“Although scientific inquiry is a dynamic give-and-take among researchers with different opinions and viewpoints, the so-called controversies surrounding low-dose effects and NMDR curves should be put to rest...These phenomena have been demonstrated time and again for a sufficient number of endocrine-related endpoints, and they no longer merit being considered “controversial” topics.”

Vandenberg et al. Endocrine Reviews 2009, 30, 75.
(authors from Tufts University School of Medicine)
Vapor Pressure Ranges

vp versus C-number

Figure 4.5 Vapor pressure at 25°C of n-alkanes as a function of chain length.

Intermolecular Forces and VPs

Nonpolar & polar, & H-accepting (HA)

H-accepting & donating (HDA)

$\propto \text{LDF}$

Experimental log $P^0$ vs. $1/T$
Clausius-Clapeyron Example

Consider 1,2,4,5-tetramethylbenzene (TeMB). In an old CRC, you find the following data

\[ T_m = 79.5 \, ^\circ C \]
\[ T_b = 195.9 \, ^\circ C \]
\[ MW = 134.2 \, g/mol \]

1. Estimate \( v_p \) (Pa) of TeMB at 20 \( ^\circ C \) and at 150 \( ^\circ C \).
2. Also, express your answer in g/m\(^3\).

<table>
<thead>
<tr>
<th>( T ) (( ^\circ C ))</th>
<th>( P ) (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>45</td>
<td>133.3</td>
</tr>
<tr>
<td>75</td>
<td>1333</td>
</tr>
<tr>
<td>104</td>
<td>5332</td>
</tr>
<tr>
<td>128</td>
<td>13330</td>
</tr>
<tr>
<td>172</td>
<td>53320</td>
</tr>
<tr>
<td>196</td>
<td>101308</td>
</tr>
</tbody>
</table>

Beware of P & T units!!
\[ \Delta_{\text{vap}} H_{iL(T1)} = a \log p_i^{o\text{L}(T1)} + b \]

\[ \Delta_{\text{vap}} H_{iL(298K)} \text{(kJ/mol)} = -8.80 \log p_i^{o\text{L}(298K)}(Pa) + 70.0 \]
Vapor Pressure Estimations

1. What is the vapor pressure of benzene at 30 °C? Given, $P_o (25^\circ C) = 10^{-0.9}$ atm?

2. What is the vapor pressure of benzyl alcohol at 25 °C, given $T_b = 205.3 \, ^\circ C$; $T_m = 15 \, ^\circ C$; 108.14 g/mol

3. What is the vapor pressure of benzene at 3 °C? $T_b = 80.1 \, ^\circ C$; $T_m = 5.5 \, ^\circ C$; 78.1 g/mol

1 atm = 101325 Pa

$R = 8.314 \, J/(mol \, K)$
Toxic Contamination From Natural Gas Wells

“While the existence of the toxic wastes has been reported, thousands of internal documents obtained by The New York Times from the Environmental Protection Agency, state regulators and drillers show that the dangers to the environment and health are greater than previously understood.”

Kevin Moloney, New York Times
February 26, 2011
“The only thing that I’ve heard is if you take a plastic bottle and put it in the microwave and you heat it up, it gives off a chemical similar to estrogen. So the worst case is some women may have little beards.”


Paul LePage, Governor of ME
February 2011
“But both the birth and the afterlife of the duck, Hohn soon learns, are toxic. Adrift on the ocean, the toys can become coated with “persistent organic pollutants” like polyvinyl chloride, bisphenol A and phthalates. Photodegraded into smaller pieces, they can be fatally ingested by sea creatures and will endure, in swirling gyres, for years.”

Ny Times Book Review “Moby Duck”

February 2011
Empirical VP Estimations

1. Calculate $\tau$ & HBN for
   - Benzene
   - benzyl alcohol
   - Dichlorodiphenyl trichloroethane (DDT)
   - 2,4,7,8-tetrachlorodibenzodioxin
   - 2,4,7,8-tetrachloro diphenyl ether
Empirical VP Estimation: benzyl alcohol

1. What is the vapor pressure of benzyl alcohol at 25 °C?

\[ T_b = 205.3 \, ^\circ C; \, T_m = 15 \, ^\circ C; \, 108.14 \, \text{g/mol} \]

\[
\ln P_{iL}^\circ = -\left[21.2 + 0.3(1.5) + 177(0.00925)\right] + \frac{205.3 + 273K}{298K} - 1 + \\
\left[10.8 + 0.25(1.5)\right]\ln\left(\frac{205.3 + 273K}{298K}\right) = -8.80
\]

\[
P_{iL}^\circ = e^{-8.80} = 0.000150\text{bar}
\]

\[
P_{iL} = 0.000150\text{bar} \times \frac{100000\text{Pa}}{1\text{bar}} = 15.0\text{Pa}
\]

1 bar = 100,000 Pa
Empirical VP Estimation: benzene

1. What is the vapor pressure of benzene at 3 °C?

\[ T_b = 80.1 \degree C; \ T_m = 5.5 \degree C; \ 78.1 \text{ g/mol} \]

\[
\ln P_i^\circ (\text{bar}) = -\left[ (21.2 + 0.30) + 177(0) \right] \left( \frac{80.1 + 273K}{276K} \right) - 1 + \\
+ \left[ (10.8 + 0.25) \ln \left( \frac{80.1 + 273K}{276K} \right) \right] = -3.26
\]

\[
P_i^\circ (\text{bar}) = e^{-3.26} = 0.0383 \text{bar}
\]

Is this really the \( P^0 \) for benzene at 3 °C?
Theoretical states...strange but useful

\[ \ln P = \frac{1}{T (K^{-1})} \]

Crossover point = \( T_m \)

Supercooled liquid \( v_p \neq \) solid \( v_p \)