Modelling and control summaries

by Anthony Rossiter

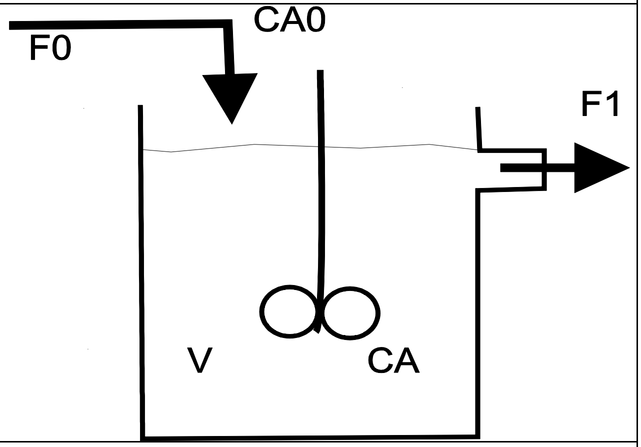
1st order modelling 10: mixing tank with reaction

This note looks at a simple mixing tank system which has flow in at a concentration C_{A0} and flow out a different concentration C_A. The aim is to model how the outlet concentration depends upon the inlet concentration, flow rates and tank volume.

ASSUMPTIONS

1. For simplicity here we assume that the flow in F0 and the flow out F1 are equal. This means the volume V in the tank is fixed.
2. The tank is well mixed so the concentration in the tank matches the outlet concentration.
3. The solvent and product A have the same density.
4. There is a reaction in the tank involving A.

MODELLING is done using a **mass or molar balance** (these are equivalent). To be more precise, we balance the rate of change of mass A within the tank.



MASS BALANCE

Accumulation of A = A (input) – A (output) + generation of A – expenditure of A

Note that the assumption here is that generation and expenditure (say from reactions) are non-zero due to the reaction.

DEFINE M_A as mass per mole for pure A, so mass of A per m^3 within solvent is $C_A M_A$

- The rate of A coming into the tank is determined by inlet flow F0 and inlet concentration. Mass flow rate in = $F_0 C_{A0} M_A$
- The rate of A leaving the tank is determined by outlet flow f1 and outlet concentration. Mass flow rate out = $F_1 C_A M_A$
- The rate of A being consumed/generated is assumed to have some dependence on the concentration in the tank, say $f(C_A)$ per unit volume. The function may vary with context.
- The total mass in the tank= $VC_A M_A$ so, given V and M_A are constant. Therefore the rate of change of mass in the tank is given by

$$VM_A \frac{dC_A}{dt} = (M_A F_0 C_{A0} - M_A F_1 C_A) + M_A V f(C_A)$$

It is noted that the term M_A is a common factor throughout and so can be removed. Also, the assumption is that $F_1 = F_0 = F$ and hence:

$$\left\{ \frac{V}{F} \frac{dC_A}{dt} + C_A = C_{A0} + \frac{V}{F} f(C_A) \right\}$$

We can do no more with this model until the function f(.) is provided.

Using deviation variables

1. Deviation variables are useful for nonlinear processes and will be required when a mixing tank contains a reaction. Therefore it is useful to introduce the concept here.
2. The idea is to define states **relative to a known steady-state** (for example degrees Celsius is relative to the freezing point of water, altitude is relative to ground level on the earth, etc.).
3. This concept is useful as the deviation variable tells you how far you have moved from a specified steady-state. Moreover, it links in with the use of Taylor series for linearization (which implicitly uses deviation variables).

STEP 1: Define a known steady-state. Note this means the derivative must be zero.	$C_{A,s}=C_{A0,s};\ \frac{dC_{A,s}}{dt}=0$
STEP 2: Define the deviation variables as deviations from the selected steady-state.	$C_A=C_A'+C_{A,s}$ $C_{A0}=C_{A0}'+C_{A0,s};$
STEP 3: Substitute expressions above into the model without a reaction.	$\frac{V}{F}\frac{d[C_A'+C_{A,s}]}{dt}+[C_A'+C_{A,s}]=[C_{A0}'+C_{A0,s}]$
STEP 4: Use the observations of STEP 1 to remove redundant terms.	$\frac{V}{F_0}\frac{dC_A'}{dt}+C_A'=C_{A0}'$
REMARK: In this example, because the underlying model is linear, superposition holds. Consequently the model with deviation variables matches the model with the original variables.	

Numerical example with a reaction

Find the response of a mixing tank with the following data and subject to a step increase in C_{A0} of magnitude 0.6mole/m^3. F=0.1m^3/min; V=2m^3; C_{A0}=0.9mole/m^3

There is a reaction inside the tank which consumes A at the following rate; the units of r_A are (mol m^{-3}*min*)$^{-1}$

$$r_A=0.2C_A+0.1C_A^2$$

Assume the system is initially at steady state before the step change in C_{A0}.

ANSWER:

1. First we need to express the model in deviation form. To do this the initial steady-state is required which can be determined from the underlying model with derivatives equal to zero. Also define the deviations variables as distances from the steady-state.

$$\left\{\frac{V}{F}\frac{dC_A}{dt}+C_A=C_{A0}+\frac{V}{F}(0.2C_A+0.1C_A^2)\right\}\quad\Rightarrow\quad C_{A,s}=C_{A0,s}+\frac{V}{F}(0.2C_{A,s}+0.1C_{A,s}^2)$$

$$C_{A0,s}=0.9\quad\Rightarrow\quad C_{A,s}=0.169;$$

$$C_A=C_{A,s}+C_A';\quad C_{A0}=C_{A0,s}+C_{A0}'$$

2. Next linearise the nonlinear term about the steady-state using a Taylor series and substitute in the deviation variables where appropriate.

$$0.2C_A + 0.1C_A^2 \approx (0.2C_{A,s} + 0.1C_{A,s}^2) + (C_A - C_{A,s})\frac{d}{dC_A}(0.2C_A + 0.1C_A^2)$$

$$0.2C_A + 0.1C_A^2 \approx (0.2C_{A,s} + 0.1C_{A,s}^2) + C_A'[0.2 + 0.2C_{A,s}]$$

3. Substitute the Taylor series expansion and deviation variables into the original model

$$\left\{\frac{V}{F}\frac{dC_A}{dt} + C_A = C_{A0} + \frac{V}{F}(0.2C_A + 0.1C_A^2)\right\}$$

$$\Rightarrow \left\{\frac{V}{F}\left(\frac{dC_{A,s}}{dt} + \frac{dC_A'}{dt}\right) + C_{A,s} + C_A' = C_{A0,s} + C_{A0}' + \frac{V}{F}(0.2C_{A,s} + 0.1C_{A,s}^2 + C_A'[0.2 + 0.2C_{A,s}])\right\}$$

4. Note that the definition of the steady-state in step 1, allows us to remove all the terms linked to the steady-state as they cancel each other, hence:

$$\frac{V}{F}\frac{dC_A'}{dt} + C_A' = C_{A0}' + \frac{V}{F}(C_A'[0.2 + 0.2C_{A,s}])$$

5. Substitute in the numbers provided (V=2, F=0.1, $C_{A,s}$=0.169) and hence:

$$\left\{20\frac{dC_A'}{dt} + C_A' = C_{A0}' + C_A'\underbrace{(4 + 4C_{A,s})}_{4.68}\right\} \quad \Rightarrow \quad \left\{\frac{20}{5.68}\frac{dC_A'}{dt} + C_A' = \frac{1}{5.68}C_{A0}'\right\}$$

6. Now the model is in standard time constant form, using standard responses for a 1st order model:

$$C_A'(t) = 0.169 + \frac{0.6}{5.68}\left(1 - e^{-\frac{5.68t}{20}}\right)$$

Summary

1. Where a mixing tank contains a reaction it may be necessary to resort to deviation variables and a Taylor series expansion in order to derive a linearised model around a given operating point.
2. The operating point should correspond to a steady-state.
3. The linearised model is only valid for the region within which the Taylor series is a good approximation.