Modelling, Design And Optimization of Equipment for Toluene Emissions Abatement

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Abstract

The work focuses the abatement of volatile organic compounds (VOC) in an inkjet dye colorant manufacturing process at Fujifilm Imaging Colorants. Toluene emissions from the inkjet dye manufacturing process were quantified using Environmental Protection Agency (EPA) equations and SuperPro Designer (SPD, Chemical Engineering Simulation Program). Quantification of toluene emissions with EPA equations was compared with the results from SPD in order to assess recent calculation changes to the design and simulation software. A model based in gas absorption for an existing scrubber was developed in order to calculate the efficiency in the VOC abatement. The model consisted in a multi-bed scrubber made up of a first scrubber with recirculation and a continuous second scrubber. A maximum efficiency value of 50% was found for the first scrubber. However, due to stripping, negative values were also observed. For the second scrubber a value of 34% was found. This resulted in an overall maximum efficiency value of 64%. Increasing the liquid flow rates will have the most immediate benefit in terms of removal efficiency. The current scrubber system was able to achieve insignificant levels for long term emissions but was unable to routinely achieve short term ones. Use of the existing condenser in the process reaction vessel (not considered for calculations) and/or increased liquid flow to the scrubber will ensure that overall abatement would satisfy both short and long term ground level concentrations.

Keywords: Volatile Organic Compounds, Gas Absorption, Inkjet Dye.

1. Introduction

Volatile organic components (VOCs) are common pollutants emitted from chemical processes. These emissions exceed environmental standards and thus VOC abatement is required [1]. VOCs are emitted as gases from certain solids or liquids through the volatilization of organic compounds at the liquid surface. The present case focuses on toluene emissions. Toluene emissions come from an inkjet dye manufacturing operations being a function of displacement (e.g., charging, transfer), heating, gas sweep (e.g., convective drying, inerting) and vacuum drying operations during manufacturing. Each year, new federal and state environmental regulations require higher destruction and improved capture of volatile organic compounds. For toluene the appraisal methodology for peak (short term) process contributions and long term process contributions at ground level equate to maximums of 0.738 kg/h and 4069 kg/annum respectively. The regulator can also apply solvent emission directive benchmarks with mass and concentration rates of 0.1 kg/h and 20 mg/m$^3$ for Class A VOCs or 2 kg C/h and 75 mg C/m$^3$ for Class B VOCs (emissions at the point source, vent outlet).

A VOC control system typically consists of a capture device and a removal device. The capture device (such as a hood or enclosure) captures the VOC-laden air from the emission area and ducts the exhaust air stream to removal equipment such as a recovery device or a destructive control device [2]. In
this work toluene emissions from the inkjet dye manufacturing process were quantified using Environmental Protection Agency (EPA) equations and a chemical engineering simulation program, SuperPro Designer (SPD). Emissions released from the process will be subjected to gas treatment in a multi-bed scrubber consisting of a recirculation first scrubber and a continuous second scrubber. A model is proposed to calculate the scrubbers efficiency using gas absorption theory and the ONDA method.

2. Emissions Model

2.1. Process

Toluene emissions derive from an inkjet dye manufacturing process involving a crystallization step described below.

Crystallization of Intermediate paste

Start the agitator and charge toluene (4329 kg) into reaction vessel A. Charge the intermediate paste (1669 kg @ 100 % wt) over a minimum of 2 hours. Heat the contents to 55 to 60 °C and hold at 55 to 60 °C for four hours. Whilst maintaining the temperature at 55 to 60 °C, add methanol (Methanol 1) over two hours.

Isolation and Water Wash of Intermediate

Pre-heat vessel B to 40 °C and transfer in contents vessel A using methanol (Methanol 2, 600 litres) as a follow through wash. Cool batch to 5 to 20 °C. Material is then passed to the filter for isolation and nitrogen drying. Nitrogen drying was not considered as the emissions are sent to a different scrubber from that being evaluated.

2.2. Emissions equations

Toluene emissions prior to absorption are a function of the following process: material loading emissions, heat-up losses and purge or gas sweep.

The amount of toluene emitted during the listed operations is calculated using the following EPA equations [2]:

Material loading emissions:

\[ E_{\text{episode}} = \frac{P_i \cdot x_i \cdot MW_i}{RT} \cdot V_r \quad (1) \]

Purging of filled vessels (gas sweep):

\[ E_{\text{episode}} = \frac{P_i \cdot x_i}{P - \sum_j x_j \cdot p_j} \quad (2) \]

Heating of vessels:

\[ E_{\text{episode}} = \frac{n_{\text{inert}}}{2} \left[ \frac{(p_i)_{T_1} \cdot x_i}{P_1 - \sum_j x_j \cdot (p_j)_{T_1}} + \frac{(p_i)_{T_2} \cdot x_i}{P_2 - \sum_j x_j \cdot (p_j)_{T_2}} \right] \quad (3) \]

where

\[ n_{\text{inert}} = \frac{1}{R} \left[ \frac{V_{r,1}Pa_1}{T_1} - \frac{V_{r,2}Pa_2}{T_2} \right] \quad (4) \]

\[ Pa_1 = P_1 - \sum_j x_j \cdot (p_j)_{T_1} \]

\[ Pa_2 = P_2 - \sum_j x_j \cdot (p_j)_{T_2} \quad (5) \]

3. Absorption Model

3.1. Solubility

Absorption is a unit operation used in the chemical industry to separate gases by washing or scrubbing a gas mixture with a suitable liquid. One or more of the constituents of the gas mixture are absorbed in the liquid and can thus be removed from the mixture. In air
pollution control, absorption involves the removal of specific gaseous pollutants from a process stream by dissolving them into a liquid.

Absorption is a mass-transfer operation. In any absorption process, possible removal efficiency is controlled by the concentration gradient of the pollutant being treated between the gas and the liquid phases. This concentration gradient is the driving force to mass transfer between phases. Therefore, the solubility of the given pollutant in the gas and liquid phases will determine the equilibrium concentration of the pollutant.

Solubility is the factor that affects the amount of a pollutant, or solute, that can be absorbed and it’s a function of both the temperature and the pressure of the system. Solubility data are obtained at equilibrium conditions. If equilibrium were to be reached in the actual operation of an absorption tower, the efficiency would fall to zero at that point since no net mass transfer could occur. The equilibrium concentration, therefore, limits the amount of solute that can be removed by absorption. Solubility data are analyzed by an equilibrium diagram that plots the mole fraction of solute in the liquid phase, denoted as \(x\), versus the mole fraction of solute in the gas phase, denoted as \(y\). For low concentrations of a non-reacting solute in the liquid phase, where a simple solution is formed, Henry’s Law applies:

\[ p^* = Hx \]  

(6)

Dividing both sides of Equation (6) by the total pressure of the system we obtain:

\[ y_e = H'x \]  

(7)

This is the equation of a straight line, where the slope \((m)\) is equal to \(H'\). Henry’s law can be used to predict solubility only when the equilibrium line is straight. Equilibrium lines are usually straight when the solute concentrations are very dilute. In air pollution control applications, this is usually the case as it is in the present case for toluene.

If a pollutant is readily soluble in the scrubbing liquor, the slope \(m\) of the equilibrium curve is low. An inverse relationship exists between \(m\) and driving force, the smaller the slope, the more readily the pollutant will dissolve into the scrubbing liquor. In this case the system toluene-water has a Henry constant of 258.

### 3.2. Equipment

Gas absorption is usually carried out in vertical countercurrent columns. In this case a packed tower is used. The model consisted in a multi-bed scrubber made up of a first scrubber with recirculation and a continuous second scrubber (Fig. 1). The packed-bed scrubbers consist of a chamber containing layers of polypropylene Pall rings that provide a large surface area for liquid-gas contact. The packing is held in place by wire mesh retainers and supported by a plate near the bottom of the scrubber. Scrubbing liquid is evenly introduced above the packing and flows down through the bed. The liquid coats the packing and establishes a thin film. The pollutant to be absorbed must be soluble in the fluid. In vertical designs, the gas stream flows up the chamber (countercurrent to the liquid) [3].
3.3. Absorption model equations

The height of a packed column refers to the depth of packing material needed to accomplish the required removal efficiency [4]. Where the concentration of the solute is small, the flow of gas and liquid will be essentially constant throughout the column, and the height of packing required, \( Z \), is given by [5]:

\[
Z = \frac{G_m}{K_G a P_{y_g}} \int_{y_e}^{y_l} \frac{dy}{y - y_e} \quad (8)
\]

in terms of the overall gas phase mass transfer coefficient \( K_G \) and the gas composition. The group \( \int (dy / y - y_e) \), in equation (8) has been defined by Chilton and Colburn as the number of overall gas transfer units \( N_{OG} \). The number of overall gas transfer units is an integrated value of the change in composition per unit driving force and expresses the difficulty of absorbing the solute from the gas. The group in front of the integral sign is the height of a transfer unit, \( H_{OG} \). Equation (8) can be written as:

\[
Z = H_{OG} N_{OG} \quad (9)
\]

In the transfer unit concept there is a clear separation between the number of transfer units \( N_{OG} \), which is based on driving forces, and the height of a transfer unit \( H_{OG} \), which represents the rate of mass transfer. The specification for the amount of solute transferred from the gas phase determines the number of transfer units required; the height of a transfer unit depends mainly on the choice of tower packing.

The relationship between the overall height of a transfer unit and the individual film transfer units \( H_L \) and \( H_G \), which are based on the concentration driving force across the liquid and gas films, is given by:

\[
H_{OG} = H_G + \frac{G_m}{L_m} H_L \quad (10)
\]

where \( m \) is the slope of the equilibrium line and \( G_m/L_m \) the slope of the operating line.

The number of transfer units is obtained by graphical or numerical integration of equation of the group \( \int (dy / y - y_e) \) in Equation (8). The true mean driving force is the logarithmic mean when both equilibrium and operating lines are straight, and they can usually be considered to be so for dilute systems. For this case, therefore,

\[
N_{OG} = \frac{y_l - y_e}{(y - y_e)_{lm}} \quad (11)
\]

This equation may be combined with the equilibrium relation \( y_e = mx \) (for dilute concentrations Henry’s law holds) and the material balance expression:
to eliminate the need for values of \( y_e \). The resulting equation which was proposed by Colburn is given below:

\[
N_{OG} = \frac{\ln \left( 1 - \frac{mG_M}{L_M} \frac{y_1 - m\chi_2}{y_2 - m\chi_2} + \frac{mG_M}{L_M} \right)}{1 - \left( \frac{mG_M}{L_M} \right)}
\]  

(13)

The height of a gas-film transfer unit and the height of a liquid-film transfer unit are given by, respectively:

\[
H_G = \frac{G_M}{k_G \sigma_a P}
\]  

(14)

\[
H_L = \frac{L_M}{k_L \sigma_L C_I}
\]  

(15)

Many correlations have been published for predicting the height of a transfer unit, and the mass-transfer coefficients. Among existing correlations, the Onda et al. work can be described as the first and still widely used, procedure for packed tower design in regard to mass-transfer coefficient predictions [6].

Onda et al. published correlations for the film mass-transfer coefficients \( k_G \) and \( k_L \) and the effective wetted area of the packing \( a_w \), which can be used to calculate \( H_G \) and \( H_L \). Their correlations were based on a large amount of data on gas absorption and distillation; with a variety of packings, which included Pall Rings and Berl saddles [5].

The equation for the effective area is:

\[
a_w = 1 - \exp \left[ -1.45 \left( \frac{\sigma_L}{a\mu_L} \right)^{0.75} \left( \frac{L_m}{a\mu_L} \right)^{0.1} \left( \frac{L_m^2}{\rho_L g} \right)^{0.05} \left( \frac{L_m^2}{\rho_L \sigma_L a} \right)^{0.2} \right]
\]  

(16)

And for the mass coefficients:

\[
k_L \left( \frac{\rho_L}{\mu_{L,G}} \right)^{1/3} = 0.005 \left( \frac{L_m}{a\mu_L} \right)^{2/3} \left( \frac{\mu_{L,G}}{\rho_L D_L} \right)^{-1/2} \left( \alpha_d P \right)^{0.4}
\]  

(17)

\[
k_G = k_5 \left( \frac{G_m}{a\mu_v} \right)^{0.7} \left( \frac{\mu_v}{\rho_v D_v} \right)^{1/3} \left( \alpha_d P \right)^{-2.0}
\]  

(18)

Taking into account Fig. 1 the equations for the bottom tier scrubber efficiency calculations are shown. For the liquid re-circulating around the bottom packed bed (base):

\[
t = 0 \Rightarrow x_2 = 0
\]

\[
t = t + \Delta t \Rightarrow x_2 = x_1 (t - \Delta t)
\]  

(19)

For the liquid exiting the bottom of the scrubber:

\[
t = 0 \Rightarrow \text{toluene liq. bottom} = \frac{E}{100} n_{\text{toluene out bottom}}
\]

\[
t = t + \Delta t \Rightarrow \text{toluene liq. bottom} = \frac{E}{100} n_{\text{toluene out bottom}} + \text{toluene liq. bottom} (t - \Delta t)
\]  

(20)

\[
x_1 = \frac{\text{toluene liq. out bottom}}{n_{\text{toluene mix}} + \text{toluene liq. out bottom}}
\]  

(21)

A model was developed to determine how the toluene absorption within the multi-bed scrubber varies with time. The calculations were made accordingly with the absorption theory and ONDA’s method, and using the following equations for the mole fraction of toluene exiting the scrubbers and for scrubber efficiency, respectively:

\[
y_2 = \frac{\left( y_1 - m\chi_2 \right) \left( 1 - \frac{mG_M}{L_M} \right)}{\exp \left[ \left( 1 - \frac{mG_M}{L_M} \right) N_{OG} \right] - \frac{mG_M}{L_M}} + m\chi_2
\]  

(22)

\[
\text{Efficiency (\%)} = 100 \left( 1 - \frac{y_2}{y_1} \right)
\]  

(23)
Equation (22) is equation (13) for the number of transfer units, rearranged for the mole fraction of solute in the gas phase exiting the scrubber. The number of transfer units ($N_{OG}$) is calculated using equation (9), being $H_{OG}$ from this equation calculated using equation (10).

4. Results and discussion

Emissions model

Toluene emissions prior to any chilled condensation at the reactor (not considered) and scrubber abatement applied are tabulated below (table 1). The calculations were compared with SPD ones.

Table 1. Toluene emissions from process (before condensation & abatement).

<table>
<thead>
<tr>
<th>Operation</th>
<th>Time (h)</th>
<th>Emissions (kg/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Excel spreadsheet</td>
</tr>
<tr>
<td>1 Charge toluene</td>
<td>0.64</td>
<td>0.36</td>
</tr>
<tr>
<td>2 Gas Sweep 1</td>
<td>0.64</td>
<td>1.20</td>
</tr>
<tr>
<td>3 Charge Intermediate paste</td>
<td>2.55</td>
<td>0.06</td>
</tr>
<tr>
<td>4 Gas sweep 2</td>
<td>2.55</td>
<td>0.53</td>
</tr>
<tr>
<td>5 Heating 1</td>
<td>0.61</td>
<td>2.14</td>
</tr>
<tr>
<td>6 Charge methanol</td>
<td>0.9</td>
<td>0.19</td>
</tr>
<tr>
<td>7 Gas sweep 3</td>
<td>0.9</td>
<td>0.44</td>
</tr>
<tr>
<td>8 Heating 2</td>
<td>2</td>
<td>0.23</td>
</tr>
<tr>
<td>9 Transfer batch</td>
<td>1.2</td>
<td>0.60</td>
</tr>
<tr>
<td>10 Transfer line wash</td>
<td>0.1</td>
<td>0.22</td>
</tr>
</tbody>
</table>

The previous table show that the highest emissions are from the vessel first heating. Due to the heating effect toluene vapors are formed in a larger quantity. The temperature at which the vessel is heated has an important effect on the toluene emissions, a temperature of 50°C instead of the 55°C would lead to a value of 1.5 kg/h in the Heating 1 operation. This effect can also be observed in the gas sweep calculations. If the second gas sweep were conducted at the same time as the first heating and considering a temperature of 55°C instead of the 20°C we would have a value of 3 kg/h of toluene emissions instead of the 0.53 kg/h.

The results from SPD are in close agreement with those from the Excel spreadsheet (model) and small discrepancies can be due to small differences in some of the parameters used by SPD to do the calculations.

Absorption model

The results for the recirculation scrubber are given in Fig. 2.

Fig. 2. First scrubber efficiency variation with time (negative absorption efficiency values are due to stripping).

The previous graph shows us that the first scrubber switches between absorption and stripping depending on the amount of toluene in the feed gas and toluene already accumulated. Stripping effect occurs when some of the toluene absorbed by the water ($x_2$, Fig. 1) goes to the gas phase ($y_2$). If this amount is higher than the toluene coming in ($y_1$) the efficiency will be negative. As we can see by Fig. 2 the maximum toluene removal efficiency for the first scrubber is about 50% and as the concentration of toluene in the gas stream decreases (Table 2) the absorption driving force reduces and stripping takes effect (Fig. 3).
Table 2. Gas mixture entering the first scrubber.

<table>
<thead>
<tr>
<th></th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Q_{in} ) (m³/h)</td>
<td>120.36</td>
<td>120.36</td>
<td>120.14</td>
<td>120.14</td>
<td>120.51</td>
<td>120.15</td>
<td>120.06</td>
<td>120.06</td>
<td>120.14</td>
<td>120.14</td>
<td>120.05</td>
</tr>
<tr>
<td>( n_{m\text{ in total}} ) (kmol/h)</td>
<td>5.006</td>
<td>5.006</td>
<td>4.996</td>
<td>4.996</td>
<td>4.996</td>
<td>5.013</td>
<td>4.996</td>
<td>4.992</td>
<td>4.992</td>
<td>4.995</td>
<td>4.991</td>
</tr>
<tr>
<td>( G_{m} ) (kmol/(m².s))</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
</tr>
<tr>
<td>( G_{m} ) (kg/(m².s))</td>
<td>0.078</td>
<td>0.078</td>
<td>0.078</td>
<td>0.078</td>
<td>0.078</td>
<td>0.078</td>
<td>0.078</td>
<td>0.077</td>
<td>0.077</td>
<td>0.078</td>
<td>0.077</td>
</tr>
<tr>
<td>( y_{\text{N2 in}} )</td>
<td>0.997</td>
<td>0.997</td>
<td>0.999</td>
<td>0.999</td>
<td>0.999</td>
<td>0.999</td>
<td>0.999</td>
<td>0.999</td>
<td>0.999</td>
<td>0.999</td>
<td>1.000</td>
</tr>
<tr>
<td>( y_{\text{Toluene in}} ) (( y_{1} ))</td>
<td>0.00339</td>
<td>0.00339</td>
<td>0.00135</td>
<td>0.00135</td>
<td>0.00135</td>
<td>0.00475</td>
<td>0.00137</td>
<td>0.00052</td>
<td>0.00052</td>
<td>0.00131</td>
<td>0.00048</td>
</tr>
</tbody>
</table>

Fig. 3. Operating lines of the first scrubber system

Fig. 4 indicates that the amount of toluene being absorbed (liquid phase) is not increasing, despite the recirculation, due to the negative efficiency (amount of gas exiting the column, \( y_{2} \), is higher than what is coming in, \( y_{1} \), due to stripping).

For the efficiency in the second scrubber, Fig. 5, one can see that it practically remains constant at approximately 34% as there is no recirculation, being a once-through scrubbing. The efficiency in the second scrubber is lower due to the lower L/G ratio, as the liquid flow rate is lower (8 m³/h instead of 12 m³/h).

Fig. 5. Second scrubber efficiency variation with time.
The results for toluene emissions from the second scrubber are given in Fig. 6 and 7.

![Fig. 6. Toluene emissions variation with time (mg/m$^3$).](image)

Fig. 6 show that the concentration rate of emissions exiting the scrubber will be above the benchmark guidance. The latter is due to the very low carrier gas flow compared to other chemical installation scrubbers, where the volumetric flow of carrier gas (air) through a scrubber used to provide through-pan draughting is typically 10-500 times higher than the carrier gas (nitrogen) flow through the existing scrubber. This is because the existing plant is fully enclosed & nitrogen-blanketed – where it is important to exclude air (safety) & to minimise nitrogen usage (due to cost, environmental & N$_2$ supply limitations). As a result, the very small mass flows of toluene leaving the scrubber result in disproportionately high outlet concentrations.

![Fig. 7. Toluene emissions variation with time (kg/h).](image)

Toluene emissions are directly related with the amount of toluene that is being released in the gas phase by the first scrubber and with the efficiency in the second scrubber, as was expected. Emissions are higher for higher amounts of toluene coming in and for lower efficiencies. Analyzing Fig. 7 one can see that the environmental limits for toluene emissions without further abatement measures (e.g., chilled condensation) will on occasions exceed the maximum short term rate.

Overall efficiency, Fig. 8, has a minimum value of about 30% (without taking into account the negative values) and a maximum of 67%.

![Fig. 8. Overall efficiency variation with time.](image)

Model sensitivity

Calculations were made to understand the sensitivity of the model to the changes in liquid, inert gas and toluene concentrations. Two toluene flow rates scenarios entering the recirculation scrubber were considered; 10 kg/batch and 50 kg/batch on a 12h batch simulation analysis (0.833 kg/h and 4.16 kg/h respectively). Due the high Henry’s constant (m=258), the scrubber efficiency is likely to be function of the G/L ratio, therefore, a range of gas and liquid flow rates were assessed to understand the sensitivity within the model. For Nitrogen, since the normal flow rate is 120 m$^3$/h, calculations were carried out with a range of lower (20 and 60 m$^3$/h) and higher values (200, 250, 300, 400, 500, 700, 1000 and 10000 m$^3$/h).
Liquid flow rates of 10, 15, 20 and 25 m3/h were carried out for the continuous bed.

The results for the first and second scrubber efficiency are given in Fig. 9. Fig. 9 indicates that the amount of toluene coming in doesn’t affect efficiency values within both scrubbers at the various nitrogen flow rates. The decreasing effect for the first scrubber efficiency is a result of the recirculation/accumulation as previously mentioned. Efficiency is lower for higher nitrogen flow rates.

Since the nitrogen flow rate is fixed due to safety reasons, an analysis was made to see how does the water flow rate for the second scrubber (with the actual toluene flow rates from table 2) affects the efficiency and toluene emissions.

![Graphs showing scrubber efficiency](image)

**Fig. 9.** Comparison between first and second scrubber efficiency variation with time for first scrubber toluene constant flow rate of 0.833 kg/h (on the left) and 4.16 kg/h (on the right). Calculations were made for several nitrogen flow rates.
As we can see by the previous graphs increasing the water flow rate to the continuous scrubber will have a major impact to the removal efficiency and consequently to the toluene emissions. Increasing the water to the continuous packed bed will decrease toluene emissions by 2.25x that for a doubling of the liquid flow rate (10 to 20 m$^3$/h).

5. Conclusions

A crystallization process from a Fujifilm Inkjet Dye produces toluene emissions that are minimized by gas absorption using a multi-bed scrubber.

Emissions from the process vessels were calculated using EPA equations and the heating process with toluene only in the vessel is the one who produces major emissions. The final process emissions were used to assess recent emission calculation changes to SuperPro Designer.

Final results for the toluene emissions calculations from SPD are in close agreement with the ones from the Excel spreadsheet and small discrepancies are likely to be due to differences in some of the parameters used by SPD to do the calculations.

The process emissions were then fed into a new toluene scrubbing model that used the ONDA equations. Toluene is only partially soluble in water (520 ppm), with a Henry’s constant of 258 at 20ºC. The efficiency of very dilute systems will be dependent on the L/G flow rate, and this dependency was shown to be the case for toluene scrubbing (Fig. 9 to 12). Accumulation in the first scrubber is limited due to poor solubility and gas stripping. The first scrubber appears to be smoothing out the toluene released to second scrubber, potentially reducing the extent of any peak emissions.

Lower nitrogen flow rates will greatly improve toluene absorption efficiency (Fig. 9). However, nitrogen in the process is used to maintain an inert atmosphere for safety reasons and cannot be changed. Increasing the liquid flow rates will have the
most immediate benefit in terms of removal efficiency, as seen in Fig. 10 to 12. The existing scrubber system using water has limited potential for toluene abatement, due to the poor solubility. The current scrubber system was able to achieve insignificance levels for long term emissions but unable to routinely achieve short term insignificance levels and either Class A or B benchmarks without additional measures. Failure to meet the concentration benchmarks is due in part to the very low carrier gas flow compared to other chemical installation scrubbers, where the volumetric flow of carrier gas [air] through a scrubber used to provide through-pan draughting is typically 10-500 times higher than the carrier gas [nitrogen] flow through the existing scrubber.

Use of the existing condenser and/or increased liquid flow to the scrubber will ensure the overall abatement measures satisfy both short and long term ground level concentrations. Potential improvement measures to be assessed include:

- Chilled condensation on the process vessel
- Increasing the second scrubber liquid flow rate
- Alternative process solvent
- Alternative scrubbing medium
- Additive to water to increase toluene solubility

6. List of symbols

- \(a\) Packing surface area per unit volume (m\(^2\)/m\(^3\))
- \(a_w\) Effective interfacial area of packing per unit volume (m\(^2\)/m\(^3\))
- \(C_t\) Total molar concentration (kmol/m\(^3\))
- \(D_L\) Liquid diffusivity (m\(^2\)/s)
- \(D_v\) Diffusivity of vapor (m\(^2\)/s)
- \(d_p\) Packing size (m)
- \(E\) Efficiency (%)
- \(G_m\) flow rate of gas per unit area (kmol/m\(^2\).s or kg/m\(^2\).s)
- \(g\) Gravitational acceleration (m/s\(^2\))
- \(H\) Henry’s law constant (dimensionless or atm)
- \(H_G\) Height of gas film transfer unit (m)
- \(H_L\) Height of liquid film transfer unit (m)
- \(H_{OG}\) Height of overall gas phase transfer unit (m)
- \(K_G\) Overall gas phase mass transfer coefficient (kmol/m\(^2\).s.atm)
- \(K_L\) Overall liquid phase mass transfer coefficient (kmol/m\(^2\).s.atm)
- \(K_5\) Constant in equation (15) (5.23 for packing sizes above 15 mm, and 2.00 for sizes below 15 mm)
- \(k_G\) Gas film mass transfer coefficient (m/s)
- \(k_L\) Liquid film mass transfer coefficient (m/s)
- \(L_m\) flow rate of liquid per unit area (kmol/m\(^2\).s or kg/m\(^2\).s)
- \(M_W\) Molecular weight of \(i\)th component
- \(m\) Slope of equilibrium line
- \(N_{OG}\) Number of overall gas-phase transfer units
- \(n_{inert}\) Inert gas leaving the vessel during the operation (kmoles)
- \(P\) Column operating pressure (atm or bar)
- \(P^*\) Vapor pressure of solute (atm)
- \(P_1\) initial vessel pressure (Pa)
- \(P_2\) final vessel pressure (Pa)
- \(P_{a1}\) initial pressure (Pa)
- \(P_{a2}\) final vessel pressure (Pa)
- \(p_i\) vapor pressure of \(i\)th component \(i\) at the exit temperature (Pa)
- \((p_i)_{T1,T2}\) vapor pressure of component \(i\) at \(T_1\) or \(T_2\) (Pa)
- \((p_j)_{T1,T2}\) vapor pressure of component \(j\) at \(T_1\) or \(T_2\) (Pa)
- \(R\) ideal gas constant (8314 J/kmol.K)
- \(T_1\) initial vessel temperature (K)
- \(T_2\) final vessel temperature (K)
- \(V_r\) volume of displaced gas (m\(^3\))
- \(V_{r,1}\) initial gas space volume (m\(^3\))
- \(V_{r,2}\) final gas space volume (m\(^3\))
- \(x_2\) concentration of solute in solution at column top
the concentration in the liquid that would be in equilibrium with the gas concentration at any point

\( x_i \) mole fraction of component \( i \) in the liquid mixture

\( x_j \) mole fraction of component \( j \) in the liquid mixture

\( y_1 \) concentration of solute in gas phase at column base

\( y_2 \) concentration of solute in gas phase at column top

\( y_e \) the concentration in the gas that would be in equilibrium with the liquid concentration at any point

\( Z \) Height of package (m)

6.1. Greek letters

\( \sigma_C \) Critical surface tension for packing material (N/m)

\( \mu_L \) Viscosity of liquid (Pa.s)

\( \mu_v \) Viscosity of vapor (Pa.s)

\( \rho_L \) Density of liquid (kg/m\(^3\))

\( \rho_v \) Density of vapor (kg/m\(^3\))

\( \sigma_L \) Liquid surface tension (N/m)

References


