SECTION II
(Modeling for Control)

II.1 Consider a continuous blending process where the water is mixed with slurry to give slurry the desired consistency (Figure II.1). The streams are mixed in a constant volume (*V*) blending tank, and the mass fraction of the solids in the inlet slurry stream is given as x_s, with a volumetric flow rate of q_s. Since x_s and q_s vary, the water make-up mass flow rate *w* is adjusted to compensate for these variations. Develop a model for this blender that can be used to predict the dynamic behavior of the mass fraction of solids in the exit stream x_e for changes in x_s, q_s, or *w*. What is the number of degrees of freedom for this process?
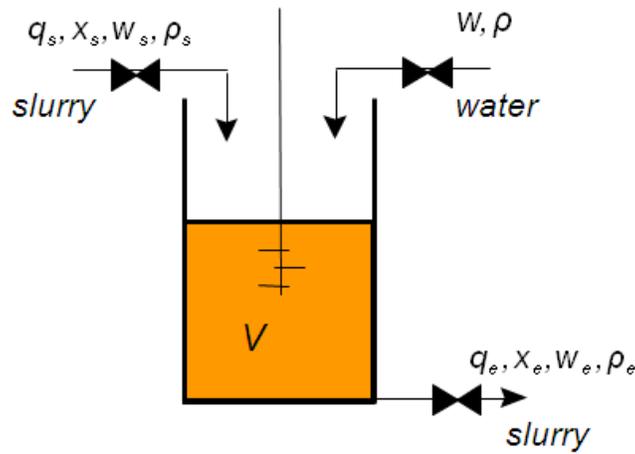

Figure II.1: Schematic of the blending process

Solution:

Let us assume that we have perfect mixing and no volume changes due to mixing. Water stream is considered to be pure water and ρ_t is the density of solid. The mass flow rates of each stream are designated by w and the volumetric rates are by q. Then, by definition, we have the following,

$$w_s = \rho_s q_s$$

$$\rho_s = \frac{w_s}{\left(\dfrac{x_s w_s}{\rho_t} + \dfrac{(1-x_s)w_s}{\rho}\right)} = \frac{1}{\left(\dfrac{x_s}{\rho_t} + \dfrac{(1-x_s)}{\rho}\right)}$$

$$\rho_e = \frac{1}{\left(\dfrac{x_e}{\rho_t} + \dfrac{(1-x_e)}{\rho}\right)}$$

The total mass balance yields the following equation,

$$\frac{d(\rho_e V)}{dt} = w_s + w - w_e$$

And since the volume is constant, we have,

$$V\frac{d(\rho_e)}{dt} = w_s + w - w_e$$

A component balance on the solids will give,

$$\frac{d(x_e \rho_e V)}{dt} = w_s x_s - w_e x_e$$

Or,

$$V\frac{d(x_e)}{dt} = -V\frac{d(\rho_e)}{dt} + w_s x_s - w_e x_e = -x_e(w_s + w - w_e) + w_s x_s - w_e x_e$$

This equation along with the definitions of the densities, forms the model of this process to help predict the variations in the mass fraction of solids in the exit slurry as a function of other process variables.

For a degree of freedom analysis, we have,

- Constants: V, ρ, ρ_t
- Number of Equations: 4 (one mass balance + one component balance + two algebraic relations)
- Number of variables: ρ_s, ρ_e, w, w_e, w_s, x_e, x_s

The number of degrees of freedom is 3. Note that one usually needs to specify the upstream solids content (density or solids fraction) and the flow rate as well as the water flow rate to fully define the system.

II.2. A binary mixture at its saturation point is fed to a single-stage flash unit (Figure II.2), where the mixture is heated at an unknown rate (Q). The feed flow rate and feed mole fractions are known and may vary with time. Assume that x represents the mole fraction of the more volatile component (e.g., x_f is the mole fraction of the more volatile component in the feed stream) and the molar heat of vaporization is the same for both components. Flow rate is given in moles per unit time. H represents the molar liquid holdup.
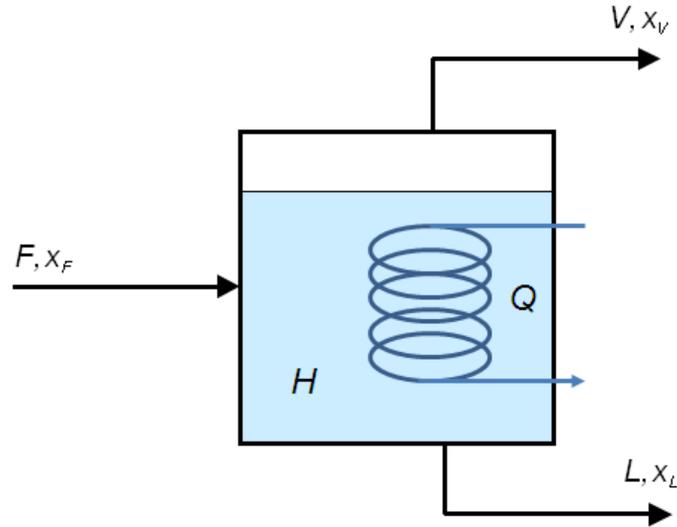
Figure II.2: Schematic of a flash unit.

1. Derive the modeling equations for this system. State your assumptions clearly and explicitly.
2. Derive the transfer function between the overhead mole fraction of the more volatile component and its feed mole fraction. (*Hint:* Assume constant molar holdup.)

Solution:

The control volume is the flash tank. We make the following assumptions:

- Negligible vapor holdup in the unit
- Constant stage temperature and pressure
- No heat loss to surroundings
- Negligible heat transfer resistance for transfer of Q.

The equilibrium relationship is given by:

$$x_D = K(T,P)x_B$$

where is K the equilibrium constant

For the energy balance, the quantity of interest is:

$$\text{Total Energy} = U + K + P$$

Here, U, K, P represent the internal, kinetic and potential energies of the system, respectively. Assuming thermal equilibrium between the vapor and the liquid streams, we can also neglect the energy balance on the vapor phase.

Since the liquid in the tank can be considered stationary

$$\Rightarrow \quad \frac{dK}{dt} = \frac{dP}{dt} = 0 \quad \text{and} \quad \frac{dE}{dt} = \frac{dU}{dt}$$

For liquid systems, one can assume that

$$\frac{dU}{dt} \cong \frac{d\mathbf{H}}{dt}$$

$\mathbf{H}$ denotes the total enthalpy of the liquid in the tank (vapor holdup neglected). Furthermore,

$$\mathbf{H} = H c_{p,B,av} (T - T_{ref})$$

Where:

$c_{p,B,av}$: average molar heat capacity of the liquid in the tank
T_{ref}: reference temperature where the specific enthalpy of the liquid is assumed to be zero.

The average molar heat capacities of the liquid streams can be expressed as:

$$c_{p,F,av} = x_F \, c_{p,A} + (1 - x_F) \, c_{p,C}$$
$$c_{p,B,av} = x_B \, c_{p,A} + (1 - x_B) \, c_{p,C}$$

Total energy balance can be formulated as:

$$\frac{[Accumulation \ of \ total \ energy]}{time} = \frac{[Input \ of \ total \ energy]}{time} - \frac{[Output \ of \ total \ energy]}{time}$$
$$+ \frac{[Energy \ supplied \ by \ steam]}{time}$$

Or

$$\frac{d[H c_{p,B,av}(T - T_{ref})]}{dt} = F c_{p,F,av}(T_{in} - T_{ref}) - B c_{p,B,av}(T - T_{ref}) - D[c_{p,D,av}(T - T_{ref}) + \lambda] + Q$$

where λ is the molar heat of vaporization, and $T_{in} = T$. At steady-state, this reduces to,

$$Q = D\lambda$$

Overall material balance yields,

$$\frac{d(H_M)}{dt} = M_F - M_D - M_B$$

where H_M is the mass holdup of the unit and M_i are the mass flow rates. We can express the mass flow rate as, for example:

$$M_F = MW_A F x_F + MW_C F(1 - x_F) = F[MW_C + x_F(MW_A - MW_C)]$$

This results in the following material balance (molar balance) expression:

$$\frac{d(H[MW_C + x_B(MW_A - MW_C)])}{dt} = F[MW_C + x_F(MW_A - MW_C)]$$
$$- B[MW_C + x_B(MW_A - MW_C)]$$
$$- D[MW_C + x_D(MW_A - MW_C)]$$

The component balance for component A yields,

$$\frac{d(Hx_B MW_A)}{dt} = Fx_F MW_A - Bx_B MW_A - Dx_D MW_A$$

$$\frac{d(Hx_B)}{dt} = Fx_F - Bx_B - Dx_D$$

II.3. An oil stream is heated as it passes through two well-mixed tanks in series (Exercise I.11). Assuming constant physical properties, develop the nonlinear state-space model for this process to predict the time evolution of the temperatures in both tanks. State your assumptions clearly and explicitly.

Solution:

In this problem the state variables are T_1, T_2. Possible time-varying inputs are the heat input and the oil flow rate.

Since the **volumes are assumed constant** we only need to perform an energy balance around each tank

Total energy balance can be formulated as:

$$\frac{[Accumulation\ of\ total\ energy]}{time} = \frac{[Input\ of\ total\ energy]}{time} - \frac{[Output\ of\ total\ energy]}{time}$$
$$+ \frac{[Energy\ supplied\ by\ the\ coil]}{time}$$

$$E = U + KE + PE,$$

where U is the internal energy, KE is the kinetic energy and PE is the potential energy. Since the tank is not moving,

$$\frac{dKE}{dt} = \frac{dPE}{dt} = 0 \, .$$

Thus

$$\frac{dE}{dt} = \frac{dU}{dt} \, ,$$

and for liquid systems,

$$\frac{dU}{dt} = \frac{dH_T}{dt}$$

where, H_T is the total enthalpy of material in the tank. H may be written as,

$$\rho A h C_p \left(T - T_{ref} \right)$$

where $T_{ref \, :}$ is the reference temperature. The energy balance for Tank 1 may be written as:

$$\frac{d\left(\rho V_1 C_p \left(T_1 - T_{ref} \right) \right)}{dt} = \rho F C_p \left(T_{in} - T_{ref} \right) - \rho F C_p \left(T_1 - T_{ref} \right) + Q$$

Assuming $T_{ref} = 0$, we will have:

$$V_1 \frac{d\left(T_1 \right)}{dt} = F T_{in} - F T_1 + \frac{Q}{\rho C_p}$$

$$\frac{dT_1}{dt} = \frac{F}{V_1} \left(T_{in} - T_1 \right) + \frac{Q}{\rho C_p V_1}$$

Similarly for Tank 2 we have

$$\frac{dT_2}{dt} = \frac{F}{V_2} \left(T_1 - T_2 \right)$$

Thus the set of Equation representing the dynamic of the temperatures in the tanks is given by

$$\boxed{\begin{aligned} \frac{d\left(T_1 \right)}{dt} &= \frac{F}{V_1} T_{in} - F T_1 + \frac{Q}{\rho C_p V_1} \\ \frac{d\left(T_2 \right)}{dt} &= \frac{F}{V_2} \left(T_1 - T_2 \right) \end{aligned}}$$

The equations are 'slightly' nonlinear due to the multiplication between the flow rate and the temperatures. Rearranging and taking the Taylor series expansion,

$$\frac{dT_1}{dt} = \frac{F}{V_1}(T_{in} - T_1) + \frac{Q}{\rho c_p V_1} = f_1(F,T_1,Q)$$

$$\approx \left[\frac{F}{V_1}(T_{in} - T_1) + \frac{Q}{\rho c_p V_1}\right]_{ss} + a_1(F - F_s) + a_2(T_1 - T_{1s}) + a_3(Q - Q_s)$$

$$\frac{dT_2}{dt} = \frac{F}{V_2}(T_1 - T_2) = f_2(F,T_1,T_2)$$

$$\approx \left[\frac{F}{V_2}(T_1 - T_2)\right]_{ss} + b_1(F - F_s) + b_2(T_1 - T_{1s}) + b_3(T_2 - T_{2s})$$

We can see that the constant coefficients are given as:

$$a_1 = \frac{\partial f_1}{\partial F}\bigg|_{ss} = \frac{(T_{in} - T_{1s})}{V_1}; a_2 = \frac{\partial f_1}{\partial T_1}\bigg|_{ss} = \frac{-F_s}{V_1}; a_3 = \frac{\partial f_1}{\partial Q}\bigg|_{ss} = \frac{1}{\rho c_p V_1}$$

$$b_1 = \frac{\partial f_2}{\partial F}\bigg|_{ss} = \frac{(T_{1s} - T_{2s})}{V_2}; b_2 = \frac{\partial f_2}{\partial T_1}\bigg|_{ss} = \frac{F_s}{V_2}; b_3 = \frac{\partial f_2}{\partial T_2}\bigg|_{ss} = \frac{-F_s}{V_2}$$

By subtracting the steady-state equation and defining deviation variables (like $\bar{F} = F - F_s$), we obtain the following equations:

$$\frac{d\bar{T}_1}{dt} = a_1\bar{F} + a_2\bar{T}_1 + a_3\bar{Q}$$

$$\frac{d\bar{T}_2}{dt} = b_1\bar{F} + b_2\bar{T}_1 + b_3\bar{T}_2$$

II.4. Consider the stirred-tank heater shown in Figure II.3. The steam is injected directly in the liquid. A_1 is the cross sectional area of the tank. Assume that the effluent flow rate is proportional to the liquid static pressure that causes its flow.

1. Identify the state variables of the system.
2. Determine what balances you should perform.
3. Develop the state model that describes the dynamic behavior of the system.
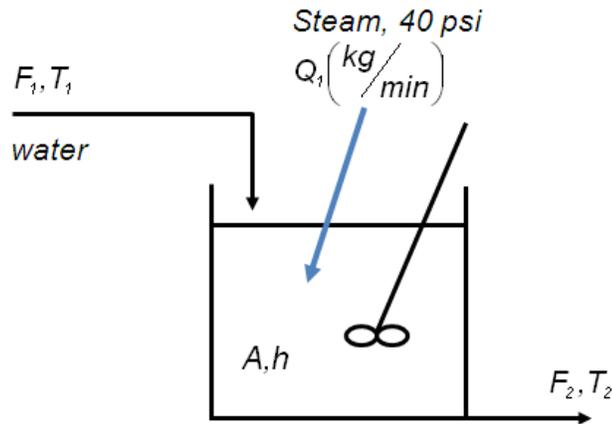
Figure II.3: Stirred tank heater

Solution:

a) State Variables: h , T_2
b) Total mass and energy balance.

Total mass balance

$$\frac{accumulation}{time} = \frac{input}{time} - \frac{output}{time}$$

$$\frac{d(\rho Ah)}{dt} = \rho F_1 - \rho F_2 + Q$$

At constant density:

$$A\frac{dh}{dt} = F_1 - F_2 + \frac{Q}{\rho} \qquad\qquad \textbf{\textit{Equation 1}}$$

Total energy balance

$$\frac{accumulation}{time} = \frac{input}{time} - \frac{output}{time}$$

$$E = U + KE + PE,$$

where U is the internal energy, KE is the kinetic energy and PE is the potential energy. Since the tank is not moving,

$$\frac{dKE}{dt} = \frac{dPE}{dt} = 0 \,.$$

Thus

$$\frac{dE}{dt} = \frac{dU}{dt} \,,$$

and for liquid systems,

$$\frac{dU}{dt} = \frac{dH_T}{dt}$$

where, H_T is the total enthalpy of material in the tank. Total mass in the tank is

$$\rho V = \rho A h \,.$$

H may be written as,

$$\rho A h C_p \left(T - T_{ref} \right)$$

where T_{ref} is the reference temperature. The input of total energy into the tank is:

$$\rho F_1 H_1 + \Delta H$$

where, ΔH is the heat supplied by 40 psi steam per unit volume. The output of total energy from the tank is: $\rho F_2 H_2$. The energy balance may be written as:

$$\frac{d\left(\rho V C_p \left(T_2 - T_{ref} \right) \right)}{dt} = \rho F_1 C_p \left(T_1 - T_{ref} \right) - \rho F_2 C_p \left(T_2 - T_{ref} \right) + \Delta H$$

Substituting for $\rho V = \rho A h$, we get

$$\frac{d\left(\rho A h C_p \left(T_2 - T_{ref} \right) \right)}{dt} = \rho F_1 C_p \left(T_1 - T_{ref} \right) - \rho F_2 C_p \left(T_2 - T_{ref} \right) + \Delta H$$

Assuming $T_{ref} = 0$, we will have:

$$A \frac{d\left(h T_2 \right)}{dt} = F_1 T_1 - F_2 T_2 + \frac{\Delta H}{\rho C_p}$$

Using the product rule:

$$A \frac{d\left(h T_2 \right)}{dt} = A h \frac{dT_2}{dt} + A T_2 \frac{dh}{dt}$$

Substituting this into the above equation, we get:

$$Ah\frac{dT_2}{dt} = F_1T_1 - F_2T_2 + \frac{\Delta H}{\rho C_p} - AT_2\frac{dh}{dt}$$

From Equation 1, we have the term $A\frac{dh}{dt}$ in the above equation. Therefore, the energy balance results in the following equation:

$$Ah\frac{dT_2}{dt} = F_1T_1 - F_2T_2 + \frac{\Delta H}{\rho C_p} - T_2\left(F_1 - F_2 + \frac{Q}{\rho}\right)$$

Simplifying results in the following equation:

$$\boxed{Ah\frac{dT_2}{dt} = F_1T_1 - F_1T_2 + \frac{\Delta H}{\rho C_p} - T_2\frac{Q}{\rho}} \qquad \textit{Equation 2}$$

II.5. Most separation processes in the chemical industry consist of a sequence of stages. For example, sulfur dioxide present in combustion gas may be removed by the use of a liquid absorbent (such as dimethylalanine) in a multistage absorber. Consider the three-stage absorber displayed in Figure II.4.
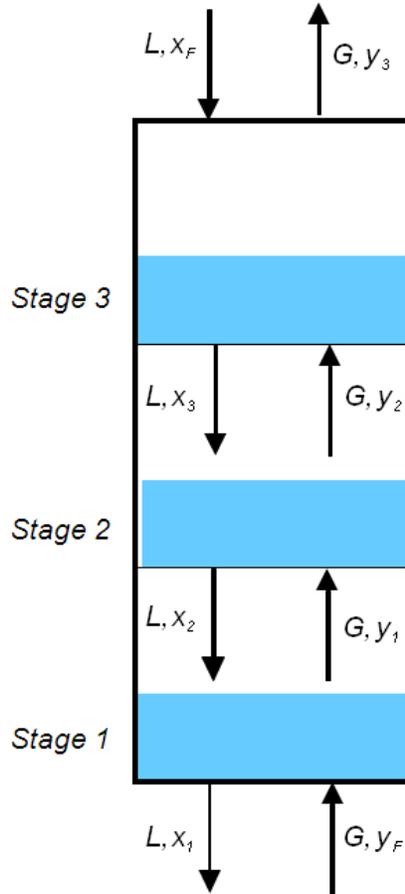
Figure II.4: Schematic of a three-stage absorber.

This process is modeled through the following equations[2]:

$$\tau \frac{dx_1}{dt} = K(y_f - b) - (1 + S)x_1 + x_2$$

$$\tau \frac{dx_2}{dt} = Sx_1 - (1 + S)x_2 + x_3$$

$$\tau \frac{dx_3}{dt} = Sx_2 - (1 + S)x_3 + x_f$$

H is the liquid holdup in each stage and assumed to be constant, and x and y represent liquid and vapor compositions, respectively. Also, $\tau = H/L$ is the liquid residence time, $S = aG/L$ is the stripping factor and $K = G/L$ is the gas-to-liquid ratio. A and b are constants.

      a. How many variables are there? How many equations (relationships)? What is the degree of freedom?

      b. Is this system underdetermined or overdetermined? Why?

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[2] Seborg, D.E, T.F. Edgar. D.A. Mellichamp, *Process Dynamics and Control*, Wiley

c. What additional relationships, if necessary, can you suggest to reduce the degrees of freedom to zero?

Solution:

All relevant symbols are given below:

a, b, H (Constants)

$x_1, x_2, x_3, x_f, y_1, y_2, y_3, y_f, S, K, G, L, \tau$ (13 variables)

Here we also included the gas phase compositions (of SO_2) although they do not appear explicitly in the modeling equations. We have three equations that result from the application of the component balances in each stage and three defining equations for three variables (given in the problem statement). One can also write the following equilibrium relationships that must be satisfied at each stage:

$$x_i = f_i(y_i) \quad i = 1,2,3$$

With these, we have a total of nine equations. The degree of freedom analysis yields:

$$F = 13 - 9 = 4$$

This is an underdetermined system. To fully define the system and have a feasible control problem, we need to remove four degrees of freedom. We can do that by the following specifications:

1. The SO_2 content of the liquid feed should be zero (there is no reason why dimethylalanine should contain any SO_2). $x_f = 0$
2. The feed gas composition y_f can be considered as a disturbance as it would be defined by the operation of upstream units.
3. Similarly, the flow rate of the gas stream may be a considered as a disturbance because the operation of upstream units (furnaces) may vary.
4. A control problem can be defined. One can suggest a feedback control mechanism that would measure the SO_2 composition in the gas phase, y_3, and according to the specified target, $y_{3,target}$, manipulate the flow rate of the liquid, L. That establishes a relationship through the feedback mechanism as follows:
$$L = f(y_3)$$

Hence, we now have one specification, two disturbances, and a feedback mechanism, resulting in four new relationships, thereby reducing the degrees of freedom to zero.

II.6. Consider a liquid chromatography for the separation of a mixture containing N components. Assuming that the process is isothermal, and there are no radial

concentration gradients, the following governing equations for solute j in the mobile phase and on the adsorbent can be obtained:

$$u_0 \frac{\partial c_j}{\partial z} + \varepsilon_t \frac{\partial c_j}{\partial t} + (1-\varepsilon)\frac{\partial q_j}{\partial t} = \varepsilon D_L \frac{\partial^2 c_j}{\partial z^2}$$

$$\frac{\partial q_j}{\partial t} = k_{a,j} c_j q_{m,j}\left(1 - \sum_{i=1}^{N} \frac{q_i}{q_{m,i}}\right) - k_{d,j} q_j$$

In this model, c is the concentration of solute in the mobile phase, and q is the adsorbate concentration. Also, u_0 is the superficial velocity, ε and ε_t are column void fraction and total void fraction respectively, D_L is the axial dispersion coefficient, q_m is the maximum adsorbate concentration, and $k_{a,j}$ and $k_{d,j}$ are the adsorption and desorption rate constants for solute j respectively.

1. How would you classify this system of equations? Why?
2. How many variables are there? How many equations (relationships)? What is the number of degrees of freedom?
3. Is this system underdetermined or overdetermined? Why?
4. What additional relationships, if necessary, can you suggest to reduce the degrees of freedom to zero?

Solution:

a. This model should be classified as a *nonlinear, distributed* model. Distributed models provide relationships for state variables as functions of both space and time, whereas a non-distributed (lumped) model will only depend on time. It is also *nonlinear* as one can see the terms involving multiplication of state variables.

a. For N components, we have c_j and q_j as the state variables. One can also consider the velocity u_0 to be a variable as the throughput for the chromatography column may change. Then, we have the following parameters:
$$k_{a,j}, k_{d,j}, q_{m,j}, \varepsilon, \varepsilon_t, D_L$$

This yields $5N+4$ variables. We have $2N$ equations. The degrees of freedom at this point are:
$$F = (5N+4) - 2N = 3N+4$$
Can we come up with more relationships? Following assumptions are appropriate:
- Void fractions ($\varepsilon, \varepsilon_t$) are constant.
- Maximum adsorbate concentration $q_{m,j}$ is a constant.

This yields $N+2$ additional relationships. The adsorption and desorption rate constants can vary with time during the chromatographic process. They can also be related to the

intrinsic adsorption/desorption rate constants (Lin et al., *Ind. & Eng. Chem. Research*, 1998). We will assume that they can be expressed as:

$$k_{d,j} = f(k_{d,j}, q_{m,j}, c_{0,i}, ...)$$
$$k_{a,j} = f(k_{a,j}, q_{m,j}, c_{0,i}, ...)$$

This yields $2N$ more relationships. Finally, the dispersion coefficient can be expressed as:

$$\frac{d_p u_0}{D_L} = 0.2 + 0.011 \text{Re}^{0.48}$$

In summary, we have

$$F = (3N + 4) - (N + 2) - 2N - 1 = 1$$

Thus, the degree of freedom is one.

b. The system is underdetermined because $F = 1 > 0$.

c. What we, as process control engineers, would do is to use a controller to affect one variable by manipulating another variable, thus providing one additional relationship and reducing F to 0. For example, it might be advantageous to control the exit concentration of one of the species by manipulating the velocity (or the flow through) u_0. The feedback yields one additional relationship between two variables, thus reducing the degrees of freedom to zero.

II.7. Consider a distillation process (Figure II.5) with the following assumptions: binary mixture, constant pressure, constant relative volatility, constant molar flows, no vapor holdup, equilibrium on all stages, and a total condenser. The modeling equations are given as follows:
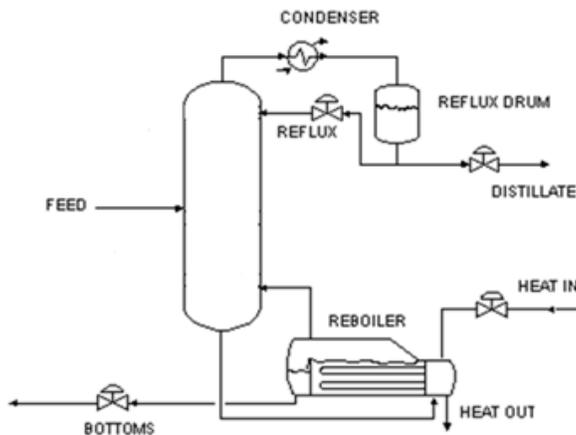

Figure II.5: Schematic of the distillation column

Total material balance on stage i:

$$\frac{dm_i}{dt} = L_{i+1} - L_i + V_{i-1} - V_i$$

Material balance for light component on stage i:

$$\frac{d(m_i x_i)}{dt} = L_{i+1} x_{i+1} - L_i x_i + V_{i-1} y_{i-1} - V_i y_i$$

The above equations apply to all stages except the top (condenser), the feed and the bottom (reboiler) stages.

From the assumption of constant molar flows and no vapor dynamics, we arrive at the following expression for the vapor flows:

$$V_{i-1} = V_i = V$$

The liquid flows depend on the liquid holdup on the stage above. We may use Francis' Weir formula:

$$L_i = f(m_i)$$

The vapor composition y_i is related to the liquid composition x_i on the same stage through the vapor-liquid equilibrium relationship:

$$y_i = \frac{\alpha x_i}{1 + (\alpha - 1)x_i}$$

Feed Stage: $i = n_F$

$$\frac{dm_i}{dt} = L_{i+1} - L_i + V_{i-1} - V_i + F$$

$$\frac{d(m_i x_i)}{dt} = L_{i+1} x_{i+1} - L_i x_i + V_{i-1} y_{i-1} - V_i y_i + F z_F$$

Total Condenser: $i = n_T$

$$\frac{dm_i}{dt} = -L_i + V_{i-1} - D = V_{i-1} - R - D$$

$$\frac{d(m_i x_i)}{dt} = -L_i x_i + V_{i-1} y_{i-1} - D x_D = V_{i-1} y_{i-1} - (R + D) x_D$$

Reboiler: i=1

$$\frac{dm_i}{dt} = L_{i+1} - V_i - B = L_{i+1} - B - V$$

$$\frac{d(m_i x_i)}{dt} = L_{i+1} x_{i+1} - V_i y_B - B x_B = L_{i+1} x_{i+1} - (B+V) x_B$$

1. How many variables are there in this model? How many equations (relationships)? What is the degree of freedom?
2. Is this system underdetermined or overdetermined? Why?
3. What additional relationships, if necessary, can one suggest to reduce the degrees of freedom to zero?

Solution:

Variables:

$$m_i; L_i; x_i; y_i; V; B, D; F; z_F; R$$

Thus, we have *4N+6* variables and α is a parameter to be specified.

Equations:

2N differential equations and *2N* algebraic equations →*4N* Equations

Degrees of freedom *DOF=6*

System is underdetermined since DOF>0

We need to specify some variables and/or define possible control loops to reduce the DOF to zero.

Feed conditions *F* and z_F are specified from conditions elsewhere in the plant (disturbances) this reduces the degrees of freedom to 4.

We can define the following control loops which will add additional relationships among the variables:

- Distillate flow rate (*D*) can be adjusted to control the level of the condenser drum
- Bottom flow rate (*B*) can be adjusted to control the level of the reboiler
- Reboiler heat duty can be adjusted to control the amount of vapor in the system
- Reflux flow rate can be adjusted to control the composition on the top of the column

This will reduce the degrees of freedom (DOF) to ***zero***

II.8. For the single-stage flash unit introduced earlier in Exercise II.2, derive the transfer function between the overhead mole fraction of the more volatile component and its feed mole fraction.

Solution:

We assumed constant molar holdup, hence, we have the following component balance:

$$H\frac{d(x_B)}{dt} = Fx_F - Bx_B - Dx_D$$

Using the equilibrium relationship (and also the fact that T and P are constant), we have:

$$x_D = Kx_B$$

This results in,

$$\frac{H}{K}\frac{d(x_D)}{dt} = Fx_F - \frac{B}{K}x_D - Dx_D$$

$$= Fx_F - \left(\frac{B}{K} + D\right)x_D$$

In standard form

$$\frac{H}{K}\frac{d(x_D)}{dt} = Fx_F - \left(\frac{B}{K} + D\right)x_D$$

$$= Fx_F - \left(\frac{B + KD}{K}\right)x_D$$

$$\frac{H}{B + KD}\frac{d(x_D)}{dt} = \frac{KF}{B + KD}x_F - x_D$$

$$\tau\frac{d(x_D)}{dt} + x_D = kx_F$$

where $\tau\dfrac{H}{B + KD}$ *and* $k = \dfrac{KF}{B + KD}$.

This is a linear equation (as all flows are constant now). Defining deviation variables,

$$\bar{x}_D = x_D - x_{D,s}$$
$$\bar{x}_F = x_F - x_{F,s}$$

And taking Laplace transform and rearranging, we have the following transfer function:

$$\tau s x_D(s) + x_D(s) = k x_F(s)$$

$$x_D(s) = \frac{k}{\tau s + 1} x_F(s)$$

$$\boxed{g(s) = \frac{x_D(s)}{x_F(s)} = \frac{k}{\tau s + 1}}$$

where we have

$$\tau \frac{H}{B + KD} \quad and \quad k = \frac{KF}{B + KD}$$

II.9. A liquid-phase isothermal reaction takes place in a continuous stirred-tank reactor. The reaction is first-order,

$$A \rightarrow B \qquad r = kC_A$$

We assume that the vessel has a constant volume, operates isothermally (constant temperature) and is well mixed.

For this system:
1. Derive the process transfer function between the outlet (tank) concentration and the feed concentration of component A.
2. Obtain the time evolution of the concentration as function of the feed concentration and the process parameters. *Hint:* use partial fraction expansion.
3. For the design and operating parameters, $F_0 = 0.1 \, \text{mol/m}^3$, $V = 2 \, \text{m}^3$, $C_{A0} = 0.1 \, \text{mol/m}^3$, $k = 0.050 \, 1/\text{min}$ and $\Delta C_{A0} = 1 \, \text{mol/m}^3$, calculate the outlet concentration when $t = V/(F + Vk)$ and when $t = 40 \, \text{min}$.

Solution:

From Example 4.5 in the book, the state equation for our reactor that provides the time evolution of the reactant composition is given as

$$\frac{dC_A}{dt} = \frac{F}{V} C_{A0} - \frac{F}{V} C_A - kC_A$$

Rewriting

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

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

$$\tau\frac{dC_A}{dt} + C_A = kC_{A0}$$

Note that k in the last equation is the steady-state gain. Defining deviation variables and taking Laplace transform to both sides of the equation

$$\tau s\overline{C}_A(s) + \overline{C}_A(s) = k\overline{C}_{A0}(s)$$
$$(\tau s + +1)\overline{C}_A(s) = k\overline{C}_{A0}(s)$$

$$\overline{C}_A(s) = C_A - C_{As} \quad and \quad \overline{C}_{A0} = C_{A0} - C_{A0s}$$

Finally,

$$\boxed{\frac{\overline{C}_A(s)}{\overline{C}_{A0}(s)} = g(s) = \frac{k}{(\tau s + +1)}}$$

where: $\tau = \dfrac{V}{F_0 + V\alpha}$ and $k = \dfrac{F_0}{F_0 + V\alpha}$.

To obtain the time domain solution, we use partial fraction technique

$$\overline{C}_{A0}(s) = \frac{M}{s} = \frac{\Delta C_{A0}}{s} \qquad \overline{C}_A(s) = \frac{k}{(\tau s + +1)}\frac{M}{s}$$

$$\frac{1}{(\tau s + 1)s} = \frac{A}{s} + \frac{B}{(\tau s + 1)}$$

s=0 $\qquad \dfrac{s}{(\tau s + 1)s} = \dfrac{As}{s} + \dfrac{Bs}{(\tau s + 1)} = A \qquad \dfrac{1}{(1)} = A$

s=-1/τ $\qquad \dfrac{(\tau s + 1)}{(\tau s + 1)s} = \dfrac{A(\tau s + 1)}{s} + \dfrac{B(\tau s + 1)}{(\tau s + 1)} = B \qquad \dfrac{1}{-1/\tau} = -\tau = B$

$$\overline{C}_A(s) = kM\left(\frac{A}{s} + \frac{B}{(\tau s + 1)}\right) = kM\left(\frac{1}{s} - \frac{\tau}{(\tau s + 1)}\right)$$

Inverting (using Table of Laplace functions)

$$\overline{C}_A(t) = kM\left(1 - \tau\frac{e^{-t/\tau}}{\tau}\right) = kM\left(1 - e^{-t/\tau}\right)$$

Substituting

$$\boxed{C_A(t) = C_{As} + \frac{F_0}{F_0 + V\alpha}\Delta C_{A0}\left(1 - e^{-t/\tau}\right)}$$

For the conditions

$$F = 0.1 m^3/\text{min} \quad V = 2m^3 \quad C_{A0} = 0.8 \text{mol/m}^3 \quad \alpha = 0.050 \, 1/\text{min} \quad \Delta C_{A0} = 1 \, \text{mol/m}^3$$

First we need to find the steady-state value for the concentration C_{As}.

$$\tau\frac{dC_A}{dt} + C_A = kC_{A0}$$

At steady-state

$$C_{As} = kC_{A0s} = \frac{0.1}{0.1 + 2\,0.05}\, 0.8 = 0.4$$

Substituting for this value

$$C_A(t) = 0.4 + \frac{0.1}{0.1 + 2\,0.05}\,1\left(1 - e^{-t/\tau}\right)$$

$$C_A(t) = 0.4 + 0.5\left(1 - e^{-t/\tau}\right)$$

For $t = \tau$ $\quad C_A(t) = 0.4 + 0.5\ (1 - 0.3679) = 0.7161$

$$\tau = \frac{V}{F + Vk} = \frac{2}{0.1 + 2\,0.05} = 10$$

$$C_A(t) = 0.4 + 0.5\left(1 - e^{-t/10}\right) = 0.4 + 0.5\left(1 - e^{-40/10}\right)$$

For t=40 min
$$= 0.4 + 0.5(1 - 0.0183)$$
$$= 0.4 + 0.498 = 0.8908$$

Figure II.S1 illustrates a plot of the concentration as function of time.
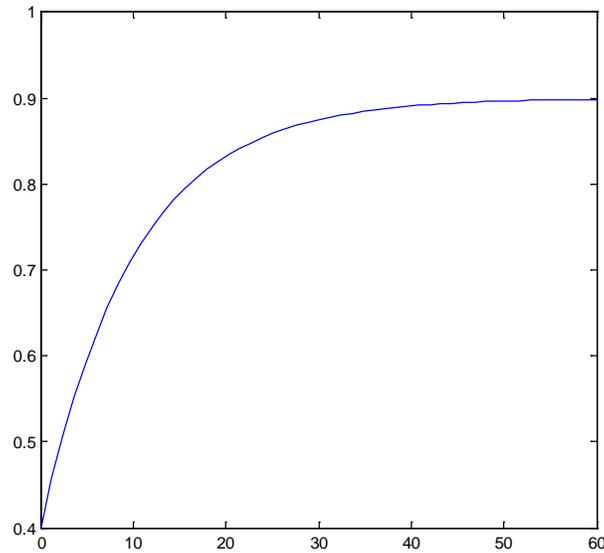
Figure II.S1: Concentration response as function of time.

II.10. Consider the same liquid-phase, isothermal, continuous stirred-tank reactor as in Exercise II.9 where the component balance can also be expressed in terms of the product concentration.

1. Derive the process transfer function between the outlet (tank) concentration for component B (product) and the feed concentration of component A.
2. Obtain the time evolution of the concentration as a function of the feed concentration and the process parameters and compare your results with those of Exercise II.9.
3. Assuming the same design and operating conditions as before what is the value of the concentration when $t = V/(F + Vk)$ and $t = 40\,\text{min}$?

Solution:

Balance on C_B

$$\frac{dC_B}{dt} = -\frac{F}{V}C_B + kC_A$$

$$\frac{dC_B}{dt} + \left(\frac{F}{V}\right)C_B = kC_A$$

$$\left(\frac{V}{F}\right)\frac{dC_B}{dt} + C_B = \frac{Fk}{V}C_A$$

$$\tau_1\frac{dC_B}{dt} + C_B = k_1C_A$$

where k_1 is the new steady-state gain.

$$\tau_1 s C_B + C_B = k_1 C_A$$

$$(\tau_1 s + 1)C_B = k_1 C_A$$

$$\frac{C_B}{C_A} = \frac{k_1}{(\tau_1 s + 1)}$$

$$\tau_1 = \frac{V}{F} \qquad k_1 = \frac{Fk}{V}$$

$$\frac{\overline{C}_A(s)}{\overline{C}_{A0}(s)} = \frac{k}{(\tau s + +1)}$$

Thus,

$$\frac{C_B}{C_A} \frac{\overline{C}_A(s)}{\overline{C}_{A0}(s)} = \frac{k}{(\tau s + +1)} \frac{k_1}{(\tau_1 s + 1)}$$

$$\frac{C_B}{\overline{C}_{A0}(s)} = \frac{kk_1}{(\tau s + +1)(\tau_1 s + 1)}$$

$$\overline{C}_{A0}(s) = \frac{M}{s} = \frac{\Delta C_{A0}}{s}$$

$$\overline{C}_B(s) = \frac{kk_1}{(\tau s + +1)(\tau_1 s + 1)} \frac{M}{s}$$

Inverting using the Laplace Table,

$$\overline{C}_B(t) = kk_1 M \left(1 + \frac{\tau_1}{\tau_2 - \tau_1} e^{-t/\tau_1} - \frac{\tau_2}{\tau_2 - \tau_1} e^{-t/\tau_2} \right)$$

$$= kk_1 M \left(1 + \frac{1}{\tau_2 - \tau_1} \left(\tau_1 e^{-t/\tau_1} - \tau_2 e^{-t/\tau_2} \right) \right)$$

$$\overline{C}_B(t) = \frac{F}{(F + Vk)} \frac{F}{Vk} \Delta C_{A0} \left(1 + \frac{1}{\tau_2 - \tau_1} \left(\tau_1 e^{-t/\tau_1} - \tau_2 e^{-t/\tau_2} \right) \right)$$

$F = 0.1 m^3/\text{min} \quad V = 2m^3 \quad C_{A0} = 0.8 \text{mol/m}^3 \quad \alpha = 0.050 \, 1/\text{min} \quad \Delta C_{A0} = 1 \, \text{mol/m}^3$

$$\tau = \frac{V}{F + Vk} = \frac{2}{0.1 + 2\,0.05} = 10$$

$$\tau_1 = \frac{V}{F} = \frac{2}{0.1} = 20$$

$$\overline{C}_B(t) = \frac{0.1}{(0.1 + 2\ 0.05)} \frac{0.1}{(2\ 0.05)} \left(1 + \frac{1}{20 - 10} \left(10e^{-t/10} - 20e^{-t/20} \right) \right)$$
$$= 0.5 \left(1 + 0.1 \left(10e^{-t/10} - 20e^{-t/20} \right) \right)$$

Steady-state value
$$C_{Bs} = kC_{As}$$

C_{As}=0.4 then
$$C_{Bs} = \frac{F}{Vk} C_{As} = \frac{0.1}{2\ 0.05} 0.4 = 0.4$$

For t=τ
$$C_B(t) = 0.4 + 0.5 \left(1 + 0.1 \left(10e^{-10/10} - 20e^{-10/20} \right) \right) = 0.4774$$

For t=40
$$C_B(t) = 0.4 + 0.5 \left(1 + 0.1 \left(10e^{-40/10} - 20e^{-40/20} \right) \right) = 0.7738$$
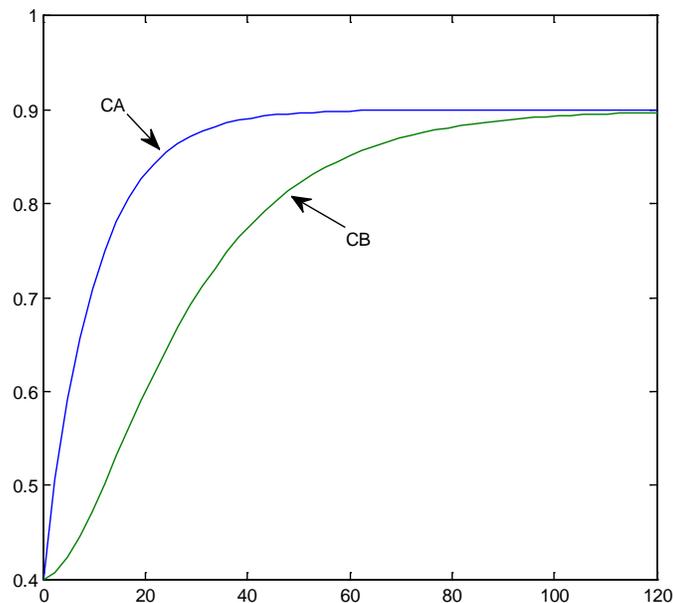
Figure II.S2: Plot of the concentrations as function of time.

II.11. Consider the same liquid-phase isothermal continuous stirred-tank reactor as in Exercise II.9 but now the reaction is second-order,
$$A \rightarrow B \qquad r = kC_A^2$$

1. Obtain a linear state-space model for this system.
2. Derive the process transfer function between the outlet (tank) concentration and the feed concentration of component A.
3. Compare the characteristic parameters with those of Exercise II.9 and discuss.

Solution:

From Example 4.5 in the book, the state equation for our reactor that provides the time evolution of the reactant composition is given as

$$\frac{dC_A}{dt} = \frac{F}{V}C_{A0} - \frac{F}{V}C_A - kC_A^2$$

We have to linearize,

$$VkC_A^2 = (VkC_{As}^2) + (2VkC_{As})(C_A - C_{As})$$

Substituting

$$V\frac{dC_A}{dt} = F(C_{A0} - C_A) - (VkC_{As}^2) + (2VkC_{As})(C_A - C_{As})$$

At steady-state,

$$0 = F(C_{A0s} - C_{As}) - VkC_{As}^2$$

Substracting

$$V\frac{dC_A}{dt} = F\left[(C_{A0} - C_A) - (C_{A0s} - C_{As})\right] + (2VkC_{As})(C_A - C_{As})$$

$$V\frac{d\overline{C}_A}{dt} = F\left[(\overline{C}_{A0} - \overline{C}_A)\right] + (2VkC_{As})\overline{C}_A$$

$$V\frac{d\overline{C}_A}{dt} = F\overline{C}_{A0} - F\overline{C}_A + (2VkC_{As})\overline{C}_A$$

$$= F\overline{C}_{A0} - \left[F + (2VkC_{As})\right]\overline{C}_A$$

$$\frac{V}{F + 2VkC_{As}}\frac{d\overline{C}_A}{dt} + \overline{C}_A = \frac{F}{F + 2VkC_{As}}\overline{C}_{A0}$$

$$\tau\frac{d\overline{C}_A}{dt} + C_A = kC_{A0}$$

where:

$$\tau = \frac{V}{F + 2VkC_{As}} \quad \text{and} \quad k = \frac{F}{F + 2VkC_{As}}$$

and the definition of the steady-state gain should be clear. Taking Laplace transform of both sides of the equation

$$\tau s\overline{C}_A(s) + \overline{C}_A(s) = k\overline{C}_{A0}(s)$$

$$(\tau s + +1)\overline{C}_A(s) = k\overline{C}_{A0}(s)$$

Finally,

$$\boxed{\frac{\overline{C}_A(s)}{\overline{C}_{A0}(s)} = g(s) = \frac{k}{(\tau s + +1)}}$$

To obtain the time domain solution, we use partial fraction technique

$$\overline{C}_{A0}(s) = \frac{M}{s} = \frac{\Delta C_{A0}}{s} \qquad \overline{C}_A(s) = \frac{k}{(\tau s + +1)}\frac{M}{s}$$

$$\frac{1}{(\tau s + 1)s} = \frac{A}{s} + \frac{B}{(\tau s + 1}$$

s=0 $\qquad \frac{s}{(\tau s + 1)s} = \frac{As}{s} + \frac{Bs}{(\tau s + 1} = A \qquad \frac{1}{(1)} = A$

s=-1/☐☐ $\qquad \frac{(\tau s + 1)}{(\tau s + 1)s} = \frac{A(\tau s + 1)}{s} + \frac{B(\tau s + 1)}{(\tau s + 1} = B \qquad \frac{1}{-1/\tau} = -\tau = B$

$$\overline{C}_A(s) = kM\left(\frac{A}{s} + \frac{B}{(\tau s + 1)}\right) = kM\left(\frac{1}{s} - \frac{\tau}{(\tau s + 1)}\right)$$

Inverting (using Table of Laplace functions),

$$\overline{C}_A(t) = kM\left(1 - \tau\frac{e^{-t/\tau}}{\tau}\right) = kM\left(1 - e^{-t/\tau}\right)$$

Substituting

$$C_A(t) = C_{As} + \frac{F}{F + 2VkC_{As}}\Delta C_{A0}\left(1 - e^{-t/\tau}\right)$$

For the conditions

$$F = 0.1 m^3/\text{min} \quad V = 2\text{m}^3 \quad C_{A0} = 0.8\text{mol/m}^3 \quad \alpha = 0.050 \, 1/\text{min} \quad \Delta C_{A0} = 1\,\text{mol/m}^3$$

First we need to find the steady-state value for the concentration C_{As}. At steady-state,

$$0 = \frac{F}{V}C_{A0} - \frac{F}{V}C_A - kC_A^2$$

$$0 = FC_{A0s} - FC_{As} - kVC_{As}^2$$

$$0 = 0.08 - 0.1C_{As} - 0.1C_{As}^2$$

Roots are -1.5247 and 0.5247, Thus $C_{As}=0.5247$ since the other root is negative. Substituting this value

$$C_A(t) = 0.5247 + \frac{0.1}{0.1 + 2\ 2\ 0.05\ 0.5247}\left(1 - e^{-t/\tau}\right)$$

$$C_A(t) = 0.5247 + 0.4879\left(1 - e^{-t/\tau}\right)$$

II.12. Consider the same liquid-phase isothermal, continuous, stirred-tank reactor as in Exercise II.11 and now allow for the possibility that the vessel volume may also change. The reaction is still second-order and the outlet flow rate depends linearly on the liquid volume in the tank.
1. What are the state variable(s), input variable(s) and output variable(s)? Obtain a linear state-space model for this system.
2. Derive the process transfer function between the outlet (tank) concentration of component A and the feed flow rate.
3. What are the poles and zeros of this transfer function?

Solution:

The model equations are given as:

$$\frac{dC}{dt} = \frac{F_0}{V}(C_0 - C) - kC^2$$

$$\frac{dV}{dt} = F_0 - F = F_0 - \beta V$$

Here C is the tank concentration, V is the tank volume, F is the flow rate, and the subscript 0 refers to inlet conditions. k and β are constants.

The state variables are composition C and volume V. Input variables would be inlet concentration and inlet flow rate. The output variables would depend on control objectives. We would typically be interested in maintaining a constant yield in the reactor (hence constant outlet composition) and constant level (or volume) to ensure constant residence time. Outputs can be the outlet composition and the volume (the state variables).

The first equation (component balance) can be classified as nonlinear, hence requiring the application of Taylor expansion. The second equation (total mass balance) is already in linear form.

$$\frac{dC}{dt} = \frac{F_0}{V}(C_0 - C) - kC^2 = f_1(F_0, C_0, V, C)$$

$$\frac{dV}{dt} = F_0 - F = F_0 - \beta V = f_2(F_0, C_0, V, C)$$

The Taylor expansion of the first equation yields:

$$\frac{dC}{dt} \cong f_1(F_{0,s}, C_{0,s}, V_s, C_s) + \left.\frac{\partial f_1}{\partial C_0}\right|_{F_{0,s}, C_{0,s}, V_s, C_s} (C_0 - C_{0,s}) + \left.\frac{\partial f_1}{\partial F_{in}}\right|_{F_{0,s}, C_{0,s}, V_s, C_s} (F_0 - F_{0,s})$$

$$\left.\frac{\partial f_1}{\partial C}\right|_{F_{0,s}, C_{0,s}, V_s, C_s} (C - C_s) + \left.\frac{\partial f_1}{\partial V}\right|_{F_{0,s}, C_{0,s}, V_s, C_s} (V - V_s)$$

The derivatives can be calculated as follows:

$$\left.\frac{\partial f_1}{\partial C_0}\right|_{F_{0,s}, C_{0,s}, V_s, C_s} = \left[\frac{F_{0,s}}{V_s}\right] = a$$

$$\left.\frac{\partial f_1}{\partial F_0}\right|_{F_{0,s}, C_{0,s}, V_s, C_s} = \left[\frac{C_{0,s} - C_s}{V_s}\right] = b$$

$$\left.\frac{\partial f_1}{\partial C}\right|_{F_{0,s}, C_{0,s}, V_s, C_s} = \left[-\frac{F_{0,s}}{V_s} - 2kC_s\right] = c$$

$$\left.\frac{\partial f_1}{\partial V}\right|_{F_{0,s}, C_{0,s}, V_s, C_s} = \left[-\frac{F_{0,s}(C_{0,s} - C_s)}{V_s^2}\right] = d$$

The first equation becomes

$$\frac{dC}{dt} \cong f_1(F_{0,s}, C_{0,s}, V_s, C_s) + a(C_0 - C_{0,s}) + b(F_0 - F_{0,s}) + c(C - C_s) + d(V - V_s)$$

By defining deviation variables like $\overline{C} = C - C_s$, and recognizing that $0 = f_1(F_{0,s}, C_{0,s}, V_s, C_s)$, we have,

$$\frac{d\overline{C}}{dt} = a\overline{C}_0 + b\overline{F}_0 + c\overline{C} + d\overline{V}$$

The second equation can also be manipulated by subtracting the steady-state equation,

$$\frac{dV}{dt} = F_0 - \beta V - (F_{0,s} - \beta V_s) = (F_0 - F_{0,s}) - \beta(V - V_s)$$

And by defining deviation variables,

$$\frac{d\overline{V}}{dt} = \overline{F}_0 - \beta\overline{V}$$

To define the state-space model, define $x_1 = \overline{C}, x_2 = \overline{V}, u_1 = \overline{C}_0, u_2 = \overline{F}_0, y_1 = x_1, y_2 = x_2$. This leads to

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} c & d \\ 0 & -\beta \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} a & b \\ 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

$$y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Taking the Laplace transform of both linear equations, we get,

$$s\overline{C}(s) = a\overline{C}_0(s) + b\overline{F}_0(s) + c\overline{C}(s) + d\overline{V}(s)$$
$$s\overline{V}(s) = \overline{F}_0(s) - \beta\overline{V}(s)$$

We need to find the transfer function,

$$\frac{\overline{C}(s)}{\overline{F}_0(s)} = g(s)$$

From the second equation,

$$\overline{V}(s) = \frac{1}{s+\beta}\overline{F}_0(s)$$

Substitute in first equation,

$$s\overline{C}(s) = a\overline{C}_0(s) + b\overline{F}_0(s) + c\overline{C}(s) + d\frac{1}{s+\beta}\overline{F}_0(s)$$

Collecting terms,

$$\overline{C}(s) = \frac{a}{s-c}\overline{C}_0(s) + \frac{b}{s-c}\overline{F}_0(s) + \frac{d}{s-c}\frac{1}{s+\beta}\overline{F}_0(s)$$

$$\overline{C}(s) = \frac{a}{s-c}\overline{C}_0(s) + \frac{1}{s-c}\left[b + \frac{d}{s+\beta}\right]\overline{F}_0(s)$$

Hence,

$$g(s) = \frac{1}{s-c}\left[b + \frac{d}{s+\beta}\right] = \frac{bs + b\beta + d}{(s-c)(s+\beta)}$$

The poles and zeros come from the roots of the following polynomials:

$$bs + b\beta + d = 0 \quad and \quad (s-c)(s+\beta) = 0$$

II.13. A bioreactor is represented by the following model that uses the Monod kinetics:

$$\frac{dx_1}{dt} = (\mu - D)x_1$$

$$\frac{dx_2}{dt} = (4 - x_2)D - 2.5\mu x_1$$

Here x_1 is the biomass concentration, x_2 is the substrate concentration, and D is the dilution rate. The specific growth rate μ depends on the substrate concentration as follows:

$$\mu = \frac{0.53x_2}{0.12 + x_2}$$

In this system, we are interested in controlling the biomass concentration using the dilution rate, at the steady-state defined by, $x_{1s} = 1.4523, x_{2s} = 0.3692, D_s = 0.4$.

1. Obtain a linear state-space model for this system.
2. Derive the process transfer function for this system.
3. What is the order of this process?

Solution:

We start with the following expansion,

$$\frac{dx_1}{dt} = (\mu - D)x_1 = f_1(x_1, x_2, D) \cong f_1(x_{1s}, x_{2s}, D_s) + \left.\frac{\partial f_1}{\partial x_1}\right|_{ss} (x_1 - x_{1s}) +$$

$$+ \left.\frac{\partial f_1}{\partial x_2}\right|_{ss} (x_2 - x_{2s}) + + \left.\frac{\partial f_1}{\partial D}\right|_{ss} (D - D_s)$$

$$\frac{dx_2}{dt} = (4 - x_2)D - 2.5\mu x_1 = f_2(x_1, x_2, D) \cong f_2(x_{1s}, x_{2s}, D_s) + \left.\frac{\partial f_2}{\partial x_1}\right|_{ss} (x_1 - x_{1s}) +$$

$$+ \left.\frac{\partial f_2}{\partial x_2}\right|_{ss} (x_2 - x_{2s}) + + \left.\frac{\partial f_2}{\partial D}\right|_{ss} (D - D_s)$$

The derivative terms can be calculated as follows,

$$a_{11} = \left.\frac{\partial f_1}{\partial x_1}\right|_{ss} = \left[\frac{0.53x_2}{0.12 + x_2} - D\right]_{ss} = 0$$

$$a_{12} = \left.\frac{\partial f_1}{\partial x_2}\right|_{ss} = \left[\frac{0.53x_1(0.12 + x_2) - 0.53x_1x_2}{(0.12 + x_2)^2}\right]_{ss} = 0.3866$$

$$b_1 = \left.\frac{\partial f_1}{\partial D}\right|_{ss} = \left[-x_1\right]_{ss} = -1.4523$$

$$a_{21} = \left.\frac{\partial f_2}{\partial x_1}\right|_{ss} = \left[-\frac{2.5(0.53x_2)}{0.12+x_2}\right]_{ss} = -1$$

$$a_{22} = \left.\frac{\partial f_2}{\partial x_2}\right|_{ss} = \left[-0.4 + \frac{2.5x_1(0.53(0.12+x_2)-0.53x_2)}{(0.12+x_2)^2}\right]_{ss} = -1.3649$$

$$b_2 = \left.\frac{\partial f_2}{\partial D}\right|_{ss} = [4-x_2]_{ss} = 3.6308$$

This yields the following state space form of the model, after defining the deviation variables:

$$\bar{x}_1 = x_1 - x_{1s}, \bar{x}_2 = x_2 - x_{2s}, \bar{u} = D - D_s$$

$$\dot{\bar{x}} = \begin{bmatrix} \dot{\bar{x}}_1 \\ \dot{\bar{x}}_2 \end{bmatrix} = \begin{bmatrix} 0 & 0.3866 \\ -1 & -1.36 \end{bmatrix}\begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \end{bmatrix} + \begin{bmatrix} -1.4523 \\ 3.6308 \end{bmatrix}\bar{u} = A\bar{x} + b\bar{u}$$

$$\bar{y} = \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \end{bmatrix} = c\bar{x}$$

To obtain the transfer function model, we need to take Laplace transform of the linear model,

$$sx_1(s) = a_{11}x_1(s) + a_{12}x_2(s) + b_1u(s) = a_{12}x_2(s) + b_1u(s)$$

$$sx_2(s) = a_{21}x_1(s) + a_{22}x_2(s) + b_2u(s)$$

Solve the second equation for $x_2(s)$ and replace in the second,

$$x_2(s) = \frac{a_{21}x_1(s)}{s-a_{22}} + \frac{b_2u(s)}{s-a_{22}}$$

$$sx_1(s) = \frac{a_{12}a_{21}x_1(s)}{s-a_{22}} + \frac{a_{12}b_2u(s)}{s-a_{22}} + b_1u(s)$$

Now, we have to collect the terms for the transfer function, and recognize that

$$y(s) = x_1(s),$$

$$\frac{y(s)}{u(s)} = g(s) = \frac{b_1s + (b_2a_{12} - b_1a_{22})}{s^2 - a_{22}s - a_{12}a_{21}}$$

This is a second-order system.

II.14. A process model is given:

$$\frac{d^2x}{dt^2} + a\frac{dx}{dt} + x = 1$$

with the initial conditions, $x(0) = x'(0) = 0$.

1. Using Laplace transformation, find the solutions of this model when $a = 1$ and $a = 3$.
2. Plot the solution $x(t)$ on one graph and discuss the effect of the parameter a on the solution.

Solution:

Taking the Laplace transform of this expression yields

$$s^2 X(s) + asX(s) + X(s) = \frac{1}{s}$$

$$X(s)(s^2 + as + 1) = \frac{1}{s}$$

And,

$$X(s) = \frac{1}{s(s^2 + as + 1)}$$

When $a = 1$, using the quadratic formula for the second order polynomial, we have the complex roots,

$$s = -\frac{1}{2} \pm \frac{\sqrt{3}}{2}j$$

Thus, the Partial Fraction Expansion will look like:

$$X(s) = \frac{1}{s\left(s + \frac{1}{2} + \frac{\sqrt{3}}{2}j\right)\left(s + \frac{1}{2} - \frac{\sqrt{3}}{2}j\right)} = \frac{A}{s} + \frac{B}{\left(s + \frac{1}{2} + \frac{\sqrt{3}}{2}j\right)} + \frac{C}{\left(s + \frac{1}{2} - \frac{\sqrt{3}}{2}j\right)}$$

Multiplying both sides by s and evaluating the expression at $s = 0$,

$$A = \frac{1}{\left(0 + \frac{1}{2} + \frac{\sqrt{3}}{2}j\right)\left(0 + \frac{1}{2} - \frac{\sqrt{3}}{2}j\right)} = 1$$

Multiplying both sides by $\left(s + \frac{1}{2} - \frac{\sqrt{3}}{2}j\right)$, and evaluating the expression at this root, we have,

$$B = -\frac{1}{2} - \frac{\sqrt{3}}{6} j$$

And similarly,

$$C = -\frac{1}{2} + \frac{\sqrt{3}}{6} j$$

Thus, we have,

$$X(s) = \frac{1}{s} + \frac{-\frac{1}{2} - \frac{\sqrt{3}}{6} j}{\left(s + \frac{1}{2} + \frac{\sqrt{3}}{2} j \right)} + \frac{-\frac{1}{2} + \frac{\sqrt{3}}{6} j}{\left(s + \frac{1}{2} - \frac{\sqrt{3}}{2} j \right)} = \frac{1}{s} + \frac{-\frac{1}{2}}{\left(s + \frac{1}{2} + \frac{\sqrt{3}}{2} j \right)} - \frac{\frac{\sqrt{3}}{6} j}{\left(s + \frac{1}{2} + \frac{\sqrt{3}}{2} j \right)} + \dots$$

From the Laplace Transform tables, we observe that,

$$\mathcal{L}^{-1}\left[\frac{p}{s+r} \right] = p e^{-r}$$

Thus, we have

$$\mathcal{L}^{-1}\left[\frac{-\frac{1}{2}}{\left(s + \frac{1}{2} + \frac{\sqrt{3}}{2} j \right)} \right] = -\frac{1}{2} e^{-\left(\frac{1}{2} + \frac{\sqrt{3}}{2} j \right)}$$

We also note the identity,

$$e^{(C_1 + C_2 j)t} = e^{C_1 t}\left(\cos C_2 t + j \sin C_2 t \right)$$

By completing the inverse transform, this results in,

$$\boxed{x(t) = 1 + 2e^{-t/2}\left[-0.5 \cos \frac{\sqrt{3}}{2} t - \frac{\sqrt{3}}{6} \sin \frac{\sqrt{3}}{2} t \right]}$$

The case with $a = 3$ can be done in a similar manner. The result will be:

$$\boxed{x(t) = 1 + 0.17 e^{-2.62t} - 1.17 e^{-0.38t}}$$

Figure II.S3 shows the behavior of $x(t)$ as a function of time for both cases. Note the oscillatory response when $a = 1$ (blue line).
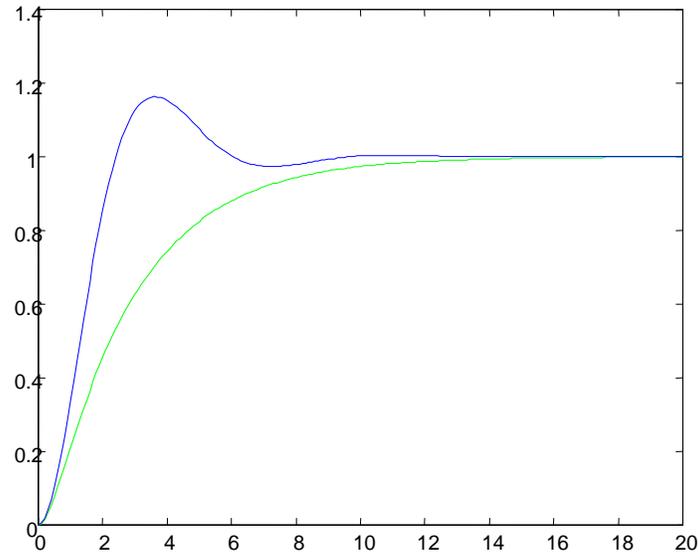
Figure II.S3: Plot of $x(t)$ for the cases in Exercise II.14.

II.15. For the process discussed earlier in Exercises I.11 and II.3, where an oil stream is heated as it passes through two well-mixed tanks in series and assuming constant physical properties, develop the transfer functions between the second tank temperature (output), T_2, and the heat input (manipulated variable), Q and the flow rate (disturbance), F . T_0 can be assumed as constant (what if it is not?).

<u>Solution:</u>

The equations are 'slightly' nonlinear due to the multiplication between the flow rate and the temperatures. Rearranging and taking the Taylor series expansion,

$$\frac{dT_1}{dt} = \frac{F}{V_1}(T_0 - T_1) + \frac{Q}{\rho c_p V_1} = f_1(F, T_1, Q)$$

$$\approx \left[\frac{F}{V_1}(T_0 - T_1) + \frac{Q}{\rho c_p V_1} \right]_{ss} + a_1(F - F_s) + a_2(T_1 - T_{1s}) + a_3(Q - Q_s)$$

$$\frac{dT_2}{dt} = \frac{F}{V_2}(T_1 - T_2) = f_2(F, T_1, T_2)$$

$$\approx \left[\frac{F}{V_2}(T_1 - T_2) \right]_{ss} + b_1(F - F_s) + b_2(T_1 - T_{1s}) + b_3(T_2 - T_{2s})$$

We can see that the constant coefficients are given as:

$$a_1 = \left.\frac{\partial f_1}{\partial F}\right|_{ss} = \frac{(T_0 - T_{1s})}{V_1}; a_2 = \left.\frac{\partial f_1}{\partial T_1}\right|_{ss} = \frac{-F_s}{V_1}; a_3 = \left.\frac{\partial f_1}{\partial Q}\right|_{ss} = \frac{1}{\rho c_p V_1}$$

$$b_1 = \left.\frac{\partial f_2}{\partial F}\right|_{ss} = \frac{(T_{1s} - T_{2s})}{V_2}; b_2 = \left.\frac{\partial f_2}{\partial T_1}\right|_{ss} = \frac{F_s}{V_2}; b_3 = \left.\frac{\partial f_2}{\partial T_2}\right|_{ss} = \frac{-F_s}{V_2}$$

By subtracting the steady-state equation and defining deviation variables (like $\overline{F} = F - F_s$), we obtain the following equations:

$$\frac{d\overline{T_1}}{dt} = a_1\overline{F} + a_2\overline{T_1} + a_3\overline{Q}$$

$$\frac{d\overline{T_2}}{dt} = b_1\overline{F} + b_2\overline{T_1} + b_3\overline{T_2}$$

Taking the Laplace transformation,

$$s\overline{T_1}(s) = a_1\overline{F}(s) + a_2\overline{T_1}(s) + a_3\overline{Q}(s)$$

$$s\overline{T_2}(s) = b_1\overline{F}(s) + b_2\overline{T_1}(s) + b_3\overline{T_2}(s)$$

and rearranging,

$$\overline{T_1}(s) = \frac{a_1}{s - a_2}\overline{F}(s) + \frac{a_3}{s - a_2}\overline{Q}(s)$$

$$\overline{T_2}(s) = \frac{b_1}{s - b_3}\overline{F}(s) + \frac{b_2}{s - b_3}\overline{T_1}(s)$$

Replacing the first equation into the second equation and rearranging again,

$$\overline{T}_2(s) = \frac{b_1}{s-b_3}\overline{F}(s) + \frac{b_2}{s-b_3}\left[\frac{a_1}{s-a_2}\overline{F}(s) + \frac{a_3}{s-a_2}\overline{Q}(s)\right]$$

$$\overline{T}_2(s) = \frac{b_1}{s-b_3}\left[1 + \frac{a_1}{s-a_2}\right]\overline{F}(s) + \frac{b_2}{s-b_3}\frac{a_3}{s-a_2}\overline{Q}(s)$$

The transfer functions can now be identified,

$$\overline{T}_2(s) = g_{TF}\overline{F}(s) + g_{TQ}\overline{Q}(s)$$

$$\overline{T}_2(s) = \frac{b_1 s - a_2 b_1 + a_1 b_1}{(s-b_3)(s-a_2)}\overline{F}(s) + \frac{a_3 b_2}{(s-b_3)(s-a_2)}\overline{Q}(s)$$

II.16. A continuous pre-fermenter shown in Figure II.6 is used as the first stage of cheese manufacture[2].
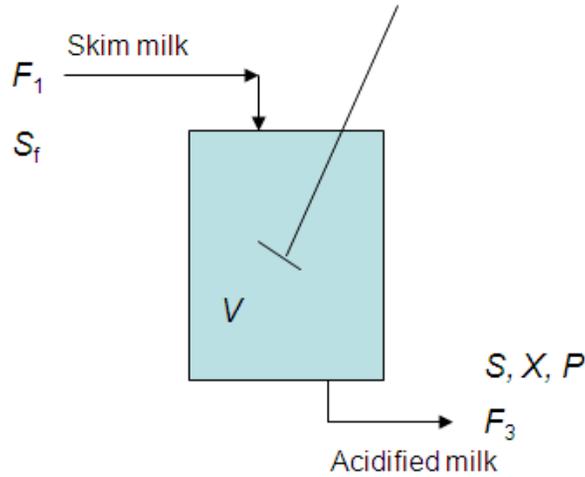
Figure II.6: Continuous pre-fermenter.

The pre-fermenter is supplied by skim milk (substrate) and the cheese starter (cells) and operated at 30^0C. The pH of the acidified skim milk is measured using a pH sensor. In Figure II.6, X_f, S_f and P_f denote the cell concentration, the lactose concentration and the lactic acid concentration in the feed stream, respectively. Since the flow rate of the cheese starter is very small compared to the skim milk flow rate, the lactose concentration in the feed is neglected. This process is modeled using the following mass balance equations:

$$V\frac{dX}{dt} = -F_3X + \mu_{max}XV$$

$$V\frac{dS}{dt} = F_1S_f - F_3S - \sigma_{max}XV$$

$$V\frac{dP}{dt} = -F_3P + \pi_{max}XV$$

The following definitions are also given:

$$\mu_{max} = \frac{\mu_0\left[H^+\right]}{K_{H1} + \left[H^+\right] + \left[H^+\right]^2/K_{H2}}$$

$$\sigma_{max} = \frac{\sigma_0\left[H^+\right]}{K_{H3} + \left[H^+\right] + \left[H^+\right]^2/K_{H4}}$$

$$\pi_{max} = \frac{\pi_0\left[H^+\right]}{K_{H5} + \left[H^+\right] + \left[H^+\right]^2/K_{H6}}$$

Here, μ_{max}, σ_{max}, π_{max} are the maximum specific growth rate, the maximum specific lactose consumption rate and the maximum specific production rate, respectively. The dependency between the pH and the lactic acid concentration is expressed through the following correlation:

$$-\log_{10}\left[H^+\right] = pH = 6.701 - 0.9564P + 0.2050P^2 - 0.02134P^3$$

The dilution rate is defined as F_3/V, and F_2/F_3 is the seed feed rate. Operating and design parameters are given in Table II.2.

1. What are the steady-state operating conditions for this process? How many of them correspond to non-trivial operation? (*Hint*: The steady-state can be considered as dependent on pH)
2. Linearize the model equations around a steady-state point determined above.
3. Comment on the stability of the system around this steady-state.

Solution:

Recognizing that the inlet flow rate needs to equal the outlet flow rate to maintain constant volume, we have,

$$F_1 = F_3$$

The dilution rate is defined as:

$$D = \frac{F_3}{V}$$

This yields the following rephrased model equations:

$$\frac{dX}{dt} = (\mu_{max} - D)X$$

$$\frac{dS}{dt} = D(S_f - S) - \sigma_{max} X$$

$$\frac{dP}{dt} = -DP + \pi_{max} X$$

The steady condition can be obtained from this equation by setting the differential terms to zero. In this case, the steady-state conditions can be gleaned from a visual inspection of these equations. The first steady-state would be the trivial (wash-out) solution with:

$$X_s = 0; S_s = S_f; P_s = 0$$

The second steady-state condition can be obtained by observing that the first equation would vanish when $\mu_{max} = D$.

The steady-state condition then is dependent on the value of D and what the fermenter pH is. We can set up a MATLAB program that would calculate the steady-state conditions as a function of pH. In fact, we can develop a plot of D vs pH. For a given value of pH, we can obtain the steady-state values of the variables X, S and P along with D. Here is the program that calculates the steady-state at a pH of 6.

```
%Steady-states for the prefermentor - Exercise II.16
%initial guesses
x0(1)=0.3; %this is X
x0(2)=45; %this is S
x0(3)=1.5; %this is P
x0(4)=0.36; %this is D
%Calculation of steady-state
x = fsolve(@prefermenterfun,x0,optimset('Display','iter'));
```

```
function F = prefermenterfun(x)
H=1e-6;
Sf=50.3;
Xf=5.4;
Pf=5.9;
mu0=0.51;
pi0=3.35;
sigma0=6.02;
kh1=9.0e-08;
kh2=6.85e-06;
kh3=1.5e-07;
kh4=3.91e-06;
```

```
kh5=4.88e-08;
kh6=4.2e-06;
mu=mu0*H/(kh1+H+H^2/kh2);
sigma=sigma0*H/(kh3+H+H^2/kh4);
pi=pi0*H/(kh5+H+H^2/kh6);
F1=(mu-x(4))*x(1);
F2=x(4)*(Sf-x(2))-sigma*x(1);
F3=-x(4)*x(3)+pi*x(1);
F4=6.701-0.9564*x(3)+0.2050*x(3)^2-0.02134*x(3)^3+log10(H);
F=[F1 F2 F3 F4];
return
```

This generates

X_s=0.1404; S_s=48.8432; P_s=0.8856   and D_s=0.4126

One can do this calculation for a range of pH values from 5.5 to 6.7. This yields the plot in Figure II.S4. It shows that for a large range of pH values there are two values of the dilution rate thus creating multiple steady-states. Thus, the conclusion would be that there are a maximum of three steady-states (including the wash-out).
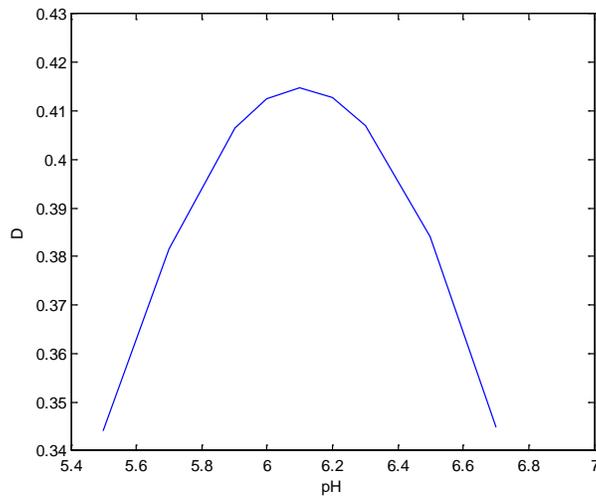
Figure II.S4: Plot of D vs pH.

The linearization can be performed around one of these states (select a pH value) and would result in the following equation:

$$
\begin{bmatrix} \dot{X} \\ \dot{S} \\ \dot{P} \end{bmatrix} = \begin{bmatrix} \mu_{max} - D & 0 & \bar{\mu}_{max} X \\ -\sigma_{max} & -D & -\bar{\sigma}_{max} X \\ \pi_{max} & 0 & -D + \bar{\pi}_{max} X \end{bmatrix} \begin{bmatrix} X \\ S \\ P \end{bmatrix}
$$

Here the state matrix is evaluated at the steady-state values and the bar notation indicates differentials with respect to P (through H^+). Of course, since we can ignore the wash-out, and recognizing $D = \mu_{max}$, the equation can be rephrased as:

$$\begin{bmatrix} \dot{X} \\ \dot{S} \\ \dot{P} \end{bmatrix} = \begin{bmatrix} 0 & 0 & \bar{\mu}_{max}X \\ -\sigma_{max} & -D & -\bar{\sigma}_{max}X \\ \pi_{max} & 0 & -D + \bar{\pi}_{max}X \end{bmatrix} \begin{bmatrix} X \\ S \\ P \end{bmatrix}$$

The stability can be inferred from the eigenvalues of the state matrix. We can write the characteristic equation as,

$$\det|A - \lambda I| = \begin{bmatrix} -\lambda & 0 & \bar{\mu}_{max}X \\ -\sigma_{max} & -D - \lambda & -\bar{\sigma}_{max}X \\ \pi_{max} & 0 & -D + \bar{\pi}_{max}X - \lambda \end{bmatrix}$$

See the paper by Funahashi and Nakamura (2007) for further discussion.

II.17. A process is modeled by the following equations:

$$2\frac{dx_1}{dt} = -2x_1 + \exp(-x_1) - 3u_1 x_2$$

$$\frac{dx_2}{dt} = -x_2 + \frac{2x_1}{1 + x_2} + 4u_2$$

The control objectives dictate the following output equations:

$$y_1 = x_1$$
$$y_2 = x_2$$

1. Find the four transfer functions relating the outputs $(y_1, \ y_2)$ to the inputs $(u_1, \ u_2)$.

2. Solve the equations with the conditions, $u_1(t) = 1, \ u_2(t) = 1, y_1(0) = 0,$ and $y_2(0) = 0$.

3. Plot the output responses. What is the steady-state reached by the outputs?

Solution:

We start by linearizing the nonlinear equations, recognizing that we have two state variables and two inputs in the state equations. The first equation yields:

$$\frac{dx_1}{dt} = f_1(x_1, x_2, u_1, u_2)$$

$$\cong f_1(x_{1s}, x_{2s}, u_{1s}, u_{2s}) + \frac{\partial f_1}{\partial x_1}\bigg|_{x_{1s}, x_{2s}, u_{1s}, u_{2s}}(x_1 - x_{1s}) + \frac{\partial f_1}{\partial x_2}\bigg|_{x_{1s}, x_{2s}, u_{1s}, u_{2s}}(x_2 - x_{2s}) +$$

$$+ \frac{\partial f_1}{\partial u_1}\bigg|_{x_{1s}, x_{2s}, u_{1s}, u_{2s}}(u_1 - u_{1s}) + \frac{\partial f_1}{\partial u_2}\bigg|_{x_{1s}, x_{2s}, u_{1s}, u_{2s}}(u_2 - u_{2s})$$

It can be put into the form,

$$\frac{dx_1}{dt} = a_{11}(x_1 - x_{1s}) + a_{12}(x_2 - x_{2s}) + b_{11}(u_1 - u_{1s}) + b_{12}(u_2 - u_{2s})$$

Also recognizing the fact that $f_1(x_{1s}, x_{2s}, u_{1s}, u_{2s}) = 0$ from the steady-state condition.
Note that the coefficients are given as follows:

$$a_{11} = \frac{\partial f_1}{\partial x_1}\bigg|_{s.s.} = \left[-1 - 0.5\exp(x_{1s})\right]$$

$$a_{12} = \frac{\partial f_1}{\partial x_2}\bigg|_{s.s.} = \left[-1.5 u_{1s}\right]$$

$$b_{11} = \frac{\partial f_1}{\partial u_1}\bigg|_{s.s.} = \left[-1.5 x_{2s}\right]$$

$$b_{12} = \frac{\partial f_1}{\partial u_2}\bigg|_{s.s.} = 0$$

One can derive the coefficients of the second equation $\frac{dx_2}{dt} = f_2(x_1, x_2, u_1, u_2)$ also as

follows:

$$a_{21} = \frac{\partial f_2}{\partial x_1}\bigg|_{s.s.} = \left[\frac{2}{1 + x_{2s}}\right]$$

$$a_{22} = \frac{\partial f_2}{\partial x_2}\bigg|_{s.s.} = \left[-1 + \frac{(2x_{1s}) - 2(1 + x_{2s})}{(1 + x_{2s})^2}\right]$$

$$b_{21} = \frac{\partial f_2}{\partial u_1}\bigg|_{s.s.} = 0$$

$$b_{22} = \frac{\partial f_2}{\partial u_2}\bigg|_{s.s.} = 4$$

We define the deviation variables:

$$\bar{x}_1 = x_1 - x_{1s}; \bar{x}_2 = x_2 - x_{2s}; \bar{u}_1 = u_1 - u_{1s}; \bar{u}_2 = u_2 - u_{2s}.$$

This results in the following linear equations:

$$\frac{d\bar{x}_1}{dt} = a_{11}\bar{x}_1 + a_{12}\bar{x}_2 + b_{11}\bar{u}_1$$

$$\frac{d\bar{x}_2}{dt} = a_{21}\bar{x}_1 + a_{22}\bar{x}_2 + b_{22}\bar{u}_2$$

If we take the Laplace transform of both equations, we have:

$$s\bar{x}_1(s) = a_{11}\bar{x}_1(s) + a_{12}\bar{x}_2(s) + b_{11}\bar{u}_1(s)$$
$$s\bar{x}_2(s) = a_{21}\bar{x}_1(s) + a_{22}\bar{x}_2(s) + b_{22}\bar{u}_2(s)$$

Note that $y_1(s) = x_1(s); y_2(s) = x_2(s)$. Rearranging, and making the substitutions,

$$\bar{y}_1(s) = \frac{a_{12}}{s - a_{11}}\bar{y}_2(s) + \frac{b_{11}}{s - a_{11}}\bar{u}_1(s)$$

$$\bar{y}_2(s) = \frac{a_{21}}{s - a_{22}}\bar{y}_1(s) + \frac{b_{22}}{s - a_{22}}\bar{u}_2(s)$$

and making the substitutions,

$$\bar{y}_1(s) = \frac{a_{12}}{s - a_{11}}\left[\frac{a_{21}}{s - a_{22}}\bar{y}_1(s) + \frac{b_{22}}{s - a_{22}}\bar{u}_2(s)\right] + \frac{b_{11}}{s - a_{11}}\bar{u}_1(s)$$

$$\bar{y}_2(s) = \frac{a_{21}}{s - a_{22}}\left[\frac{a_{12}}{s - a_{11}}\bar{y}_2(s) + \frac{b_{11}}{s - a_{11}}\bar{u}_1(s)\right] + \frac{b_{22}}{s - a_{22}}\bar{u}_2(s)$$

Collecting the terms, we end up with the following transfer functions,

$$\frac{\bar{y}_1(s)}{\bar{u}_1(s)} = \frac{b_{11}(s - a_{22})}{(s - a_{11})(s - a_{22}) - a_{12}a_{21}}$$

$$\frac{\bar{y}_1(s)}{\bar{u}_2(s)} = \frac{b_{22}a_{12}}{(s - a_{11})(s - a_{22}) - a_{12}a_{21}}$$

$$\frac{\bar{y}_2(s)}{\bar{u}_1(s)} = \frac{b_{11}a_{21}}{(s - a_{11})(s - a_{22}) - a_{12}a_{21}}$$

$$\frac{\bar{y}_2(s)}{\bar{u}_2(s)} = \frac{b_{22}(s - a_{11})}{(s - a_{11})(s - a_{22}) - a_{12}a_{21}}$$

Here are the two files needed to solve the problem in MATLAB.

_____

```matlab
%File odehmwk.m
%solution of a set of ODEs
clear all
dt=0.1;
t=[0:dt:10];
x0=[0;0];
[T Y] = ode45('odeeq',[0 10], x0);

plot (T,Y);
```

_____

```matlab
%File odeeq.m
%ODEs
function  dy=odeeq(t,y)
u1=1;
u2=1;
dy=[0.5*(-2*y(1)-3*u1*y(2)+exp(-y(1)))
    -y(2)+2*y(1)/(1+y(2))+4*u2];

return
```

_____

The plot obtained is given in Figure II.S5 (x_1 is becoming negative and x_2 is increasing):
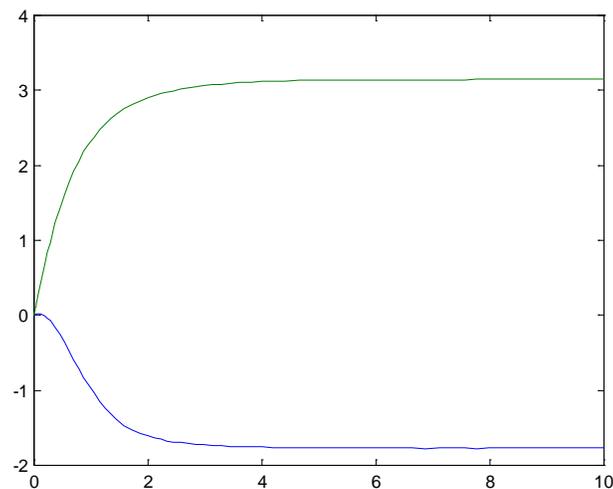
Figure II.S5: Time response for x_1 and x_2.

The steady state values can be obtained by simply typing the following on the command line (Last entries of the matrix Y):

» whos

Name	Size	Bytes	Class
T	89x1	712	double array
Y	89x2	1424	double array
dt	1x1	8	double array
t	1x101	808	double array
x0	2x1	16	double array

Grand total is 371 elements using 2968 bytes

» Y(89,1)

ans =

  -1.7727

» Y(89,2)

ans =

  3.1444

The Simulink block diagram is shown in Figure II.S6.
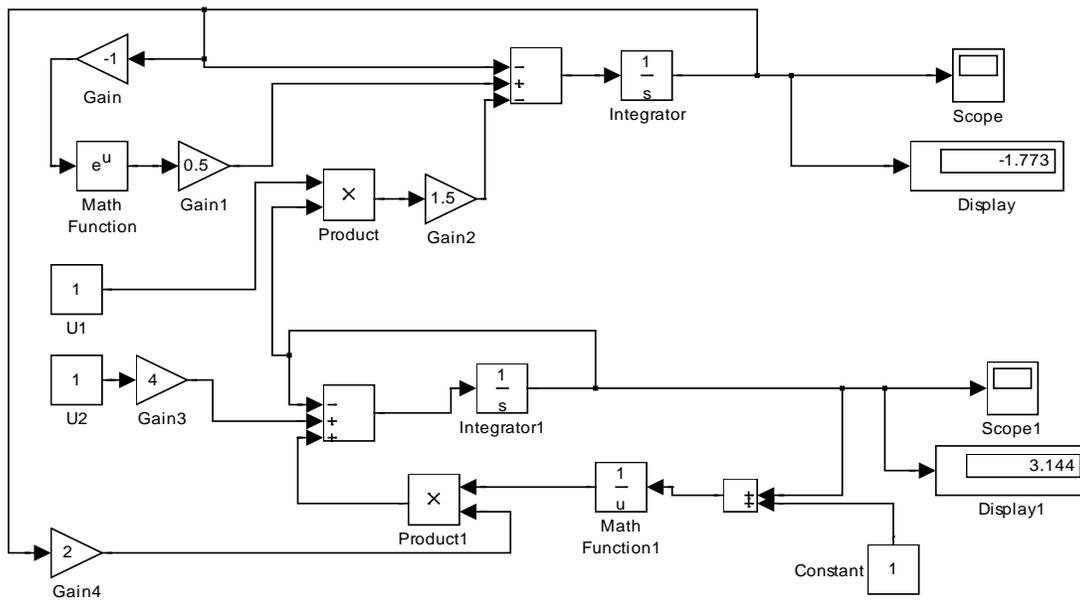
Figure II.S6: Schematic of the model implemented in Simulink.

II.18. Following state-space model is given,

$$\dot{x} = Ax + Bu$$
$$y = Cx$$
;

with

$$A = \begin{bmatrix} -2 & 1 & 0 \\ -3 & 0 & 3 \\ -1 & 0 & -3 \end{bmatrix}; B = \begin{bmatrix} 0 \\ 3 \\ 1 \end{bmatrix}; C = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}$$

Determine the eigenvalues of the state matrix. Also, find the transfer function model for this system. Report the poles and zeros of this transfer function. Obtain the response of this model to a step change in the input.

Solution:

We need to define the matrix *A* first and then issue the *eig* command in MATLAB:

```
» A=[-2 1 0;-3 0 3;-1 0 -3]
A =
  -2   1   0
  -3   0   3
  -1   0  -3

» eig(A)
ans =
 -0.8054 + 1.7006i
 -0.8054 - 1.7006i
 -3.3892
```

To find the transfer function model we can use the following sequence (after defining B and C also):

```
» [num,den]=ss2tf(A,B,C,0);
» g=tf(num,den)
```

Transfer function:

```
                  3 s + 12
g(s) =     ----------------------
           s^3 + 5 s^2 + 9 s + 12
```

The poles and zeros can be obtained in various ways. Here is one:

```
» pole(g)
ans =
 -3.3892
 -0.8054 + 1.7006i
 -0.8054 - 1.7006i
```

» zero(g)
ans =
  -4.0000

Note that the eigenvalues and the poles are the same. Here is the command for obtaining the step response and the resulting output response plot in Figure II.S7:

» step(g)
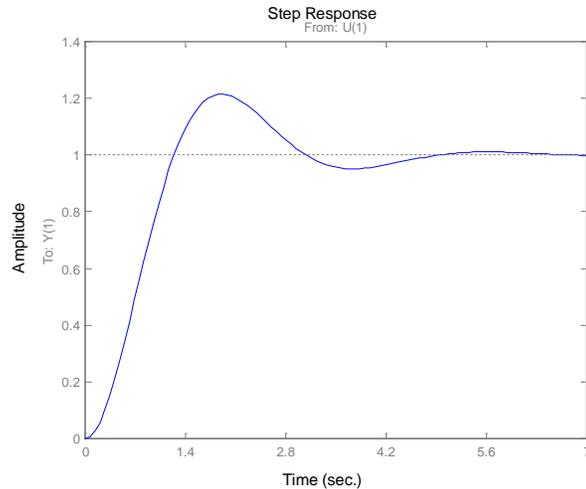
Figure II.S7: Step response of the output variable.

II.19. A state-space model is given:

$$
\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -2.405 & 0 \\ 0.833 & -2.238 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 7 \\ -1.117 \end{bmatrix} u
$$

$$
y = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}
$$

Find the transfer function $g(s)$ where $y(s) = g(s)u(s)$. Determine the poles and zeros.

Solution:

There are various methods to obtain the transfer function for this system. By taking Laplace transform of each equation, we obtain:

$$
sx_1(s) = -2.405x_1(s) + 7u(s)
$$

$$
sx_2(s) = 0.833x_1(s) - 2.238x_2(s) - 1.117u(s)
$$

The output equation yields,

$$y(s) = x_2(s)$$

By rearranging the state equations and solving for $x_2(s)$,

$$x_2(s) = \frac{1}{(s+2.238)}\left[\frac{1.117s + 3.145}{s+2.405}\right]$$

Thus,

$$y(s) = \frac{-1.117s + 3.145}{(s+2.238)(s+2.405)}u(s)$$

We have the following poles and zeros:

$$z_1 = +2.8156$$
$$p_1 = -2.238$$
$$p_2 = -2.405$$

We can also obtain the transfer function thorough the following expression (that can be easily derived using the Laplace transform rules):

$$\frac{y(s)}{u(s)} = g(s) = C(sI - A^{-1})B$$

where I is the identity matrix.

Another way is to use MATLAB with the following commands:

» A=[-2.405 0;0.833 -2.238];
» B=[7;-1.117];
» C=[0 1];
» D=0;
» [num,den]=ss2tf(A,B,C,D);
» g=tf(num,den)

Transfer function:

$$g(s) = \frac{-1.117\ s + 3.145}{s^2 + 4.643\ s + 5.382}$$

II.20. A chemical reactor has been operating at steady-state for a long time with the feed flow rate kept constant at 3.5 m^3/min. To handle a projected increase in upstream capacity, the operator decides to increase the feed flow rate suddenly by 10%, resulting in a change in the outlet stream composition recorded in Table II.2. Using the process reaction curve method, obtain an empirical transfer function model for this process.

Table II.2: Composition data in response to a change in flow rate.

Time (min)	Change (gmol/m^3)	Time (min)	Change (gmol/m^3)
0	0	1.6	0.35
0.2	0	1.8	0.5
0.4	0	2	0.55
0.6	0.02	3	0.7
0.8	0.1	4	0.9
1	0.15	5	0.95
1.2	0.2	6	1
1.4	0.3	8	1

Solution:

The transfer function model that will be used in this method is given by:

$$g(s) = \frac{k}{\tau s + 1} e^{-t_D s}$$

The parameter K can be determined from the steady-state information:

$$k = \frac{\Delta y}{\Delta u} = \frac{1}{0.35} = 2.86$$

One can use either the graphical method or the method that uses the output variable solution. If you are using the equation-based method, you have to recognize the fact that the Example 6.1 is for a specific input (unit step change) only, and in this problem the change is 0.35 m^3/min. The latter gives:

$$\ln\left(\frac{kM - y}{kM}\right) = -\frac{t - t_D}{\tau} = -\frac{1}{\tau}t + \frac{t_D}{\tau}$$

Select two points on the graph:
$$t = 1.4; \; y = 0.3$$
$$t = 3; \; y = 0.7$$

We have the following equations:

$$-0.357 = -\frac{1.4}{\tau} + \frac{t_D}{\tau}$$

$$-1.2 = -\frac{3}{\tau} + \frac{t_D}{\tau}$$

They result in:

$$\tau = 1.9\,\text{min}; t_D = 0.38\,\text{min}$$

So the transfer function is:

$$g(s) = \frac{2.86}{1.9s+1}e^{-0.38s}$$

Graphically, one can show the result in Figure II.S8.
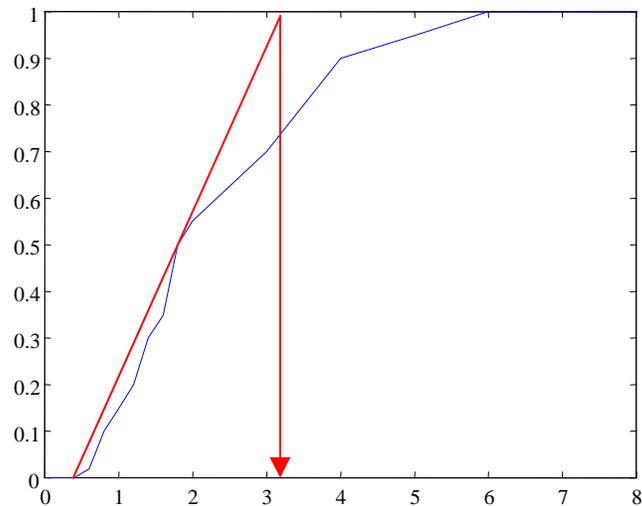
Figure II.S8: Plot of the composition data as in Table II.2.

Note that this method yields, $t_D = 0.5\,\text{min}; \tau = 3.2 - 0.5 = 2.7\,\text{min}$. The discrepancy results from the uncertainties built into each method.

II.21. An experiment is performed on a shell-and-tube heat exchanger that heats a process stream with medium-pressure steam. In the experiment, the steam valve is opened an additional 5% in a stepwise manner. The resulting temperature response of the process outlet stream is given in Figure II.7. Determine the process model parameters using the reaction curve method, and estimate the inaccuracies due to the data and calculation methods as discussed in Chapter 6.
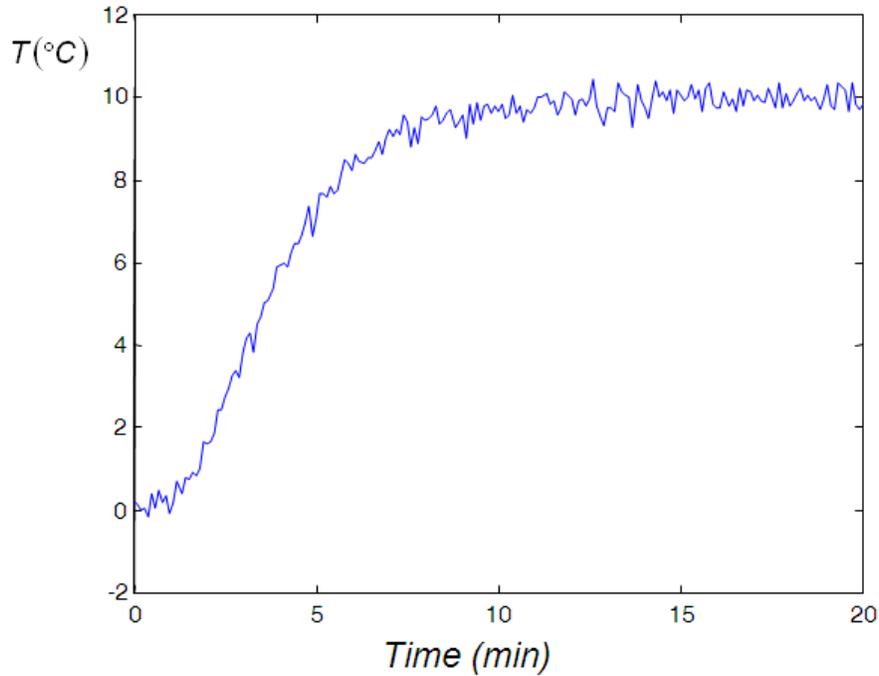
Figure II.7: Temperature response of the outlet process stream.

Solution:

Using the Process Reaction Curve Method, we first identify the constant k by considering the ultimate value of the temperature and the magnitude of the input change,

$$k = \frac{10^0 C}{5\%} = 2\ ^0C/\%$$

Then, we draw an estimated tangent to the inflection point of the response and two points on the graph are noted as shown below (Figure II.S9).
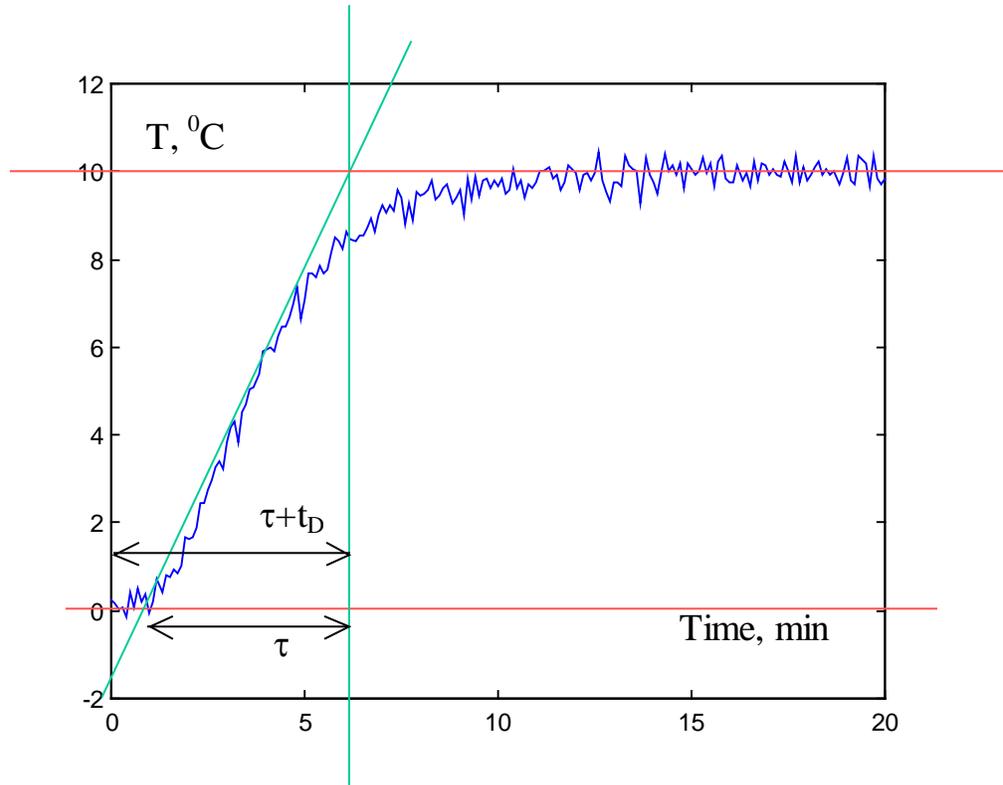
Figure II.S9: Illustration of the graphical approach.

This yields the following estimates of the other parameters:

$$\tau + t_D = 6$$
$$\tau = 5$$
$$t_D = 1$$

The transfer function representing the response of the process stream temperature with respect to the steam flow rate, then, looks like,

$$g(s) = \frac{2e^{-s}}{5s + 1}$$

II.22. For the vertical tube double-pipe heat exchanger in Exercise I.12, a set of open-loop experiments are carried out to study the system dynamics. The data can be downloaded from the authors' web pages (see Preface) and consists of:

- Outlet temperature of the vertical tube heat exchanger (stream 2) under variations of the flow rate of stream 1 (manipulated variable).
- Outlet temperature of the vertical tube heat exchanger (stream 2) under variations of the flow rate of stream 2 (disturbance).

- Outlet temperature of the vertical tube heat exchanger (stream 2) under variations of the feed temperature (stream 2) (disturbance).

The data are normalized as follows:
- Flow rate % = (actual flow rate - 0)/7800*100
  (7800 is the span range on the DCS)
- Temperature % = (actual temperature-32)/(212-32)*100

For this system:

1. Obtain the process transfer functions between the inputs (manipulated variable, disturbance) and the outlet temperature.
2. Try alternative model structures and discuss the results.

Solution:

Changes in flow rate F602

Using the complete data file for all changes in the input variable we obtain the following fit (Figure II.S10)
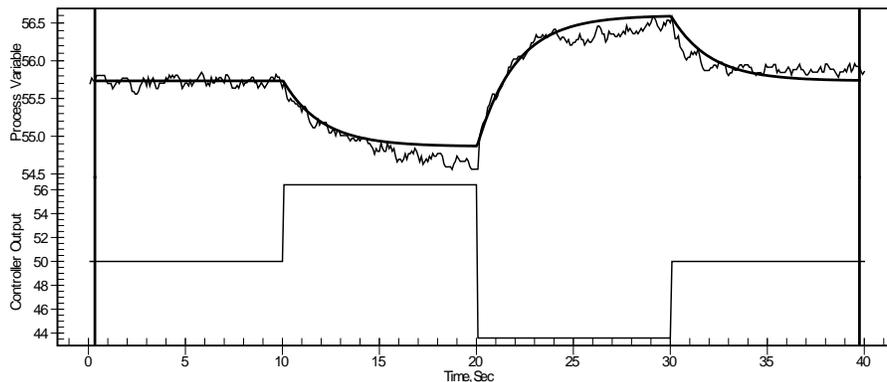
Figure II.S10: Fit of the model to the data.

The corresponding transfer function is given by (using nonlinear regression)

$$g_p(s) = \frac{T602(s)}{F602(s)} = \frac{0.138e^{-0.1s}}{(1.99s+1)}$$

However, if we use only the first portion of the data, corresponding to the first step test up to time 20 seconds), we obtain a fit as illustrated in Figure II.S11.
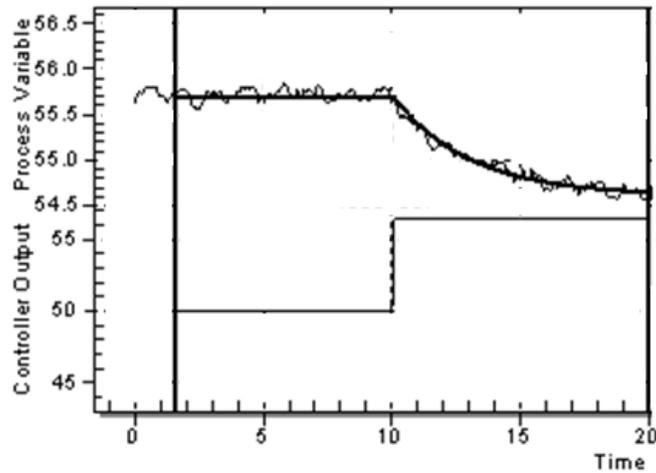
Figure II.S11: Fit of the model to the data.

The corresponding transfer function is given by

$$g_p(s) = \frac{T602(s)}{F602(s)} = \frac{0.173e^{-0.1s}}{(3.01s+1)}$$

Using the middle portion of the data we have (Figure II.S12)
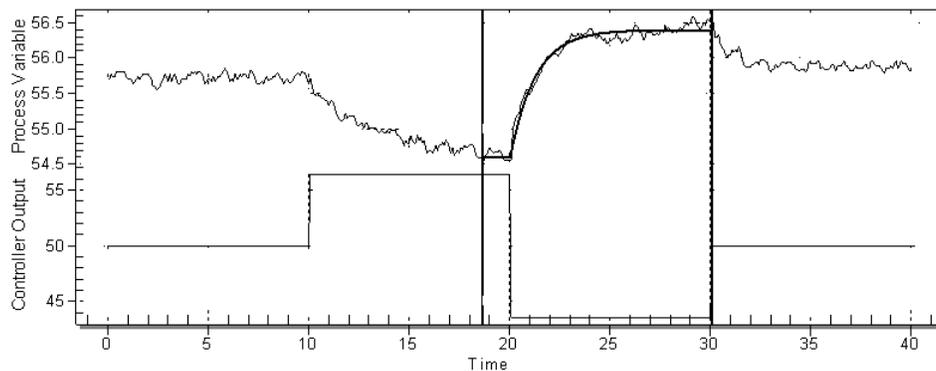
Figure II.S12: Fit of the model to the data.

$$g_p(s) = \frac{T602(s)}{F602(s)} = \frac{0.14e^{-0.213s}}{(1.25s+1)}$$

Similar studies can be performed using the other two portions of the data to analyze the variability of the process dynamic against positive and negative changes as well as the magnitude of the step.

The differences are due to the nonlinear characteristics of the process. We can also appreciate that the transfer function obtained using the whole data set provides some kind of average for the systems dynamics when dealing with positive and negative changes and should be used for control design purposes.

Using as a test a second order plus delay model (SOPTD) we obtain (Figure II.S13)
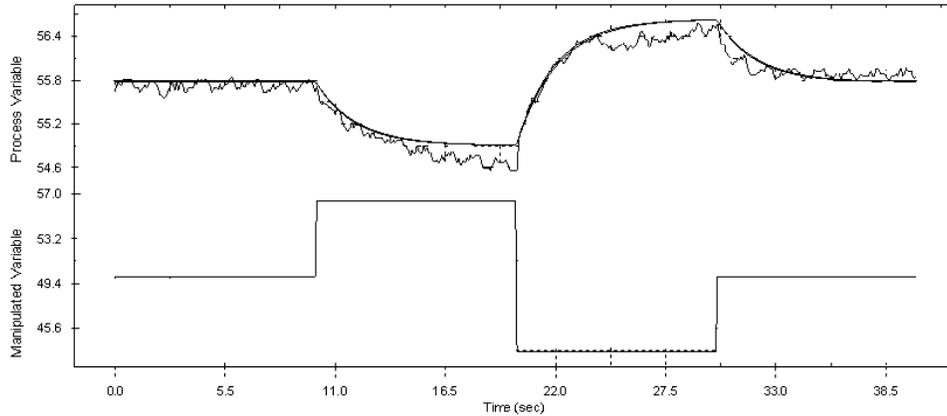
Figure II.S13: Fit of the model to the data

$$g_p(s) = \frac{T602(s)}{F602(s)} = \frac{0.135e^{-0.1s}}{(2.009s + 1)(0.0083s + 1)}$$

However, the addition of complexity into the model does not add accuracy into the prediction thus a FOPTD model will be used for further processing. Also notice that tone of the time constants is very small compared to the other meaning that a first order plus delay model is a good choice for the process.

<u>Changes in flow rate F601</u>

Assuming a FOPTD model we obtain the fit as shown in Figure II.S14.
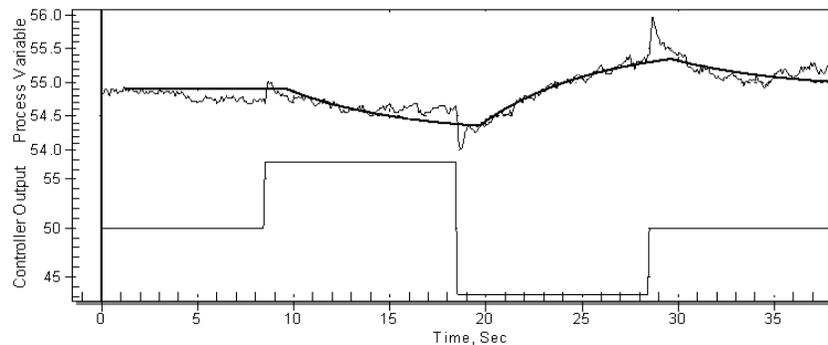
Figure II.S14: Fit of the model to the data.

This response clearly is not appropriate for the system's dynamics.

Selecting a second order model plus delay and lead element and after some manual adjustment of the model parameters, we have he fit shown in Figure II.S15.
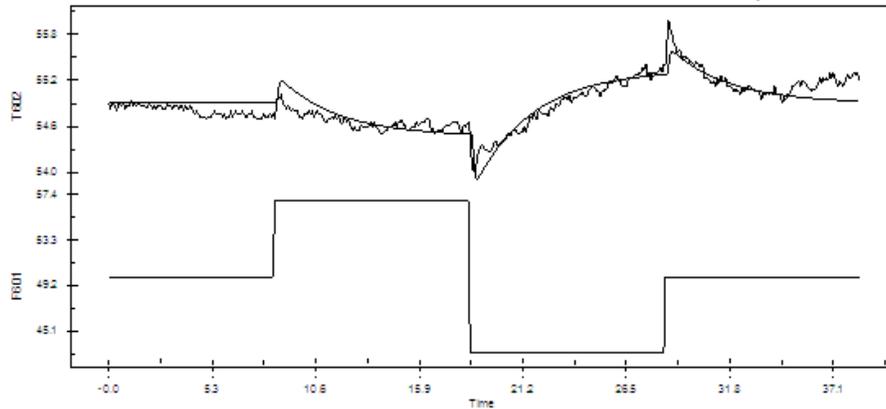
Figure II.S15: Fit of the model to the data.

$$g_{d1}(s) = \frac{T602(s)}{F601(s)} = \frac{-0.0572(-2.5s+1)e^{-0.2752s}}{(3.693s+1)(0.0296)}$$

which provides a more proper representation of the process dynamics and more importantly allows us to match the inverse response behavior of the process.

<u>Changes in the inlet process stream temperature (T601)</u>

We have for the overall fitting (using the whole data set), Figure II.S16.
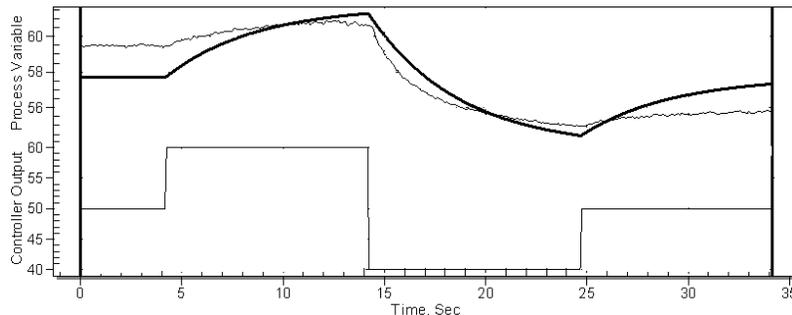
Figure II.S16: Fit of the model to the data.

$$g_{d2}(s) = \frac{0.3996e^{-0.1s}}{(4.43s+1)}$$

Using the first portion of the data we obtain the fit as shown in Figure II.S17.
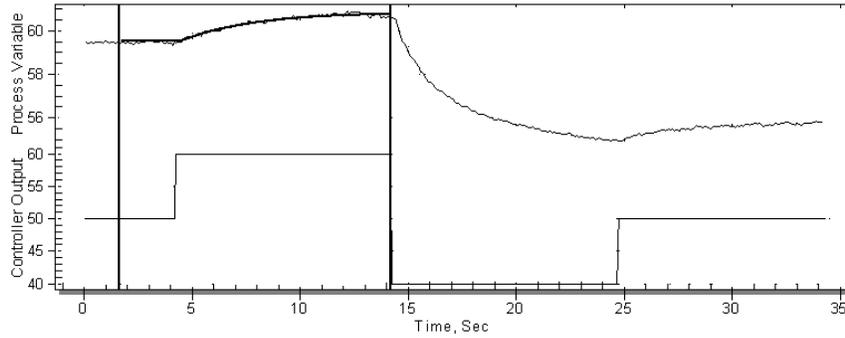
Figure II.S17: Fit of the model to the data.

With

$$g_{d2}(s) = \frac{T602(s)}{T601(s)} = \frac{0.133e^{-0.15s}}{(3.35s+1)}$$

Using the middle portion of the data we have a fit a shown in Figure II.S18.
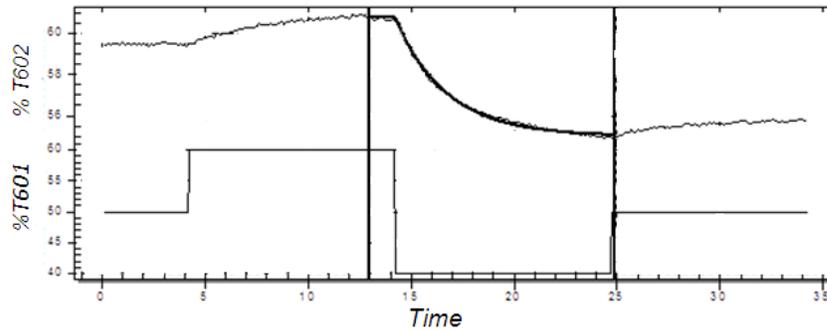
Figure II.S18: Fit of the model to the data.

$$g_{d2}(s) = \frac{T602(s)}{T602(s)} = \frac{0.2874e^{-0.1s}}{(2.466s+1)}$$

The best model in this case is an average between the last two cases, that is

$$g_{d2}(s) = \frac{T602(s)}{T601(s)} = \frac{0.20e^{-0.12s}}{(3.0s+1)}$$

Thus finally the model for the VTHX unit is given as follows

$$T602(s) = \frac{0.138e^{-0.1s}}{(1.99s+1)}F602(s) + \frac{(-0.0572)(-2.54s+1)e^{-0.2752s}}{(3.693s+1)(0.0296s+1)}F601(s)$$
$$+ \frac{0.20e^{-0.12s}}{(3.0s+1)}T601(s)$$

Final verdict on model selection:

For the manipulated variable changes, a simple FOPDT model is enough.

For the disturbances in inlet process stream flow rate, to be able to represent the more complex dynamics involved, a first-order model with a lead and a delay term is necessary. This is the only model to be able to represent the inverse response behavior.

Why these types of response for a disturbance change?

We have two effects acting together in opposite ways and at different time scales. One is a convective effect because the change of the amount of total flow coming into the heat exchanger and the other is a thermal effect since the temperature of the incoming feed has changed. The convective effect is immediate (incompressible fluid) and acts in the first instance, and the thermal effect takes some time to have an impact on the system (the time for the change to travel through the heat exchanger).

II.23. Bioreactors are used to produce a variety of pharmaceuticals, and food products. A simple bioreactor model involves biomass and substrate. The biomass consists of cells that consume the substrate. Following material balance equations are derived for a bioreactor[3],

$$\frac{dx_1}{dt} = (\mu - D)x_1$$
$$\frac{dx_2}{dt} = D(x_{2f} - x_2) - \frac{\mu x_1}{Y}$$

Here, D is the dilution rate, x_1 is the biomass concentration, x_2 is the substrate concentration, x_{2f} is the feed concentration of the substrate, and Y is the yield with $Y = 0.4$. The specific growth rate μ for a system with substrate inhibition is given as,

$$\mu = \frac{\mu_{max} x_2}{k_m + x_2 + k_1 x_2^2}$$

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[3] Bequette, B.W., *Process Dynamics: Modeling, Analysis and Simulation*, Prentice Hall (1998).

The constants are given as, $k_m = 0.12\,g/L; k_1 = 0.4545\,L/g; \mu_{max} = 0.53\,hr^{-1}$.   The steady-state values of the input and the state variables are, $D_s = 0.3\,hr^{-1}; x_{1s} = 1.5302; x_{2s} = 0.1745$.

Construct a simulation of this process in MATLAB/Simulink. By introducing small step changes in the dilution rate, observe the biomass response. Develop a discrete-time model (see Eq. 6.9) for this system using the step-response data.

Solution:

The Simulink block diagram for the bioreactor model is given in Figure II.S19.
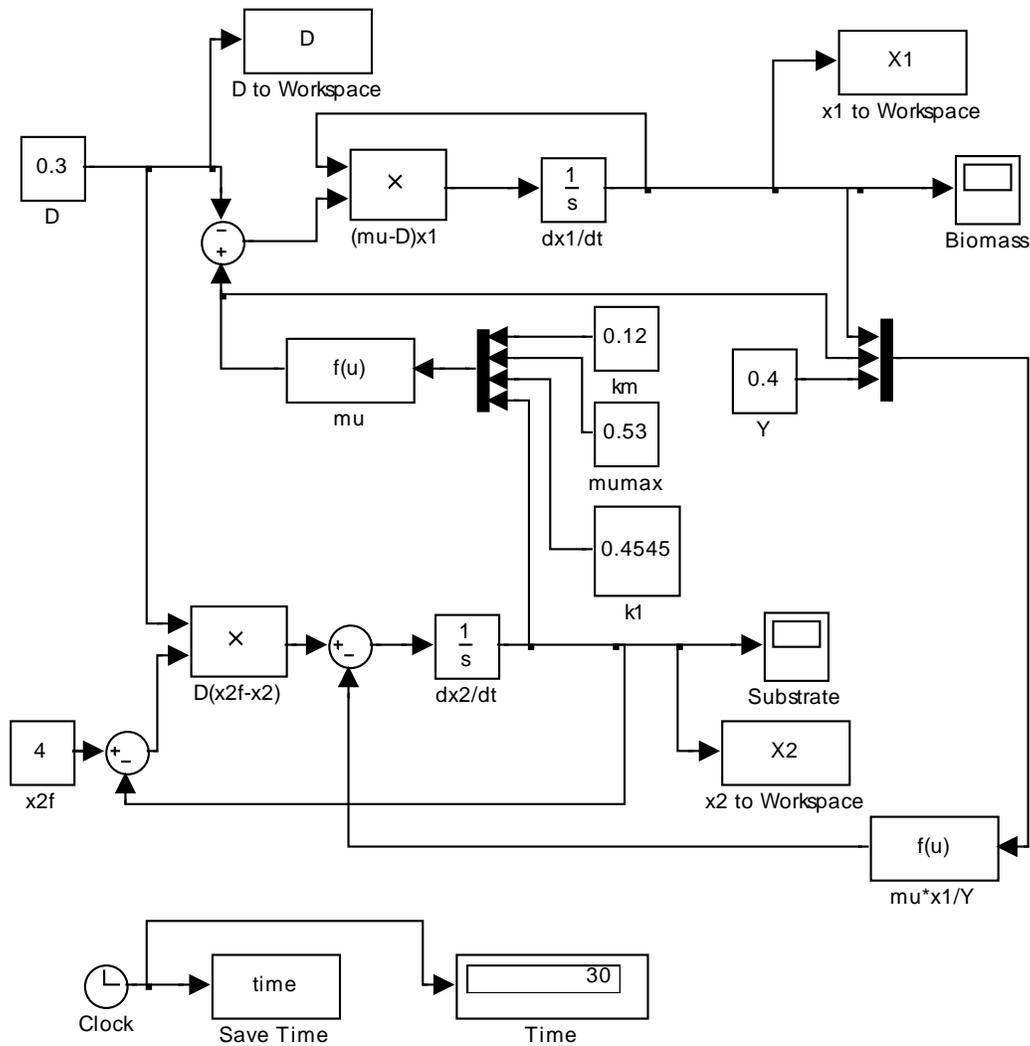
Figure II.S19: Simulink diagram for bioreactor model.

Staring from an initial condition of $x_{10} = x_{20} = 1.0$, the biomass and substrate response for $D = 0.3$ is given in Figure II.S20.
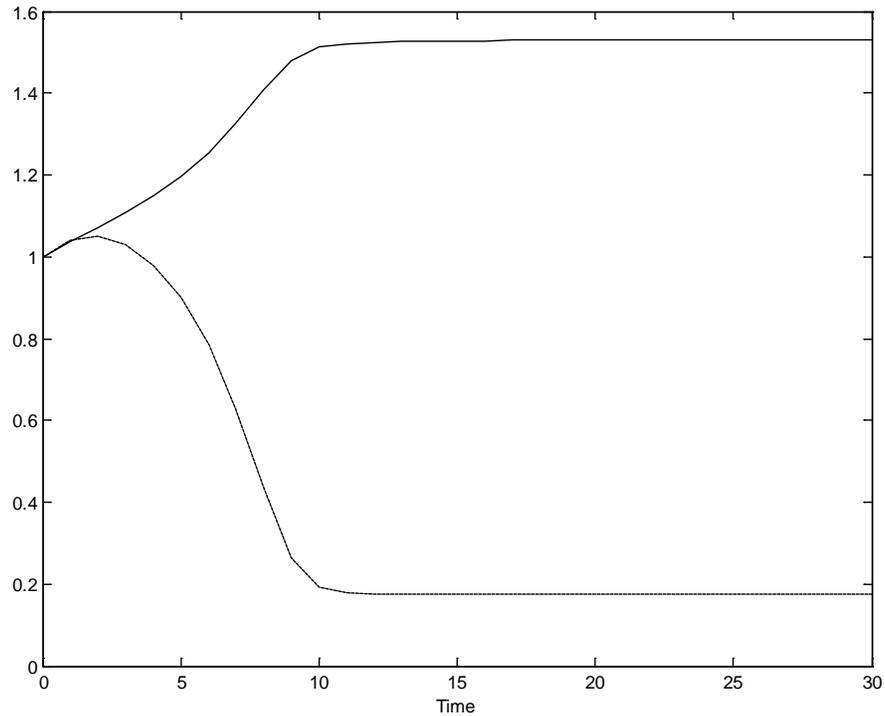
Figure II.S20: The response of biomass (solid) and substrate (dashed) from an initial condition of $x_{10} = x_{20} = 1.0$.

Figure II.S21 shows the response of the biomass concentration for a series of step changes in the dilution rate. We will use the first half of this response data for modeling and the second half for validation.
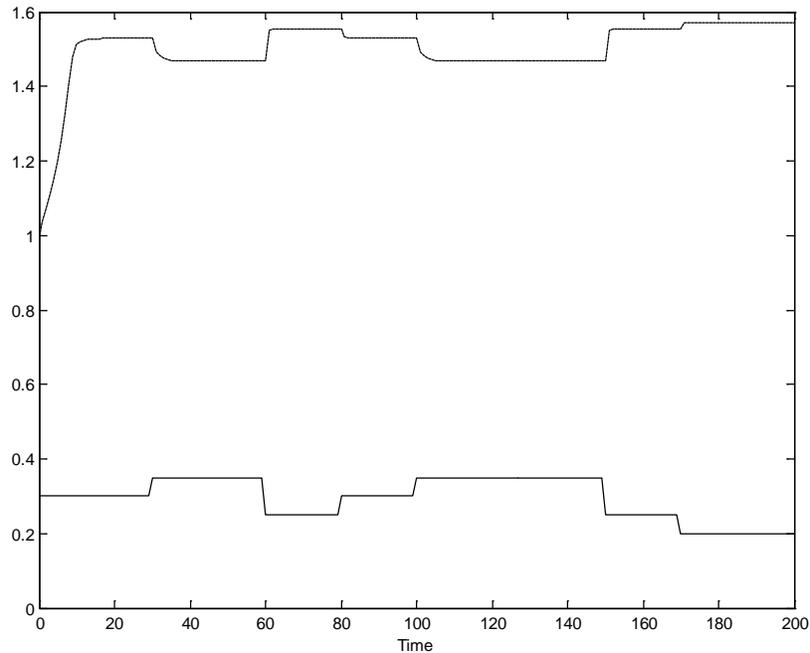
Figure II.S21: Set of step changes in dilution rate results in this biomass response.

We will show the results for a first-order and a second-order model. Following are the forms of the model:

First-order: $y(i+1) = -a_1 y(i) + b_1 u(i)$

Second-order: $y(i+1) = -a_1 y(i) - a_2 y(i-1) + b_1 u(i) + b_2 u(i-1)$

The parameter matrix is formed and calculated as follows for the second-order model,

$$\phi(i+1) = \begin{bmatrix} -y(i) & -y(i-1) & u(i) & u(i-1) \end{bmatrix}$$

$$\theta = \begin{bmatrix} a_1 & a_2 & b_1 & b_2 \end{bmatrix}^T$$

The parameters obtained using the LS algorithm are:

First-order: $a_1 = -0.4443; b_1 = -0.1157$

Second-order: $a_1 = -1.0817; a_2 = 0.1167; b_1 = -0.1673; b_2 = 0.1584$

The results of the validation and cross-validation simulations are shown in Figures II.S22 and II.S23. There is general agreement but the models perform poorly in predicting the steady-states. This is most likely due to the nonlinear nature of the actual process.
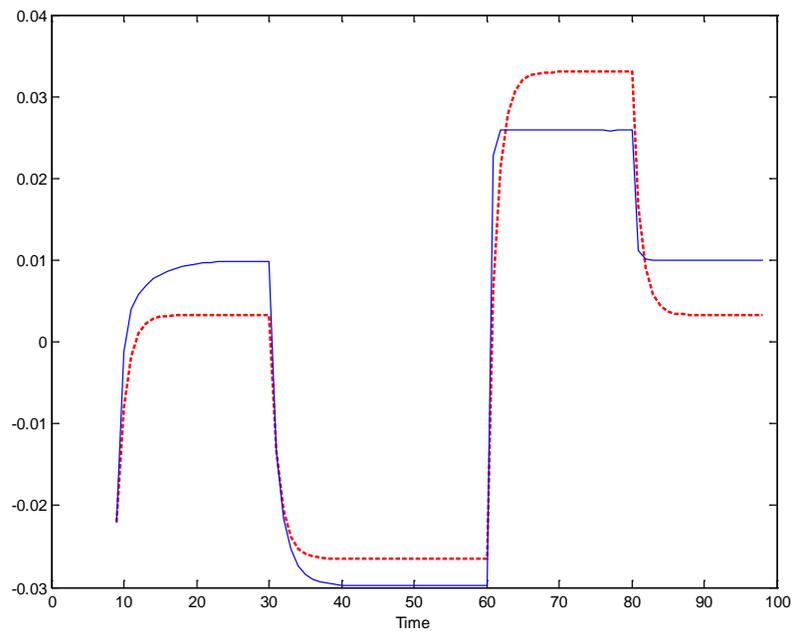
(a)
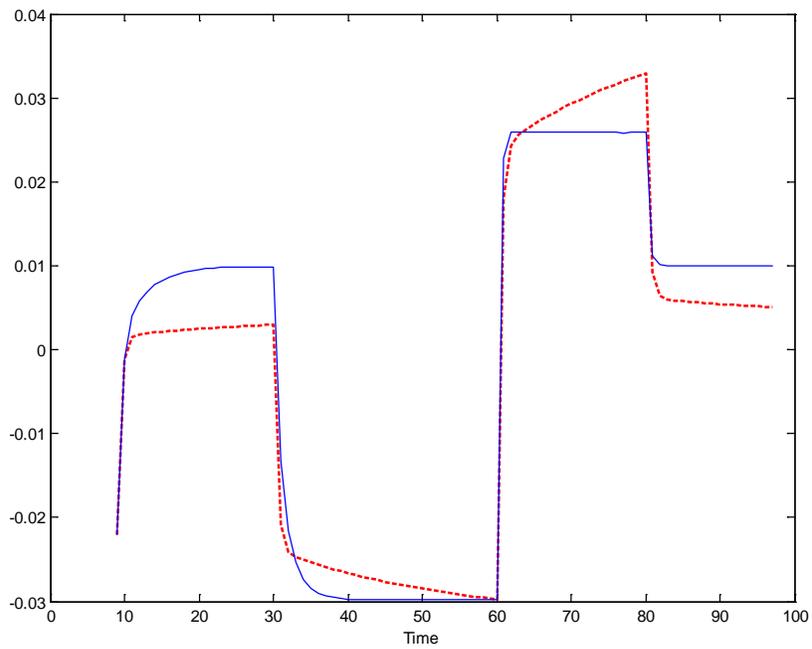
(b)

Figure II.S22. Validation of first-order model (a) and second-order model (b), actual data (line), model prediction (dashed).
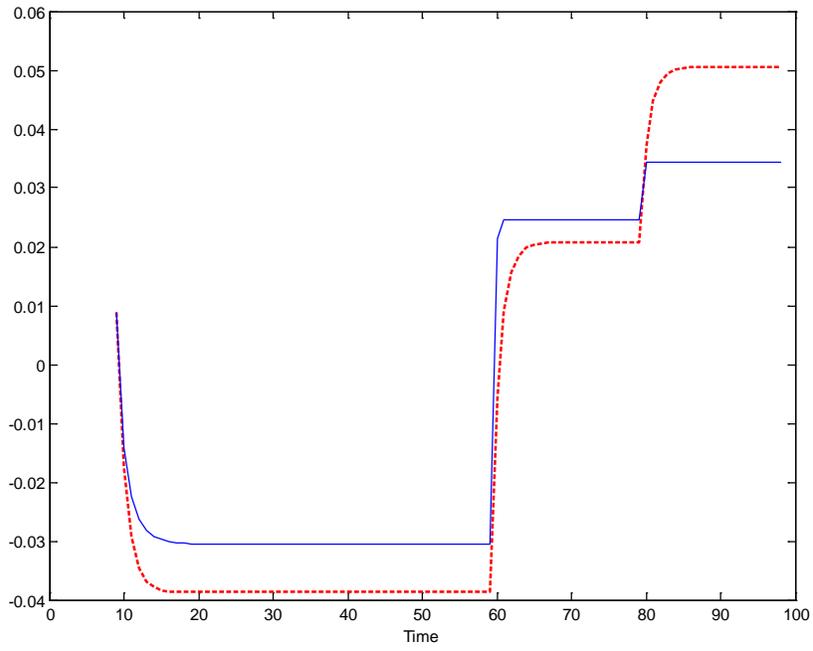
(a)
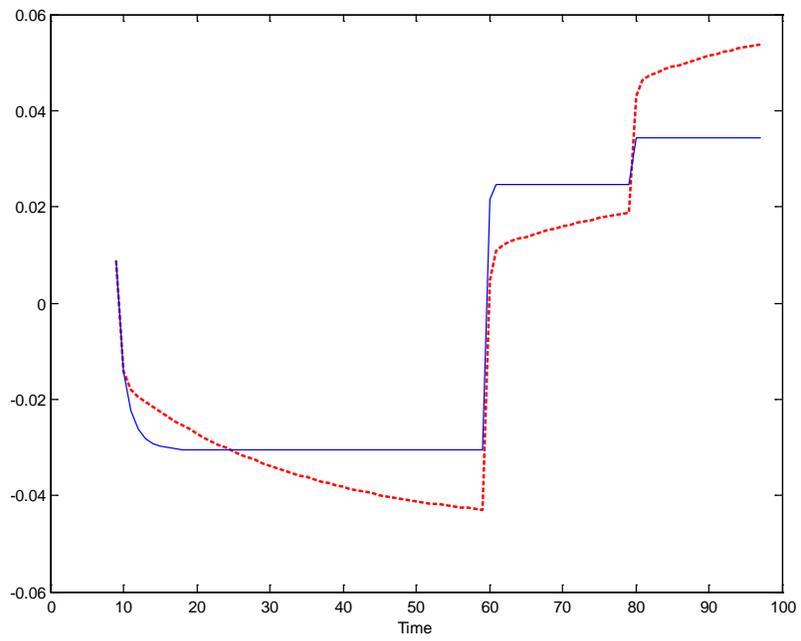
(b)

Figure II.S23. Cross-validation of first-order model (a) and second-order model (b), actual data (line), model prediction (dashed).