

Regarding LiBr-water mixture properties.

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1 Functions of vapor pressure

Equilibrium vapor pressure above a mixture as a function of solution temperature and mass fraction is given by equation 1 and constants in table 4.

1.1 Solving Temperature

To get temperature as a function of pressure and mass fraction, it would be useful to have the derivative available, and this is possible as follows. However, note that you can get θ from p and then solve T . Anyway,

$$p(T, x) = p_\sigma(\theta), \quad \theta = T - \sum_{i=1}^8 a_i x^{m_i} (0.4 - x)^{n_i} \left(\frac{T}{T_c} \right)^{t_i}$$

$$\frac{\partial p}{\partial T} = \frac{\partial p_\sigma}{\partial \theta} \frac{\partial \theta}{\partial T}$$

Now the pressure derivative should be obtained from CoolProp, whereas the adjusted temperature derivative is in closed form:

$$\frac{\partial \theta}{\partial T} = 1 - \sum_{i=1, t_i > 0}^8 a_i x^{m_i} (0.4 - x)^{n_i} t_i \left(\frac{T}{T_c} \right)^{t_i-1} T_c^{-1}$$

1.2 Solving mass fraction

Similarly, we need the derivative wrt mass fraction:

$$\frac{\partial p}{\partial x} = \frac{\partial p_\sigma}{\partial \theta} \frac{\partial \theta}{\partial x}$$

where

$$\frac{\partial \theta}{\partial x} = - \sum_{i=1, m_i > 0}^8 a_i m_i x^{m_i-1} (0.4 - x)^{n_i} \left(\frac{T}{T_c} \right)^{t_i} - \sum_{i=1, n_i > 0}^8 a_i x^{m_i} n_i (0.4 - x)^{n_i-1} (-1) \left(\frac{T}{T_c} \right)^{t_i}$$

Mass fraction (in the liquid) as a function of vapor pressure and temperature is given by equation 1 and constants in table 4. To get pressure as a function of temperature and mass fraction, it would be useful to have the derivative available, and this is possible as follows.