Exercise 2: Answer guide

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1. (a) Pages 89-92 in the book "Process Modelling and Model Analysis."

   (b) Isothermal process

   (c) Quasi-Static Processes, Isobaric Processes at constant volume and approximately zero for liquids and solids, because the volume V is relatively small for such systems.

   (d) Narrow temperature range and Ideal Gases.

2. (a) For compactness in the below $T = T_{out}$, $P = P_{out}$. As there are two phases in the system we define the vapour and liquid phases as control volumes. We assume these volumes are at phase equilibrium, are homogeneous and have the same temperature. We can write the balance equation:

$$\frac{d\phi}{dt} = J_{in} - J_{out} + R_{generated} - R_{consumed} = J_{in} - J_{out} + q \tag{1}$$

for the extensive variable of our system. For this system, our extensive variables are mass and energy. If we have N components, we can define $N - 1$ component balances, 1 total mass balance and 1 energy balance.

$$\frac{dn}{dt} = F - V - L \qquad \text{total MB}$$

$$\frac{dn_i}{dt} = Fz_i - Vy_i - Lx_i \qquad i = 1 : N - 1 \text{ component MB}$$

$$\frac{dH}{dt} = Fh_F - Vh_V - Lh_L + Q \qquad \text{total EB}$$

Current number of equations: $N + 1$.

We now define the constitutive equations. We know that mass fractions must sum to 1.

$$1 = \sum_i x_i$$

$$1 = \sum_i y_i$$

$$1 = \sum_i z_i$$

Current number of equations: $N + 4$.

We assume phase equilibrium, and that this is described by a K-value expression. If we assume that Raoult's law applies then K depends only on temperature and pressure. We assume that the saturation pressure, p_i^{sat}, is a known function of temperature.

$$y_i = K_i x_i = p_i^{sat}(T)x_i/P \qquad i = 1 : N - 1$$

We should also specify the heat transfer between the flash tank and the jacket that keeps the temperature constant.

$$Q = hA(T - T_{fluid})$$

Current number of equations: $2N + 4$.

At this point we don't have any equations describing the amount of gas or liquid in the tank – to add this information we define hold-up equations for the mass and energy:

$$n = n_V + n_L$$
$$n_i = n_V x_i + n_L y_i \qquad i = 1 : N - 1$$
$$H = n_V h_V + n_L h_L$$

Current number of equations: $3N + 5$.

(b) Counting the variables defined so far: $n, n_V, n_L, H, F, V, L, T, Q, P, V_{tank}, n_i, x_i, y_i, z_i = 4N + 11$ So before variable specification, the degrees of freedom are: $DOF = N + 6$.

Note that we don't have any algebraic equations that describe the outlet flow rates from the tank! One could assign these as known variables (in reality this means specifying a set-point for some controller on the outflow), or introduce new equations that relate the flow rates to the tank operation, e.g. $L = f(n_L, P, V_{tank})$ or $G = f(t)$.

Say that we use these two equations for L, and G, and that the tank volume is known. The number of variables to specify is $DOF = 4N + 10 - 3N - 7 = N + 3$.

If we have a two component flash, $N = 2$, so we need to specify 5 variables to solve the system.

(c) If the process is at steady state then the hold-up equations are not nescessary to solve for the outflows of the system.

(d) No. The degrees of freedom are satisfied, however this specification over-specifies the phase equilibrium part of the system, i.e. specifying y_A and x_B, species the two other mole fractions. Specifying T, P specifies the equilibrium $y_i = K_i x_i = p_i^{sat}(T)x_i/P$.

(e) Yes, one can specify the system to have mostly linear equations.

3. (a) Model boundary: storage tank; Modelling goal: describe how fast the solvent flows out on the ground.

(b) Short time scale: high outflow of solvent; long time scale: zero outflow of solvent if the rupture is in the side part of the storage tank.

(c) Level of the liquid and outflow of liquid. Assumption: only liquid phase

(d) Level of the liquid and temperature inside the tank. Assumption: no liquid outflow and steady-state

(e) Anything reasonable