Solutions for Tutorial 4
Modelling of Non-Linear Systems

4.1 Isothermal CSTR: The chemical reactor shown in textbook Figure 3.1 and repeated in the following is considered in this question. The reaction occurring in the reactor is

$$A \rightarrow B \qquad\qquad r_A = -kC_A^{0.5}$$

The following assumptions are appropriate for the system.
(i) the reactor is well mixed,
(ii) the reactor is isothermal,
(iii) density of the liquid in the reactor is constant,
(iv) flow rates are constant, and
(v) reactor volume is constant.

a. Formulate the model for the dynamic response of the concentration of A in the reactor, $C_A(t)$.
b. Linearize the equation(s) in (a).
c. Solve the linearized equation analytically for a step change in the inlet concentration of A, ΔC_{A0}.
d. Sketch the dynamic behavior of $C_A(t)$.
e. Discuss how you would evaluate the accuracy of the linearized model.

Goal → Variable System→ Balance→ DOF → Linear?
(or constitutive equation)

Again, we apply the standard modelling approach, with a check for linearity.

a. Goal: Determine composition of A as a function of time.

Variable: C_A in the reactor

System: The liquid in the reactor.

Balance: Component balance on A.

Accumulation = in - out + generation

(1) $$MW_A\left(VC_A|_{t+\Delta t} - VC_A|_t\right) = MW_A \Delta t\left(FC_{A0} - FC_A - VkC_A^{0.5}\right)$$

Divide by delta time and take the limit to obtain

$$(2) \qquad V\frac{dC_A}{dt} = F(C_{A0} - FC_A) - VkC_A^{0.5}$$

Are we done? Let's check the degrees of freedom.

DOF = 1 - 1 = 0 Yes!

b. Is the model linear? If we decide to solve the model numerically, we do not have to linearize; in fact, the non-linear model would be more accurate. However, in this problem we seek the **insight** obtained from the approximate, linear model.

All terms involve a constant times a variable (linear) except for the following term, which is linearized using the Taylor series..

$$(3) \qquad C_A^{0.5} \approx \left(C_A^{0.5}\right)_s + 0.5\left(C_A^{-0.5}\right)_s (C_A - C_{As}) + \text{higher order terms}$$

This approximation can be substituted into equation 2, and the initial steady-state model subtracted to obtain the following, with $C'_A = C_A - C_{AS}$.

$$(4) \qquad V\frac{dC'_A}{dt} = F(C'_{A0} - FC'_A) - Vk(0.5C_{As}^{-0.5})C'_A$$

This linear, first order ordinary differential equation model can be arranged into the standard form, given in the following.

$$(5) \qquad \tau\frac{dC'_A}{dt} + C'_A = KC'_{A0} \quad \text{with} \quad \tau = \frac{V}{F + 0.5VkC_{As}^{-0.5}} \qquad K = \frac{F}{F + 0.5VkC_{As}^{-0.5}}$$

c. Let's solve this equation using the Laplace transform method. We can take the Laplace transform of equation (5) to obtain

$$(6) \qquad \tau\left(sC'_A(s) - C'_A(t)|_{t=0}\right) + C'_A(s) = KC'_{A0}(s)$$

Note that equation (6) is general for any function $C_{A0}(t)$. We can rearrange this equation and substitute the Laplace transform of the step change in feed composition ($C'_{A0}(s) = \Delta C_{A0}/s$ to give.

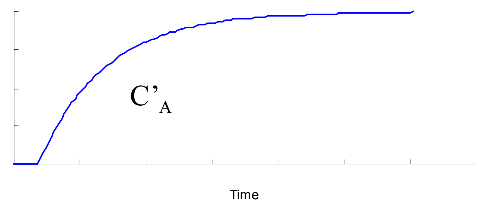
$$(7) \qquad C'_A(s) = \frac{K}{\tau s + 1}\frac{\Delta C_{A0}}{s}$$

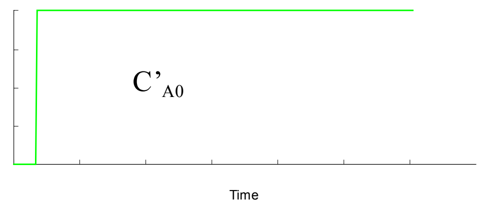
We can take the inverse Laplace transform using entry 5 in textbook Table 4.1 to give

(8) $C'_A(t) = \Delta C_{A0} K (1 - e^{-t/\tau})$

d. A typical sketch is given here. We already have experience with the step response to a linear, first order system. We know that

- the output changes immediately after the step is introduced.
- the maximum slope appears when the step is introduced
- the curve has a smooth (non-oscillatory response)
- 63% of the change occurs when $t = \tau$ (past the step)
- the final steady state is K(Δinput)





e. We should always investigate the accuracy of our mathematical models! We can estimate the accuracy of the parameters used based on

Laboratory data used in developing the constitutive model	- Is the rate expression accurate - uncertainty in k
Construction of equipment	V (cross sectional area)
Accuracy of measurements used to achieve desired values	V (level) and F (flow)

In addition, we should estimate the error introduced by the linearization. No error is introduced if the process stays exactly at the initial steady state, and the errors generally increase as the process deviates further from the initial steady state. Here, two methods are suggested. (Remember, we do not seek highly accurate models – we seek simple, approximate models for control design, which will be explained shortly.)

1. **Evaluate the key parameters over the range of operation**. We can evaluate the gain (K) and the time constant (τ) at different values over the range of operation. If these parameters do not change much, the linearization would be deemed accurate.

2. **Steady-state prediction**. Compare the steady-state output values from the non-linear model with steady-state output values from the linearized model (KΔinput). This method will check the gain only, not the time constant.

4.2 Controlling the Reactor Concentration by Feed Flow Rate: The reactor in question 3.1 above is considered again in this question. Component A is pumped to the reactor from the feed tank. The inlet concentration of A, C_{A0}, is *constant*, and the feed flow rate varies with time.

a. Develop the dynamic model to predict the concentration of A.
b. Linearize the equation and solve the linearized equation analytically for a step change in the feed flow rate, ΔF.
c. Sketch the dynamic behavior of the effluent concentration, $C_A(t)$.
d. Describe the equipment required to maintain the feed flow rate at a desired value.

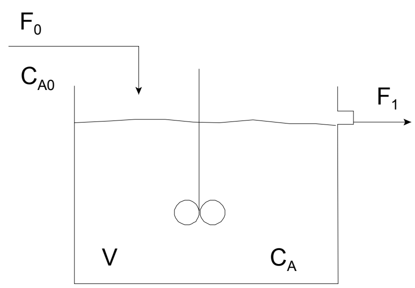


Figure 3.1

Motivation: Why are we interested in this model? Often, the feed composition cannot be adjusted easily by mixing streams. Therefore, we sometimes adjust the feed flow rate to achieve the desired reaction conversion. (We do not like to do this, because we change both the production rate and the conversion when we adjust feed flow rate.)

a. We begin by applying our standard method for modelling.

a. Goal: Determine composition of A as a function of time.

Variable: C_A in the reactor

System: The liquid in the reactor.

Balance: Component balance on A.

Accumulation = in - out + generation

(1) $$MW_A\left(VC_A|_{t+\Delta t} - VC_A|_t\right) = MW_A \Delta t\left(FC_{A0} - FC_A - VkC_A^{0.5}\right)$$

Divide by delta time and take the limit to obtain

(2) $$V\frac{dC_A}{dt} = F(C_{A0} - FC_A) - VkC_A^{0.5}$$

Are we done? Let's check the degrees of freedom.

DOF = 1 - 1 = 0 Yes!

b. Is the model linear? If we decide to solve the model numerically, we do not have to linearize; in fact, the non-linear model would be more accurate. However, in this problem we seek the **insight** obtained from the approximate, linear model.

We see that several terms are non-linear. In fact, when flow is a variable, we would usually find terms (F)(variable), where "variable" is temperature, compositions, etc. The following terms will be linearized by expanding the Taylor series.

(3) $$FC_{A0} \approx (FC_{A0})_s + F_s C'_{A0} + C_{A0s}F' + \text{higher order terms}$$

(4) $$FC_A \approx (FC_A)_s + F_s C'_A + C_{As}F' + \text{higher order terms}$$

(5) $$C_A^{0.5} \approx \left(C_A^{0.5}\right)_s + 0.5\left(C_A^{-0.5}\right)_s (C_A - C_{As}) + \text{higher order terms}$$

Substituting the approximations, subtracting the initial steady state, and rearranging gives the following.

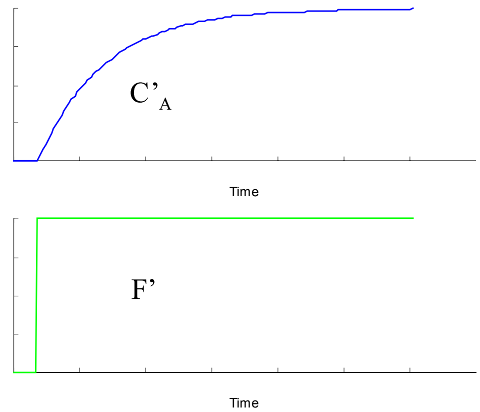
(6) $$\tau\frac{dC'_A}{dt} + C'_A = KF' \qquad \text{with } \tau = \frac{V}{F_s + 0.5VkC_{As}^{-0.5}} \qquad K = \frac{(C_{A0s} - C_{As})}{F_s + 0.5VkC_{As}^{-0.5}}$$

We can solve this equation for step change in flow rate by taking the Laplace transform, substituting F'(s) = ΔF/s, and taking the inverse Laplace transform. The result is given in the following equation.

(7) $$C'_A(t) = (\Delta F)K\left(1 - e^{-t/\tau}\right)$$

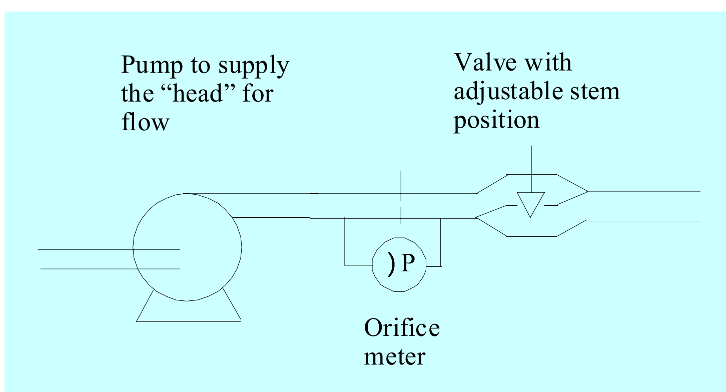
c. The plot and qualitative properties are the same as for other first order systems.

- the output changes immediately after the step is introduced.
- the maximum slope appears when the step is introduced
- the curve has a smooth (non-oscillatory response)
- 63% of the change occurs when $t = \tau$ (past the step)
- the final steady state is $K(\Delta \text{input})$



Does this make sense? As we increase the feed flow, the "space time" in the reactor decreases. (See Fogler (1999) or other textbook on reaction engineering for a refresher.) When the space time decreases, the conversion decreases, and the concentration of reactant increases. **Yes, the model agrees with our qualitative understanding!**

d. **Equipment** is required to control the flow is needed if we are to adjust the flow to achieve the desired reactor operation, e.g., conversion. Any feedback controller requires a sensor and a final element. (See Chapter 2.) The sensor could be any of the sensors described in the Instrumentation Notes. The most common sensor in the process industries is the orifice meter, which measures flow based on the pressure drop around an orifice restriction in a pipe. The final element would be a control valve that can adjust the restriction to flow.



4.3 Isothermal CSTR with *two* input changes: This question builds on the results from tutorial Questions 3.1 and 3.2. Consider a CSTR with the following reaction occurring in the reactor

$$A \rightarrow B \qquad -r_A = kC_A^{0.5}$$

Assuming 1) the reactor is isothermal, 2) the reactor is well mixed, 3) density of the reactor content is constant, and 4) the reactor volume is constant.

a. Derive the linearized model in deviation variables relating a change in C_{A0} on the reactor concentration, C_A.

b. Derive the linearized model in deviation variables relating a change in F on the reactor concentration, C_A.

c. Determine the transfer functions for the two models derived in parts a and b.

d. Draw a block diagram relating C_{A0} and F to C_A.

e. The following input changes are applied to the CSTR:

   1. A step change in feed concentration, C_{A0}, with step size ΔC_{A0} at t_C, and
   2. A step change in feed flow rate, F, with step size ΔF at t_F.> t_C.

   Without solving the equations, sketch the behavior of $C_A(t)$.

a/c. The model for the change in C_{A0} (with the subscript meaning the input change C_{A0}). The model for this response has been derived in previous tutorial question 3.1, and the results are repeated in the following.

$$\tau_{CA0}\frac{dC'_A}{dt} + C'_A = K_{CA0}C'_{A0} \quad \text{with} \quad \tau_{CA0} = \frac{V}{F + 0.5VkC_{As}^{-0.5}} \qquad K_{CA0} = \frac{F}{F + 0.5VkC_{As}^{-0.5}}$$

(1) $$(C'_A(s))_{CA0} = \frac{K_{CA0}}{\tau_{CA0}s + 1}C'_{A0}(s) \qquad \text{transfer function} \qquad \frac{(C_A(s))_{CA0}}{C_{A0}(s)} = \frac{K_{CA0}}{\tau_{CA0}s + 1}$$

$$C'_A(t) = \Delta C_{A0}K_{CA0}\left(1 - e^{-t/\tau_{CA0}}\right)$$

b/c. The model for a change in F (with the subscript meaning the input change F) The model for this response has been derived in previous tutorial question 3.2, and the results are repeated in the following.

$$\tau_F \frac{dC'_A}{dt} + C'_A = K_F F' \quad \text{with} \quad \tau_F = \frac{V}{F_s + 0.5VkC_{As}^{-0.5}} \qquad K_F = \frac{(C_{A0s} - C_{As})}{F_s + 0.5VkC_{As}^{-0.5}}$$

(2) $$(C'_A(s))_F = \frac{K_F}{\tau_F s + 1} F'(s) \qquad \text{transfer function} \qquad \frac{(C_A(s))_F}{F(s)} = \frac{K_F}{\tau_F s + 1}$$

$$C'_A(t) = (\Delta F) K_F \left(1 - e^{-t/\tau_F}\right)$$

c. The transfer functions are given in the results above.

Remember that a transfer function simply gives the relationship between the input and output.

INPUT → TRANSFER FUNCTION → OUTPUT

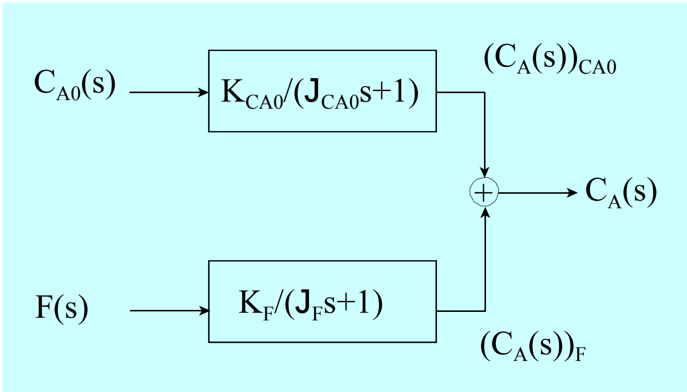
Since the system is linearized, we can add the output changes in C'_A to determine the overall affect.

(3) $$(C'_A(s)) = (C'_A(s))_{CA0} + (C'_A(s))_F$$

d. The block diagram is given in the figure.

Note that the primes (') to designate deviation variables are not used in transfer functions or block diagrams. This is because transfer functions and block diagrams ALWAYS use deviation variables.

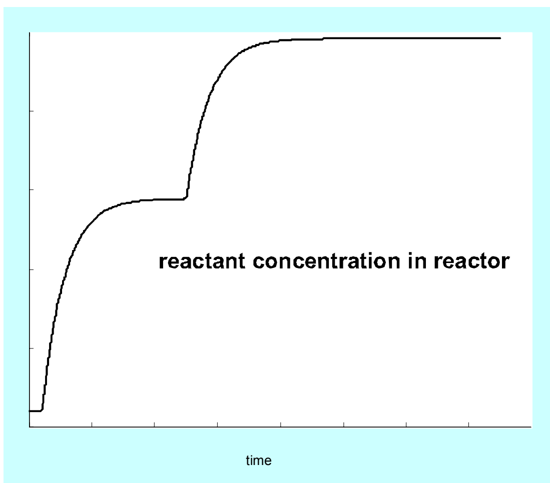
Remember that the block diagram is simply a picture of equations (1) to (3).



e. We can sketch the shape of the response without knowing the numerical values of many parameters because we understand dynamic systems. Let's list some aspects of the response that we know.

1. K_F is positive
2. K_{CA0} is positive
3. Both systems are first order
4. The two time constants are equal
5. Both systems are stable (time constants are positive)

The figure below was generated with 1) a positive step change in CA0 and after a long time, a positive step change in F.



What would the plots look like with

a. a positive change in C_{A0} and a negative in F?
b. both changes introduced at the same time?
c. A slow ramp introduced in C_{A0}?

Can you think of other types of input changes and sketch the output concentration?

4.4 Let's consider the usefulness of the transfer functions that we just derived. From the transfer function $C_A(s)/C_{A0}(s)$, answer the following questions.

a.	Does a causal relationship exist?	**Hint:** How could the process gain help?
b.	What is the order of the system?	**Hint:** How many differential equations are in the model?
c.	Is the system stable?	**Wow:** we sure need to know if a process is unstable!
d.	Could $C_A(t)$ exhibit oscillations from a step change in C_{A0}?	**Question:** Why would we like to know this?
e.	Would any of your answer change for any values of the parameters of the model (F, V, k, etc.)?	**Important:** We can learn general types of behavior for some processes!

a. A causal relationship exists if the transfer function is NOT zero. While this is not *exactly* correct, we will test for the existence of a causal relationship by evaluating the steady-state gain.

$K = 0 \Rightarrow$ no causal relationship $K \neq 0 \Rightarrow$ causal relationship

We should also look at the magnitude of the gain.

The answer for $C_A(s)/C_{A0}(s)$ is yes; a causal relationship exists!

Follow-up question: Can you think of a situation in which the steady-state gain is zero, but a causal relationship exists?

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b. The order of the system is the number of first order differential equations that relate the input to the output.

One quick way to check this is to evaluate the highest power of "s" in the denominator of the transfer function.

The answer for $C_A(s)/C_{A0}(s)$ is one, or first order.

Follow-up question: Are the order of all input/output pairs the same for any processes? Hint: What is the order of $C_B(s)/C_{A0}(s)$ for the same reactor?

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c. The system is stable if the output is bounded for a bounded input. (Any real input is bounded, but a ramp could become infinite when we overlook the physical world, where valves open completely and mole fractions are bounded between 0 and 1.)

We determine stability by evaluating sign of the exponent relating the variable to time. Recall that $y = A\, e^{-\alpha t} = A\, e^{-t/\tau}$. The value of alpha is the root(s) of the denominator of the transfer function!

$\alpha = 1/\tau > 0$ $\Rightarrow$ stable **$\alpha = 1/\tau \leq 0$ $\Rightarrow$ stable**

The answer for $C_A(s)/C_{A0}(s)$ is $\tau > 0$; therefore, the system is stable.

Follow-up question: If one variable in a system is stable (unstable), must all other variables in the system be stable (unstable)?

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d. The function form of the time dependence of concentration is given in the following.

$$C'_A(t) = \Delta C_{A0} K_{CA0} \left(1 - e^{-t/\tau_{CA0}}\right)$$

When the roots of the denominator of the transfer function are real, the system will be over damped (or critically damped).

The answer for $C_A(s)/C_{A0}(s)$ is no.

Follow-up question: If one variable in a system is overdamped (underdamped), must all other variables in the system be overdamped (underdamped)?

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e. We can determine possible types of behavior by looking at the range of (physically possible) values for the parameters in a process. (We must assume that the model structure, i.e., the equations, is correct.)

The parameters in the model are all positive; none can change sign. For this and the equations for the gain and time constant, we conclude that

The answer for $C_A(s)/C_{A0}(s)$ is no, the qualitative features (causal, first order, stable) cannot change.

You can test your understanding by answering these questions for any other model in the course!

Now, you can apply your analysis skills to another process!

4.5 Process plants contain many interconnected units. (As we will see, a control loop contains many interconnected elements as well.) Transfer functions and block diagrams help us combine individual models to develop an overall model of interconnected elements.

Select some simple processes that you have studied and modelled in this course.

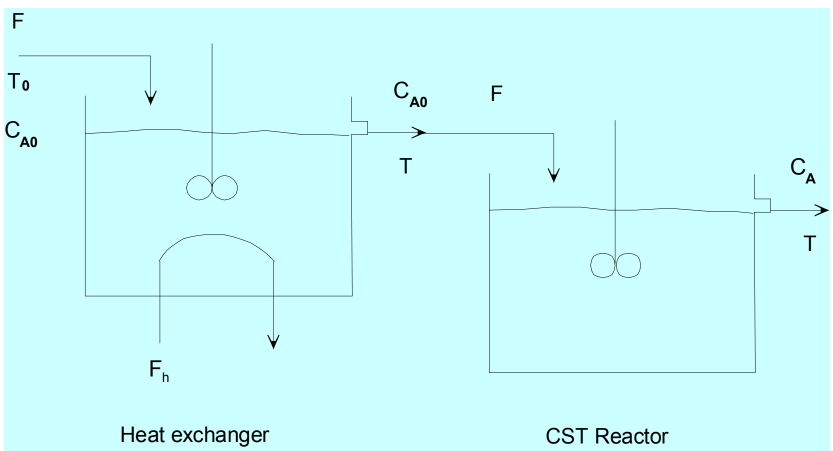
a. Connect them is series.

b. Derive an overall input-output model based on the individual models.

c. Determine the gain, stability and damping.

d. Sketch the response of the output variable to a step in the input variable.

a. Series process - As a sample problem, we will consider the heat exchanger and reactor series process in the following figure. This is a common design that provides flexibility by enabling changes to the reactor temperature. As we proceed in the course, we will see how to adjust the heating medium flow to achieve the desired reactor operation using feedback control.



In this example, the heating medium flow, F_h, (valve opening) is manipulated, and the concentration of the reactant in the reactor, C_A, is the output variable.

As we proceed in the course, we will see how to adjust the heating medium flow to achieve the desired reactor operation using automatic feedback control.

Heat exchanger: The heat exchanger model is derived in the textbook Example 3.7, page 76. The results of the modelling are summarized in the following, with the subscript "c" changed to "h", because this problem involves heating.

Energy balance: (with $C_p \approx C_v$)

$$V_{ex} \rho C_p \frac{dT}{dt} = F\rho Cp(T_0 - T) + Q - W$$

with $Q = UA(T - (T_{hin} + T_{hout})/2)$ and $UA = \frac{aF_c^{b+1}}{F_c + aF_c^b / 2\rho_h C_{ph}}$

Linearized model:

$$\tau_{ex} \frac{dT'}{dt} + T' = K_{pex} F_c'$$ with the subscript "ex" for exchanger.

Transfer function: (Taking the Laplace transform of the linearized model)

$$\frac{T(s)}{F_h(s)} = \frac{K_{pex}}{\tau_{ex} s + 1} = G_{ex}(s)$$ a first order system!

Non-isothermal CSTR: The basic model of the CSTR is given in textbook equations (3.75) and (3.76), which represent the component material and energy balances. They are repeated below, with **typographical errors corrected here**!

$$V \frac{dC_A}{dt} = F(C_{A0} - C_A) - Vk_0 e^{-E/RT} C_A$$

$$V\rho C_p \frac{dT}{dt} = F\rho C_p (T_0 - T) - UA(T - T_{cin}) + (-\Delta H_{rxn}) Vk_0 e^{-E/RT} C_A$$

These equations are linearized in Appendix C to give the following approximate model, with only input T_0 varying.

$$\frac{dC'_A}{dt} = a_{11} C'_A + a_{12} T'$$
$$\frac{dT'}{dt} = a_{21} C'_A + a_{22} T' + a_{25} T'_0$$

We can take the Laplace transform of the linearized equations and combine them by eliminating the reactor temperature, T', to give the following transfer function.

$$\frac{C'_A(s)}{T'_0(s)} = \frac{a_{25}}{s^2 - (a_{11} + a_{22})s + (a_{11}a_{22} - a_{12}a_{21})} = G_r(s)$$ a second order system

Note that the reactor is a second order system because the energy balance relates inlet temperature to reactor temperature and the component material balance relates temperature to concentration, because of the effect of temperature on reaction rate.

b. Combining the linearized models: The block diagram of this system is given in the following figure. This is a series connection of two processes, a first order exchanger and a second order reactor, which gives the overall third order transfer function given in the following equation.

$$\frac{C'_A(s)}{T'_0(s)} = \frac{T'(s)}{T'_0(s)}\frac{C'_A(s)}{T'(s)} = G_{ex}(s)G_r(s) = \frac{K_{pex}}{(\tau_{ex}s+1)}\frac{a_{25}}{\left(s^2-(a_{11}+a_{22})s+(a_{11}a_{22}-a_{12}a_{21})\right)}$$

Note that heat exchanger and reactor are a third order system.

c. Model analysis –

Gain: The steady-state gain can be derived from this model by setting s=0. (Recall that this has meaning only if the process is stable.) The gain in this system is none zero, as long as the chemical reaction depends on temperature.

Damping: We cannot be sure that the roots of the denominator of the transfer function are real. If fact, the analysis of the CSTR in textbook Appendix C shows that the dynamics can be either over or underdamped, depending on the design and operating parameters.

Stability: We cannot be sure that the CSTR is stable, i.e., roots of the denominator of the transfer function have negative real parts. If fact, the analysis of the CSTR in textbook Appendix C shows that the dynamics can be either stable or unstable, depending on the design and operating parameters.

d. Step response: Many different responses are possible for the CSTR, and only one case is sketched here. Recall the dynamic response between T_0 and T_1 is first order. Since we have copious experience with this step response, it is not given in a sketch. An example of the response between T_0 and T_3 are given in the following figure. The plot is developed for an example without heat of reaction. In this situation, the third order system is guaranteed to be stable and overdamped; as we expect, the response has an "s-shaped" output response to a step input, with the reactant concentration decreasing in response to an increase in heating fluid to the exchanger.

Reactant concentration

Heating fluid valve opening