Mixing gases

"Exact" value (Viacheslav maple's calculus)

$\rho'_o := 2.231 \frac{kg}{m^3}$

Data

$P := 1\ atm$ $T := 300\ K$

$Fluids := \text{stack}(\text{"Helium"}, \text{"Xenon"})$ $\nu := \text{length}(Fluids)$

$x := \text{stack}(0.6, 0.4) \frac{mol}{mol}$ $\sum x = 1$

Props

$Mix := \text{""}$ for $k \in [1..\nu]$

$Mix := \text{concat}\left(Mix, \text{"\&"}, Fluids_k, \text{"["}, \text{var2str}\left(x_k\right), \text{"]"}\right)$

$Mix := \text{substr}(Mix, 2) = \text{"Helium[0.6]\&Xenon[0.4]"}$

$\text{CoolProp\_Props}(\text{"D"}, \text{"T"}, T, \text{"P"}, P, Mix) = ▮$

lastError = "Initialize failed for backend: "?", fluid: "Helium&Xenon" fractions "[0.6000(

$\rho := \overrightarrow{\text{CoolProp\_Props}(\text{"D"}, \text{"T"}, T, \text{"P"}, P, Fluids)} = \begin{bmatrix} 0.1625 \\ 5.3612 \end{bmatrix} \frac{kg}{m^3}$

$Tc := \overrightarrow{\text{CoolProp\_Props1}(\text{"TCRIT"}, Fluids)} = \begin{bmatrix} 5.1953 \\ 289.733 \end{bmatrix} K$

$Pc := \overrightarrow{\text{CoolProp\_Props1}(\text{"PCRIT"}, Fluids)} = \begin{bmatrix} 0.2276 \\ 5.842 \end{bmatrix} MPa$

Notation:
prime is for the mixture

$M := \overrightarrow{\text{CoolProp\_Props1}(\text{"M"}, Fluids)} = \begin{bmatrix} 4.0026 \\ 131.293 \end{bmatrix} \frac{g}{mol}$

$M' := \sum_{k=1}^{\nu} x_k \cdot M_k = 54.9188 \frac{g}{mol}$

Method 1: As ideal gases

From $P \cdot V = n \cdot R \cdot T$ $\rho = \frac{m}{V}$ $m = MM \cdot n$

$\rho' := M' \cdot \frac{P}{R_m \cdot T} = 2.230907 \frac{kg}{m^3}$

$err := \left|\frac{\rho'_o - \rho'}{\rho'_o}\right| = 0.0042\ \%$

Method 2: Using mixing density formula

Mole to mass fractions

$y := \overrightarrow{\frac{x \cdot M}{M'}} = \begin{bmatrix} 0.04372934 \\ 0.95627066 \end{bmatrix}$

$\rho' := \frac{1}{\sum_{k=1}^{\nu} \frac{y_k}{\rho_k}} = 2.234906 \frac{kg}{m^3}$

$err := \left|\frac{\rho'_o - \rho'}{\rho'_o}\right| = 0.1751\ \%$

Method 3: Using Redlich-Kwong formula

$$b := \overrightarrow{\frac{\sqrt[3]{2}-1}{3} \frac{\text{mol K}}{\text{J}} R_m^{\ 2} \cdot \frac{Tc}{Pc}} = \begin{bmatrix} 0.1367 \\ 0.297 \end{bmatrix} \frac{\text{L}}{\text{mol}}$$

volume constant correction for each compound

$$b' := \sum_{k=1}^{\nu} x_k \cdot b_k = 0.2009 \frac{\text{L}}{\text{mol}}$$

volume constant correction for the mixture. Notice that it is lineal in x

$$a := \overrightarrow{\frac{1}{9 \cdot \left(\sqrt[3]{2}-1\right)} R_m^{\ 2} \cdot \frac{Tc^{2.5}}{Pc}} = \begin{bmatrix} 0.008 \\ 7.228 \end{bmatrix} \frac{\text{J}^2 \cdot \sqrt{\text{K}}}{\text{mol}^2\ \text{Pa}}$$

attractive potential of molecules coefficient for each compound

for $k \in [1..\nu]$
  for $j \in [1..\nu]$
    $\alpha_{k\,j} := \sqrt{a_k \cdot a_j}$

$$\alpha = \begin{bmatrix} 0.008 & 0.2403 \\ 0.2403 & 7.228 \end{bmatrix} \frac{\text{J}^2 \cdot \sqrt{\text{K}}}{\text{mol}^2\ \text{Pa}}$$

The "a" coefficient for the mixture is not lineal in x, assuming that α(i,j) is the geometric mean of a(i) & a(j)

$$a' := \sum_{k=1}^{\nu} \sum_{j=1}^{\nu} x_k \cdot x_j \cdot \alpha_{k\,j} = 1.2747 \frac{\text{J}^2 \cdot \sqrt{\text{K}}}{\text{mol}^2\ \text{Pa}}$$

attractive potential of molecules coefficient for the mixture

Now we can solve the Redlich-Kwong for the mixture like it was a compound

$$v' := \text{FindRoot}\left(P = \frac{R_m \cdot T}{v' - b'} - \frac{a'}{\sqrt{T} \cdot v' \cdot (v' + b')},\ v' = 1 \frac{\text{L}}{\text{mol}} \right)$$

$$v' = 24.7893 \frac{\text{L}}{\text{mol}}$$

$$\rho' := \frac{M'}{v'} = 2.2154 \frac{\text{kg}}{\text{m}^3}$$

$$err := \left| \frac{\rho'_o - \rho'}{\rho'_o} \right| = 0.6981\ \%$$

Alvaro

appVersion(4) = "1.0.8348.30405"