

Vapor-Liquid Equilibrium of Benzene and Toluene

This application calculate the vapor-liquid equilibrium of a benzene-toluene mixture. Specifically, the application calculates the

- temperature, given the composition of the liquid phase and pressure
- dew point and composition of the liquid phase given composition of the vapor phase and pressure

The application employs the empirical Antoine equation to calculate the vapor pressures of benzene and toluene. The parameters are sourced from the [NIST Chemistry Webbook](#).

The techniques used here can be applied to many other mixtures - you just need to find the right data for the Antoine equation.

restart :

with(Units[Simple]) :

Antoine Equations for Vapor Pressures of Benzene and Toluene

Vapor pressure of benzene (from the [NIST webbook for benzene](#) and valid from 421.46 K to 554.8 K)

$$p_1 := 10^{4.60362 - \frac{1701.073 \text{ K}}{T + 20.806 \text{ K}}} \text{ bar} :$$

Vapor pressure of toluene (from the [NIST webbook for toluene](#) and valid from 420.00 K to 580.99 K)

$$p_2 := 10^{4.54436 - \frac{1738.123 \text{ K}}{T + 0.394 \text{ K}}} \text{ bar} :$$

Total pressure

$$P_{total} := 4500 \text{ mmHg} :$$

Temperature Given Composition of Liquid Phase and Pressure

Fraction of benzene in liquid phase

$$x_1 := 0.6 :$$

Fraction of toluene in liquid phase

$$x_2 := 1 - x_1 = 0.4$$

Sum of partial pressures

$$P := x_1 \cdot p_1 + x_2 \cdot p_2 = \left(0.6 \cdot 10^{4.60362 - \frac{1701.073 \text{ K}}{T + 20.806 \text{ K}}} + 0.4 \cdot 10^{4.54436 - \frac{1738.123 \text{ K}}{T + 0.394 \text{ K}}} \right) \text{ bar}$$

Hence the temperature of the mixture is

$$T_{mix} := \text{fsolve}(P = P_{total}, T = 200 \text{ K}) = 435.94 \text{ K}$$

Dew Point and Composition of Liquid Phase Given Composition of Vapor Phase and Pressure

Fraction of benzene in vapor phase

$$y_1 := 0.5 :$$

Fraction of toluene in vapor phase

$$y_2 := 1 - y_1 = 0.5$$

Dew point temperature

$$T_{dew} := \text{fsolve}\left(y_1 \cdot \frac{P_{total}}{p_1} + y_2 \cdot \frac{P_{total}}{p_2} = 1, T = 400 \text{ K}\right) = 445.99 \text{ K}$$

Hence the partial pressures are

$$\text{eval}(p_1, T = T_{dew}) = 910.89 \text{ kPa}$$

$$\text{eval}(p_2, T = T_{dew}) = 447.27 \text{ kPa}$$

The composition of the liquid phase is

$$x_1 := \text{eval}\left(\frac{y_1 \cdot P_{total}}{p_1}, T = T_{dew}\right) = 0.329$$

$$x_2 := \text{eval}\left(\frac{y_2 \cdot P_{total}}{p_2}, T = T_{dew}\right) = 0.671$$