u = \arccos \left( \frac{u_x}{|u|} \right)$$

where $u_x$ is the axial velocity component. The angle expressed in this way is well-defined for any cell but if one wants to assign more weight to the cells filled with liquid phase and corresponding to larger flow velocity, the following weight coefficient was proposed as:

$$\omega = \alpha_i \left( \frac{|u|}{u_x} \right)$$

where $\alpha_i$ is liquid volume fraction. The resulting PDF distribution is shown in figure 1c. It is worth to note, that the distribution is dominated by low angles corresponding to small deflections of velocity vectors from vertical direction. It should be also mentioned that the distribution includes the peak located in the neighbourhood of 90°, resulting from the occurrence of corresponding peak in the PDF distribution of Raschig rings orientation. Due to the duality of PDF distribution shown in figure 1c it was decided to split it into two subranges with $\varphi_u^*$ as a border value.
The PDF distribution presented in figure 1c was fitted with the following two functions:

\[
f(\varphi) = \begin{cases} 
  \frac{a + b \varphi}{1 + B \varphi^2} & \text{for } \varphi \in \left[0; \varphi^*_b\right] \\
  0 & \text{for } \varphi \in \left(\varphi^*_b; \pi/2\right) 
\end{cases}
\]  

where \(a, b, q, A, B\) are constants specific for the particular configuration of the packed bed. For the purpose of Eulerian two-fluid modelling strategy it was necessary to express the liquid velocity vector orientation angle as a function of its cumulative distribution function \(D\) [18]. At first \(D\) has to be determined by integration of PDF distribution given by expression (3) leading to:

\[
D(\varphi) = \begin{cases} 
  \int_0^{\varphi^*_b} f d\varphi = \frac{qA}{2B} \ln(1 + B \varphi^2) & \text{for } \varphi \in \left(0; \varphi^*_b\right) \\
  \int_0^{\varphi^*_b} f d\varphi = -a \varphi^*_b + \frac{1}{2} b \varphi^*_b^2 - a \varphi^*_b - \frac{1}{2} b \varphi^*_b^2 + D(\varphi^*_b) & \text{for } \varphi \in \left(\varphi^*_b; 90^\circ\right) 
\end{cases}
\]

The desired formulas for the orientation angle may be then derived from expressions (4) yielding:

\[
\varphi = \begin{cases} 
  \left[1 - \frac{1}{B} \left(1 + \exp\left(\frac{2B}{qA} - 1\right)\right) \right]^{0.5} & \text{for } D \in \left(0; D(\varphi^*_b)\right) \\
  -a + \left(\frac{a^2}{b^2} + \frac{2}{b} \left(D - D(\varphi^*_b) + a \varphi^*_b + b \varphi^*_b^2\right)\right)^{0.5} & \text{for } D \in \left(D(\varphi^*_b); 1\right) 
\end{cases}
\]

Expressions (5) were implemented in CFD model described in the following section.

2.2. Eulerian approach

The model of the packing column was developed as a 3-dimensional laminar, unsteady, multiphase gas-liquid flow with the use of the two-fluid Euler-Euler approach allowing for the slip between countercurrently moving phases (corresponding for the Stokes number regime \(Sk>>1\)). All conservation equations are solved for each phase separately. Conservation of mass for \(k^{th}\) phase yields:

\[
\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla(\alpha_k \rho_k \bar{u}_k) = 0
\]
where $\rho_k$ is the $k^{th}$ phase density. The momentum equation for $k^{th}$ phase with respect to the Eulerian multiphase model (assuming flow incompressibility) has the following form:

$$\frac{\partial}{\partial t}(\alpha_i \rho_i \bar{u}_i) + \nabla (\alpha_i \rho_i \bar{u}_i \cdot \bar{u}_i) = -\nabla (\alpha_i p) + \nabla \left[ \alpha_i \mu_i \left( \nabla \bar{u}_i + \nabla \bar{u}_i^T \right) \right] + \alpha_i \rho_i \bar{g} + M_B + \bar{M}_f \quad (7)$$

where $p$ is the static pressure shared by all phases, $\mu_k$ stands for dynamic viscosity, $g_k$ is the gravity vector and $M_B$ describes an interaction force between phases taking into account the characteristics of the packing elements of porous zone, fluids properties and their flow rates [19]. The detailed description of the computational algorithm can be found in [20]. The last term of equation (7), i.e. $M_f$, reflects the liquid momentum change due to its interactions with packing elements being the geometrical constraints for the flow (as a consequence resulting in change of liquid flow direction), and in general it can be expressed in the following form:

$$M_f = f(u_{o,B}, \varphi_{o,B}, \Theta, \varphi_{o,B}(u_{o,B})) \quad (8)$$

where $u_{o,B}$ is the mean axial velocity of liquid phase determined according to [19] and $\varphi_{o,B}(u_{o,B})$ represents the orientation angle corresponding to the $u_{o,B}$ given by:

$$\varphi_{o,B}(u_{o,B}) = \arccos \left( \lim_{u \to u_{o,B}} \sum_{i=1}^{n} \cos \varphi_{o,i} \right) \approx 40^\circ \quad (9)$$

In order to model the liquid spreading in porous region satisfying formula (3) the orientation angle was generated according to equation (5) with cumulative distribution function $D$ replaced by the random number characterized by uniform PDF distribution (white noise) taking its values from the range $<0;1>$. The angle $\theta$ was generated according to the uniform distribution. Having the instantaneous orientation angle (represented by both generated angles) the local instantaneous flow velocity components were then calculated taking into account velocity vector magnitude corresponding to previous time step. In this way axial velocity varied within domain giving, however, the prescribed flow rate (resulting from velocity $u_{o,B}$) at each cross section. The test simulations have shown, that the PDF distribution of the velocity vector orientation calculated according to the procedure described in the present section fits the distribution received with the use of VOF simulation presented in section 2.1 with very good agreement.

2.3. Model geometry and boundary conditions

The numerical model of liquid spreading in the porous zone was applied to simulate the flow in a cylindrical column of diameter 0.1m containing packed bed section 0.5m high and filled with 6mm Raschig rings. The column was supplied with 15l/h water flux delivered by 5mm pipe located 50mm above the packing section at column axis. For the present simulation gas was assumed not to flow. Such a model geometry reflects the existing test rig currently being used for the corresponding experimental trials. The inlet and outlet boundary conditions were applied at the bottom and the top of the column respectively (see figure 2a) allowing gas to flow up. The liquid was supplied to the column with the use of the source boundary condition and then it was driven by gravity flowing countercurrently to the gas phase and leaving the column at its bottom. The non-slip boundary condition was applied at column wall. The computational domain was discretized with unstructured mesh with local refinement reflecting the regions of excessive gradients of flow parameters. Series of simulations was conducted for meshes of different sizes and the final mesh of appr. 0.5mln cells was accepted as providing the grid independent solution.

ANSYS FLUENT version 13 was used as a solver of the flow governing equations and ANSYS GAMBIT for geometry and mesh generation. Second-order discretization schemes were used to solve the flow equations. The SIMPLE algorithm was applied for the pressure-velocity coupling. The algorithm for the liquid spreading process as well as the phase interaction in porous zone was
implemented in a form of user defined functions, i.e. the own-developed subroutines linked to the solver. The rigorous criteria were used to ensure the full convergence of the solution. All the residua of governing equations had to fall down below the $10^{-4}$ level. Moreover, the liquid volume fraction at various cross sections was monitored to show whether the flow in a porous region has reached the steady state.

3. Results

The analysis of simulation results was started from the qualitative insight into the flow spreading process. For that purpose the magnified views of the flow structure in form of velocity vector chart and the volume fraction contour map are presented in figure 2b and figure 2c, respectively. As can be seen from the instantaneous velocity vector map (see figure 2b), the orientation angle varies in a wide range giving impression of chaotic motion satisfying, however, the distribution described by equation (3). The chaotic nature of the liquid motion is much less pronounced if the volume fraction distribution (see figure 2c) is analyzed in the corresponding region. White colour corresponds to no gas present in the mixture while black one to pure gas. One can easily notice, that the chaotic nature of the flow disappears as the volume fraction distribution depends on the time history of the liquid redistribution process, leading finally to the spreading of the jet-like flow with easily noticeable irregularities. The highest volume fraction values occur just downstream the entrance to the porous region and moving downstream its values decrease as liquid is redistributed in transverse directions. The results collected in figure 2 indicate the reasonable behaviour of liquid in a randomly generated porous region and proves the relevance of the spreading model implemented in Eulerian approach.

![Figure 2](image_url)

**Figure 2.** Model geometry and boundary conditions (a), instantaneous velocity vector map (b) and corresponding liquid volume fraction distribution (c).

In order to analyze the liquid spreading process the flow statistics have to be taken into account to reduce irregularities resulting from random orientation of packing elements. As the most suitable parameter the liquid volume fraction was selected and the corresponding distributions are shown in figure 3 as a system of isolines (in figure 3a) and in the form of radial profiles for selected cross sections (see figure 3b). The data in figure 3a are presented for upper half of the packing section and numbers correspond to the liquid volume fraction expressed as a percentage. As can be seen the most intense spreading is observed just downstream the top edge of the porous region what is manifested by high radial gradient of volume fraction $\partial \alpha_l / \partial r$. In the following cross sections i.e. for increasing x-coordinate the spreading rate is gradually decreasing as can be deduced from the divergence of $\alpha_l$.
isolines. It should be remarked, that the volume fraction distribution shown in figure 3a corresponds to particular vertical cross section and that is why the view is not symmetrical. As a complement to figure 3a the radial profiles of liquid volume fraction for a number of cross-sections (located at dimensionless coordinate x/h where h is the total height of the packing) are presented in figure 3b. The data shown here were averaged not only in time but also in circumferential direction. The volume fraction profile at the cross section closest to the packing top (x/h=0.14) indicates the existence of a core flow resulting from the small-diameter liquid jet entering the packed bed. The maximum volume fraction value of 22.5% confirms, that the most efficient spreading rate occurs in the initial region of the packed bed as it decreased from the initial level of 100% at (at x/h≈0). The core flow is surrounded by a region (r/D≥0.25) with a negligible presence of liquid (α_l<3%). Volume fraction profiles at consecutive cross sections (displaced by constant interval) become more and more uniform. The decrease of volume fraction maximum values is due to the gradual reduction of the spreading rate in radial direction. At the last analyzed cross section (x/h=0.9) the volume fraction at the column axis is appr. 6.5% while at the column wall it reaches appr. 3%. It shows that the packing section 0.5m high and of 0.1m diameter is not able to uniformly redistribute the liquid in cross section. One should note, that the previous statement is valid for the considered packed bed configuration only and has no general character.

Figure 3. Averaged liquid volume fraction distribution in a packed bed (a) and its radial profiles for selected cross sections (b).

4. Summary
The paper presents the combined VOF-Eulerian two-fluid modelling strategy applied to the two-phase flow in an unstructured packed bed composed of 6mm Raschig rings. As the first step, the detailed geometry of porous region was considered allowing to recover the detailed flow structure with the use of conventional conservation laws and the liquid free surface tracking method (VOF). The flow statistics obtained in this way allowed to determine the probability density function of the velocity vector orientation which was then implemented into the Eulerian-Eulerian model in ANSYS FLUENT environment to simulate the flow in a column with the packed bed. The test simulations have shown the reasonable model behaviour and the flow redistribution which followed the VOF approach with high precision. The results of computations provided an insight into the liquid spreading process along and across the packing section. The spreading rate has been found to be large at the top of porous zone and rapidly decreasing downstream and towards the wall. The Eulerian two-fluid approach developed
in present paper will be used in future work for the parametric analysis of the packing beds providing the characteristics needed for their optimisation. In further research work the model will be incorporated into the carbon capture and storage (CCS) model including additionally carbon dioxide capture chemistry, heat transfer and phase change phenomena [21]. The reliable and physically based model of liquid spreading in the packed bed is a crucial point to simulate such a complex physio-chemical system in an adequate way.

5. References

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