# Modeling Phase Separation of Toluene-water in a Horizontal settler

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**Abstract:** The mixer-settler principle is commonly used for industrial extraction processes. This is done by mixing the two immiscible liquids to perform mass transfer and subsequently separating them in gravity settler. However, when drop size becomes small, separation in a settler becomes difficult and entrainment of valuable chemical occurs. Moreover, entrained impurities dilute the product. Consequently, the settler should be designed and optimized in such a way that entrainment is minimized. Computational fluid dynamics is a useful tool to study the separation behavior in a settler and can be used to optimize the design and operation of settler. The fluid flow pattern inside the settler and its consequence for entrainment can be evaluated. The mixture-model and the two-phase level set model in COMSOL multiphyiscs are used for simulation of phase separation of toluene and water. The results describe fluid recirculation and sedimentation of drops in a settler. However, the entrainment values obtained are rather low (< 4 ppm) compared to experimental values in the range of 100 ppm.

**Key words:** Mixer-settler, entrainment, mixture-model and two phase level set model.

## 1. Introduction

In industrial liquid-liquid extraction processes, phase separation is a vital process step that limits the throughput of the process. Phase separation among others depends on the physical properties of the system under consideration and the drop size created during mixing. To increase the mass transfer area during extraction, small size drops are preferred. However, separation of these small drops becomes prohibitive with a consequence of entrainment.

To study the separation behavior in a settler under different flow conditions and for various drop sizes as well as when the settler geometry is modified, computational fluid dynamics can be useful in evaluating the separation performance and prediction of entrainment. The availability of a reliable predictive model that captures the fluid mechanics in the settler means entrainment data from experiment can be validated and also extended to study separation behavior when external fields such as electric field is applied.

Two approaches in COMSOL Multiphysics are used in simulating the phase separation behavior of toluene –water in a horizontal settler; the mixture model and the two-phase level set model. Each of the models is explained below.

### 1.1 Mixture model

In mixture model, the dynamics of the immiscible liquid system is modeled by a momentum transport equation for the mixture, a continuity equation and a transport equation for the dispersed phase volume fraction [1].

$$\rho\frac{\partial u}{\partial t}+\rho(u.\nabla)u=-\nabla p-\nabla.\left(\frac{\rho\phi_d\rho_d}{\rho(1-\frac{\phi_d\rho_d}{\rho})}\right)u_{slip}u_{slip}+\nabla.(\eta[\nabla u+\nabla u^T])+\rho g+F \tag{1}$$

Equation (1) represents the momentum transport equation for the mixture. The first term on the left side represents a momentum accumulation term while the second term represents momentum transport by convection. The terms on the right hand side represent external forces acting on the system; pressure forces ($-\nabla p$), drag forces ($\nabla.\left(\frac{\rho\phi_d\rho_d}{\rho(1-\frac{\phi_d\rho_d}{\rho})}\right)u_{slip}u_{slip}$), viscous forces ($\nabla.(\eta[\nabla u+\nabla u^T])$, gravity forces ($\rho g$) and any other external force such as electric field ($F$).

The continuity equation for the mixture can be written as:

$$(\rho_c - \rho_d)[\nabla.(\phi_d(1-\frac{\phi_d \rho_d}{\rho})u_{slip}) + \frac{m_{dc}}{\rho_{dc}}] + \rho_c(\nabla.u) = 0 \quad (2)$$

And, the continuity equation for the dispersed phase can be written as:

$$\frac{\partial \phi_d}{\partial t} + \nabla.[\phi_d u + \phi_d(1-\frac{\phi_d \rho_d}{\rho})u_{slip}] = \frac{-m_{dc}}{\rho_{dc}} \quad (3)$$

The slip velocity $u_{slip}$ is calculated by Hadamard-Rybczynski correlation for drag coefficient.

$$(3c_d \rho_c / 4d_d) / u_{slip} / u_{slip} = -(\rho - \rho_d) / (\rho \nabla p) \quad (4)$$

$$c_d = (24 / \mathrm{Re}_p) / (1 + (\eta_c / 3\eta_d)) / (1 + \eta_c / \eta_d) \quad (5)$$

$$\mathrm{Re}_p = \rho_c d_d / u_{slip} / / \eta \quad (6)$$

### 1.2 Level-set method

In level-set method, the interface of separation of two immiscible liquid systems is tracked by the Cahn-Hilliard equation [2]:

$$\frac{\partial \varphi}{\partial t} = \frac{\nabla.\gamma\lambda\nabla\psi}{\varepsilon^2} \quad (7)$$

where $\gamma$ is the interface mobility, the quantity $\lambda$ is the mixing energy and $\varepsilon$ is the capillary width that scales with the thickness of the interface. The latter two quantities are related to surface tension coefficient

$$\sigma = \frac{2\sqrt{2}}{3}\frac{\lambda}{\varepsilon} \quad (8)$$

The level-set equation is then coupled with Navier-stoke equation for the momentum balance.

## 2. Methods and procedure

The previously mentioned methods are used to model phase separation of toluene and water. The flow regime is laminar. In table 1, the data needed for the simulation is given. Initially the upper section of the settler is filled with toluene and the remaining part is filled with water. Due to transient behavior, the input variables are initialized by a step function. The differential equations used with each method are solved by putting appropriate boundary conditions. At the entrance section, inlet values of variables (inlet velocity, volume fraction) are specified as boundary condition. At the exit of settler, the pressure boundary condition is specified for the mixture. At the other sections of the settler, the no-slip boundary condition is specified for the momentum equation while insulation/symmetry is specified for the dispersed phase volume fraction.

Table 1: Values of different variables used in a simulation

| Variable name | Value |
|---|---|
| Inlet velocity [m/s] | 0.02 |
| Volume fraction of dispersed water phase in the inlet stream in volume [v/v] | 0.1 |
| Drop diameter [ $\mu m$ ] | 100 |
| Length of settler [cm] | 15 |
| Height of settler [cm] | 10 |

## 3. Results and discussion

In figure 1, we show the results obtained for the level-set method. The top figure represents the separation behavior obtained without any modification of the settler while in the second case a baffle is included at the exit. It can be seen that there is recirculation across the settler length when no baffles are used. In the later case the included baffle was able to break the recirculation at the distance it was inserted in the settler. This helps to reduce the entrainment. This can be seen from the concentration of the aqueous and toluene phases at the exit of the settler (1.554e-6 v/v % with out baffle compared to 3.476e-8 v/v % with baffle).

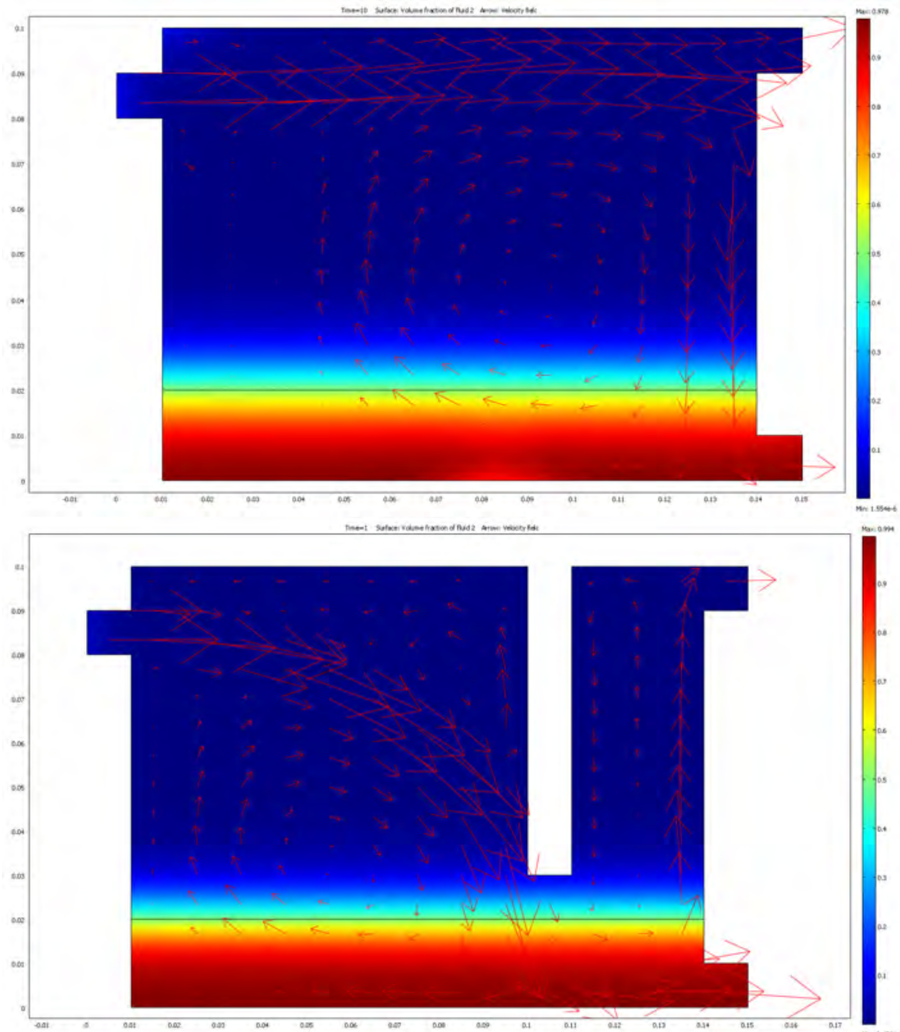

Figure 1: Comsol level-set model for settler without baffle (top) with baffle (bottom).

In Figure 2 the results of modeling with the mixture model in COMSOL are depicted. The following important differences from the mixture method can be observed. First, the calculated exit volume fractions of the dispersed phase have values greater than 1 and less than 0. These are not possible values in reality. Secondly, the calculated velocity profiles do not show much recirculation behavior as in case of level-set. The droplets simply follow horizontal and vertical motion in the direction of the flow. In addition, at the upper exit of the settler, the flow turns back.

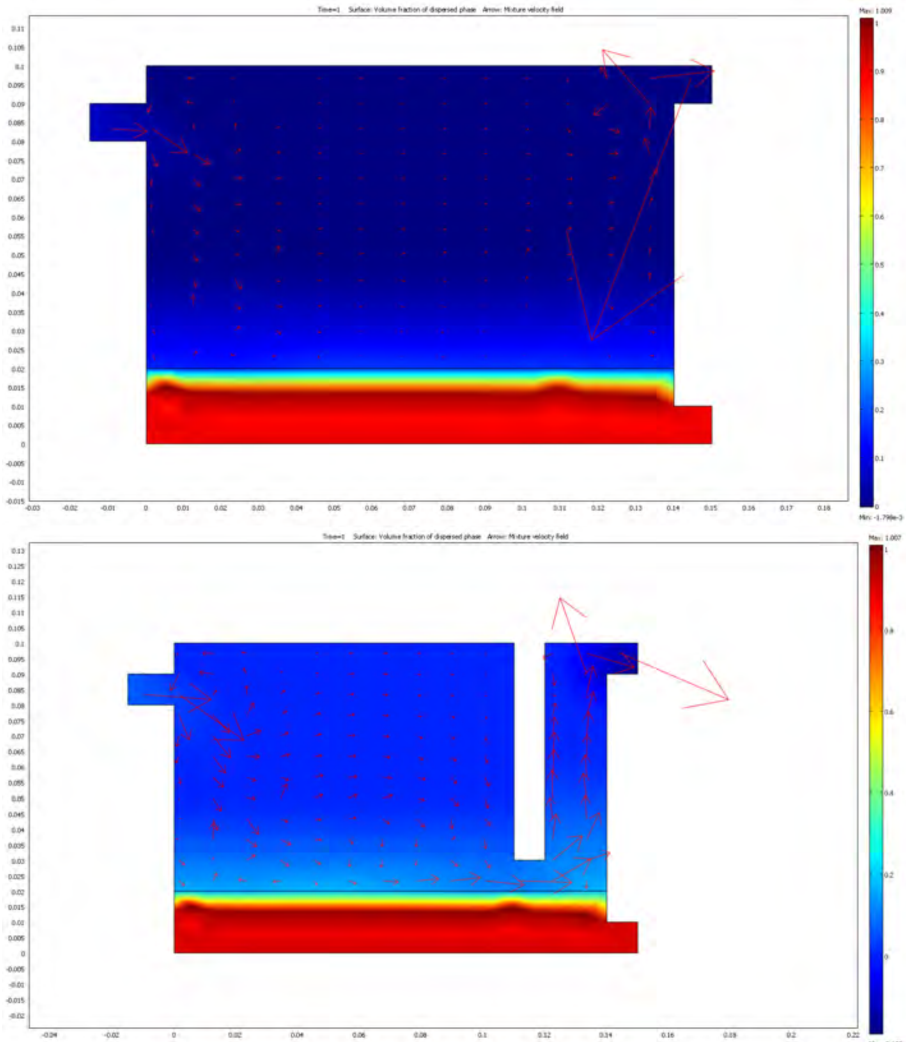

Figure 2: Comsol mixture model for settler without baffel (top) and with baffle (bottom).

## 4. Conclusion and Future Work

In this paper, we have demonstrated CFD modeling of a settler using COMSOL multiphysics. We considered two different methods; the level-set and mixture model methods. It was shown that modification of settler design such as by including baffle at the exit alters the fluid flow pattern in the settler which decreases the entrainment level. Hence, the level set method could further be extended to optimize the settler design.

## 5. Reference


1. Contaminant-Removal from waste water in a secondary clarifier, *COMSOL manual*, 211- 221
2. Phase separation, *COMSOL manual*, 178- 184