Example 9: CSTR Dynamic Model

Example 9 uses information from Example 8 which is in the reference file below.

Reference:C:\Users\Harvey\OneDrive\documents\ebook single phase\Mathcad version - 3\Example 8.xmcd

The optimal feed temperature in Example 8, 300 K, is very near ambient temperature. Temperatures near ambient are difficult to control, and precise control will be needed to prevent a "runaway" to the high conversion solution. Therefore, cooling will be added in this example to raise the inlet temperature requirement. Using Fig E8.4, a cooling rate of -250,000 J/kg was selected. The desired feed temperature for this rate of cooling is 320 K. However, in order to reach the intermediate solution, the feed rate needs to first be raised to 335 K, and then lowered to 320 K. These changes in feed temperature may need to be done manually, or the temperature controller for the feed temperature needs to be well damped to prevent overshoot. For the simulation, a cubic ramp function will be used for setting the feed temperature history.

The model does not include temperature controllers or level control. These elements can be added as needed.

Flow rate is a more convenient variable than space time for the dynamic model because it can be directly controlled. Therefore, a flow rate is assumed and the reactor volume, and heat exchanged/time are calculated from the optimal space time determined in Ex. 8.

$$q\_design := 200 \cdot \frac{L}{min} \qquad Qm := -2.5 \cdot 10^5 \cdot \frac{J}{kg}$$

$$Vr := q\_design \cdot \tau_{opt} = 2 \times 10^3 \, L$$

$$Qt := Qm \cdot q\_design \cdot \rho = -8.333 \times 10^5 \cdot \frac{J}{s} \qquad A(t) := act$$

constant activity

Forcing functions in time

The ODE and PDE routines (e.g. Rkadapt) don't accept abrupt changes in a variable when the routine includes an error criteria. One of two things may happen: the integration stops with an error, or the step size gets very, very small. This can happen even when the change is from a constatnt value to a linear ramp between two values, not a step change. To most integration routines, the change to a ramp from a constant value is still an abrupt change in slope. The real world doesn't have as many abrupt changes as we often believe. There is often a capacitance in the system or a lag in the controller elements that make the variable of interest change smoothly to the new value.

The cubic function below is used to smooth the transition from one value to another for the variable of interest. The function arguments are described below, and then the function is applied to the feed temperature, feed and cooling rates.

cubic transition function

$$SR(x, x1, y1, x2, y2) := if\left[x \le x1, y1, if\left[x > x2, y2, y1 + \left[3 \cdot \left(\frac{x - x1}{x2 - x1}\right)^2 - 2 \cdot \left(\frac{x - x1}{x2 - x1}\right)^3\right] \cdot (y2 - y1)\right]\right]$$

x = independent variable
x1 = value of x where change in y is to start
y1 = value of dependent variable for x<x1
x2 = value of x where change in y is to end
y2 = value of dependent variable for x>x2

The independent variable, t , used below is the time in seconds used in the integration routine. The unit "s" needs to be added for the conversion to the time values used in the SR functions.

$Tin1(t) := SR(t \cdot s, 0, 298 \cdot K, 10 \cdot min, 335 \cdot K)$ Initial ramp in feed temperature

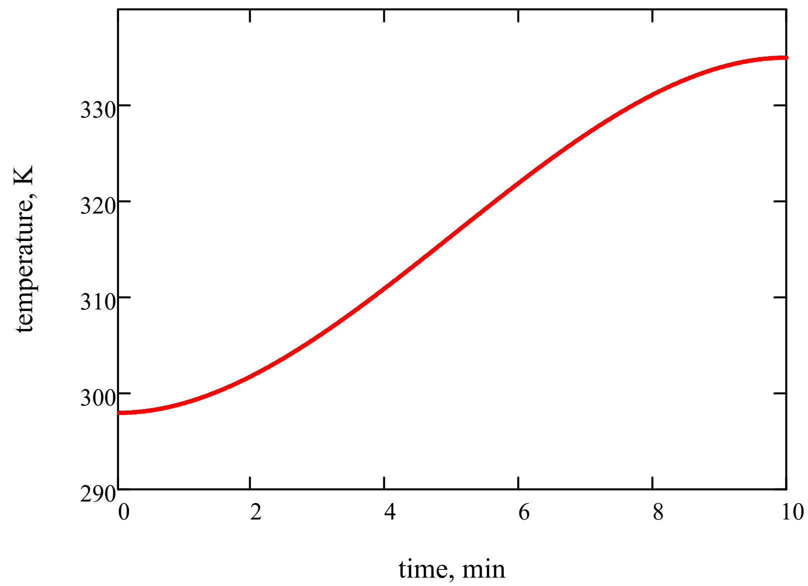
The reactor contents need time to reach the steady state temperature at the first feed temperature. In $Tin(t)$ definition, 360 minutes is allowed for this to occur. Then, the temperature is lowered over a 10 min period to the desired operating temperature.

$Tin(t) := SR(t \cdot s, 360 \cdot min, Tin1(t), 370 \cdot min, 320 \cdot K)$ Add the ramp down to lower temperature to allow for greater variability in feed temperature or cooling rate. This example demonstrates how more than one change in a variable can be defined using embedded SR functions.

$Q(t) := SR(t \cdot s, 60 \cdot min, 0, 80 \cdot min, Qt)$

$q(t) := SR(t \cdot s, 0, 0, 1 \cdot min, q\_design)$ Start flow with a 1 min ramp time.

Fig E9.1: Cubic Transition for Feed Temperature



The initial increase in the inlet temperature shown in Fig E9.2 below appears as a steep ramp. When the time scale is expanded, as shown in Fig E9.1 on the left, the gradual changes at the start and end of the transition period for the inlet temperature are evident.

The Differential equations

$$D(t,Y) := \begin{bmatrix} \dfrac{q(t)\cdot\left(\omega_{0_0} - Y_0\right)}{Vr} + \dfrac{Mw_0\cdot Rxn\left(submatrix(Y,0,NC-1,0,0),Y_{NC},1,A(t)\right)_0}{\rho} \\ \dfrac{q(t)\cdot\left(\omega_{0_1} - Y_1\right)}{Vr} + \dfrac{Mw_1\cdot Rxn\left(submatrix(Y,0,NC-1,0,0),Y_{NC},1,A(t)\right)_1}{\rho} \\ \dfrac{q(t)\cdot\left(\omega_{0_2} - Y_2\right)}{Vr} + \dfrac{Mw_2\cdot Rxn\left(submatrix(Y,0,NC-1,0,0),Y_{NC},1,A(t)\right)_2}{\rho} \\ \dfrac{q(t)\cdot\left(\omega_{0_3} - Y_3\right)}{Vr} + \dfrac{Mw_3\cdot Rxn\left(submatrix(Y,0,NC-1,0,0),Y_{NC},1,A(t)\right)_3}{\rho} \\ \dfrac{-\rho\cdot q(t)\cdot Del\_H\left(Tin(t),Y_{NC}\cdot T_0,\omega_0,submatrix(Y,0,NC-1,0,0)\right) + Q(t)}{Vr\cdot\rho\cdot Cp\left(submatrix(Y,0,NC-1,0,0),Y_{NC}\right)\cdot T_0} \end{bmatrix}\cdot s$$

The differential equations have not been converted to dimensionless time. The ODE integration routines in Mathcad require dimensionless expressions. Therefore, all of the derivatives have been multiplied by the default time unit, seconds.

initial conditions

$$Y_0 := stack\left(\omega_0, \frac{298 \cdot K}{T_0}\right)$$

$NT := 1000$ number of time steps for printing (also may affect convergence, increase if integration does not converge)

$tend := 15 \cdot hr$ end of simulation

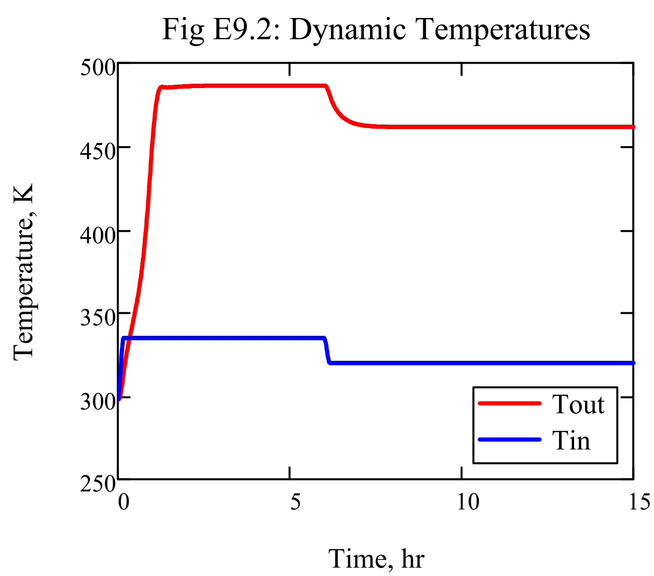
$$S := Rkadapt\left(Y_0, 0, \frac{tend}{s}, NT, D\right)$$

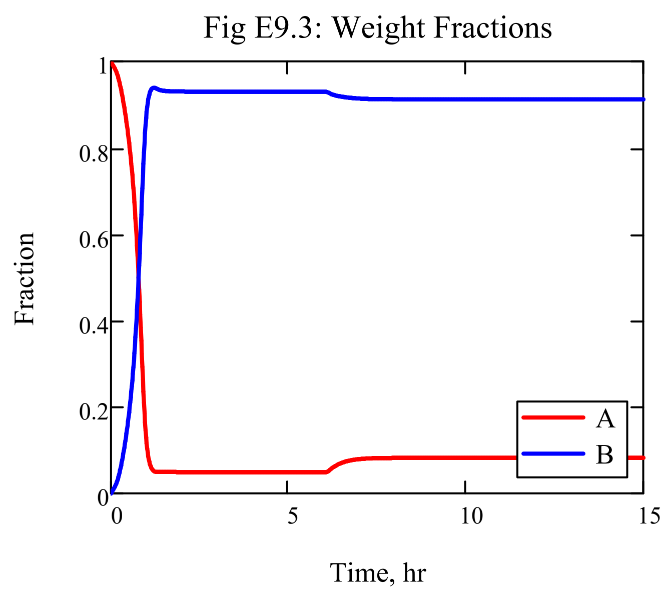
Results

$i := 0 .. NC - 1$ component index $j := 0 .. NT$ time index

$t := S^{\langle 0 \rangle} \cdot s$ The independent variable is the first column in the solution matrix for Rkadapt.

$\omega_{i,j} := \left(S^{\langle i+1 \rangle}\right)_j$ $Tout := S^{\langle NC+1 \rangle} \cdot T_0$





result is high conversion of A and high selectivity to B

Summary

This example has demonstrated the dynamic CSTR model. Inerts could be used to eliminate the multiple steady states. If the C product is desired, then the CSTR would be suitable without the inerts because a feed temperature could be chosen that results in a single solution.

This example provided an operating challenge: how to operate at the desirable stable solution. This challenge was due to the extra multiple solutions for the system. Even single reactions result in multiple solutions. However, for single reactions, the stable solutions are at the low and high conversions which can easily be reached from an operating standpoint. The intermediate solution is unstable and therefore of no interest. The additional solutions in this problem were due to the addition of another reaction.

Exercise for Example 9

This example has shown one startup scenario. The reactor was started up at ambient temperature with the reactor full of reactant. It was assumed that a catalyst was added at time 0. Instead of starting the reactor full of the reactant, it could be initially filled with the inert. An inert feed could then be used to heat the reactor contents before switching to the reactant feed composition. Also, catalyst could be withheld until the reactant is present and it is at a temperature near the desired outlet temperature. Explore these startup options with the goal of reducing the amount of reactant A leaving the reactor during the startup period.

References

Fogler, H.S., "Elements of Chemical Reaction Engineering", 3rd Ed., Prentice-Hall (1999).

Parulekar, S.J., Illinois Inst. of Technology, Chemical Engineering Education, Winter (2007)