CFD simulation and optimization of the settler of an industrial copper solvent extraction plant: A case study

Roohollah Sadeghi, Ali Mohebbi, Amir Sarrafi, Ataallah Soltani, Mazyar Salmanzadeh, Shahram Daneshpojoo

Abstract

A computational fluid dynamics simulation based on Eulerian–Eulerian two-phase method accompanied by experimental field measurements has been applied to study the behavior of aqueous–organic dispersion in the copper solvent extraction settler in the Sarcheshmeh copper complex, Iran. This simulation takes into account multiple-size group (MUSIG) model for droplet dispersion and droplet size distribution, which is based on a population balance equation and considers the break-up and coalescence models of the droplets. Fluid flow field has been calculated by solving the continuity and Navier Stokes equations along with the standard k-ε turbulence model. The turbulence model included buoyancy, drag, lift and turbulent dispersion forces. The simulation results have been compared with the experimental field measurements to validate the accuracy of the CFD work. Effects of the number of rows of picket fences and also their structure on the performance of the settler have been investigated. The results showed that the phase separation was achieved more effectively when two rows of picket fences with a distance of 1.3 m from each other are set into the inlet of the settler. The inspection of distribution of droplet size at different points in the settler showed that the presence of picket fences increases the size of droplets. Finally, the effect of closed to opened (C/O) area ratio of the picket fences on the performance of the settler was studied. The results showed that by increasing the C/O ratio, some circulation appears in the flow which causes a negative effect on phase separation.

1. Introduction

Liquid–liquid extraction is a process for separating components in solution by their distribution between two immiscible liquid (Robbimins, 1984; Skelland and Tedder, 1987). Solvent extraction has many applications in the petrochemical and pharmaceutical industries as well as in hydrometallurgy (copper, cobalt, nickel and zinc). In hydrometallurgy the most applied solvent extraction equipment is a mixer–settler (Ritcey and Ashbrook, 1984). The main ideas in the development of the solvent extraction mixer–settler focused on achieving clean phase separation, minimizing the loss of the reagents and decreasing the surface area of the settlers (Pekkala et al., 1999; Lewis, 1979; and Mizrahi and Barnea, 1973). We recently studied effect picket fences on launder of Settler in Sarcheshmeh copper complex (Sadeghi et al., 2011). This study showed that by setting the picket fences, flow pattern becomes uniform, and turbulent eddies disappear.

In the mixer–settler aqueous and organic phases are pumped into a mixer to achieve homogeneous dispersion. After mixing, the dispersion is fed into a settler where the aqueous and organic phases are separated by gravity. The performance of a settler depends on distribution of feed into the settler. Feed distribution has a large effect on flow pattern in the settler. Undesirable feed distribution leads to production of macro eddies and circulation flow in the settler. Macro eddies can be eliminated by baffles and packed media.

The most common method to make phase separation more effective is to use picket fences, which are installed in different locations in the settler. The idea of the picket fences is to retain a deep and dense dispersion layer in the first part of the settler (Nyman et al., 1996). Several studies have been reported on the effect of picket fences in the settler. Kankaanpää (2005) confirmed that the flow field can be propagated with using at least two picket fences before impressing of viscous effect. It was also confirmed that without picket fences the feed spouting velocity was propagated for long distances in the settler. According to Kankaanpää’s (2005) work the feed model without full depth resulted in a reverse flow of the aqueous from half way down the settler back to the feed end. Stanbridge and Sullivan (1999) studied inlet feed arrangement distribution to settler. They showed that feed arrangement distribution has a great effect on settler performance. Their study showed that perfect flow in the settler can be obtained by uniform feed distribution along the width of the settler.

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Miller (2006) reported that performance of a settler can increase by up to 30–50% by improving the feed distribution and coalescence systems. These systems also increase settler performance when an emulsion band is not present due to fast breaking emulsions.

In our previous work (Sadeghi et al., 2011), a computational fluid dynamics modeling accompanied by experimental field measurements was applied to study the performance of the launder of settler in the Sarcheshmeh copper complex, Iran. Our results showed that by installing two picket fences without dam in the launder, the phase separation improves and the performance of the launder is optimized. In the present study, which is a continuation of our previous simulation (Sadeghi et al., 2011), three dimensional CFD modeling has been used to predict the performance of a copper solvent extraction settler in the Sarcheshmeh copper complex. The performance of the model has been compared with the experimental field measurement data and the effect of picket fences on phase separation in the settler has been studied.

2. Experimental measurements

Lack of experimental measurements for this type of settler forced us to do experimental field measurements for the current situation of the settler in Sarcheshmeh copper complex. The measured physical properties of the phases (organic and aqueous) are presented in Table 1. One of the important parameters in the performance of a settler is droplet size distribution of dispersed phase in the settler inlet. In the settler of the Sarcheshmeh copper complex, organic phase is continuous and aqueous phase is dispersed.

For measuring droplet sizes (Singh et al., 2008), a dispersion sample (i.e. a mixture contains aqueous phase droplets dispersed in an organic phase) was poured in a Petri dish containing surfactant (Sorbitan mono-oleate) and organic phase. The surfactant prevented the coalescence of droplets and thus stabilized the dispersion. The dish was kept under a microscope with a camera, which connected to a personal computer. For measuring adequate numbers of droplets several images from different locations of the dish were taken. Fig. 1 shows a typical image of the stabilized dispersion which was analyzed by image processing software. Fig. 2 shows a graphical droplet size distribution of dispersed aqueous phase in the settler inlet.

In order to validate the results of simulation, the measured data for volume fraction of organic phase at different points of the settler were used. A glass tube having a diameter of 3 cm and a length of 1 m was used for this purpose. One end of the glass tube contained a rotating disc set an angle to the incoming flow. The tube was situated in different heights in the settler inside the liquid. After incoming the liquid into the tube, the disc was closed and there was no liquid passing through. Thereafter, phase separation occurs and the volume fraction of organic phase in that point of the settler was measured based on the height of the organic phase in the tube.

3. CFD simulation

3.1. Governing equations

The Eulerian–Eulerian multiphase model has been used because of high volume fraction of dispersed phase. Furthermore, the droplet coalescence and the break-up models have been implemented in the Eulerian–Eulerian model of the commercial ANSYS CFX-11 software. It is assumed that the flow is turbulent incompressible and isothermal.

Table 1

<table>
<thead>
<tr>
<th>Aqueous dynamic viscosity (mPa.s)</th>
<th>Organic dynamic viscosity (mPa.s)</th>
<th>Aqueous density (kg m⁻³)</th>
<th>Organic density (kg m⁻³)</th>
<th>Interfacial tension (mN m⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3</td>
<td>3.3</td>
<td>1100</td>
<td>806</td>
<td>26.1</td>
</tr>
</tbody>
</table>

The calculated Reynolds number at the inlet of the settler based on hydraulic diameter was about 11000.

3.1.1. Continuity equations

The continuity equations for continuous (c) and dispersed (d) phases are as follows (Versteeg and Malalasekera, 1995; White, 1991):

\[
\nabla \cdot (\rho_c \alpha_c \mathbf{U}_c) = 0, \quad (1)
\]

\[
\nabla \cdot (\rho_d \alpha_d \mathbf{U}_d) = 0, \quad (2)
\]

where \( \rho \), \( \alpha \), and \( \mathbf{U} \) are density, volume fraction and mean velocity vector respectively.

3.1.2. Momentum equations

The time averaged governing equation for a steady incompressible, turbulent flow form as (White, 1991; Soo, 1999; Lunder and Spalding, 1974):

\[
\begin{align*}
\rho_c \left[ \nabla \left( \alpha_c \mathbf{U}_c \mathbf{U}_c \right) \right] & = -\nabla \rho_c + (\mu_c + \mu_t) \nabla^2 \left( \alpha_c \mathbf{U}_c \right) + S_{Mc}, \quad (3) \\
\rho_d \left[ \nabla \left( \alpha_d \mathbf{U}_d \mathbf{U}_d \right) \right] & = -\nabla \rho_d + (\mu_d + \mu_t) \nabla^2 \left( \alpha_d \mathbf{U}_d \right) + S_{Md}. \quad (4)
\end{align*}
\]

here \( \mu, \mu_t, \rho \), and \( S \) are dynamic viscosity, turbulent viscosity, density and source term respectively. \( \mathbf{U}_c \) and \( \mathbf{U}_d \) are the time averaged mean vectorial velocities. The \( k-\varepsilon \) turbulent model has been used to calculate the turbulent viscosity (Lunder and Spalding, 1974):

\[
\mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon}. \quad (5)
\]

where \( k \) and \( \varepsilon \) are turbulent kinetic energy and turbulent dissipation rate respectively and the related transport equations are as follows:

\[
\begin{align*}
\rho \left[ \frac{\partial (\alpha \mathbf{U})}{\partial x} + v \frac{\partial (\alpha \mathbf{U})}{\partial y} + w \frac{\partial (\alpha \mathbf{U})}{\partial z} \right] & = \nabla \left[ \alpha \left( \mu + \mu_t \frac{\partial}{\partial z} \right) \nabla k \right] \quad (6) \\
& + 2 \omega \mu_t E_{ij} E_{ij} - \alpha \varepsilon,
\end{align*}
\]

\[
\begin{align*}
\rho \left[ \frac{\partial (\alpha \mathbf{U})}{\partial x} + v \frac{\partial (\alpha \mathbf{U})}{\partial y} + w \frac{\partial (\alpha \mathbf{U})}{\partial z} \right] & = \nabla \left[ \alpha \left( \mu + \mu_t \frac{\partial}{\partial z} \right) \nabla \varepsilon \right] \quad (7) \\
& + C_{1\varepsilon} \frac{\varepsilon}{k} 2 \omega \mu_t E_{ij} E_{ij} - C_{2\varepsilon} \alpha \varepsilon \frac{\varepsilon^2}{k}.
\end{align*}
\]
The mean rate of strain tensor $E_{ij}$ is:

$$E_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).$$  \hspace{1cm} (8)

The model coefficients used were the defaults values of the CFX 11, which are as follows: $C_1 = 0.09$, $C_{12} = 1.44$, $C_2 = 1.92$, $\delta_t = 1.0$ and $\delta_k = 1.22$.

Source term included the buoyancy, drag, lift and turbulent dispersion. The buoyancy force for the continuous phase is zero, ($F_{buo} = 0$). The lift force on the continuous phase is equal but opposite in sign.

The lift force. Lift force depends on the relative velocity and the curl of the continuous phase due to velocity gradient in the droplet due to velocity gradient in the fluid. This condition makes the lift force. Lift force depends on the relative velocity and the curl of the continuous phase in the following way:

$$F_{\text{lift}} = \rho \omega |U_{rel}| A_p C_l,$$

where $A_p$ is the projected area of the droplet and $C_l$ is the drag coefficient. The drag coefficient depends on the droplet diameter, the flow regime and the Reynolds number which is given by:

$$Re = \frac{\rho_d U_d d_i}{\mu_c},$$  \hspace{1cm} (11)

where $d_i$ is Sauter mean diameter. In this study, Ishii and Zuber’s (1979) drag coefficient was used.

There is a pressure distribution on the upper and lower surfaces of the droplet due to velocity gradient in the fluid. This condition makes the lift force. Lift force depends on the relative velocity and the curl of the continuous phase in the following way:

$$\rho_d \nabla \cdot (\alpha_d \rho_d C_l (U_C - U_d)) \times \nabla U_C,$$

where $C_l$ is lift coefficient and was set on 0.1 according to Behzadi et al. (2004). The lift force on the continuous phase is equal but opposite in sign.

The effect of turbulent fluctuation on the droplets dispersion was taken into account by the turbulent dispersion force. Turbulent dispersion depends on fluctuations and volume fraction gradient of the continuous phase. The dispersion force for the continuous phase can be written as follows (Soo, 1999):

$$k_c \nabla \alpha_c = \frac{\rho_c}{\Delta t},$$  \hspace{1cm} (13)

where $C_{TD}$ is the turbulent dispersion coefficient which was set on 0.1 according to Olmos et al. (Olmos et al., 2001). $k_c$ is the turbulent kinetic energy of the continuous phase. For the dispersed phase, this force is equal but opposite in sign.

The droplets that enter to the settler have size distribution and their size vary along the settler. Therefore, the droplet size distribution is taken into account in the calculations. The multiple-size-group (MUSIG) model that was developed by Lo (1996) was used to model the size distribution of droplets in the dispersed phase. This model contains break-up and coalescence rate terms. Population balance is a well-establish method for calculating size distribution in the dispersed phase. MUSIG provides a framework in which the population balance method can be incorporated into the three-dimensional CFD calculations. The model has been incorporated into CFX 11 software. The MUSIG model considers a number of droplet size groups to give a better representation of the size distribution (Kankaanpää, 2007).

Continuity equation for one MUSIG-size group-i can be written as (ANSYS CFX-11; Kankaanpää, 2007):

$$\rho_i \nabla \cdot (\alpha_i U_i) = S_i,$$  \hspace{1cm} (14)

where $S_i$ is the source term of the rate of mass transfer into the MUSIG-size group due to the break-up and coalescence processes. Eq. (14) can be applied to all MUSIG-size groups because the sum of all droplet volume fractions equals the volume fraction of the dispersed phase, i.e:

$$\sum_{i=1}^{N} \alpha_{d,i} = 1,$$  \hspace{1cm} (15)

where $N$ is the total number of MUSIG-size groups.

The individual volume fraction of MUSIG-size-group-i can be written as:

$$\alpha_{d,i} = \alpha_{d},$$  \hspace{1cm} (16)

where $f_i$ is the fraction of the dispersed phase volume fraction in MUSIG-size group-i. When Eq. (16) is substituted into Eq. (14), the continuity equation for the MUSIG-size group-i is yielded:

$$\rho_i \nabla \cdot (\alpha_{d,i} U_i) = S_i.$$  \hspace{1cm} (17)

Fig. 2. Droplet size distribution in the inlet of the settler.
The source term $S_i$ can be calculated from the population balance Eq. (19) when the product of the droplet number density of MUSIG-size group-$i$ ($n_i$) and the droplet volume of MUSIG-size group-$i$ ($v_i$) are related to the volume fraction of MUSIG-size group-$i$ by:

$$\eta v_i = \alpha d_f.$$  (18)

In this way, the normal population balance equation can be related to the continuity equation of the dispersed phase, Eq. (17) became identical to Eq. (17) when the dispersed phase density multiples both sides (ANSYS CFX-11; Kankaanpää, 2007)

$$\nabla .(U_d n_i) = \nabla .(\alpha d_f U_d j) = \delta_i = B_B - D_B - B_c - D_c,$$  (19)

where $\delta_i$ is source term of the rate of mass transfer into the MUSIG-size group due to break-up and coalescence processes with unit of $1/(m^3\cdot s)$. The birth rate of the MUSIG-size group-$i$ droplets due to break-up of larger droplets can be given by (ANSYS CFX-11; Kankaanpää, 2007):

$$B_B = \frac{N}{j+1} \begin{cases} g(v_j; v_i), \\ \end{cases}  (20)$$

the function of $g$ is the droplet break-up kernel. The death rate of the MUSIG-size group-$i$ droplet due to break-up to smaller droplet droplets can be given by:

$$D_B = g_i n_i.$$  (21)

The birth rate of the MUSIG-size group-$i$ droplet due to coalescence of group-$j$ and group-$k$ droplets can be given by (ANSYS CFX-11; Kankaanpää, 2007)

$$B_c = \sum_j^{N} \sum_k^{N} Q_{j,k}^n n_j n_k,$$  (22)

where the function of $Q$ is the specific droplet coalescence rate. The death rate of the MUSIG-size group-$i$ droplet due to coalescence with other droplets can be given by (ANSYS CFX-11; Kankaanpää, 2007):

$$D_c = n_i \sum_j^{N} Q_{j}^n n_j.$$  (23)

During the normal iteration, additional transport Eq. (17) is solved for the scalar variable $f_i$ after that, the size distribution of the dispersed phase can be defined from the solution of $f_i$ and the Sature mean diameter ($d_f$), which is used in computing the drag force between the continuous phase and dispersed phase and also momentum equation can be calculated from (ANSYS CFX-11; Kankaanpää, 2007):

$$d_f = \frac{1}{\sum_i^{N} f_i d_i},$$  (24)

where $d_i$ is the droplet diameter of the MUSIG-size group-$i$.

Luo and Svendson (1996) developed a theoretical model for the break-up of drops and bubbles in turbulent suspensions. The model is based on the theory of isotropic turbulence and probability. The break-up kernel is modeled as (ANSYS CFX-11; Kankaanpää, 2007):

$$g(v_j; v_i) = 0.923 F_{B} (1 - \alpha_d) \left( \frac{v_j}{d_i^3} \right)^{1/3} f_{\ell_{\eta \ell}} \int_{\xi_{\ell\eta}}^{1} \left( 1 + \xi \right)^{2} e^{-\xi} d\xi, \quad (25)$$

$$\chi = \frac{12}{\beta \rho \sigma \ell_{\eta}^{2}/2} \left( 1 - F_{B} \ell_{\eta}^{2/3} \right) \left( \frac{v_j}{d_i^3} \right)^{1/3} \xi^{11/3}, \quad (26)$$

$$F_{B} = \frac{v_j}{v_i}.$$  (27)

where $v_i$ and $v_j$ are the volumes of droplet with sizes of $d_i$ and $d_j$ respectively. $\xi$ is the dimensionless size of eddies in the inertial subrange of isotropic turbulence and $\sigma$ is the surface tension coefficient. The lower limit of the integration is given by :

$$\xi_{\min} = 11.4 \frac{\eta}{d_i^3}.$$  (28)

where

$$\eta = \left( \frac{1}{\varepsilon_c} v_c \right)^{1/4}.$$  (29)

In addition, $F_B$ is a calibration coefficient, $\beta = 2$, $\varepsilon_c$ is the continuous-phase eddy dissipation rate, $v_c$ is the continuous-phase kinematic viscosity.

The model of Prince and Blanch (1999) assumes that the coalescence of two droplets occurs in three steps. First, the droplets collide trapping a small amount of liquid between them. This liquid film then drains until the liquid film separating the droplets reaches a critical thickness. The film then ruptures and the droplets join together. The implemented coalescence model only includes the turbulence collision mechanism between the two droplets; the turbulence is assumed to be isotropic and droplet sizes lie in the inertial sub-range. Buoyancy-driven collision and laminar shear collision rates are ignored. Actually, ignoring the buoyancy-driven collision due to the difference in rise velocities of droplets of different sizes is acceptable, because the MUSIG model assumes that all the droplets have the same velocity. However, the buoyancy force is taken into account when it controls the phase separation by density difference of the dispersed and continuous phase via the body forces.

The coalescence kernel is therefore modeled by a collision rate of two droplets and a collision efficiency relating to the time required for coalescence. The coalescence kernel for the turbulence collision mechanism can be given by (ANSYS CFX-11; Kankaanpää, 2007):

$$Q(v_j; v_i) = \left( \theta_j + \theta_j^3 + \theta_j^5 \right) \eta_j,$$  (30)

where $\theta_j$ is collision efficiency and it modeled by comparing the time required for coalescence, $t_{ij}$ with the actual time during the collision, $t_{ij}$

$$\eta_j = \frac{1}{2} \frac{1}{t_j},$$  (31)

$$t_j = \frac{16 \gamma \xi_j \eta_j}{16 \sigma \ell_{\eta}},$$  (32)

$$t_j = \frac{h_i}{\varepsilon_c},$$  (33)

where $h_i$ is the initial film thickness, $h_j$ is the critical film thickness when rupture occurs, and $t_{ij}$ is the equivalent radius:

$$t_{ij} = \left( \frac{1}{2} \left( \frac{1}{t_{i}} + \frac{1}{t_{j}} \right) \right)^{-1}.$$  (34)

The turbulent contributions to collision frequency are modeled as (ANSYS CFX-11):

$$\theta_j^3 = F_{c} \eta_j \left( \frac{u_j^2 + \frac{v_j^2}{2}}{u_j^2} \right)^{1/2},$$  (35)

where the collision cross-sectional area of the droplets is defined by (ANSYS CFX-11):

$$S_j = \frac{\pi}{4} \left( d_i + d_j \right)^2.$$  (36)
The turbulent velocity is given by (ANSYS CFX-11):

$$u_t = \sqrt{2\varepsilon_0^{1/3}d_i^{1/3}},$$  \hspace{1cm} (37)$$

and $F_C$ is a calibration factor.

ANSYS CFX-11 code calculates the collision area four times higher than the actual value because it uses the diameter instead of radius in Eq. (36). However, this error does not affect the final results, because the coalescence model is optimized by the calibration coefficient. In this study, the buoyancy ($\theta_i^B$) and shear ($\theta_i^S$) contributions to collision frequency were neglected.

**Table 2**
Breakdown percentage for size distribution of droplets at inlet.

<table>
<thead>
<tr>
<th>Number of size group (i)</th>
<th>Size group (μm)</th>
<th>Breakdown percentage (%)</th>
<th>Number of size group (i)</th>
<th>Size group (μm)</th>
<th>Breakdown percentage (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>100</td>
<td>18.8</td>
<td>9</td>
<td>1000</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>175</td>
<td>32.3</td>
<td>10</td>
<td>1150</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>250</td>
<td>30.9</td>
<td>11</td>
<td>1300</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>350</td>
<td>12.4</td>
<td>12</td>
<td>1450</td>
<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>450</td>
<td>4.6</td>
<td>13</td>
<td>1800</td>
<td>0.0</td>
</tr>
<tr>
<td>6</td>
<td>600</td>
<td>1.0</td>
<td>14</td>
<td>2000</td>
<td>0.0</td>
</tr>
<tr>
<td>7</td>
<td>700</td>
<td>0.0</td>
<td>15</td>
<td>850</td>
<td>0.0</td>
</tr>
</tbody>
</table>

**Fig. 3.** Settler geometry and picket fence geometry.

**Fig. 4.** Comparison between measured data of organic phase volume fraction at different heights from the bottom of the settler with those of predicted by CFD simulation. ($z = 1.5$ m, $z$ is vertical to flow direction in a horizontal plane).
4. Physical domain

Fig. 3 shows the settler geometry of the Sarcheshmeh copper complex, which has been used in this study. The settler includes 25 columns. Its dimensions are 11 m x 11 m x 0.9 m with two outlets at the end of the settler, positioned on the top and bottom of the end wall. Flow rate in the settler is 1100 m³/h and organic to aqueous flow rate ratio is 0.95. In the settler, organic phase is continuous and aqueous phase is dispersed. The fluid height in the settler is 0.85 m. In Fig. 3, the x axis is the flow direction, z is vertical to the flow direction in a horizontal plane and y is the vertical axis.

5. Calculations procedure

The settler process was studied in steady state. The governing mass and momentum equations were solved by using commercial ANSYS CFX-11 software package. ANSYS CFX is a commercial multi-purpose CFD code currently developed by ANSYS Inc. The CFX numerical kernel uses the element based finite volume method (EBFVM) to treat generalized unstructured meshes in Cartesian coordinates. The discrete system of linearized equations is solved using the algebraic multi-grid (AMG) method accelerated by the incomplete lower upper (ILU) factorization technique. The pressure–velocity coupling is carried out in a single cell of the co-located grid using a Rhie and Chow (1983) like formulation. This solution approach uses a fully implicit discretization of the equations. In steady state solutions, the false time step technique is applied to the solution relaxation.

Upwind differencing scheme was employed for volume fraction and the high resolution scheme was used for the other terms. The hydrostatic pressure, frictionless and no-slip boundary conditions at the upper outlet, free fluid surface and walls have been applied respectively. Moreover, the boundary conditions at the inlet and the lower outlet were mass flow rate boundary conditions.

The grid independency test was carried out with three different three-dimensional meshes, which contained 500,000, 600,000 and 700,000 cells respectively. Comparison between simulation results and experimental data showed that 600,000 cells were needed to produce the grid-independent solution. The denser grid was used in the entrance of the settler due to intensive variations of the gradient of some variables in this region.

Several parameters should be selected before calculations in MUSIG model. These parameters are the numbers of the droplet size groups, the minimum droplet diameter, the maximum droplet diameter, and the coalescence and break-up calibration coefficients. Fig. 2 shows that the minimum droplet size in the inlet is about 100 μm. Therefore, the minimum size in the MUSIG model was selected at 100 μm. The coalescence calibration coefficients of 0.01, 0.005 and 0.001 were used in the different simulation runs with maximum droplet size of 1200 μm and the number of the droplet size in groups of 10. When the coalescence calibration coefficient was 0.1, effective coalescence occurred in the entrance of the settler and the separated aqueous phase contained only the maximum size group. When the coalescence calibration coefficient was 0.005, the droplet size distribution became uniform but the amount of aqueous phase in the upper outlet was much. Weak phase separation occurred in the settler for coalescence calibration coefficient of 0.001 because the separation of phases in the settler was controlled by the coalescence rather than break-up; therefore, the calibration coefficient of break-up did not affect the process. Different simulation runs were done for determining the maximum droplet size. The maximum droplet sizes of 1000, 1200, 1400, 1600, 1800, 2000 and 2200 μm were used. The results of simulations showed that with increasing maximum droplet size, proper droplet size distribution in different regions in the settler is obtained.

Different simulation runs were carried out with number of droplet size groups of 10, 15 and 20. When the number of droplet size groups increased, increasing the droplet size from minimum to maximum values could be smoother and it was possible that the droplet sizes in the inlet of settler were distributed in the adequate size groups according to the measured droplet distribution in Fig. 2. On the other hand as the numbers of size groups increase, the calculation time increases. After these test calculations, for effective phase separation, the coalescence and break-up calibration coefficients, maximum droplet size and number of droplet size groups were selected as 0.005, 0.1, 2000 μm and 15 respectively. When the number of droplet size groups was 15, this value for proper distribution of droplets in the inlet could be six (see Table 2).

6. Results and discussion

6.1. Validation of the model

The developed CFD model was checked by some criteria for the calculation converging, which were used in the previous works (Kankaanpää; 2007) and ensured that the results could be confirmed

<table>
<thead>
<tr>
<th>x = 8 m</th>
<th>x = 6 m</th>
<th>x = 4 m</th>
<th>Fluid height (cm) from the bottom of the settler</th>
</tr>
</thead>
<tbody>
<tr>
<td>z = 1.5 m (z is vertical to flow direction in a horizontal plane)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Experimental data</td>
<td>Simulation results</td>
<td>Error (%)</td>
<td>Experimental data</td>
</tr>
<tr>
<td>0.047</td>
<td>0.0511</td>
<td>5.1</td>
<td>0.091</td>
</tr>
<tr>
<td>0.071</td>
<td>0.0781</td>
<td>7.8</td>
<td>0.133</td>
</tr>
<tr>
<td>0.472</td>
<td>0.4623</td>
<td>2.1</td>
<td>0.355</td>
</tr>
</tbody>
</table>

Fig. 5. The velocity vectors of the organic phases in the settler at z = 4.5 m.
as converged. In this work, scaled residuals were smaller than $10^{-4}$, total mass flow rate error of each phase was less than 0.1% and the mass ratio of phases in the settler was constant. The results have also been compared with experimental data. Fig. 4 shows the simulation results of volume fraction of organic phase at different points of the settler. The measured experimental data have also been added to the Fig. 4 for comparison. Table 3 shows the related errors. As it can be seen the CFD results are in good agreement with the experimental data.

Fig. 5 shows the organic phase velocity vectors at $z = 4.5$ m ($z$ is vertical to flow direction in a horizontal plane). This figure indicates that the phases flow towards the central section after entering the settler, this causes an increase in velocity in that section and formation of the dispersion band. An important point regarding this band is that its velocity vectors are more along the length of the settler and the band’s thickness reduces when the dispersion flows toward the end of the settler.

### 6.2. Effect of picket fences on the settler performance

Increasing the performance of the existing settler in the Sarcheshmeh copper complex has been the main goal of this research. To achieve this goal, the settler operation has been optimized by testing different arrangements of picket fences with the aid of CFD modeling. Picket fences geometry in three rows is shown in Fig. 3. The dimensions of each picket fence are $0.9 \times 0.1 \times 0.025$ m and the distance between the two plates of picket fences in $x$ and $z$ directions are 0.05 m and 0.025 m respectively. Location and number of picket fences, distance between the picket fences and their effect on droplet size distribution have been the case studies. Closed to opened area...
ratio (C/O) was considered equal to 2 for the picket fences as one can see from Fig. 3. The operating conditions for simulation of the settler with and without picket fences were the same.

**6.2.1. Effect of one picket fence row**

The effect of location of picket fences on settler performance has been tested by installing the picket fence rows at three locations. **Fig. 6a** shows the organic phase velocity vectors for the case of one picket fence row. The distance of this row from the inlet of the settler was 1.75 m, which was the closest possible distance allowed for installation of the picket fences. As it can be seen in Fig. 6a, the picket fence causes to increase the movement of fluid particles in all directions, or on the other hand, velocity vectors are propagated in all directions. The organic phase volume fraction versus the height of the settler at two locations before and after the picket fence row is shown in **Fig. 7.** As one can see there is a sharp variation in the volume fraction of organic phase due to installation of the picket fence. This means that the thickness of the dispersion band reduces considerably after installation of the picket fence. The variation of the organic phase volume fraction with the height at the end of the settler ($x = 9$ m) has been illustrated in **Fig. 8.** From this figure, it can be observed that the existence of one picket fence row causes a reduction in the dispersion band at the end of the settler.

We have tested the presence of picket fences at two other locations of 3.55 m and 7.95 m from the inlet. **Fig. 6b and c** show the velocity vectors of the organic phase along the settler on the plane $z = 4.5$ m for these locations respectively. As can be seen in these figures, by moving the picket fences toward the end of the settler, the dispersion band continues to the end of the settler.

The organic phase volume fraction versus the height at the end of the settler for different locations of picket fence rows and also without picket fence is shown in **Fig. 8.** According to this figure when the picket fence is located in $x_1 = 1.75$ m, there is a sharper slope in the graph. This means that the dispersion band becomes thinner. This figure also shows that the graph without picket fence coincides with the graph of one picket fence in $x_1 = 7.95$ m. This confirms that the dispersion band does not change when picket fence is located in $x_1 = 7.95$ m. It can be concluded that when the picket fences are set close to the inlet of the settler, the phase separation becomes more effective and the performance of the settler is better.

The main function of picket fences is propagation of velocity vectors. This propagating increases the possibility for more droplets.

<table>
<thead>
<tr>
<th>Distance of picket fence row from inlet (m)</th>
<th>Pressure drop over the picket fences (Pa)</th>
<th>Pressure drop over the picket fences (mm)</th>
<th>Organic volume fraction at upper outlet (%)</th>
<th>Aqueous entrainment (ppm) at upper outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.75</td>
<td>57.21</td>
<td>6.29</td>
<td>99.93</td>
<td>700</td>
</tr>
<tr>
<td>3.55</td>
<td>49.03</td>
<td>5.39</td>
<td>99.83</td>
<td>1300</td>
</tr>
<tr>
<td>7.95</td>
<td>24.14</td>
<td>2.56</td>
<td>99.74</td>
<td>1400</td>
</tr>
</tbody>
</table>

**Fig. 9.** The effect of two picket fence rows on the velocity vectors of the organic phase a) $D = 1.3$ m, b) $D = 0.6$ m ($z = 4.5$ m, $x_1 = 1.75$ m).

**Fig. 10.** Comparison of the organic phase volume fraction versus the height at end of the settler ($x = 9$ m) for different numbers of picket fences.
collision and causes coalescence among droplets with a growth in size and an increase in buoyancy force which in turn makes the settling process faster. The coalescence process consists of droplet–droplet and droplet–interface mechanisms. The dominant mechanism at the inlet of the settler is the droplet–droplet mechanism whereas; the dominant mechanism at the end of the settler is the droplet–interface mechanism. Therefore, the installation of picket fences at the inlet of the settler is essential.

The pressure drop values over the picket fences, the organic phase volume fraction and the aqueous phase entrainment at the upper outlet for different distances of the picket fence from the inlet of the settler are given in Table 4. This table shows that by moving the picket fences from the inlet to the end of the settler, the pressure drop over the picket fences decreases. This is due to the reduction of velocity in the dispersion band. Moreover, this table indicates that when one row of the picket fence is set in distance of 1.75 m from the inlet of the settler, the volume fraction of the organic phase reaches to 99.93%, which shows the aqueous entrainment at the upper outlet is 700 ppm. While this entrainment for other distances, is more than 700 ppm.

6.2.2. Effect of two picket fence rows

After evaluating the effect of one picket fence and its proper location on the performance of the settler, the effect of two picket fence rows was evaluated. The velocity vectors of the organic phase for two picket fence rows in the settler are shown in Fig. 9a. It is observed from this figure that the velocity vectors are fully propagated after the second row of the picket fences. Fig. 10 compares the effect of different numbers of picket fences on the dispersion band at the end of the settler (x = 9 m). As one can see from this figure, the curve of organic phase volume fraction versus the height of the settler for two picket fences has a sharper slope than that of one picket fence row. This means the thickness of the dispersion band is reduced more for two picket fences at the end of the settler.

The pressure drop values, the organic phase volume fraction and the aqueous phase entrainment at the upper outlet of the settler for two rows of picket fences are given in Table 5. This table shows that when two rows of picket fences are set the volume fraction of the organic phase at the upper outlet reaches to 99.95%, which corresponds to the aqueous entrainment of 500 ppm. These results indicate that utilizing two picket fence rows have a better performance than one.

The increasing the distance between installation locations of two picket fence rows causes the second picket fence row set far from the entrance and separation efficiency decreases. Therefore, the mentioned distance was not increased, but the effect of reduction of the distance was investigated. For this evaluation, the distance between the picket fences was assigned equal to 0.6 m. The velocity vectors of the organic phase for this case (D = 0.6 m) are shown in Fig. 9b. In this figure, the existence of an intensive circulation flow between the picket fences is observed. This circulation flow causes disturbance in the separation process, because this flow increases the breaking up of the bigger droplets and destroys the separated layers after the first row of picket fences. This fact is shown in Fig. 11 quantitatively. As one can see in this figure the slope of the curve for the case with distance between picket fences of 1.3 m is sharper than in the case with D = 0.6 m. As the slope becomes sharper the phase separation is better.

6.2.3. Droplet size distribution around picket fences

The distribution of droplet size in the settler was evaluated at different points in order to verify the main function of picket fences, which is to develop bigger droplets. The locations of the selected five points were as shown in Fig. 12, distributed at the inlet, in between the picket fence rows and after the last picket fence row. The size distribution of droplets at the points (1) and (2) are shown in Fig. 13a. This figure shows that percentage of size group 2 increases and those of size groups 3, 4 and 5 decreases, while other bigger size groups increase in the point (2) than point (1). These results prove that both droplets break-up and coalescence are the controlling process at the inlet of the settler.

The distribution of droplet size after the first picket fence at the point (3) is shown in Fig. 13b. From this figure, it can be observed clearly that when the picket fences are set into the settler, the growth of the droplet sizes increases. This figure also shows that when there are two picket fence rows in the settler, the size of droplets is bigger. Whereas point (3) is located before the second picket fence row, it can be concluded that the picket fences will be effective even in the region before where they are located. The distribution of droplet size at the point (4) is shown in Fig. 13c. This figure also shows, the picket fences cause an increase in droplet size. The droplet size at this point is bigger because this point is located close to the bottom of the settler and there is no droplet smaller than 600 μm at this location. The distribution of droplet size at the point (5) is shown in Fig. 13d. From this figure, it can be observed that in the case without the picket fence, the size group 3 has the highest percentage. This means that at this height the dominant droplet size is 250 μm (see Table 3).

**Table 5**

<table>
<thead>
<tr>
<th>Pressure drop over the first picket fence row (x1 = 1.75 m)</th>
<th>Pressure drop over the second picket fence row (D = 1.1 m)</th>
<th>Organic phase volume fraction at upper outlet (%)</th>
<th>Aqueous phase entrainment (ppm) at upper outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pa mm</td>
<td>Pa mm</td>
<td>99.95</td>
<td>500</td>
</tr>
<tr>
<td>55.42</td>
<td>5.55</td>
<td>45.53</td>
<td>5.01</td>
</tr>
</tbody>
</table>

![Fig. 11. Comparison of the organic phase volume fraction versus the height at the end of the settler (x = 9 m) for different distances between picket fences.](image-url)
6.2.4. Effect of picket design — closed to opened area

One of the important parameters in design of the picket fences is the ratio of the closed to opened (C/O) area. In all previous simulations, this ratio was assigned equal to 2. Since a reduction in C/O ratio leads to a reduction in velocity vector propagation and efficiency of the picket fence, so the increasing of this ratio has been evaluated. The velocity vectors of the organic phase for C/O = 4 are shown in Fig. 14. This figure shows an intensive circulation flow behind the picket fences in the settler, which continues to the end of the settler. This fact is shown in Fig. 15 quantitatively. As one can see in this figure when C/O = 4 an increase in the thickness of the dispersion band at the end of the settler is observed. Therefore, increasing C/O ratio has a bad effect on the performance of the settler.

7. Conclusions

In this study, for the first time in our knowledge, a three dimensional computational fluid dynamics accompanied by experimental field measurements have been applied to predict the performance of an industrial mixer–settler in the Sarcheshmeh copper complex, Iran. The simulation results were validated by the experimental data. The simulation of the settler without the picket fence showed that the dispersion band continued to the end of the settler. By installing one picket fence row near the inlet of the settler, velocity vectors were propagated resulting in an increase in droplet size and a reduction in the dispersion band thickness. The dispersion band almost vanished when two rows of picket fences were set into the settler. When the distance between picket fences decreased, intensive circulation flow between picket fences was formed; this caused a reduction in the phase separation. Increasing the ratio of the closed to opened (C/O) area in the picket fences caused a circulation flow behind the picket fences and this circulation flow continued to the end of the settler. With the aid of CFD simulation, the precise location and arrangements of the picket fences, as well as the geometry of the picket fences can be optimized. This means that the industrial settler can be designed easier, cheaper and with a shorter lead-time.

Acknowledgments

The authors would like to acknowledge Sarcheshmeh copper complex for their financial support.
Fig. 15. Comparison of the organic phase volume fraction versus the height at end of the settler (x = 9 m) for different C/O ratios.

References


