Experimental Determination of Steady-State and Transient Behavior of Non-Isothermal and Non-Adiabatic Continuous Stirred-Tank Reactors

**Computer Project** 

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## I. Introduction

In this project, we investigate how the steady-state and transient behavior of chemical reactors are modeled. We derive the mass and energy balance equations from which we build the model. We show how steady-states are solutions to a system of nonlinear algebraic equations. We show how the transient behavior of the reactor is a solution to a system of nonlinear ordinary differential equations.

This project requires the ability to

- solve a system of nonlinear algebraic equations and
- solve a system of nonlinear ordinary differential equations.

#### **II.** Objective:

The objective of this project is to model the steady-state and transient behavior (temperature and concentration of reactants and products in the reactor effluent) of a homogeneous liquid-phase reaction of the form

$$\upsilon_{A}A + \upsilon_{B}B \to \upsilon_{C}C + \upsilon_{D}D \tag{B.1}$$

taking place in a continuous stirred-tank reactor (CSTR) under non-isothermal and non-adiabatic conditions.

#### **III.** Project Description

In the first project of the semester, we obtained the reaction rate prefactor constant,  $k_o$ , the activation energy,  $E_a$ , and the heat of reaction,  $\Delta H_r$ , for a reaction of the type given in equation (A.1) These reaction parameters were obtained under isothermal conditions in a batch reactor. However, they are constants and can be used to describe the reaction in any type of reactor under any sort of conditions. (In truth, these factors may be functions of temperature. For the purposes of this project, we neglect this functionality.)

In this project we are going to examine the reaction in a continuous stirred-tank reactor (CSTR). CSTR's can operate continuously and provide several advantages over batch reactors. The CSTR of interest is jacketed and has some degree of temperature control, therefore the reactor is not adiabatic. However, the temperature control is not so perfect that the temperature remains constant in the reactor, therefore the reactor is not isothermal.

A schematic of our process is shown in Figure One. The nomenclature used in the diagram will be used through-out the project. Further definition of the nomenclature is given in the next section.



Figure 1. Process diagram for non-isothermal, non-adiabatic ideal stirred-tank Reactor with homogeneous liquid-phase reaction.

## **IV. Nomenclature and Units**

Species: component A is reactant 1 component B is reactant 2 component C is product 1 component D is product 2 component S is non-reactive solvent component X is coolant in jacket of reactor

## Flow Streams:

stream 1 is feed stream of reactant A stream 2 is feed stream of reactant B stream E is reactor effluent stream X is reactor coolant

Flowrates:  $F_1$ ,  $F_2$ ,  $F_E$ ,  $F_X$  [liters/minute] (subscript indicates stream)

Concentrations:  $C_{A,1}$ ,  $C_{A,E}$ ,  $C_{B,2}$ ,  $C_{B,E}$ ,  $C_{S,1}$ ,  $C_{S,2}$ ,  $C_{S,E}$ ,  $C_{C,E}$ ,  $C_{D,E}$ ,  $C_{X,X}$  [moles/liter] (first subscript indicates species, second subscript indicates stream)

Temperatures:  $T_1$ ,  $T_2$ ,  $T_E$ ,  $T_{X,in}$ ,  $T_{X,out}$  [Kelvin] (subscript indicates stream)

Volume of the reactor: V [liters]

Heat transfer rate (from jacket to reactor): Q [Joules/minute]

Stream Volumetric Enthalpies:  $\tilde{H}_1$ ,  $\tilde{H}_2$ ,  $\tilde{H}_E$ ,  $\tilde{H}_X$  [Joules/liter]

Component Molar Heat Capacities:  $\hat{C}_{p,A}$ ,  $\hat{C}_{p,B}$ ,  $\hat{C}_{p,C}$ ,  $\hat{C}_{p,D}$ ,  $\hat{C}_{p,X}$  [Joules/mole/K]

Reactor-Jacket heat transfer area: A  $[m^2]$ 

Reactor-Jacket heat transfer coefficient: U [Joules/sec/K/m<sup>2</sup>]

## **V. Reaction Specifications**

You are modeling the same reaction as in the first computer project.

$$\upsilon_{A}A + \upsilon_{B}B \to \upsilon_{C}C + \upsilon_{D}D \tag{B.1}$$

You are to use the same stoichiometric coefficients that you used in computer project 01. The rate of reaction per unit volume, r(t), is of the form:

$$\mathbf{r}(\mathbf{t}) = \mathbf{C}_{\mathsf{A}}^{|\upsilon_{\mathsf{A}}|} \mathbf{C}_{\mathsf{B}}^{|\upsilon_{\mathsf{B}}|} \mathbf{k}_{\mathsf{o}} \mathbf{e}^{\frac{-\mathbf{E}_{\mathsf{a}}}{\mathsf{RT}}}$$
(B.2)

where A is the concentration of species A in moles/liter, B is the concentration of species B in moles/liter,  $k_o$  is the reaction rate prefactor constant,  $E_a$  is the activation energy, R is the gas constant, 8.314 J/mol/K, and T is the temperature in K. The units of r(t) are moles/liter/sec.

The rate of production or consumption of an individual species is, for example for species A,

$$\frac{dA}{dt} = v_A r(t) = v_A C_A^{|v_A|} C_B^{|v_B|} k_o e^{\frac{-E_a}{RT}}$$
(B.3)

where the stoichiometric coefficient,  $v_A$ , is negative for reactants and positive for products. The units of equation (B.3) are moles/liter/sec. We can write equation (B.3) for all components of interest. The rate of heat production/consumption per unit volume is given by

$$\frac{dH}{dt} = -\Delta H_r r(t) = -\Delta H_r C_A^{|\nu_A|} C_B^{|\nu_B|} k_o e^{\frac{-E_a}{RT}}$$
(B.4)

where  $\Delta H_r$  is the heat of reaction. An exothermic reaction has a negative  $\Delta H_r$  so we include a negative sign in (B.4) to ensure that an exothermic reaction generates heat, a positive  $\frac{dH}{dt}$ . The units of equation (B.4) are Joules/liter/sec.

The change in total moles per unit volume in the reactor is proportional to the number of moles created or destroyed.

$$\frac{dN}{dt} = \sum_{i=1}^{4} \upsilon_{i} r(t) = \left(\sum_{i=1}^{4} \upsilon_{i}\right) C_{A}^{|\upsilon_{A}|} C_{B}^{|\upsilon_{B}|} k_{o} e^{-\frac{E_{a}}{RT}}$$
(B.5)

The units of equation (B.5) are Joules/liter/sec. If this change in the number of moles is non-zero, it causes a change in the volume of material inside the reactor. This change in the volume per unit volume is given as

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$$\frac{dV}{dt} = \frac{1}{C_{T}} \sum_{i=1}^{4} \upsilon_{i} \mathbf{r}(t) = \frac{1}{C_{T}} \left( \sum_{i=1}^{4} \upsilon_{i} \right) C_{A}^{|\upsilon_{A}|} C_{B}^{|\upsilon_{B}|} \mathbf{k}_{o} \mathbf{e}^{-\frac{E_{a}}{RT}}$$
(B.6)

The units of equation (B.6) are inverse sec.  $C_{T}$  is the inverse molar volume of the mixture. It has units of concentration. In this model we assume it is a function neither of composition nor of temperature.

You are to use the same values of the reaction rate prefactor constant,  $k_o$ , the activation energy,  $E_a$ , and the heat of reaction,  $\Delta H_r$ , that you calculated in computer project 01.

## **VI. Material Balances:**

We can write molar balances for each of the five species in the reactor. They all follow the general balance equation form.

accum. = in - out + generation

A: 
$$V \frac{dC_{A}}{dt} = F_{1}C_{A,1} - F_{E}C_{A,E} + v_{A}C_{A}^{|v_{A}|}C_{B}^{|v_{B}|}k_{o}e^{-\frac{E_{a}}{RT}}$$
 (B.7)

B: 
$$V \frac{dC_{B}}{dt} = F_{2}C_{B,2} - F_{E}C_{B,E} + v_{B}C_{A}^{|v_{A}|}C_{B}^{|v_{B}|}k_{o}e^{-\frac{E_{a}}{RT}}$$
 (B.8)

C: 
$$V \frac{dC_{c}}{dt} = 0 - F_{E}C_{C,E} + \upsilon_{C}C_{A}^{|\upsilon_{A}|}C_{B}^{|\upsilon_{B}|}k_{o}e^{-\frac{E_{a}}{RT}}$$
(B.9)

D: 
$$V \frac{dC_{D}}{dt} = 0 - F_{E}C_{D,E} + v_{D}C_{A}^{|v_{A}|}C_{B}^{|v_{B}|}k_{o}e^{-\frac{E_{a}}{RT}}$$
 (B.10)

S: 
$$V \frac{dC_s}{dt} = F_1 C_{s,1} + F_2 C_{s,2} - F_E C_{s,E} + 0$$
 (B.11)

The units of equations (B.7.1) to (B.7.5) are moles/sec.

#### **VII. Energy Balances:**

We can write energy balance for the reactor. It follows the general balance equation form.

$$V\frac{d\widetilde{H}}{dt} = F_1\widetilde{H}_1 + F_2\widetilde{H}_2 - F_E\widetilde{H}_E - \Delta H_r C_A^{|\nu_A|} C_B^{|\nu_B|} k_o e^{-\frac{E_a}{RT}} + \dot{Q}$$
(B.12)

The units of equation (B.7.6) are Joules/sec. The enthalpies are per unit volume. The heat transferred from the jacket to the reactor,  $\dot{Q}$ , will be negative if the jacket is cooling the reactor. The heat transferred can be determined with an energy balance on the jacket.

$$V_{j} \frac{d\widetilde{H}_{x}}{dt} = F_{x}\widetilde{H}_{x,in} - F_{x}\widetilde{H}_{x,out} - \dot{Q}$$
(B.13)

where

$$\dot{\mathbf{Q}} = \mathbf{U}\mathbf{A}\Delta\mathbf{T}_{\mathsf{Im}} = \mathbf{U}\mathbf{A}\frac{\left(\mathbf{T}_{\mathsf{X},\mathsf{in}} - \mathbf{T}_{\mathsf{rxtr}}\right) - \left(\mathbf{T}_{\mathsf{X},\mathsf{out}} - \mathbf{T}_{\mathsf{rxtr}}\right)}{\mathsf{In}\left[\frac{\left(\mathbf{T}_{\mathsf{X},\mathsf{in}} - \mathbf{T}_{\mathsf{rxtr}}\right)}{\left(\mathbf{T}_{\mathsf{X},\mathsf{out}} - \mathbf{T}_{\mathsf{rxtr}}\right)}\right]}$$
(B.14)

This formulation of the log mean temperature difference will be undefined for the case where cases:

- $T_{x,in} = T_{rxtr}$ , in which case  $\Delta T_{lm} = 0.0$
- $T_{X,out} = T_{rxtr}$ , in which case  $\Delta T_{Im} = 0.0$
- $T_{x,out} = T_{x,in}$ , in which case  $\Delta T_{Im} = T_{x,out} T_{rxtr}$

## **VIII. Constraints:**

When we use moles we know: the sum of the mole fractions for any stream must be one.

$$\sum_{i=1}^{n} x_{i} = 1$$
 (B.15)

When we use concentrations, we know

$$\mathbf{x}_{i} = \frac{\mathbf{C}_{i}}{\sum_{i=1}^{n} \mathbf{C}_{i}} = \frac{\mathbf{C}_{i}}{\mathbf{C}_{T}}$$
(B.16)

$$C_{A,1} + C_{S,1} = C_T$$
 (B.16.1)

$$C_{B,2} + C_{S,2} = C_T$$
 (B.16.2)

 $C_{A,E} + C_{B,E} + C_{C,E} + C_{D,E} + C_{S,E} = C_{T}$  (B.16.3)

$$\mathbf{C}_{\mathbf{X},\mathbf{X}} = \mathbf{C}_{\mathsf{T}} \tag{B.16.4}$$

We have assumed that  $C_{\tau}$  is the same for each stream.  $C_{\tau}$  is the inverse molar volume of the mixture. It has units of concentration. In this model we assume it is a function neither of composition nor of temperature.

#### **IX.** Assumptions

- 1. Heat Capacities are independent of temperature.
- 2. The volumetric enthalpy of a mixture [Joules/liter] for stream k, is:

$$\widetilde{\mathbf{H}}_{k} = \left(\mathbf{T}_{k} - \mathbf{T}_{o}\right)\sum_{i=1}^{n} \widehat{\mathbf{C}}_{p,i} \mathbf{C}_{i,k}$$
(B.17)

Thus, for example, the following streams have enthalpies given by:

$$\widetilde{H}_{E} = (T_{E} - T_{o}) (\hat{C}_{p,A} C_{A,E} + \hat{C}_{p,B} C_{B,E} + \hat{C}_{p,C} C_{C,E} + \hat{C}_{p,D} C_{D,E} + \hat{C}_{p,S} C_{S,E})$$
(B.18.1)

$$\tilde{H}_{1} = (T_{1} - T_{o})(\hat{C}_{p,A}C_{A,1} + \hat{C}_{p,S}C_{S,1})$$
(B.18.2)

$$\tilde{H}_{2} = (T_{2} - T_{o}) (\hat{C}_{p,B} C_{B,2} + \hat{C}_{p,S} C_{S,2})$$
(B.18.3)

$$\widetilde{\mathsf{H}}_{\mathsf{X},\mathsf{in}} = (\mathsf{T}_{\mathsf{X},\mathsf{in}} - \mathsf{T}_{\mathsf{o}}) \hat{\mathsf{C}}_{\mathsf{p},\mathsf{X}} \mathsf{C}_{\mathsf{X},\mathsf{X}} \text{ and } \widetilde{\mathsf{H}}_{\mathsf{X},\mathsf{out}} = (\mathsf{T}_{\mathsf{X},\mathsf{out}} - \mathsf{T}_{\mathsf{o}}) \hat{\mathsf{C}}_{\mathsf{p},\mathsf{X}} \mathsf{C}_{\mathsf{X},\mathsf{X}}$$
(B.18.4)

3. The heat exchange between the coolant jacket and the reactor is 100% effective. (There is no heat loss. Therefore the Therefore  $\dot{Q}$  in the reactor energy balance equation (B.12) is the same as the  $\dot{Q}$  in the jacket energy balance equation (B.13).

4. All species have the same molar volume. Molar volumes are independent of temperature and composition. The molar volume is designated  $\frac{1}{C_T}$ , where  $C_T$  is the total concentration of any stream in [moles/liter].

5. The reactor is well stirred so the concentrations and temperatures of the exit stream are the same as those inside the reactor tank.

$$C_A = C_{A,E}, C_B = C_{B,E}, C_C = C_{C,E}, C_D = C_{D,E}, C_S = C_{S,E}, T = T_E$$

and therefore

$$\widetilde{H}_{A} = \widetilde{H}_{A,E} \ , \ \widetilde{H}_{B} = \widetilde{H}_{B,E} \ , \ \widetilde{H}_{C} = \widetilde{H}_{C,E} \ , \ \widetilde{H}_{D} = \widetilde{H}_{D,E} \ , \ \widetilde{H}_{S} = \widetilde{H}_{S,E}$$

#### X. KNOWN Physical Properties and Problem Specifications

Flowrates:  $F_1 = 20$ ,  $F_2 = 10$ ,  $F_X = 100$  [liters/min] (need to convert these to per second) Concentrations:  $C_{A,1} = 4.0$ ,  $C_{B,2} = 3.0$  [moles/liter]

 $C_{S,1}, C_{S,2}, C_{X,X}$  - known from equation (B.16.1), (B.16.1), & (B.16.4) [moles/liter]

Temperatures:  $T_1 = 298$ ,  $T_2 = 350$ ,  $T_{x,in} = 273$  [Kelvin]

Volume of the reactor: V = 200 [liters]

Volume of the jacket:  $V_i = 20.0$  [liters]

Area for heat transfer: A = 0.0615 [meters<sup>2</sup>]

Heat transfer coefficient U = 1000.0 [Joules/sec/K/meters<sup>2</sup>]

Heat transfer rate: Q - known from equation (B.14) [Joules/sec]

Stream Volumetric Enthalpies:  $\tilde{H}_1$ ,  $\tilde{H}_2$ ,  $\tilde{H}_E$ ,  $\tilde{H}_C$  functional forms known from equations (B.18.1), (B.18.2), (B.18.3), & (B.18.4) [Joules/liter]

Component Molar Heat Capacities:  $\hat{C}_{p,A} = 3.0$ ,  $\hat{C}_{p,B} = 5.0$ ,  $\hat{C}_{p,C} = 6.0$ ,  $\hat{C}_{p,D} = 7.0$ ,  $\hat{C}_{p,S} = 4.184$ ,  $\hat{C}_{p,X} = 4.184$  [Joules/mole/K]

Molar Volume:  $\frac{1}{C_T} = \frac{1}{55.5556} = 0.018$  liters/mole (the molar volume of water)

stoichiometric coefficients:  $\upsilon_A$ ,  $\upsilon_B$ ,  $\upsilon_C$ ,  $\upsilon_D$ , reaction rate prefactor:  $k_0$ , reaction activation energy:  $E_a$ , and heat of reaction:  $\Delta H_r$  - given or obtained in computer project 01.

Initial Conditions: (We need 7 because we have 7 ordinary differential equations.)

- concentrations in reactor:  $C_A(t_o) = C_B(t_o) = C_C(t_o) = C_D(t_o) = 0$ ,  $C_S(t_o) = C_T$
- temperature in reactor:  $T(t_o) = T_{x,in}$
- outlet temperature of coolant:  $T_{X,out}(t_o) = T_{X,in}$

## XI. UNKNOWN Variables

We have eight independent unknowns. The flowrate of the reactor effluent, the composition of the reactor effluent (5), the temperature of the reactor effluent, and the temperature of the jacket exit stream.

$$F_{E}, C_{A}, C_{B}, C_{C}, C_{D}, C_{S}, T, T_{X,out}$$

The enthalpies are not independent unknowns because, if we know the 8 variables above, then we can calculate the enthalpies. Similarly, the rate of heat transfer from the reactor to the jacket,  $\dot{Q}$ , is not an unknown. If we know the reactor and jacket temperatures, we can calculate the heat transfer.

If we have 8 independent unknowns, then we need 8 independent equations. These equations are five material balances, equations (B.7) to (B.11); a reactor energy balance equation (B.12); a jacket energy balance, equation (B.13); and a constraint on the mole fractions in the reactor, equation (B.16.3).

Of these equations 7 are first-order nonlinear ordinary differential equations. One is a linear algebraic equation.

#### XII. STEADY-STATE ANALYSIS

At steady state, all time derivatives in our 8 independent equations are zero. The 8 equations then become:

A: 
$$0 = F_1 C_{A,1} - F_E C_{A,E} + v_A C_A^{|v_A|} C_B^{|v_B|} k_o e^{-\frac{E_a}{RT}}$$
(B.19)

B: 
$$0 = F_2 C_{B,2} - F_E C_{B,E} + v_B C_A^{|v_A|} C_B^{|v_B|} k_o e^{-\frac{E_a}{RT}}$$
(B.20)

C: 
$$0 = -F_{E}C_{C,E} + v_{C}C_{A}^{|v_{A}|}C_{B}^{|v_{B}|}k_{o}e^{-\frac{E_{a}}{RT}}$$
(B.21)

D: 
$$0 = -\mathbf{F}_{\mathsf{E}}\mathbf{C}_{\mathsf{D},\mathsf{E}} + \upsilon_{\mathsf{D}}\mathbf{C}_{\mathsf{A}}^{|\upsilon_{\mathsf{B}}|}\mathbf{C}_{\mathsf{B}}^{|\upsilon_{\mathsf{B}}|}\mathbf{k}_{\mathsf{o}}\mathbf{e}^{-\frac{\boldsymbol{L}_{\mathsf{a}}}{\mathsf{R}\mathsf{T}}}$$
(B.22)

-

S: 
$$0 = F_1 C_{s,1} + F_2 C_{s,2} - F_E C_{s,E}$$
 (B.23)

$$0 = F_1 \tilde{H}_1 + F_2 \tilde{H}_2 - F_E \tilde{H}_E - \Delta H_r C_A^{|\nu_A|} C_B^{|\nu_B|} k_o e^{-\frac{E_a}{RT}} + \dot{Q}$$
(B.24)

$$0 = F_{X}\tilde{H}_{X,in} - F_{X}\tilde{H}_{X,out} - \dot{Q}$$
(B.25)

$$C_{A,E} + C_{B,E} + C_{C,E} + C_{D,E} + C_{S,E} = C_{T}$$
 (B.26)

This is a set of 8 nonlinear algebraic equations, with 8 unknowns. We know how to solve this. Your task is to determine the steady-state values of the six unknowns:  $F_E$ ,  $C_A$ ,  $C_B$ ,  $C_C$ ,  $C_D$ ,  $C_S$ , T, and  $T_{out}$ . State what initial guesses you used to converge to the steady state solution. Provide as an appendix to your report a copy of the input file you used for syseqn.m. You do not need to include a copy of syseqn.m, unless you changed it substantially.

Note: This technique will always work in theory. However, in some cases, there is a problem that arises depending upon which numerical method you use to solve the system of equations. The problem is due to the fact that the right hand side of energy balances equation (B.24) and (B.25) can deviate from zero by 100,000 times the magnitude of the mass balances. Therefore, the solver tries only to minimize the energy balances, ignoring the mass balances. This is a problem of poor scaling. It can be remedied in a variety of ways. One way is to make all of the equations dimensionless. A second, less systematic but quicker method, is to look after one iteration at the deviations from 0 for the 8 equations and stick in constant factors to account for the differences in magnitudes. For this case, only the energy balances need these factors and would result in energy balances of the form:

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$$0 = 10^{-5} \cdot \left( F_1 \tilde{H}_1 + F_2 \tilde{H}_2 - F_E \tilde{H}_E - \Delta H_r C_A^{|\upsilon_A|} C_B^{|\upsilon_B|} k_o e^{-\frac{E_a}{RT}} + \dot{Q} \right)$$
(B.24)

$$0 = 10^{-5} \cdot \left( F_{X} \widetilde{H}_{X,\text{in}} - F_{X} \widetilde{H}_{X,\text{out}} - \dot{Q} \right)$$
(B.25)

The equations are still true since multiplying zero by a constant is still zero. What it does do is make the deviation from zero on the same order of magnitude for all eight equations.

Your second task, is to find the steady states for the adiabatic system (Use U=0.0.)

#### XIII. TRANSIENT ANALYSIS

We have our eight equations.

A: 
$$V \frac{dC_{A}}{dt} = F_{1}C_{A,1} - F_{E}C_{A,E} + v_{A}C_{A}^{|v_{A}|}C_{B}^{|v_{B}|}k_{o}e^{-\frac{E_{a}}{RT}}$$
 (B.7)

B: 
$$V \frac{dC_B}{dt} = F_2 C_{B,2} - F_E C_{B,E} + v_B C_A^{|v_A|} C_B^{|v_B|} k_0 e^{-\frac{E_a}{RT}}$$
 (B.8)

C: 
$$V \frac{dC_{c}}{dt} = 0 - F_{E}C_{C,E} + v_{c}C_{A}^{|v_{A}|}C_{B}^{|v_{B}|}k_{o}e^{-\frac{E_{a}}{RT}}$$
 (B.9)

D: 
$$V \frac{dC_{\rm D}}{dt} = 0 - F_{\rm E}C_{\rm D,E} + \upsilon_{\rm D}C_{\rm A}^{|\upsilon_{\rm A}|}C_{\rm B}^{|\upsilon_{\rm B}|}k_{\rm o}e^{-\frac{E_{\rm a}}{RT}}$$
(B.10)

S: 
$$V \frac{dC_s}{dt} = F_1 C_{s,1} + F_2 C_{s,2} - F_E C_{s,E} + 0$$
 (B.11)

$$V\frac{d\widetilde{H}}{dt} = F_1\widetilde{H}_1 + F_2\widetilde{H}_2 - F_E\widetilde{H}_E - \Delta H_r C_A^{|\nu_A|} C_B^{|\nu_B|} k_o e^{-\frac{E_a}{RT}} + \dot{Q}$$
(B.12)

$$V_{j} \frac{d\tilde{H}_{x}}{dt} = F_{x}\tilde{H}_{x,in} - F_{x}\tilde{H}_{x,out} - \dot{Q}$$
(B.13)

$$\mathbf{C}_{\mathsf{A}} + \mathbf{C}_{\mathsf{B}} + \mathbf{C}_{\mathsf{C}} + \mathbf{C}_{\mathsf{D}} + \mathbf{C}_{\mathsf{S}} = \mathbf{C}_{\mathsf{T}} \tag{B.16.3}$$

There are two practical problems with this formulation. First, equation (B.16.3) is not an ODE. We can rearrange it

$$\mathbf{C}_{\mathrm{S}} = \mathbf{C}_{\mathrm{T}} - \mathbf{C}_{\mathrm{A}} - \mathbf{C}_{\mathrm{B}} - \mathbf{C}_{\mathrm{C}} + \mathbf{C}_{\mathrm{D}} \tag{B.27}$$

If we do this, then the ODE for  $\frac{dC_s}{dt}$ , equation (B.11), is redundant. The solution is to discard equation (B.16.3) in favor of (B.11) because we will need  $\frac{dC_s}{dt}$  later on. Moreover, we have no way to determine the flowrate,  $F_E$ . We need some other way to calculate the volumetric flowrate of the effluent stream. We can do this simply enough by writing a consistent volume balance. There is no accumulation of volume in the tank so

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$$F_{E} = F_{1} + F_{2} + \frac{1}{C_{T}} \left( \sum_{i=1}^{4} v_{i} \right) C_{A}^{|v_{A}|} C_{B}^{|v_{B}|} k_{o} e^{-\frac{E_{a}}{RT}}$$
(B.28)

We can solve this algebraic equation at each time step so we then have a value of  $F_E$ , needed to solve the ODEs. Equation (B.28) must be evaluated before we try to evaluate the time derivatives.

The second problem is discovered when we look at the reactor energy balance. If we substitute in for the enthalpy we obtain:

$$V \frac{d(T - T_{o})(\hat{C}_{p,A}C_{A} + \hat{C}_{p,B}C_{B} + \hat{C}_{p,C}C_{C} + \hat{C}_{p,D}C_{D} + \hat{C}_{p,S}C_{S})}{dt} = F_{1}\tilde{H}_{1} + F_{2}\tilde{H}_{2} - F_{E}\tilde{H}_{E} - \Delta H_{r}C_{A}^{|\nu_{A}|}C_{B}^{|\nu_{B}|}k_{o}e^{-\frac{E_{a}}{RT}} + \dot{Q}$$
(B.29)

We take the derivative on the left hand side of the equation and we eliminate the reference temperature, To, by setting it to 0 Kelvin, on the right hand side of the equation to obtain:

$$VT\left(\hat{C}_{p,A}\frac{dC_{A}}{dt} + \hat{C}_{p,B}\frac{dC_{B}}{dt} + \hat{C}_{p,C}\frac{dC_{C}}{dt} + \hat{C}_{p,D}\frac{dC_{D}}{dt} + \hat{C}_{p,S}\frac{dC_{S}}{dt}\right) + V\left(\hat{C}_{p,A}C_{A} + \hat{C}_{p,B}C_{B} + \hat{C}_{p,C}C_{C} + \hat{C}_{p,D}C_{D} + \hat{C}_{p,S}C_{S}\right)\frac{dT}{dt}$$
(B.30)  
$$= F_{1}\tilde{H}_{1} + F_{2}\tilde{H}_{2} - F_{E}\tilde{H}_{E} - \Delta H_{r}C_{A}^{|\nu_{A}|}C_{B}^{|\nu_{B}|}k_{o}e^{-\frac{E_{a}}{RT}} + \dot{Q}$$

We arrange this in the following form:

$$\frac{dT}{dt} = \frac{\left[-VT\left(\hat{C}_{p,A}\frac{dC_{A}}{dt} + \hat{C}_{p,B}\frac{dC_{B}}{dt} + \hat{C}_{p,C}\frac{dC_{C}}{dt} + \hat{C}_{p,D}\frac{dC_{D}}{dt} + \hat{C}_{p,S}\frac{dC_{S}}{dt}\right)\right]}{V\left(\hat{C}_{p,A}C_{A} + \hat{C}_{p,B}C_{B} + \hat{C}_{p,C}C_{C} + \hat{C}_{p,D}C_{D} + \hat{C}_{p,S}C_{S}\right)}$$
(B.31)

This equation requires that you already know the time derivatives of the concentrations.

Performing the same substitution and rearranging the energy balance on the jacket we obtain:

$$V_{j} \frac{d(T_{X,out} - T_{o})\hat{C}_{p,X}C_{X,X}}{dt} = F_{X}(T_{X,in} - T_{o})\hat{C}_{p,X}C_{X,X} - F_{X}(T_{X,out} - T_{o})\hat{C}_{p,X}C_{X,X} - \dot{Q}$$
(B.32)

We take the derivative on the left hand side of the equation and we eliminate the reference temperature, To, by setting it to 0 Kelvin, on the right hand side of the equation to obtain:

$$V_{j}\hat{C}_{p,X}C_{X,X} \frac{dT_{X,out}}{dt} = F_{X}T_{X,in}\hat{C}_{p,X}C_{X,X} - F_{X}T_{X,out}\hat{C}_{p,X}C_{X,X} - \dot{Q}$$
(B.33)

We didn't encounter the same trouble with the energy balance on the jacket as we did with the energy balance on the reactor because there is only one component in the jacket so the concentration doesn't change with time.

We can solve this system of equations using the standard sysode.m code if we order the equations properly in the input file. First we put equation (B.28) to obtain  $F_E$ . Then we put equations (B.7) through (B.11) and (B.13) to obtain all of the concentration time derivatives and the jacket temperature time derivative. Lastly, we put equation (B.31) to obtain the reactor temperature time derivative.

The task here is to solve the system of nonlinear ODEs. Generate plots of

$$\mathsf{C}_{\mathsf{A}},\,\mathsf{C}_{\mathsf{B}},\,\mathsf{C}_{\mathsf{C}},\,\mathsf{C}_{\mathsf{D}},\,\mathsf{C}_{\mathsf{S}},\mathsf{T},\mathsf{T}_{\mathsf{X},\mathsf{out}}$$

as a function of time for the non-isothermal, non-adiabatic case. Comment on your physical understanding of the plots. You will need to determine the duration of your solution (the time at which you quit solving the ODEs) based upon how long it takes for your particular system to reach steady-state. You should show the unambiguous approach to a steady-state.

## References

- 1. Smith, J.M., "Chemical Engineering Kinetics", J.M. Smith, McGraw-Hill, 3rd Edition, New York, 1981, Example 5.4, page 249-250.
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- 4. Weber, F., Bruns, D., "Writing Guidelines for ChE 310 & 410", University of Tennessee, Department of Chemical Engineering, http://clausius.engr.utk.edu/che310