Modelling and Simulation of a Batch Packed Column for Fruit Wine Distillations

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APENDIX - PHYSICAL PROPERTIES OF THE MIXTURES

The physical and transport properties of the mixture were obtained from [1].

The bulk liquid mixture density is given by,

$$\rho = \frac{x_1 \cdot MW_1 + (1 - x_1) \cdot MW_3}{V_{ap} \cdot x_1 + \dfrac{(1 - x_1) \cdot MW_3}{\rho_3}} \tag{1}$$

which requires the apparent molar volume,

$$V_{ap} = 5.1214 \cdot 10^{-2} + 6.549 \cdot 10^{-3} \cdot x_1 + \cdots \\ 7.406 \cdot 10^{-5} \cdot (T - 273.15) \tag{2}$$

The liquid density of pure ethanol and water are, respectively,

$$\rho_1 = \frac{MW_1}{\left(57.763 + 7.406 \cdot 10^{-2} \cdot (T - 273)\right)} \tag{3}$$

$$\rho_3 = 3.3 \cdot 10^{-6} \cdot T^2 + 1.689 \cdot 10^{-3} + 0.785 \tag{4}$$

The bulk liquid viscosity is given by,

$$\mu = \eta \cdot \rho \tag{5}$$

where the kinematic viscosity is,

$$\eta = \frac{x_{1,vol} \cdot \mu_1 \cdot exp\left(\dfrac{565.67 \cdot \left(1 - x_{1,vol}\right)}{T}\right)}{\rho_1} + \frac{\left(1 - x_{1,vol}\right) \cdot \mu_3 \cdot exp\left(\dfrac{101.84 \cdot \left(1 - x_{1,vol}\right)}{T}\right)}{\rho_3} \tag{6}$$

This expression requires the volumetric ethanol molar fraction, pure ethanol and water viscosity, which are represented by the following equations:

$$x_{1,vol} = \left(1 + \left(\frac{1 - x_1}{x_1}\right) \cdot \frac{MW_3 \cdot \rho_1}{MW_1 \cdot \rho_3}\right)^{-1} \tag{7}$$

$$\mu_1 = \exp\left(-6.21 + \frac{1.1614 \cdot 10^3}{T} + 6.18 \cdot 10^{-3} \cdot T \ldots - 1.13 \cdot 10^{-5} \cdot T^2\right) \tag{8}$$

$$\mu_3 = \exp\left(-24.76 + \frac{4.21 \cdot 10^3}{T} + 4.53 \cdot 10^{-3} \cdot T - 3.38 \cdot 10^{-5} \cdot T^2\right) \tag{9}$$

The diffusion coefficients, D_{ij}, is required to calculate the mass transfer coefficients for each binary system [2]. For ethanol-methanol is,

$$D_{21} = \frac{5.527 \cdot 10^{-8} \cdot T}{\mu_1} \tag{10}$$

for methanol-water is,

$$D_{23} = \frac{6.2585 \cdot 10^{-8} \cdot T}{\mu_3} \cdot \left(\frac{\sigma_3}{\sigma_2}\right)^{0.15} \tag{11}$$

which depends on the superficial tension of methanol and water, given respectively by,

$$\sigma_2 = (-0.0921 \cdot T + 49.961) \cdot 10^{-3} \tag{12}$$

$$\sigma_3 = (-0.1681 \cdot T + 122.05) \cdot 10^{-3} \tag{13}$$

and, for the pair ethanol-water is,

$$D_{13} = 0.0208 \cdot exp(\frac{-2534.5}{T}) \tag{14}$$

The enthalpies of the vapor, H, and liquid, h, depend on the temperature and the corresponding ethanol molar fraction:

$$\begin{aligned} H = {} & -2919.83 \cdot y_1 + (31.46 - 11.98 \cdot y_1) \cdot T + 36172.03 \\ & + (4.063 \cdot 10^{-4} + 0.073 \cdot y_1) \cdot T^2 \end{aligned} \tag{15}$$

$$h = (55.678 \cdot x_1 + 75.425) \cdot T - 15208.44 \cdot x_1 - 20602.34 \tag{16}$$

Finally, the water heat capacity, $c_{p,w}$, thermal conductivity, λ, and Prandtl number are given by the following expressions:

$$c_{p,w} = 8.94 \cdot 10^{-6} \cdot T^2 - 5.5 \cdot 10^{-3} \cdot T + 5.02 \tag{17}$$

$$\lambda = -8.07 \cdot 10^{-6} \cdot T^2 + 6.35 \cdot 10^{-3} \cdot T - 0.57 \tag{18}$$

$$Pr = exp\left(-8.92 + 6.2 \cdot 10^{-7} \cdot T^{2.5} + \frac{2915.88}{T}\right) \tag{19}$$

References

[1] H. J. Neuburg and J. R. Perez-Correa, “Dynamic and steady state modelling of a pilot binary tray distillation column,” *Latin American Applied Research*, vol. 24. pp. 1–15, 1994.

[2] O. J. P. Poling B.E., Prausnitz J.M., *The Properties of Gases and Liquids*, vol. 12, no. 4. 2000.