Highlights

1. Two-phase CFD models for a novel hybrid pulsed sieve plate solvent extraction column as well as a standard pulsed sieve plate column were developed.
2. Holdup for both columns were predicted with CFD and comparisons were made with literature data.
3. Axial dispersion coefficients for both columns were predicted with CFD and comparisons were made with literature data.

Graphical abstract

CFD Simulation of Two-phase Flow in a Hybrid Pulsed Sieve Plate Solvent Extraction Column: Prediction of Holdup and Axial Dispersion Coefficients

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ABSTRACT:

Two-phase computational fluid dynamics (CFD) models for a hybrid pulsed sieve plate solvent extraction column as well as a standard pulsed sieve plate column have been developed with commercial software ANSYS FLUENT. Hydrodynamic performance including two-phase distribution and velocity fields are generated with the models and comparisons are made between two columns. Important parameters including holdup and axial dispersion coefficients are studied systematically, and CFD successfully predicts the higher holdup and lower axial dispersion coefficients for the hybrid pulsed sieve plate column as measured in the experiments. CFD also gives reasonable predictions for the effect of pulsation intensity, dispersed phase velocity and continuous phase velocity on holdup, except for the effect of pulsation intensity in low pulsation region, and the cause has been discussed from the perspective of droplet breakage and coalescence. Comparison with literature data shows that CFD underestimates the holdup of

hybrid pulsed sieve plate column and standard pulsed sieve plate column by 23.3% and 31.4% respectively, and the cause has been discussed from the perspective of drag law. CFD gives good prediction of axial dispersion coefficients for the hybrid pulsed sieve plate column and the standard pulsed sieve plate column with ARD of 12.0% and 14.3% respectively. This study shows CFD to be a useful tool to predict performance for the novel hybrid pulsed sieve plate column as well as the standard pulsed sieve plate column.

Key words:

CFD, Hybrid pulsed sieve plate column, Hydrodynamics, Axial dispersion, Solvent extraction

1. Introduction

Liquid-liquid extraction is an important separation process. An extraction column has advantages such as high volume efficiency, small footprint and environmentally friendly features over other solvent extraction contacting devices, so they have been used for a range of applications in chemical, petroleum, nuclear, hydrometallurgical and other industries for many years^[1-3]. Among different types of extraction columns, the pulsed sieve plate column is characterized by the absence of moving mechanical parts which avoids frequent maintenance, and the mode of providing energy which makes remote operation possible^[4, 5]. Because of these advantages, pulsed sieve plate columns are widely applied especially in the nuclear fuel reprocessing field^[6, 7]. Extraction of lithium from chloride brine in salt lakes is another important field^[8], where pulsed sieve plate columns are likely to be applied. In order to solve the corrosion problem with traditional stainless steel sieve plates resulting from high chloride content brine, two types of novel ceramic internals, the ceramic sieve plate and the hybrid ceramic internal, have been designed based on standard sieve plates and tested in a pilot plant^[9, 10]. The hybrid ceramic internal is designed by adding ceramic packing on ceramic sieve plates, so that the axial dispersion and droplet diameter can be reduced, hence the mass transfer can be intensified.

Hydrodynamic parameters, especially holdup, are important to determine the column throughput, while mass transfer parameters including axial dispersion coefficients are important to determine separation efficiency^[11, 12]. Researchers have investigated the hydrodynamic^[13-16] and mass transfer performance^[15, 17, 18] of standard pulsed sieve plate columns. Additionally experiments have been performed to test the hydrodynamic^[9] and mass transfer^[10] performance

of the two types of novel ceramic internals. Hydrodynamic experiments show that the hybrid ceramic internal has higher holdup and smaller drop size which both contribute to higher mass transfer area^[9]. Mass transfer experiments show lower axial dispersion coefficients and higher overall mass transfer efficiency for the hybrid ceramic internal^[10].

In the studies mentioned above, axial dispersion model is used to interpret the experimental data, while key parameters are modeled with classical empirical correlations. The axial dispersion model assumes 1D counter-current flows for the two phases and takes into account the deviation from plug flow with axial dispersion coefficients^[19]. This model is limited as it cannot provide detailed information about the two-phase flow occurring inside the column. Recently computational fluid dynamics (CFD) has emerged as a promising method to assist extraction column design and performance modeling^[20]. CFD can give detailed information such as velocity field, phase distribution and turbulence parameters inside the column by solving partial differential equations given by fluid mechanics theory. It is expected that future developments of this modeling method will significantly save time and cost in extraction column design by reducing expensive physical experiments ^[21].

In the past decades researchers have made efforts to apply CFD to extraction columns such as Disc and Doughnut Column^[22, 23] and Rotating Disc Column (RDC)^[21, 24-26] which can be simplified with central symmetry of their structures. The CFD modeling of pulsed sieve plate columns is more difficult due to the complexity in its structure and the non-steady feature from pulsation. In 2009, Yadav et al.^[27] first applied CFD in the modeling of pulsed sieve plate columns, and the two-phase simulation results including the thickness of the dispersed

phase layer and holdup agree well with literature values. In the simulation a 2D mesh was constructed and downcomers were set on each plate for the continuous phase, however there are no downcomers in a standard pulsed sieve plate column. The Eulerian-Eulerian method and $k - \varepsilon$ model were used to model two-phase flow and turbulence respectively, while pulsation was modelled with a sinusoidal velocity boundary condition. These approaches are widely used by later researchers. Din et al.^[16] performed two-phase simulation in a standard pulsed sieve plate column by using layers of porous media to model sieve plates. They only ran one simulation and found the simulated holdup is 72.17% of the experimental value. Tang et al.^[28] performed a single-phase CFD simulation in a standard sieve plate column and a “disperse-coalescence” sieve plate column with 3D meshes. They used single-phase flow in two directions under non-pulsation conditions to describe two phases respectively. They used the variation of velocity on a cross section to explain the difference in axial dispersion for both internals. Kolhe et al.^[29] performed single-phase simulation in 3D mesh of a standard pulsed sieve plate column. They used the tracer injection method to calculate axial dispersion coefficients and found good agreement with experimental data. Sen et al.^[5] performed a single-phase simulation in a standard pulsed sieve plate column. They compared two approaches to construct the 2D mesh, i.e. keeping the pitch the same as in the actual geometry, varying the hole diameter and keeping the hole diameter the same as in the actual geometry and varying the pitch, and found the latter approach gives a better prediction. They also found the simulation of a few compartments gives as good prediction as the simulation of the whole column, and can save much of the computation cost. Later Sen et al.^[4] further performed a two-phase simulation based on the

approaches above, and compared the holdup with literature data. They found that when using different drag models the Kumar-Hartland model gave the best prediction and they further modified this model according to literature data.

Although a number of efforts have been made in this field, only Din et al.^[16] and Sen et al.^[4] reported two-phase CFD simulation for standard pulsed sieve plate column. Din et al.^[16] used porous media to model sieve plates but the simulation results deviate much with experiments. Sen et al.^[4] modeled sieve holes directly in 2D CFD, which approach would be applied in this study, however, they didn't study the newly developed hybrid pulsed sieve plate column. A few researchers have worked on the mass transfer performance and axial dispersion in two-phase simulation of pulsed sieve plate columns under pulsation conditions. Hence the main objectives of this work are:

1. To develop two-phase CFD models under pulsation conditions for a hybrid pulsed sieve plate column, as well as a standard pulsed sieve plate column for comparison.
2. To predict holdup for both columns with CFD, compare the results with experimental data and explain the difference between two columns.
3. To calculate axial dispersion coefficients with tracer injection method in CFD, compare the results with experimental data and explain the difference between two columns.

2. Mathematical models

2.1. Two-phase CFD model

The two-phase flow in this study is described by the Eulerian-Eulerian model which mathematically treats the two phases as interpenetrating continua^[30]. The organic phase is set as the dispersed phase while the aqueous phase is the continuous phase. The conservation equations solved for each phase are shown as follows:

Continuity equation for phase I:

$$\frac{\partial(\alpha_l \rho_l)}{\partial t} + \nabla(\alpha_l \rho_l \vec{u}_l) = 0$$

Equation 1

Momentum conservation equation for phase I:

$$\frac{\partial(\alpha_l \rho_l \vec{u}_l)}{\partial t} + \nabla(\alpha_l \rho_l \vec{u}_l \vec{u}_l) - \nabla \tau_l = -\alpha_l \nabla p + \alpha_l \rho_l g + F_k$$

Equation 2

In the equations above α represents the volume fraction, ρ represents density, $\vec{u}$ is phase velocity, τ is the stress strain tensor, p is the pressure shared by all phases, g is gravitational acceleration, F_k is the momentum transport term by inter-phase interaction. The subscript l represents phase l . Because here we only consider the two-phase condition volume fractions of the two phases at every mesh unit should satisfy Equation 3:

$$\alpha_1 + \alpha_2 = 1$$

Equation 3

The phase interaction term F_k includes momentum exchange by different mechanisms, i.e. drag force, lift force and virtual mass force. It has been shown by Wang et al.^[31] that the drag force is the dominant force while the latter two mechanisms can be

neglected. The drag force term between the continuous and dispersed phase is calculated by Equation 4^[19]:

$$F_{c,d} = \frac{\rho_d \alpha_c \alpha_d f}{\tau_d} (\vec{u}_d - \vec{u}_c)$$

Equation 4

Here f represents the drag force coefficient and τ_d is the particulate relaxation time which is calculated with Equation 5 :

$$\tau_d = \frac{\rho_d d_d^2}{18\mu_c}$$

Equation 5

where d_d is the Sauter mean diameter of the dispersed phase and μ is dynamic viscosity. Coalescence and breakage phenomenon are not taken into account so the mean diameter of the dispersed phase is given according to experimental results. The Schiller and Neumann^[32] model is used to calculate the drag coefficient:

$$f = \frac{C_D Re}{24}$$

Equation 6

$$C_D = \begin{cases} \frac{24(1 + 0.15Re^{0.687})}{Re} & Re \leq 1000 \\ 0.44 & Re > 1000 \end{cases}$$

Equation 7

In which the relative Reynolds number is defined as:

$$Re = \frac{\rho_c |\vec{u}_d - \vec{u}_c| d_d}{\mu_c}$$

Equation 8

By combining the above equations, the drag force term can be represented as follows:

$$F_{c,d} = \frac{3\rho_c \alpha_c \alpha_d C_D |\vec{u}_d - \vec{u}_c| (\vec{u}_d - \vec{u}_c)}{4d_d}$$

Equation 9

2.2. Turbulence model

The realizable $k\sim\epsilon$ mixture turbulence model is used to describe multiphase turbulence, which is extended from the single-phase version. This model consists of partial differential equations for turbulence kinetic energy k and its dissipation rate^[30] :

$$\frac{\partial}{\partial t}(\rho_m k) + \nabla \cdot (\rho_l \vec{u}_m k) = \nabla \cdot \left(\frac{\mu_{t,m}}{\sigma_k} \nabla k \right) + G_{k,m} + G_{b,m} - \rho_m \epsilon$$

Equation 10

$$\frac{\partial}{\partial t}(\rho_m \epsilon) + \nabla \cdot (\rho_l \vec{u}_m \epsilon) = \nabla \cdot \left(\frac{\mu_{t,m}}{\sigma_\epsilon} \nabla \epsilon \right) + \rho_m C_1 S \epsilon - \rho_m C_2 \frac{\epsilon}{k + \sqrt{\nu \epsilon}} + C_{1\epsilon} \frac{\epsilon}{k} C_{3\epsilon} G_b$$

Equation 11

$$C_1 = \max\left(0.43, \frac{\eta}{\eta + 5}\right), \quad \eta = S \frac{k}{\epsilon}$$

Equation 12

S represents the strain rate tensor and G_k is the generation of turbulent kinetic energy caused by the mean velocity gradient. In the equations above, the density, velocity and turbulent viscosity for the mixture are defined as:

$$\rho_m = \alpha_c \rho_c + \alpha_d \rho_d$$

Equation 13

$$\vec{u}_m = \frac{\alpha_c \rho_c \vec{u}_c + \alpha_d \rho_d \vec{u}_d}{\alpha_c \rho_c + \alpha_d \rho_d}$$

Equation 14

$$\mu_{t,m} = \rho_m C_\mu \frac{k^2}{\varepsilon}$$

Equation 15

Previous research by Drumm et al.^[25] compared different turbulence models' results with PIV experiment data and suggested realizable $k \sim \varepsilon$ model is the most appropriate model to describe two-phase behaviour. Therefore this model has been used in this study with the default values for C_1 , C_2 and C_μ .

2.3. Species transport model

In order to simulate axial dispersion, the species transport model is used for the continuous phase. The continuous phase is set to be a mixture of aqueous phase (water) and a non-transferring "tracer". The transport equation for this "tracer" is:

$$\frac{\partial}{\partial t} (\rho \alpha_c c_i) + \nabla \cdot (\rho \alpha_c \vec{u}_c c_i) = \nabla \cdot \vec{J}_i$$

Equation 16

$$\vec{J}_i = \left(\rho D_m + \frac{\mu_t}{Sc_t} \right) \cdot \nabla c_i$$

Equation 17

where c_i is concentration of species i , $\vec{J}_i$ is the mass diffusion term, and D_m is the molecular diffusion coefficient. $\frac{\mu_t}{Sc_t}$ is the diffusion term caused by turbulent flow, in which μ_t is turbulent viscosity and Sc_t is turbulent Schmidt number. The default number for Sc_t of 0.7 is used.

2.4. Axial dispersion coefficient calculation

In the classical axial dispersion model, the flow patterns for both phases are simplified to 1D counter current flows with axial dispersion terms. The transport equation describing the mass balance of a species is Equation 18,

$$x_c \frac{\partial c}{\partial t} = -u_c \frac{\partial c}{\partial z} + E_c \frac{\partial^2 c}{\partial z^2}$$

Equation 18

Introducing the following dimensionless variables:

$$Pe = \frac{u_c \cdot L}{E_c} \quad C = \frac{c}{c_{max}} \quad Z = \frac{z}{L} \quad \theta = \frac{t \cdot u_c}{x_c \cdot L}$$

then Equation 18 becomes Equation 19:

$$Pe \frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z} = \frac{\partial C}{\partial \theta}$$

Equation 19

Using a two-point monitoring method the initial condition and boundary condition can be expressed as:

Initial condition:

$$\theta = 0, \quad C(Z, 0) = 0$$

Equation 20

Boundary conditions:

$$Z=L1, \quad C(L1, \theta)=C1(\theta); \quad Z=1, \quad \frac{\partial C}{\partial Z} = 0$$

Equation 21

Where $C1(\theta)$ is the recorded dimensionless “tracer” concentration - time curve at the first sampling point. $L1$ is the dimensionless position of this point.

3. Numerical procedure

The physical properties of the experimental system (30%TBP in Kerosene - Water) used in this study are measured by Yi et al.^[9] and shown in Table 1. The schematic diagram of the two columns studied is shown in Figure 1 and the key dimensions of the columns are shown in

Figure 1 Schematic diagrams and photograph of column internals (A) hybrid pulsed sieve plate column (B) standard pulsed sieve plate column (C) tie rods (D) photograph of the hybrid pulsed sieve plate column

Table 2. Sauter mean diameter of dispersed phase is set according to experimental data reported by Yi et al.^[9]

Table 1 Physical properties of the aqueous and organic phases

Property	Aqueous	Organic
Density (kg/m ³)	1008	844
Viscosity (Pa·s)	1.06x 10 ⁻³	2.05 x 10 ⁻³
Interfacial tension (N/m)	0.0101

Figure 1 Schematic diagrams and photograph of column internals (A) hybrid pulsed sieve plate column (B) standard pulsed sieve plate column (C) tie rods (D) photograph of the hybrid pulsed sieve plate column

Table 2 Geometric size of the hybrid pulsed sieve plate column and the standard pulsed sieve plate column

Geometry	Size (mm)
Column diameter	72.5
Compartment height	50
Hole diameter	3
Fractional open area	23%
Packing height	25

As shown in Figure 2, integrated triangular and quadrilateral 2D meshes are constructed with Gambit 2.4.6 to model both columns. Take hybrid pulsed sieve plate column as an example, 2mm of triangular grids are used for the middle part of compartments where more details are needed, while sparser 3mm quadrilateral grids are used for the top and bottom parts which are less important. The sizes above are chosen after preliminary consistency trials. As for the packing, corrugated boards are compressed together and cut to make the packing, while channels on neighboring boards cross each other with right angle. Hence in the simplified 2D mesh squares are evenly distributed above the plates to shape the crossing channels inside the packing. One pressure outlet condition is used at the top boundary for

organic outlet, while three velocity inlet conditions are used for the aqueous inlet, aqueous outlet and organic inlet boundaries in Figure 2. A sinusoidal velocity boundary condition is used to model the pulsing leg at right of the bottom. The rest of the surfaces of plates, packing and the column wall are defined with no-slip wall boundary conditions and the near-wall region is modelled with standard wall function. Sampling lines are set in free area of each compartment for tracer monitoring. The mesh of the pulsed sieve plate column is the same with the hybrid pulsed sieve plate column except for the lack of packing on each plate. The two phases used in the simulation are kerosene and water, while their physical properties are set according to Table 1.

Figure 2 Meshes of the hybrid pulsed sieve plate column and the standard pulsed sieve plate column

Simulations are carried out using commercial CFD software ANSYS FLUENT 14.0. The unsteady state simulation is performed with a time step of 0.002s while the first order implicit solver is used. The First order upwind scheme is used for the flow equations discretization in space. The SIMPLE algorithm is used for the pressure-velocity coupling. Convergence of the solution is considered when the residual of the equations is less than 1×10^{-4} .

4. Results and discussion

In a simulation, organic phase (dispersed phase) flows through the column from the bottom to the top and the aqueous phase (continuous phase) flows in the counter current direction, while pulsation is applied from the bottom of the column at the same time. After the two-phase distribution reaches a steady state, holdup is calculated. Then the “tracer” is injected from the continuous phase inlet boundary. The average concentration of “tracer” at the sampling lines in each compartment are then recorded and will be used to calculate axial dispersion coefficients.

4.1. Two-phase flow fields and holdup distribution

The typical simulation results of two-phase velocity fields and holdup distribution for both columns are shown in Figure 3 to Figure 5. The simulations are performed under the same operation conditions: velocity of continuous phase is $1.3 \times 10^{-3} \text{ m/s}$, velocity of

dispersed phase is $3.5 \times 10^{-3} \text{ m/s}$ and pulsation intensity is 1.2 cm/s . The continuous phase velocity field of the hybrid pulsed sieve plate column is shown in Figure 3(a), in which several small vortexes developed in the free area of each compartment, and the scale of the vortexes is restricted by the packing. The continuous phase velocity field of the standard pulsed sieve plate column is shown in Figure 3(b), in which there is a main vortex in each compartment. Scale of the main vortex is restricted by the neighboring plates and is obviously larger than that of the vortexes in the hybrid pulsed sieve plate column. Since the vortexes are the main cause of axial dispersion, the standard pulsed sieve plate column should have larger axial dispersion coefficients. The dispersed phase velocity fields are shown in Figure 4, in which the dispersed phase rises through the plates and packing directly while no vortex is found in both columns, which indicates little axial dispersion in the dispersed phase. Holdup distributions are shown in Figure 5, and holdup in the hybrid pulsed sieve plate column is obviously higher than that of the standard pulsed sieve plate column. It should be noted that one cause of the observed difference is the deceleration effect of packing to the dispersed phase.

Figure 3 Velocity fields of continuous phase for two columns: (a) hybrid pulsed sieve plate

column; (b) standard pulsed sieve plate column ($V_c=1.3 \times 10^{-3} \text{ m/s}$, $V_d=3.5 \times 10^{-3} \text{ m/s}$,

$A_f=1.2 \text{ cm/s}$)

Figure 4 Velocity fields of dispersed phase for two columns: (a) hybrid pulsed sieve plate column; (b) standard pulsed sieve plate column ($V_c=1.3 \times 10^{-3} \text{ m/s}$, $V_d=3.5 \times 10^{-3} \text{ m/s}$, $A_f=1.2 \text{ cm/s}$)

Figure 5 Holdup distribution for two columns: (a) hybrid pulsed sieve plate column; (b) standard pulsed sieve plate column ($V_c=1.3 \times 10^{-3} \text{ m/s}$, $V_d=3.5 \times 10^{-3} \text{ m/s}$, $A_f=1.2 \text{ cm/s}$)

4.2. Holdup

Holdup is defined to be the volume fraction of dispersed phase in the main part of the column:

$$x_d = \frac{v_d}{v_c + v_d}$$

Equation 22

In the simulations, holdup is calculated with integral for local volume fraction of dispersed phase in the mesh of the compartments. In experiments holdup is measured with

the volume displacement method^[33]. The effects of pulsation intensity (Af), dispersed phase velocity (V_d) and continuous phase velocity (V_c) on holdup for both columns are investigated with CFD, and the results are compared with the experimental data reported by Yi et al^[9] in Figure 6. Figure 6(a) shows simulated holdup for both columns increases when pulsation intensity is increased, while the experimental holdup decreases at first and then increases after a minimum point. CFD simulations successfully predict the increasing trend in high pulsation region where smaller sized droplets resulted from higher pulsation intensity brings lower rising velocity, longer residence time and higher holdup. However, the CFD simulation could not predict the decreasing trend observed at the low pulsation intensity region, where the increasing pulsation brings more energy, thinner layer of dispersed phase accumulated under each plate and lower holdup in experiments. A possible cause is that the CFD model doesn't take into account the droplet breakage and coalescence phenomenon, thus it fails to depict the accumulated layer under the plates in low pulsation region. Figure 6(b) shows simulated holdup for both columns increases when dispersed phase velocity is increased, which agrees with the increasing trend of experimental data. Figure 6(c) shows continuous phase velocity has little effect on simulated holdup as well as experimental data. In Figure 6(a) – (c), CFD simulations successfully predict the higher holdup in the hybrid pulsed sieve plate column compared with the standard pulsed sieve plate column, which can be explained by the deceleration effect of packing as well as the lower rising velocity resulted from smaller drop size in the hybrid pulsed sieve plate column. Figure 6(a) – (c) also show that simulated holdup from CFD for both columns is lower than experimental data under the conditions investigated. An explanation is that the most widely used Schiller and Neumann

drag model underestimates the drag coefficient, which is in agreement with the CFD model outcomes presented by Onink et al. ^[26] with a rotating disc contactor.

The deviation of simulated holdup from experimental data is measured with average relative deviation (ARD) which is defined as:

$$ARD = \frac{1}{n} \sum_{i=1}^n \frac{|predicted\ value - experimental\ value|}{experimental\ value} \times 100\%$$

Equation 23

where n is the number of data points.

The ARD of holdup is 23.3% for the hybrid pulsed sieve plate column and 31.4% for the standard pulsed sieve plate column, which means the CFD simulations underestimate the holdup of both columns by 23.3% and 31.4% respectively.

Figure 6 Effect of (a) pulsation intensity ($V_c=2.02 \times 10^{-3} \text{ m/s}$, $V_d=2.02 \times 10^{-3} \text{ m/s}$); (b) dispersed phase velocity ($V_c=1.30 \times 10^{-3} \text{ m/s}$, $Af=1.2 \text{ cm/s}$); (c) continuous phase velocity ($V_d=7.0 \times 10^{-4} \text{ m/s}$, $Af=1.2 \text{ cm/s}$) on simulated and experimental holdup

4.3. Axial dispersion coefficient

The unsteady tracer injection method is used to measure axial dispersion in this study. After the two phases reach steady state, a small amount of tracer is injected into the column through the aqueous inlet boundary, and the average tracer concentration in the compartments is then recorded. A typical set of simulation data is shown in Figure 7, in which the tracer concentration is recorded in the second to the fifth compartments from the top. The tracer distribution on the lower sampling line is wider and lower as a result of axial dispersion caused by vortices in the compartments. There are fluctuations on the curves

caused by the reciprocating movement from pulsation, thus the curves will be smoothed by choosing the data in the middle of each pulsation cycle for further analysis. To calculate axial dispersion coefficients, the curves in the middle two (i.e. the third and fourth) compartments are used to reduce end effects. As described by Yi et al.^[23] the partial differential equation shown in Equation 18 will be solved by a pre-coded MATLAB program with axial dispersion coefficient as variable to best fit the curves.

Figure 7 A typical set of tracer concentration evolution curves on sampling lines in compartments

The effects of pulsation intensity (A_f), dispersed phase velocity (V_d) and continuous phase velocity (V_c) on axial dispersion coefficients for both columns are investigated with CFD, and the results are compared with the experimental data reported by Yi et al.^[10] in Figure 8. Figure 8(a) shows simulated axial dispersion coefficient increases when pulsation

intensity is increased for both columns, which agrees with the trend of experimental data. Figure 8(b) shows simulated axial dispersion coefficient for both columns increases when dispersed phase velocity is increased, however the trend is not significant in the low dispersed phase velocity region. The experimental data collected in this low V_d region also shows a similar trend to the simulations. Figure 8(c) shows simulated axial dispersion coefficient for both columns slightly increases when continuous phase velocity is increased, and the experimental data shows the same trend. In general, in Figure 8(a) – (c) the predictions for axial dispersion coefficients by CFD agree well with experimental data especially for the hybrid pulsed sieve plate column, while for the standard pulsed sieve plate column CFD simulations underestimate the experimental data. A possible explanation is that the larger free area in the standard pulsed sieve plate column brings more complexity and uncertainty in the two-phase flow, which leads to larger deviation of CFD from experiments. The deviation of simulated axial dispersion coefficients from experimental data is measured with ARD. The ARD of axial dispersion coefficients is 12.0% for the hybrid pulsed sieve plate column and 14.3% for the standard pulsed sieve plate column, which indicates a good prediction performance for CFD.

All the simulation and experimental results in Figure 8(a) – (c) indicate that the axial dispersion coefficients of the hybrid pulsed sieve plate column are about 50% lower than that of the standard pulsed sieve plate column. This phenomenon is assumed to be a result of the smaller scale vortices from the smaller free area in the compartments of the hybrid

pulsed sieve plate column, and continuous phase velocity fields as shown in Figure 3 help prove this assumption.

Figure 8 Effect of (a) pulsation intensity ($V_c=1.30 \times 10^{-3} m/s$, $V_d=7.0 \times 10^{-4} m/s$); (b) dispersed phase velocity ($V_c=1.30 \times 10^{-3} m/s$, $Af=1.2 cm/s$); (c) continuous phase velocity ($V_d=7.0 \times 10^{-4} m/s$, $Af=1.2 cm/s$) on axial dispersion coefficients in CFD and experimental data

5. Conclusions

In this study, two-phase models were developed with CFD for a novel hybrid pulsed sieve plate solvent extraction column, as well as a standard pulsed sieve plate column for comparison. The following conclusions can be drawn from this study:

- (i) CFD successfully predicted the higher holdup of the hybrid pulsed sieve plate column compared to the standard pulsed sieve plate column.
- (ii) CFD model could not predict the trend in holdup at the low pulsation region because the models did not take into account the droplet breakage and coalescence phenomenon.
- (iii) CFD could predict the holdup of both columns within 23.3% and 31.4% respectively.
- (iv) CFD successfully predicted the higher axial dispersion coefficients for the standard pulsed sieve plate column compared to the hybrid pulsed sieve plate column.
- (v) CFD was found to give a good prediction for axial dispersion coefficients in both columns with ARD of 12.0% and 14.3% respectively.

In general, this study shows that CFD can be used to provide reasonable predictions of performance for the novel hybrid pulsed sieve plate column as well as the standard pulsed sieve plate column, which proves CFD to be a useful tool in column design and modelling.

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■ Nomenclature

Symbols

A	amplitude, m
c	species concentration, mol/m ³
C	dimensionless concentration
C _D	drag coefficient
d _d	Sauter mean diameter, m
D _m	molecular diffusion coefficient, m ² /s
E _c	axial dispersion coefficient, m ² /s
f	frequency, Hz
F	interaction force, N
g	gravitational acceleration, m/ s ²
G	generation term of turbulent kinetic energy, kg/(m ² · s ³)
k	turbulent kinetic energy, m ² /s ²
L	characteristic length, m
p	pressure, Pa
Pe	Peclet number
Re	Reynolds number
t	time, s
u	velocity, m/s
v _c	volume of the continuous phase for the effective length of the column, m ³
v _d	volume of the dispersed phase for the effective length of the column, m ³

V superficial velocity for two phases, m/s
 x_d volume fraction holdup of the dispersed phase, dimensionless
Y species concentration, mol/m³
Z dimensionless distance

Greek letters

α volume fraction
 ε turbulent energy dissipation, m²/s³
 μ dynamic viscosity, Pa · s
 μ_t turbulent viscosity, Pa · s
 ρ density, kg/ m³
 θ dimensionless time
 τ stress strain tensor, N/ m²

Subscripts

c continuous phase
d dispersed phase
l liquid phase l
m mixture

Abbreviations

CFD computational fluid dynamics
RDC rotating disc contactor
ARD average relative deviation

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