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Introduction

Prevention of flammable vapor concentrations in a waste tank can be accomplished by forced ventilation of the tank vapor space. The forced ventilation must provide a sufficient flow rate to maintain the bulk vapor space below the composite lower flammability limit (CLFL) of the combustibles, and it must also produce velocities near the liquid surface of sufficient magnitude such that the generated forced convection mass transfer rate can support the evolution rate of the combustibles. If this second criterion is not met, the combustible vapors could potentially stratify, leading to bulk vapor-space concentrations above the CLFL.

A simple steady-state forced-convection mass transfer model has been developed to calculate the combustible vapor concentration profile in the boundary layer at the liquid-vapor space interface. Mass transfer across the boundary layer is controlled by molecular diffusion in the viscous sublayer and turbulence-induced eddy diffusivity in the balance of the boundary layer. The effect of negative density gradients on eddy diffusivity are accounted for in the model.

Using estimates of the boundary-layer thickness and edge velocity from experimental data and/or other analytical methods, the model can demonstrate that the mass transfer rate across the boundary layer is greater than or equal to the evolution rate of the combustible vapors. Conversely, the model can be used to estimate the boundary-layer thickness and edge velocity necessary to sustain a given mass transfer rate.

Analytical Development

Model of Mass Transfer Across a Forced-Convection Boundary Layer

When the nitrogen purge system is operational, a boundary layer is formed at the liquid surface by forced-convection flow in the tank vapor space. Assuming for the moment a uniform velocity profile, in conjunction with isothermal conditions, the steady-state mass transfer of benzene evolved from the liquid surface across the boundary layer under turbulent flow conditions is given by
Equation (1) can be solved numerically using false time-stepping. The spatial derivatives are evaluated using centered-space finite differencing. Forward-time finite differencing is used to evaluate the false time-step. Forward- and backward-space differencing are used to evaluate the left- and right-hand side boundary conditions, respectively.

The convergence criterion used to terminate the calculation is:

\[
\max \left[ \frac{c_n^j - c_{n+1}^j}{\Delta t} \right] < \text{error}
\]

Convergence was also judged based on a comparison of the analytical solution for the concentration gradient in the viscous sublayer to that predicted by the numerical solution of (1). Logic was incorporated into the numerical algorithm that prevented the dispersive errors associated with first-order centered-space differencing from generating specious positive concentration gradients. Based on the experience of the analyst and some numerical experimentation, 151 to 301 grid points were used with a time-step size of 1.0E-04 to 1.0E-05 s. Error-values in the range of 1.0E-03 to 1.0E-05 were used.

A peaking factor on the mass flux is used account for spatial variation in mass flux and/or the velocity field. Spatial non-uniformity in either the mass flux or the velocity field will result in radial and azimuthal variations in benzene concentration. This in turn will lead to lateral benzene fluxes created by the hydrostatic head differences between regions of high and low benzene concentration. Experiments on heavy-gas dispersion indicate even small density differences will generate significant lateral spreading, hence lateral concentration gradients will tend to “smooth out”. Moreover, the bulk convection in the vapor space will also cause lateral spreading.

In terms of a simple two control-volume approximation the mass fluxes can be characterized as shown in Figure 2. Note that if a very large number of control volumes were used, this characterization becomes a CFD analysis.
If the forced convection mass transfer across the boundary layer is sufficient to handle the total mass evolution rate, a further constraint must be met

\[ m_{1,0} \leq m_{1,\text{max}} \]  

The simplest and most limiting case for (3a-f) is when \( m_{2,\text{max}} = 0 \). In terms of the ratios of the respective inventory-vapor space surface areas associated with the control volumes, the peaking factor that the mass evolution rate would be multiplied by is

\[ F_p = 1 + \frac{A_2}{A_1 + A_2} \]  

A less conservative approach would be to calculate \( m_{1,\text{max}} \). Since, via (3f),

\[ m_{1,\text{max}} \geq m_{1,i} + m_{2-i} \]  

the effective mass evolution rate that CV2 must be able to handle is found from (3e) as

\[ (m_{2,i} - m_{2-i}) = m_{\text{total}} - (m_{1,i} + m_{2-i}) = m_{\text{total}} - m_{1,\text{max}} \]  

This evolution rate for CV2 would then be used to calculate the benzene concentration profile for that velocity field. If the profile showed a small gradient across the logarithmic region it could be concluded that the combined forced convection mass transfer of the two CVs is sufficient to transport the total mass evolution rate, and hence maintain a well-mixed vapor space.
Characterization of Effective Mass Diffusivity

In order to solve (1), an expression for effective mass diffusivity as a function of position in the boundary layer has to be developed. Using the standard boundary layer wall function, the boundary layer is treated as two separate layers, the viscous sublayer and the logarithmic layer; the outer layer is conservatively treated as part of the logarithmic layer. In the viscous sublayer, molecular diffusivity limits the molar transfer rate

\[ D(y) = D_m \quad \text{for} \quad y^+ \leq 35 \]  

Brighton’s evaluation of mass transfer in a neutrally-buoyant turbulent boundary layer finds that outside of the viscous sublayer the turbulent molar diffusivity is equal to

\[ D(y) = \frac{\kappa u^* y}{Sc_T} \quad \text{for} \quad y^+ > 35 \quad y^+ = \frac{yu^*}{v} \]  

The differential transport equation for turbulent kinetic energy (KE) in the boundary layer for the conditions under consideration (i.e., steady-state, uniform boundary layer) is

\[ G_k - G_b = -\frac{d}{dy} \left[ \frac{\mu_T}{\sigma_k} \frac{dk}{dy} \right] + \rho^2 C_\mu \frac{k^2}{\mu_T} \]  

\[ G_k = \mu_T \left( \frac{du}{dy} \right)^2 \quad G_b = -g \frac{\mu_T}{\rho Sc_T} \frac{d\rho}{dy} \]  

The density gradient term in (10b) is evaluated numerically using forward-space differencing, except at \( i=n \), where backward-space differencing is used. Forward-space differencing is used where possible, as opposed to centered-space differencing, as it is a more accurate representation of the density gradient that influences the reduction of turbulent KE.

If \( G_k >> |G_b| \), the buoyancy-generation term has little impact on the turbulent KE of the differential volume. Conversely, if \( G_k \sim |G_b| \) or \( G_k \leq |G_b| \) the buoyancy-generation term, if positive, will cause a decrease the turbulent KE. In the limiting case, \( G_b > 0; |G_b| >> G_k \), the turbulent KE would be driven to zero, indicating a transition to laminar flow. The direct solution of (9) is beyond the scope of this analysis, however an order-of-magnitude evaluation of the \( G_k \) and \( G_b \) terms can be used to scale the effective molar diffusivity.

Let \( \beta \) equal the ratio the buoyancy-generation/reduction KE term to the shear stress-generation KE term, \( \beta = G_b / G_k \). When \( \beta \) approaches zero, buoyancy (either positive or negative) has a negligible effect on the boundary layer and the eddy diffusivity. When \( \beta \) approaches 1.0, negative
buoyancy starts to appreciably reduce the energy available to generate turbulence. Since the friction velocity (u-star) is proportional to the square-root of the turbulent KE, as an approximation the eddy diffusivity can be scaled by \( \sqrt{1-\beta} \).

Now the effective molar diffusivity, accounting for the viscous sublayer (7), enhanced molar diffusivity due to turbulence (8), and potential molar diffusivity reductions due to negative buoyancy (note that the positive buoyancy case is not addressed in this formulation) can be expressed as

\[
D(y) = D_m + \delta(y^+ - 35) \beta (1 - \beta) \frac{k u^* y}{S c_f} \sqrt{1 - \beta},
\]

where

\[
\delta(x) = \begin{cases} 
0 & x \leq 1 \\
1 & x > 1 
\end{cases}
\]  

(11)

Evaluation of CFD Analysis Data and its Application to the Model

Reference 5 documents a CFD analysis of the flow field in the Tank 48 vapor space under steady-state isothermal conditions. The velocity data from that analysis can be used to characterize the boundary-layer thickness and the velocity at the edge of the boundary layer. These data can be used in conjunction with the inner (logarithmic) region characterization of turbulent boundary layer velocity profile to estimate the friction velocity, \( u^* \), used in calculating the effective molar diffusivity.

Inspection of the velocity data finds that it varies across the entire liquid surface. Since the methodology developed herein treats the velocity field as spatially uniform, the data need to be appropriately simplified into a form that is amenable for use. With this in mind, it is decided to qualitatively split the velocity field into two regions, a “high velocity” region and a “low velocity” region.

Visual inspection of the velocity vector plots in Reference 5 finds the following in the plane normal to the inventory surface at a height of 12 cm: ~20% of the surface has a velocity of 70 cm/s or greater; ~30% of the surface has a velocity between 70 cm/s and 40 cm/s; ~30% of the surface has a velocity between 40 cm/s and 20 cm/s; and ~20% of the surface has a velocity of less than 20 cm/s.

The purge flow rate under which these velocities were generated was 300 scfm. The velocities are scaled by the square-root of the ratio of nitrogen purge flow rates to account for the higher velocities that would occur at the higher flow rates. At higher flow rates the boundary-layer thickness should also be reduced; however no credit is taken for boundary-layer thickness reduction, as the analyst knows of no method short of performing another CFD analysis for estimating the amount of reduction from the 300 scfm case.

Outline of How the Calculation is Performed

First, peaking factors and u-star values were calculated for the characterization of the boundary layer edge velocities corresponding to a nitrogen purge flow rate of 700 scfm. Next, well-mixed
bulk vapor space benzene concentrations are calculated for benzene evolution rates of 50, 100, 200, and 400 gm/min. Finally, the benzene concentration profile in the boundary layer is calculated by solving (1) numerically.

RESULTS

Figure 3 gives the profiles for benzene evolution rates of 50, 100, 200, and 400 gm/minute with a 700 scfm purge flow rate cases characterized by a 0.4 m/s boundary-layer edge velocity over 50% of the surface ($F_p = 2$); and 0.0 m/s over the remaining 50% of the surface.

![Figure 3. Boundary-layer benzene concentration profiles at various uniform benzene evolution rates for a 700 scfm nitrogen purge flow rate with 0.4 m/s boundary-layer edge velocity over 50% of the surface, -0 m/s over remaining 50% of the surface.](image)

The profiles show a relatively steep concentration gradient across the viscous sublayer in comparison to that in the logarithmic profile region. The gradient in the viscous sublayer is due to molecular diffusion only, hence the slope in this region should match that given by the analytical solution for (1) with a constant diffusivity. When checked, the numerical solution was found to deviate from the analytical solution by no more than +/-2%.

The shallow concentration gradient across in the logarithmic profile region shows that the effective molar diffusivity due to turbulent fluctuations in the boundary layer is much larger than the molecular diffusivity.

The “wiggles” seen in the viscous sublayer concentration are a numerical artifact caused using a centered-differencing term to evaluate the gradient between the viscous sublayer and the
logarithmic region (this same behavior is seen when centered-differencing methods are used to capture shocks (i.e. discontinuities) in compressible flow). Increasing the number of grid points would tend to mitigate this effect. Note that the “wiggles” do not adversely impact the overall solution, as seen by the good agreement between the numerical and analytical solution for the concentration gradient in the viscous sublayer.

In none of the cases evaluated was the negative density gradient of a magnitude sufficient to preclude the generation of eddy diffusivity outside of the viscous sublayer.

Finally, the very small concentration gradients in the logarithmic region of all of the cases evaluated indicates that the forced-convection mass transfer rate was sufficient to maintain a well-mixed bulk vapor space.

**CONCLUSIONS**

A simple model has been developed to evaluate benzene mass transfer across a uniform steady-state forced-convection boundary layer. The model includes the potential impact of negative density gradients on the production of eddy diffusivity.

Using characteristic velocities and boundary-layer thicknesses from Tank 48 CFD analyses, as well as a simple peaking factor method to account for non-uniformities in the boundary-layer velocity profile, benzene concentration profiles have been determined for uniform benzene evolution rates of 50, 100, 200, and 400 gm/minute with a nitrogen purge flow rate of 700 scfm.

A simple peaking factor can be applied to the benzene evolution rate to account for non-uniformities in the vapor space flow field. However, since the peaking factor approach neglects mass transfer over a portion of the surface, this method may be over-conservative in some cases. In those cases, a two-CV approach can be taken where, via crediting lateral spreading from regions of high benzene concentration to low concentration regions, more appropriate credit is taken for the mass transfer rates in the different flow regions over the surface.

The results for the cases evaluated indicate that the only significant benzene gradient in the boundary layer is in the viscous sublayer. The eddy diffusivity generated by turbulent fluctuations causes the logarithmic profile region to exhibit almost no resistance to mass transfer from the viscous sublayer to the bulk vapor space. This causes the negative density gradient to be small, and hence not adversely impact the eddy diffusivity. These conditions indicate that the forced-convection mass transfer rate in the evaluated cases is sufficient to maintain a well-mixed bulk vapor space.
References and Nomenclature


Table 1. Nomenclature Table.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c$</td>
<td>molecular concentration of benzene</td>
<td>$Sc_T$</td>
<td>turbulent Schmidt number (0.85)</td>
</tr>
<tr>
<td>$y$</td>
<td>spatial location in the boundary layer</td>
<td>$y^+$</td>
<td>nondimensional position in the boundary layer</td>
</tr>
<tr>
<td>$D(y)$</td>
<td>effective mass diffusivity</td>
<td>$v$</td>
<td>molecular kinematic viscosity</td>
</tr>
<tr>
<td>$n^*$</td>
<td>molar flux at the liquid surface</td>
<td>$F_p$</td>
<td>peaking factor</td>
</tr>
<tr>
<td>$\delta$</td>
<td>boundary layer thickness</td>
<td>$A_2$</td>
<td>surface area of low velocity region</td>
</tr>
<tr>
<td>$c_{bulk}$</td>
<td>bulk vapor space benzene concentration</td>
<td>$A_1$</td>
<td>surface area of high velocity region</td>
</tr>
<tr>
<td>$\Delta y$</td>
<td>distance between grid points</td>
<td>$k$</td>
<td>turbulent kinetic energy (KE)</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>size of false time step</td>
<td>$G_k$</td>
<td>rate of turbulent KE generation due to shear in</td>
</tr>
<tr>
<td>$i$</td>
<td>the i$^{th}$ grid point</td>
<td>$G_b$</td>
<td>rate of turbulent KE generation or reduction</td>
</tr>
<tr>
<td>$j$</td>
<td>the j$^{th}$ time step</td>
<td>$g$</td>
<td>due to buoyancy effects</td>
</tr>
<tr>
<td>$n$</td>
<td>total number of grid points</td>
<td>$\mu_T$</td>
<td>eddy viscosity</td>
</tr>
<tr>
<td>$D_m$</td>
<td>molecular diffusivity</td>
<td>$\sigma_k$</td>
<td>empirical constant</td>
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<td>$\kappa$</td>
<td>von Karman coefficient (0.41)</td>
<td>$C_\mu$</td>
<td>empirical constant</td>
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<tr>
<td>$u^*$</td>
<td>friction velocity</td>
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