



## Computational Fluid Dynamics Analysis of Gas Absorption Process in a Randomly Packed Column for Toluene Absorption from Air

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Packed towers are used extensively in the chemical industries for mass transfer operations such as gas absorption, desorption, extraction and distillation. In gas absorption process a soluble component is absorbed by contact with a liquid phase in which the component is soluble. This system is used for scrubbing gas streams of toxic components such as sulphur dioxide and carbon dioxide or volatile organic compounds such as toluene. This research studies the toluene absorption with a viscous absorbent, di(2-ethylhexyl)adipate. Hydrodynamics and mass transfer parameters of a packed column such as pressure drop and mass transfer coefficients have been investigated using computational fluid dynamics analysis. The computational fluid dynamics predictions are compared to the experimental data reported by Heymes *et al.* For validation of the computational fluid dynamics predictions, some theoretical models such as Billet model have also been used. The experimental results showed that the liquid phase mass transfer coefficients of the system depend on the gas and liquid phase velocities. This behaviour has also been observed in the computational fluid dynamics analysis. It is clear that the influence of viscosity on the phenomena is considerable, *e.g.*, under the same conditions the pressure drop of air/water system is about 30 % lower than toluene/di(2-ethylhexyl)adipate system. Comparison between the computational fluid dynamics results, experimental data and theoretical models showed a good agreement and confirms the ability of the computational fluid dynamics for design and optimization of the absorber packed columns.

**Key Words:** Absorption, Volatile organic compounds, Packed bed, Viscous absorbent, Computational fluid dynamics.

### INTRODUCTION

Up to now, absorption is still a powerful tool for the gas separation and purification. This process is used extensively to remove toxic or noxious components (pollutants) or atmospheric volatile organic compounds (VOCs) from effluent gas streams<sup>1</sup>. Volatile organic compounds are organic chemical compounds that have high enough vapour pressures under normal conditions to significantly vapourize and enter the atmosphere<sup>2,3</sup>. Many VOCs are human-made chemicals that are used and produced in the manufacture of paints, pharmaceuticals and refrigerants. Some common examples include acetone, benzene, xylene and toluene.

Volatile organic compounds are common ground-water contaminants. Various processes are available for VOCs reduction, such as absorption, photocatalytic oxidation, biological treatment, adsorption and condensation. In this paper the absorption process with high viscous absorbent *i.e.*, di(2-ethylhexyl)adipate (DEHA) has been investigated. The problems of VOC absorption by viscous fluids have not been much studied in the literature. There are a few published articles related to investigation of toluene absorption in a packed column.

Jovi<sup>4</sup> reported experimental investigation of photocatalytic oxidation of toluene. In this study heterogeneous photocatalysis for the toluene degradation in the gas phase on commercial TiO<sub>2</sub> catalyst was investigated. The influence of the gas flow rate and the toluene inlet concentration was studied in this work.

Experimental studies of adsorption process for toluene removal are reported by Mohan *et al.*<sup>5</sup> An activated carbon packed bed for toluene removal has been used in this work and effect of process conditions on toluene removal and break point time of the granular activated carbon are investigated.

Nikakhtari and Hill proposed a biological process for VOCs removal. The gas hold-up and mass transfer rate have been studied in their work<sup>6</sup>.

The absorption process for toluene removal using a viscous absorbent has been proposed by Heymes *et al.*<sup>7,8</sup>. Some important hydrodynamics and mass transfer parameters such as dry pressure drop, wet pressure drop, liquid hold-up, mass transfer coefficients and mass transfer rate are investigated in their work. Hydrodynamics and mass transfer experiments were performed in a randomly packed column.

The results of the Heymes *et al.*<sup>7,8</sup> work have been used in the current paper for validation of the CFD predictions.

The aim of this paper is the CFD analysis of the gas absorption process in a packed column. A multicomponent multiphase model has been used for simulation of hydrodynamics and mass transfer operation. Computational fluid dynamics is concerned with obtaining numerical solutions using the computer. Of the solution methods used in the CFD codes, the finite volume method is the most common. It is the method used in the commercial codes CFX-10 and CFX-11, the package used for the CFD analysis of this work<sup>9</sup>. Versteeg and Malalasekara (1995) give a good introduction to the finite volume method<sup>10</sup>.

## EXPERIMENTAL

As mentioned earlier, experimental studies of toluene absorption with a high viscous solvent in a packed bed is reported by Heymes *et al.*<sup>7,8</sup>. The experimental set-up is shown in Fig. 1.

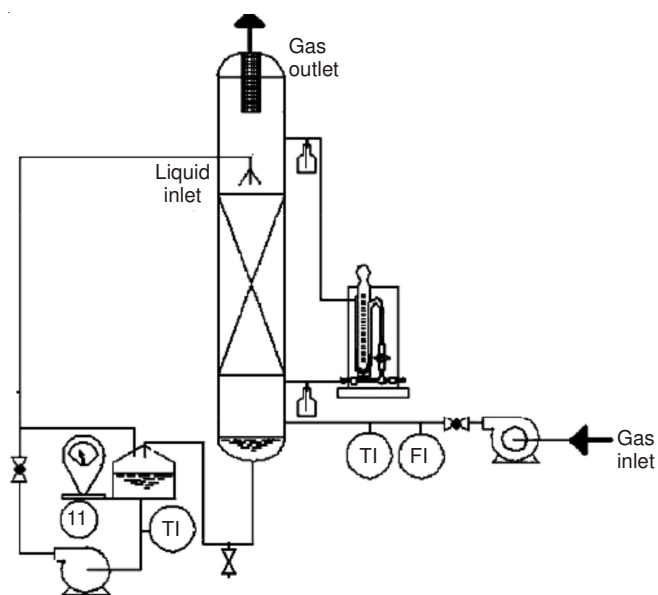


Fig. 1. Experimental set-up (Heymes *et al.*<sup>7</sup>)

The column has an internal diameter of 0.1 m and a height of 2.5 m. The hiflow rings are inserted in the column. The height of the packing, equal to 1 m and the void fraction, equal to 0.92, were used in this study. The particle diameter was 17 mm and the specific surface area was 275 m<sup>-1</sup> the liquid flow rate through the column was measured using a water-meter type volumetric counter and the gas velocity was measured using a hot-wire anemometer. The dry and wet pressure drops were read on the U tube. In the pressure drop experiments, the range of gas and liquid flow rates were 0-3.5 and 2.9-9.8 kg m<sup>-2</sup> s<sup>-1</sup>, respectively. In the mass transfer experiments, the range of toluene concentration in the gas phase (air) was 500, 1000 and 5000 mg m<sup>-3</sup>. The toluene concentration in the DEHA at top and bottom of the column was determined by means of a UV spectrometer. Finally the mass transfer coefficients in gas and liquid phases and the mass transfer rate can be calculated<sup>7</sup>.

**Mathematical models:** Optimum operation of a packed bed gas absorption system requires a thorough understanding

of hydrodynamics and mass transfer parameters. There are a lot of semi theoretical or complete theoretical relationships that describe the hydrodynamics or mass transfer parameters. For validation of the simulation result, these models can be compared to prediction results; also some of the models (mass transfer coefficients models) must be fed to CFD programs to enable the software to perform local calculations of the transport equations.

The interest of this work is limited to the hydrodynamic behaviour and mass transfer in a randomly packed column. Hence an isothermal multiphase flow system is assumed. Thus only the continuity, momentum and mass transfer equations are considered. A multiphase flow system contains a mixture of phases which are assumed to be mixed at scales much larger than the molecular scale. The computational fluid dynamics model considers the multiphase flow in the Eulerian/Eulerian framework. The Eulerian/Eulerian multi-fluid model is a popular multiphase model that each phase possesses its own flow field<sup>11,12</sup>.

The governing equations for the flow of a multiphase fluid are<sup>9</sup>:

Continuity equation:

$$\frac{\partial}{\partial t}(\phi_{\alpha}\rho_{\alpha}) + \nabla \cdot (\phi_{\alpha}\rho_{\alpha}U_{\alpha} - \Gamma_{\alpha}\nabla\phi_{\alpha}) = 0 \quad (1)$$

$\alpha = L, G.$

Momentum equation:

$$\frac{\partial}{\partial t}(\phi_{\alpha}\rho_{\alpha}) + \{\phi_{\alpha}U_{\alpha}U_{\alpha} - \mu_{e\alpha}(\nabla U_{\alpha} + (\nabla U_{\alpha})^T)\} = \phi_{\alpha}(B_{\alpha} - \nabla P) + F_{\alpha} \quad (2)$$

$\alpha = L, G.$

Mass transfer equation:

$$\frac{\partial}{\partial t}(\phi_{\alpha}\rho_{\alpha}Y_{i\alpha}) + \nabla \cdot (\phi_{\alpha}(\rho_{\alpha}U_{\alpha}Y_{i\alpha} - \Gamma_{\alpha}\nabla Y_{i\alpha})) = \sum_{\beta=1, \beta \neq \alpha}^N m_{\alpha\beta}^i \quad (3)$$

$\alpha = 1, \dots, N, \beta = 1, \dots, N_C.$

In order to solve eqns. 1-3 for velocity, pressure, volume fraction and mass fraction, we need additional equations to specify the interphase interaction terms such as interphase drag force, turbulent viscosities and mass balance.

Several correlations are available for the interphase drag force model in the CFX, such as Ishii Zuber, Schiller Naumann and Grace model<sup>9</sup>. In this paper, the drag coefficient has been estimated using the drag correlation of Ishii Zuber.

$$C_D = \frac{24}{Re}(1 + 0.15Re^{0.687}) \quad (4)$$

This model is suitable when continuous-dispersed fluid pair are available in the system.

Also the  $k-\epsilon$  model as a turbulence model has been used. For the most engineering problems, the  $k-\epsilon$  model has been used with significant success. This model uses an eddy viscosity hypothesis for the turbulence. In this model, the effective viscosity is defined as:

$$\mu_{\alpha,eff.} = \mu_{\alpha} + \mu_{T\alpha} \quad (5)$$

where  $\mu_\alpha$  = molecular viscosity and  $\mu_{T\alpha}$  = turbulent viscosity and can be calculated as:

$$\mu_{T\alpha} = C_\mu \rho_\alpha \frac{k_\alpha^2}{\varepsilon_\alpha} \quad (6)$$

where  $C_\mu$  = empirical constant,  $k$  = turbulence kinetic energy and  $\varepsilon$  is the turbulence dissipation rate.

The mass balance through the packed bed is verified by the relations as follow<sup>7</sup>:

$$Q_G(C_{G,in} - C_{G,out}) = Q_L(C_{L,out} - C_{L,in}) \quad (7)$$

$$\begin{aligned} & Q_L(C_{L,out} - C_{L,in}) \\ &= K_L a V_C \frac{(C_{G,in}/H - C_{L,out}) - (C_{G,out}/H - C_{L,in})}{\ln\left(\frac{C_{G,in}/H - C_{L,out}}{C_{G,out}/H - C_{L,in}}\right)} \quad (8) \end{aligned}$$

$$\begin{aligned} & Q_G(C_{G,in} - C_{G,out}) \\ &= K_G a V_C \frac{(C_{G,in} - HC_{L,out}) - (C_{G,out} - HC_{L,in})}{\ln\left(\frac{C_{G,in} - HC_{L,out}}{C_{G,out} - HC_{L,in}}\right)} \quad (9) \end{aligned}$$

Gas and liquid phase mass transfer coefficients,  $K_{Ga}$  and  $K_{La}$ , can be calculated by using the proposed theoretical models. Various hydrodynamics and mass transfer models in the packed columns presented such as Billet and Schultes model<sup>13-18</sup>, Olujić model<sup>19</sup> and Maskowiak model<sup>20,21</sup>. These models have been used for prediction of dry pressure drop, wet pressure drop, liquid hold-up, flooding point, loading zone, wetted surface area and mass transfer coefficients. The details of these models are presented by Heymes *et al.*<sup>7</sup>.

In present studies, the billet and Onda model have been used for mass transfer simulation. These models commonly used for predicting the surface area and the mass transfer coefficients for both gas and liquid phase. Billet proposes the flowing relations for mass transfer coefficients and wetted surface area:

$$K_{La} = C_L^* \left(\frac{\rho_G g}{\mu_G}\right)^{1/6} \left(\frac{D_L}{d_h}\right)^{1/2} \alpha^{2/3} U_L^{2/3} \left(\frac{a_{wet}}{a}\right) \quad (10)$$

$$\begin{aligned} K_{Ga} = C_G^* \frac{1}{(\varepsilon - h_T)^{1/2}} \left(\frac{a^{3/2}}{d_h^{1/2}}\right) D_G \left(\frac{U_G \rho_G}{a \mu_G}\right)^{3/4} \\ \times \left(\frac{\mu_G}{\rho_G D_G}\right)^{1/3} \left(\frac{a_{wet}}{a}\right) \quad (11) \end{aligned}$$

$$\left(\frac{a_{wet}}{a}\right) = 1.5(ad_p)^{-0.5} (Re_L)^{-0.2} (We_L)^{0.75} (Fr_L)^{-0.45} \quad (12)$$

$C_L^*$  and  $C_G^*$  are the constant of the billet equations and are 1.577 and 0.390, respectively for the hiflow rings<sup>13</sup>.

Onda proposed correlations for the wetted area and mass transfer coefficients as following relationships<sup>22</sup>:

$$\left(\frac{a_{wet}}{a}\right) = 1 - \exp\left(-1.45\left(\frac{\sigma_c}{\alpha_L}\right)^{0.75} Re_L^{0.1} Fr_L^{-0.05} We_L^{0.2}\right) \quad (13)$$

$$SH_L = 0.0051 Re_L^{4/3} Sc_L^{-1/2} (ad_p)^{0.4} \quad (14)$$

$$Sh_G = 5.23 Re_G^{0.7} Sc_G^{1/3} (ad_p)^{-2} \quad (15)$$

Relations (4)-(12) were fed to CFX software as the expressions, to enable the software to solve the mass transfer equation.

**Geometry and boundary conditions:** In the finite volume method, the computational domain is divided into small sub-regions known as control volumes. In this paper, mesh preparation for the domain was made in gambit 2.2.30.

The 3-D computational domain for CFD simulation of packed column is shown in Fig. 2. The porosity of the medium is 0.92. This model is very similar to real geometry of the packed column and the dimensions are equal.

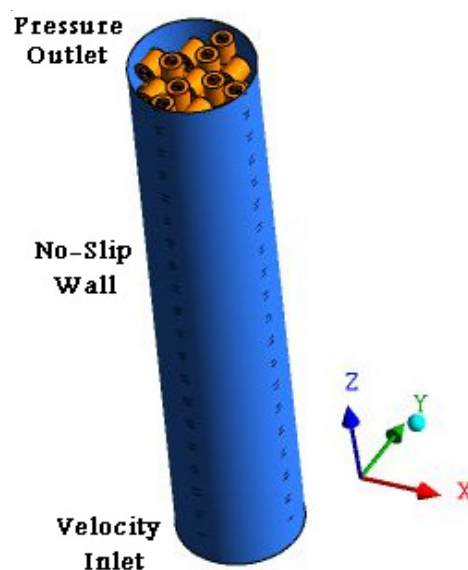


Fig. 2. Computational domain

The computational fluid dynamics simulation results after grid independence testing are considered robust computations. Grid independence is a process of gradually applying and refining grid rendering to a geometrical domain starting with coarse meshing until certain key results of interest do not change. The sensitivity of the simulation results were checked by comparing the results for 5, 4, 3 and 2 mm element sizes. The simulation results for toluene concentration at the top of the column were similar for the 3 and 2 mm cell size, so tetrahedral elements with 3 mm grid size were used.

For computational fluid dynamics simulation, the gas and liquid phases were taken to be toluene + air and di(2-ethylhexyl)adipate, respectively. The gas phase is continuous and the liquid is dispersed phase.

In this case, at the bottom of the column, a "velocity inlet" boundary condition was used. At this boundary condition the appropriate value for the velocity component, toluene mass fraction, volume fraction and turbulent quantities must be specified for gas and liquid phases. At the top of the column, the "pressure outlet" boundary was specified. At this boundary, the outlet static pressure was specified. No-slip boundary conditions were applied to the walls. Laminar flow and k-ε model were used for liquid and gas phases, respectively.

## RESULTS AND DISCUSSION

Computational fluid dynamics analysis has been carried out to obtain the dry pressure drop, wet pressure drop and mass transfer parameters. The results obtained are outlined below.

**Hydrodynamics parameters:** In the design of the packed columns, a key factor is the pressure drop of the liquid and/or vapour streams through the selected packing material. During the operation of the packed column, the pressure drop through the packing material may increase due to plugging of the packing, poor liquid or gaseous distribution, breaking of the packing material, use of incorrect packing and incorrect packing procedures, *etc.*

The pressure losses per unit packed depth accompanying the flow of fluids through packed columns are caused by simultaneous kinetic and viscous energy losses.

For computational fluid dynamics simulation of dry and wet pressure drop, only the continuity and momentum equations are considered. For dry pressure calculation, single phase model and for wet pressure drop calculation, two-phase model has been used.

The pressure drop in the absence of liquid flow is called dry pressure drop. A sample of pressure contours in a plan at the center of the column is shown in Fig. 3. The map, from bottom to top, ranges from 101325-101410 (pa) for the gas phase pressure.

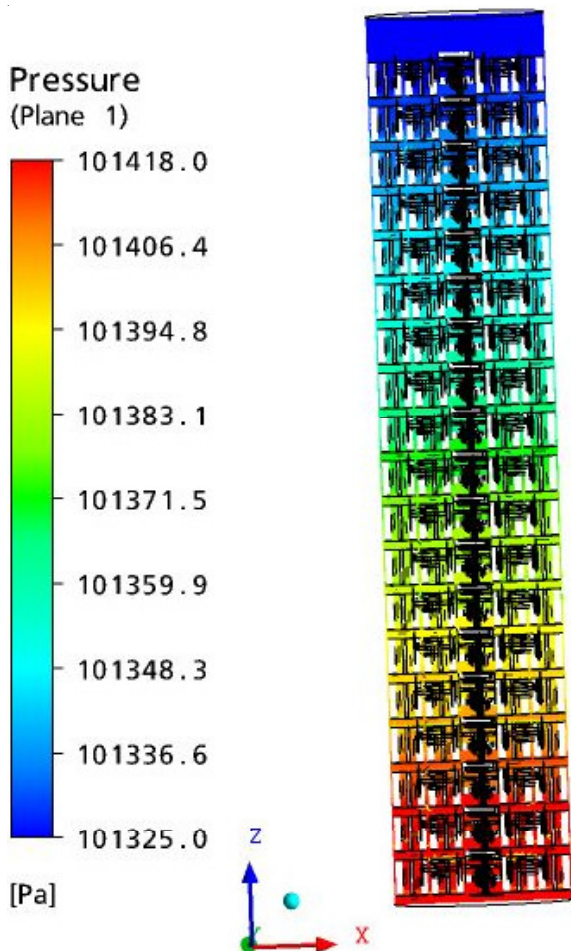


Fig. 3. Pressure contours at the center of the domain

Fig. 4 shows the variation of dry pressure drop against superficial gas velocity. The slope of the dry pressure drop line in the logarithmic scale was found to be 1.85, consistent with the values of 1.8-2.0 reported in the literature, indicating turbulent flow<sup>23,24</sup>. According to this figure, the frictional losses increase as the gas flow rate is increased.

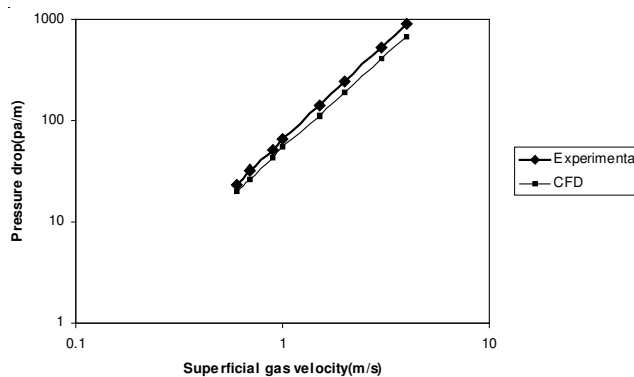


Fig. 4. Dry pressure drop versus superficial gas velocity

This figure also shows a comparison between experimental data and CFD simulation results. It can be seen that the CFD predictions show a good agreement with the experimental data. It is also clear that the pressure drops predicted from the CFD simulation are lower than the experimental data. This could be related to the gas maldistribution and channeling effects. In the CFD models we assume that the gas phase distribution in packed bed is uniform and gas maldistribution and channeling are neglected, therefore the predicted pressure drop is lower than the experimental pressure drop.

In this section, the average relative error between CFD predictions and experimental data is 14.3 %.

Since both the gas and the liquid are competing for the free cross sectional area left by packing, an increase in liquid flow rate will result in an increase in the frictional losses.

In this section, effect of liquid viscosity on wet pressure drop has been investigated. Cotte<sup>25</sup> studied the hydrodynamics of air/water and air/PEG400 systems in a packed column containing hiflow rings. Heymes *et al.*<sup>7,8</sup> also studied toluene/DEHA system. The authors have observed that the viscosity of the liquid considerably influences the pressure drop. Under the same conditions, at the pilot scale packed column, the pressure drop of the DEHA system is about 30 % higher than water system. Also the pressure drop in the PEG400 system is two times higher than water system.

In this section, the wet pressure drop in air/water and DEHA/toluene systems has been predicted by CFD analysis and compared to the experimental data reported by Heymes *et al.*<sup>7,8</sup>.

In Fig. 5, two phase pressure drop predicted by the CFD simulations is compared with the experimental data. The liquid flow rates are 2.96 and 9.87 kg/m<sup>2</sup>s. At the fixed gas velocity, the gas pressure drop increase with increased liquid rate, principally because of the reduced free cross section available for flow of gas resulting from the presence of the liquid.

It can be seen that the CFD predictions are lower than experimental data, especially at high superficial gas velocity. As mentioned earlier, this could be explained by some important

TABLE-1  
COMPARISON OF CFD PREDICTIONS WITH EXPERIMENTAL DATA

Author	System	$\mu_L$ (Pa s)	L (kg/m <sup>2</sup> s)	$U_G$ (m/s)	$\Delta P$ (pa/m) experimental	$\Delta P$ (pa/m) CFD	Relative error (%)
Cotte	Air/water	0.0010	4.2	1	77	65	15.6
Heysem	Toluene/DEHA	0.0144	4.2	1	107	90	15.8
Cotte	Air/PEG400	0.0820	3.9	1	150	125	16.6

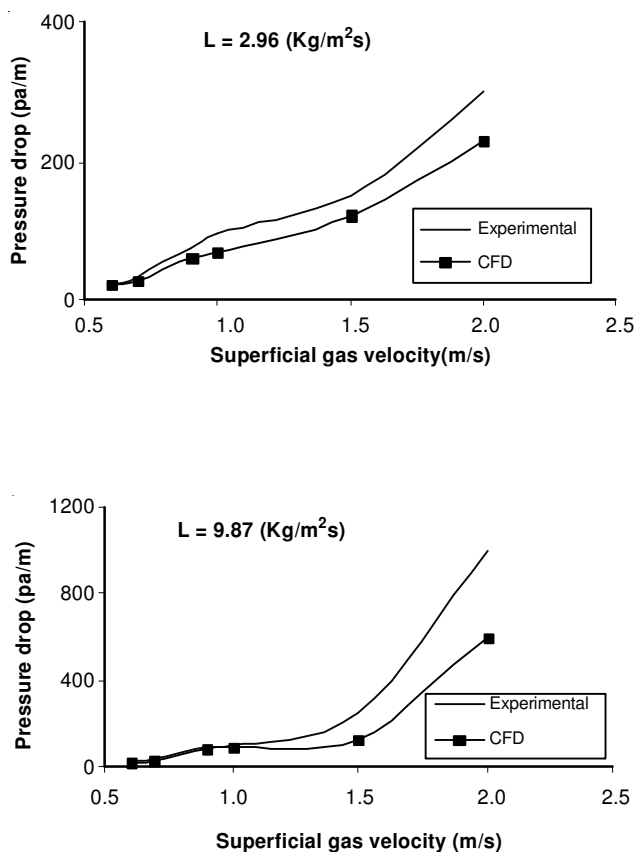


Fig. 5. Two phase pressure drop as a function of gas and liquid flow rates

phenomena such as fluid maldistribution and flow channeling, which were neglected in the CFD models. These parameters are very effective on pressure drop especially at high gas superficial velocity.

The average relative errors between the CFD predictions and the experimental data are 18.6 and 21 % for  $L = 2.96 \text{ kg/m}^2\text{s}$  and  $L = 9.87 \text{ kg/m}^2\text{s}$ , respectively.

Table-1 presents the predicted results of CFD simulation for wet pressure drop in comparison with air/water and air/PEG400 systems. Data can be compared together because there is no significant difference between the gas and liquid flow rates.

It is clear that the liquid viscosity is very effective on pressure drop. The pressure drop of the air/water system is about 38 % lower than toluene/DEHA system and 94 % lower than air/PEG400 system and the result could be predicted by CFD pretty good.

**Mass transfer parameters:** As it was mentioned earlier, this research studies the absorption process in a packed column; using a viscous absorbent (DEHA) to treat a toluene loaded vent gas. The aim is to study the mass transfer of toluene to

the di(2-ethylhexyl)adipate. For calculation of gas and liquid phase mass transfer coefficients ( $K_{La}$  and  $K_{Ga}$ ) the gas and liquid flow rates and toluene concentrations in the gas inlet should be measured<sup>26</sup>. Then the mass transfer coefficients can be calculated by eqns. 8 and 9. The experimental results<sup>7</sup> are shown in Table-2.

TABLE-2  
EXPERIMENTAL MASS TRANSFER COEFFICIENTS

Toluene conc. (mg/m <sup>3</sup> )	L (Kg/m <sup>2</sup> s)	G (Kg/m <sup>2</sup> s)	$K_{La}$ (s <sup>-1</sup> )	$K_{Ga}$ (s <sup>-1</sup> )
4990	13.16	0.51	$2.52 \times 10^{-4}$	2.75
1205	13.16	0.51	$2.51 \times 10^{-4}$	0.79
1193	9.87	0.51	$3.69 \times 10^{-4}$	1.89
5038	6.58	0.51	$3.23 \times 10^{-4}$	1.34
520	6.58	1.16	$2.28 \times 10^{-4}$	13.5
1005	6.58	1.21	$2.38 \times 10^{-4}$	13.8
1005	6.58	1.81	$2.43 \times 10^{-4}$	12.1

The mass transfer coefficients can be predicted by CFD simulations. Toluene concentration distribution in gas and liquid phase through the packed bed can be used for calculation of mass transfer coefficients. Fig. 6 shows a sample of the toluene mass fraction profile in the gas phase through the packed column obtained by CFD modeling. Decreasing of toluene concentration from bottom to top of the packed bed is clear from this figure.

Di(2-ethylhexyl)adipate is a high viscous absorbent and the Henry's constant is small, so the mass transfer resistance is mainly located in the liquid phase and the local liquid phase mass transfer coefficient is equal to overall liquid mass transfer coefficient<sup>7</sup>.

Figs. 7 and 8 show the comparisons between the predicted mass transfer coefficients from the CFD simulations and experimental data. From these figures, it can be clearly seen that the CFD simulation can predict the mass transfer coefficient pretty good over the range of gas flow rate. The average relative error for prediction of gas and liquid phase mass transfer coefficients are 12.7 and 22 %, respectively.

The differences are due to the simplifications made in the CFD models, e.g., neglecting the flow maldistribution and channeling and liquid back mixing in the CFD models. It is clear from Figs. 7 and 8 that the gas and liquid loads are effective parameters on the mass transfer coefficients.

In the Heymes *et al.* work, the  $K_{La}$  depend on the both gas and liquid phase velocities, but many authors believe that the liquid phase mass transfer depend just on the liquid velocity<sup>27,28</sup>. These unexpected results are due to the viscosity effects. In the low viscosity systems, the liquid phase mass transfer coefficient depends on liquid velocity and the mass transfer increase by increasing the liquid velocity. But in the high viscous fluids such as di(2-ethylhexyl)adipate, the viscosity effects on the phenomena are considerable.

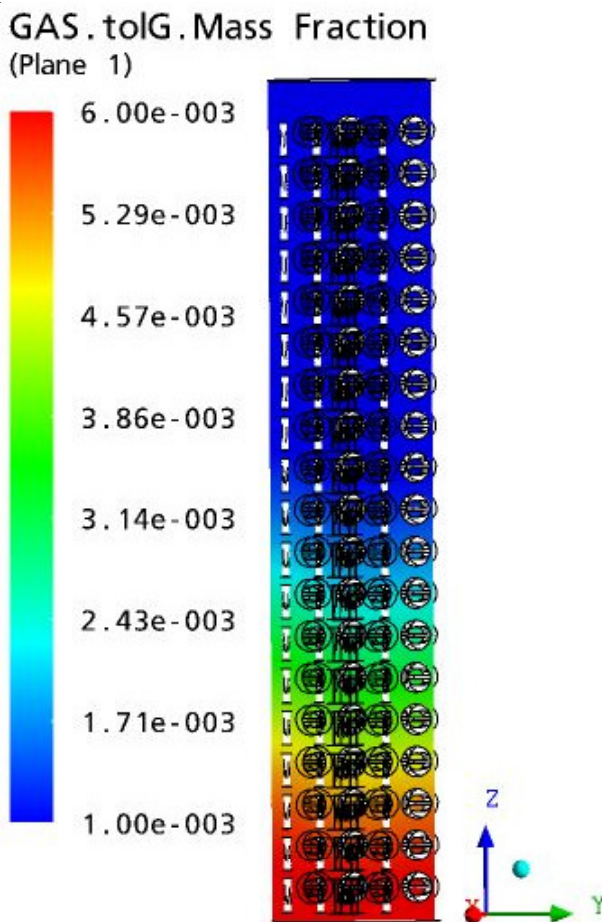


Fig. 6. Toluene mass fraction profile in the gas phase through the packed column

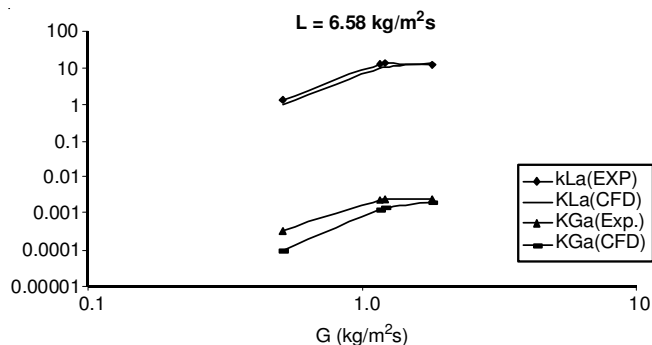


Fig. 7. Comparisons between the predicted mass transfer coefficients versus gas load from the CFD simulations and experimental data

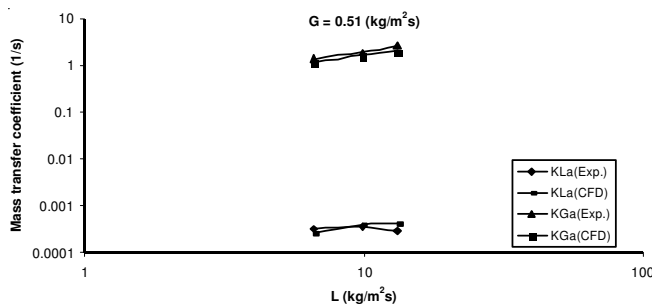


Fig. 8. Comparisons between the predicted mass transfer coefficients versus liquid load from the CFD simulations and experimental data

Fig. 9 compares the computational fluid dynamics results and Onda<sup>22</sup> and Billet *et al.*<sup>13-18</sup> predictions with the experimental data.

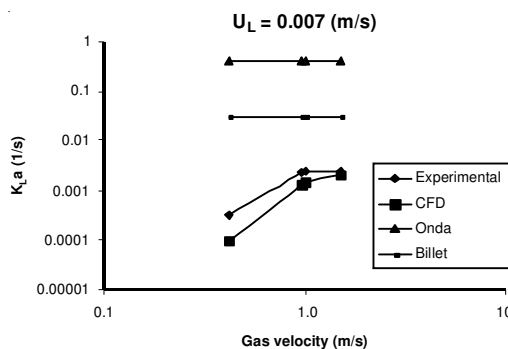


Fig. 9. Comparisons between the CFD simulation, experimental data, Onda correlation<sup>22</sup> and Billet model<sup>18</sup>

Onda's<sup>22</sup> correlation gives result very far from the experimental data, because this model is simple and old and established using the old kinds of the packings<sup>21</sup>. The Billet<sup>18</sup> model gives better results and is closer to the experimental data, because this model established using more recent and modern packing systems, but still the results are far from the experimental data. As mentioned by Heymes *et al.*<sup>13-18</sup>, the differences are due to the viscosity of the DEHA that does not fall within the range of values used by Billet<sup>13-18</sup> and Onda<sup>22</sup> to adjust their correlations. It is clear from Fig. 8 that the computational fluid dynamics predictions are closer to the reality.

**Conclusion**

Two-phase models for fluid dynamic and inter-phase gas-liquid mass transfer parameters were developed for randomly packed towers by means of computational fluid dynamics.

Governing equations such as volume averaged continuity, momentum and mass transfer equations were numerically solved using CFX version 11. The velocity distribution, pressure and mass concentration profile within an absorption packed column were predicted by CFD.

First of all, CFD modeling of the dry and wet pressure drop across the packed tower was studied. It has been shown through comparison with the experimental data that the CFD model can predict the pressure drop pretty well. The average relative error for prediction of dry pressure drop and irrigated pressure drop are 14.3 and 18.6 %, respectively. In the CFD models the gas phase distribution in packed bed was uniform and gas maldistribution and channeling were neglected, therefore the predicted pressure drops were lower than the experimental data.

For investigation and prediction of mass transfer constants ( $K_{La}$  and  $K_{Ga}$ ) in the absorption packed column a CFD model of the multiphase flow was applied. This research studied the toluene absorption with a viscous absorbent (DEHA). The mass transfer is supposed to be limited by the liquid-side resistance. When a low viscous absorber has been used, the  $K_{La}$  just depend on the liquid velocity, but in the current work the absorber is a viscous fluid and the viscosity is effective on mass transfer parameters. The experimental results and CFD predictions showed that the liquid side mass transfer coefficient depends on the both gas and liquid velocities.

The liquid viscosity is also very effective on pressure drop. For example, the pressure drop of the air/water system is about 38 % lower than toluene/DEHA system and 94 % lower than air/PEG400 system.

So the effect of viscosity on the mass transfer and pressure drop is considerable and that further research is necessary in order to better understand of this effects.

Based on the results of the simulation it can be shown that this approach can give reasonably good prediction of the gas and liquid phase mass transfer coefficients in the randomly packed column within 12.7 and 22 % errors.

In general the results are close to experimental values and small differences are due to the simplifications made in the CFD models, e.g., neglecting the flow channeling, flow maldistribution and liquid back mixing in the CFD models.

### Nomenclature

$a$	: Specific surface area of the packing per unit volume (1/m)
$a_e$	: Effective interfacial area of the packing per unit volume (1/m)
$a_{wet}$	: Wetted area of the packing per unit volume (1/m)
$B$	: Body force vector (N/m <sup>3</sup> )
$C$	: Concentration (mol/m <sup>3</sup> )
$C_D$	: Drag coefficient
$C_\mu$	: Empirical constant in eqn. 6
$C_L^*$ and $C_G^*$	: Empirical constant in eqns. 10 and 11
$D$	: Diffusivity (m <sup>2</sup> /s)
$d_h$	: Hydraulic diameter (m)
$G$	: gas flow rates (Kg/m <sup>2</sup> s)
$g$	: Acceleration due to the gravity (m/s <sup>2</sup> )
$h_L$	: Liquid hold up
$H$	: Henry's law constant
$K_{La}$	: Liquid phase mass transfer coefficient (1/s)
$K_{Ga}$	: Gas phase mass transfer coefficient (1/s)
$L$	: Liquid flow rate (Kg/m <sup>2</sup> s)
$\bullet A$	
$m_{LG}$	: Mass transfer rate (Kg/m <sup>3</sup> s)
$N$	: Number of the phases
$P$	: Pressure (Pa)
$Q$	: Flow rate (m <sup>3</sup> /s)
$t$	: Time (s)
$U$	: Interstitial velocity vector (m/s)
$V_c$	: Column volume (m <sup>3</sup> )
$Y_i$	: Mass fraction of component i

### Greek symbols

$\alpha, \beta$	: Phase index
$\gamma$	: Volume fraction
$\varepsilon$	: Porosity
$\mu$	: Viscosity (kg/m s)
$\rho$	: Density (kg/m <sup>3</sup> )
$\sigma$	: Surface tension (N/m)
$\Gamma$	: Dispersion coefficient (kg/m s)

### Dimensionless numbers

$Fr_L$	: Froude number for the liquid, $Fr_L = \frac{U_L^2 a_p}{S}$
$Re_L$	: Reynolds number for the liquid, $Re_L = \frac{\rho U_L}{a_p \mu}$
$Sh$	: Sherwood number, $Sh = d_p / \delta$
$Sc$	: Schmidt number, $Sc = \mu / \rho DL$
$We_L$	: Weber number for the liquid, $We_L = \frac{\rho U_L^2}{a_p \rho}$

### Subscripts

in	: Inlet
out	: Outlet
g	: Gas
L	: Liquid

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