# CHE656

# Process Analysis and Modeling

## Modeling and Optimizing Chemical Processes

## Exercise Problems

### Year 2021 Edition

Prepared by

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# Part I


# Process Modeling and Dynamics

## 1. *Mass Balance in a Two-Tank System*

Consider the following two vessels connected in series. We will model this system over a total time domain of 20 minutes. Initially (at $t = 0$), Tank 1 is filled with 20 kg of brine solution with 60 mass% salt, while Tank 2 is filled with 20 kg of pure water. For the first 10 minutes, pure water with a flow rate of $F_1 = 1 + t$ (in kg/min) is added to Tank 1 (assuming the added salt dissolves instantly), while $F_2$ is kept to zero. We define $M_1$ and $M_2$ as the total mass and define $x_1$ and $x_2$ as the mass fraction of salt, all respectively in Tank 1 and Tank 2.

$F_1$ (pure water)

$M_1$ $x_1$        $F_2$        $M_2$ $x_2$

Tank 1                Tank 2
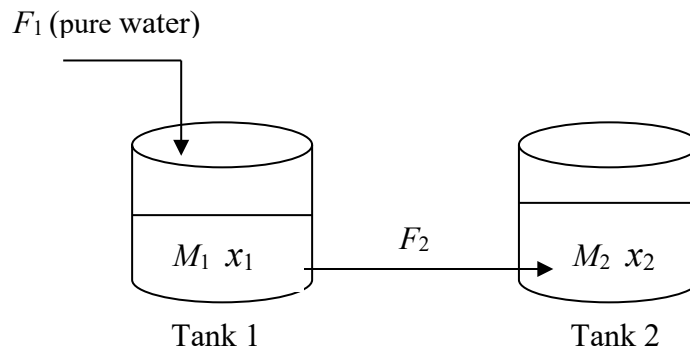
(a) Derive an analytical expression of $x_1$ as a function of time $t$, for $0 \le t \le 10$ min. Note that you must integrate your derived ODE by hand and show intermediate results using known techniques, such as separation of variables, substitution, integrating factors, etc. Do not use tables of integrals or online help or points will be deducted.

**Answers:**    $M_1$ ($t = 10$ min) = _____ kg    $x_1$ ($t = 10$ min) = _____

(b) Between $10 \le t \le 20$ min, $F_1$ is shut off (i.e. its flow rate is kept to zero now) and $F_2$ is turned on and set equal to 1 kg/min. Derive an analytical expression of $x_2$ as a function of time $t$, for $10 \le t \le 20$ min. Note that the initial time in your integration must be set to 10 min, not 0 min. Again, you must integrate your derived ODE by hand and show all intermediate results.

**Answers:**    $M_2$ ($t = 20$ min) = _____ kg    $x_2$ ($t = 20$ min) = _____

## 2. *A Two-Tank System*

A large tank is connected to a smaller tank by means of a valve, which remains closed at all times. The large tank contains nitrogen (assume it is an ideal gas) at 700 kPa, while the small tank is evacuated (vacuum). The valve between the two tanks starts to leak and the rate of gas leakage is proportional to the pressure difference between the two tanks, as given by

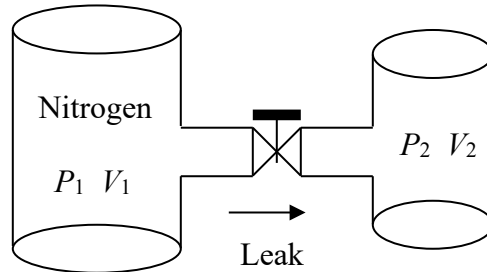$$Leak \ Flow = C_V \sqrt{P_{AVG}(P_1 - P_2)}$$

where $P_{AVG}$ = average absolute pressure across the valve = $(P_1 + P_2)/2$

Valve constant $C_V = 3.6 \times 10^{-4}$ kmol/kPa-hour.
Tank volumes are 30 m$^3$ and 15 m$^3$.
Assume constant temperature of 293.15 K in both tanks.
Universal gas constant = 8.31439 kPa-m$^3$/kmol-K.



(a) Derive an analytical expression of $dn_1/dt$ as a function of $n_1$, where $n_1$ is the number of moles of nitrogen in the large tank. This ODE of yours should contain only $n_1$ as the unknown variable. Use MATLAB to solve for $n_1$ (use *ode45* and "format short"), and run the model up until $t = 25$ hours.

**Answer:** $n_1$ ($t = 25$ hours) = _____ kmoles

(b) As a good chemical engineer, you always look for ways to simplify your engineering calculations. In this particular problem, it is possible to derive an analytical solution when $t$ is small, i.e. when $P_2 \ll P_1$. Derive an analytical expression for $n_1$ as a function of time $t$. Calculate $n_1$ after 2 hours and 4 hours, and compare these solutions with those from Part (a) by reporting the absolute % relative errors (assuming the MATLAB solutions are exact and show 4 decimal places).

**Answers:**

$n_1$ ($t = 2$ hours) = _____ kmoles     % relative error = _____

$n_1$ ($t = 4$ hours) = _____ kmoles     % relative error = _____

## 3. *Mixing Tank with 2 Feeds*
Consider the following mixing tank problem. Water is flowing into a well-stirred tank at 120 kg/hr and methanol is being added at 20 kg/hr. The resulting solution is leaving the tank at 100 kg/hr. There is 100 kg of fresh water in the tank at the start of the operation. We are interested in determining the mass fraction of methanol in the outlet as a function of time $t$.

120 kg/hr water                                    20 kg/hr methanol



100 kg/hr
solution
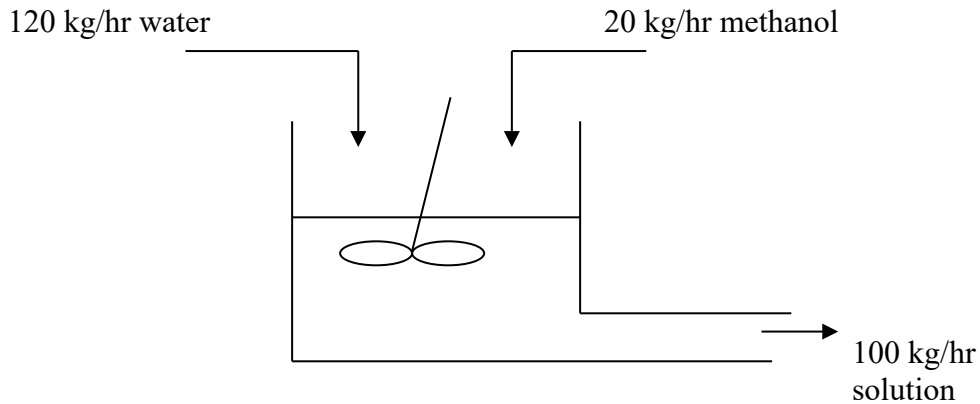
(a) Derive an analytical expression for solving the mass fraction of methanol as a function
of time $t$. An analytical solution is possible for this particular system.

(b) Use MATLAB to solve for the mass fraction of methanol in the outlet after 1 hour, and
compare the number to the exact solution in Part (a). Also, what is the methanol mass
fraction in the outlet at steady state?

(c) Of course, steady-state condition probably cannot be achieved in this system because the
inflow rate is greater than the outflow rate, and sooner or later, the tank will fill and
overflow. Assuming that the density of the solution in the tank is always constant at
1000 kg/m³ and the volume of the tank is 1.0 m³, compute the time it takes for the tank
to overflow.

4. **Mass Balance in a Two-Vesse; System**
Consider the following two closed vessels connected in series used to store gas. Initially (at
$t = 0$), Vessel 1 is filled with 100 gmoles of a mixture of methane and nitrogen, 80 mol% of
which is methane, while Vessel 2 is filled with 10 gmoles of pure nitrogen.

The gas in Vessel is gradually released into Vessel 2 via a sophisticated control valve which
allows the released molar flow rate $F$ (gmoles/minute) to be directly proportional to the
amount of gas left in Vessel 1, i.e $F = 0.01N_1$, where $N_i$ is the total number of gmoles of
gas in Vessel $i$ and $y_i$ is the mole fraction of methane in Vessel $i$.
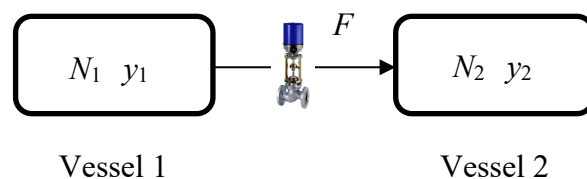


Vessel 1                                    Vessel 2

(a) Derive an analytical expression of $N_2$, the total amount of gas in Vessel 2, as a function
of time.

**Answer:**  $N_2$ $(t = 30$ min$) = $ _____ gmoles

(b) Derive an analytical expression of $y_2$, the mole fraction of methane in Vessel 2, as a function time. You must show detailed work in your integration and are not allowed to use formulas from the Internet or tables of integration.

**Answer:**  $y_2$ $(t = 30$ min$) = $ _____

(c) Verify your analytical solution in Part (b) by solving the ODE $dy_2/dt$ derived using *ode45* solver in MATLAB. Make a plot of $x_2$ as a function of time from $t = 0$ to $t = 200$ minutes. Hint: Another way to verify your MATLAB solution is to specify an initial condition of $y_2(0) = 0.8$, which will result in a flat response because $y_2$ will no longer vary with time.

## 5. *Continuous Cone-Shaped Open Vessel*

Consider a conical open vessel as shown in the following figure. The vessel has a radius R at the top and a height H. Water flows into the vessel at a rate of $F_1$ and it flows out through a valve at a rate of $F_2$. The following data are given:
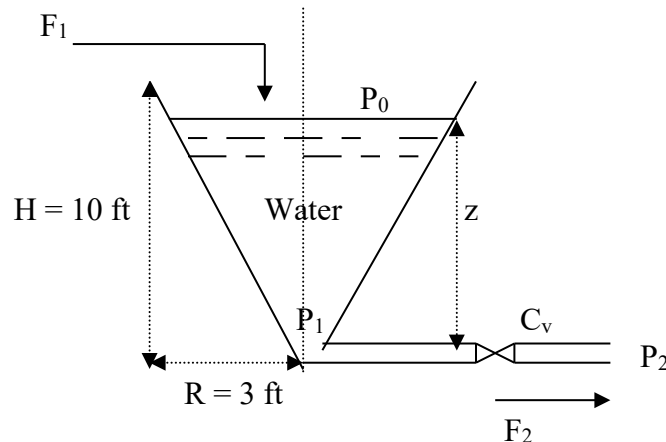


$P_0 = P_2 = 14.7$ psia
$C_v =$ characteristic valve constant $= 3.0$ ft$^3$/psia$^{1/2}$-min
$\phi =$ water mass density $= 62.4$ lbm/ft$^3$
$z_0 =$ initial liquid height $= z(t = 0) = 5$ ft

$F_1$ is not constant but is controlled such that it varies with the liquid height according to:
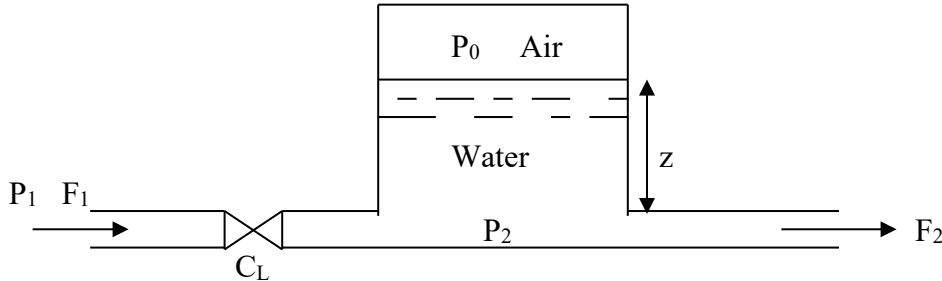
$$F_1 = 2z^{1/2} \quad \text{ft}^3/\text{min}$$

Solve for z analytically as a function of time.

**Hint:** Volume of a cone $V = \int_0^z A(z)dz$
where $A(z) =$ cone cross-sectional area and is a function of z

## 6. *Adiabatic Expansion/Compression in an Enclosed Vessel*

Consider the following system in which air is trapped inside an enclosed vessel while water flows into the vessel at a rate of $F_1$ and flows out at a rate of $F_2$.



Initially, the air is at 25°C and $1.01325 \times 10^5$ Pa (Pascal), and the liquid height is 5.0 meter. The following data are available:

Gravitational acceleration $g$ = 9.80665 m/s²
Air $C_V$ (heat capacity at constant volume) = $2.0731 \times 10^4$ J/kmol°C

| | |
|---|---|
| Vessel volume =10.0 m³ | Vessel cross-sectional area = 1.0 m² |
| Water density = 1000 kg/m³ | Gas constant R = 8314 m³Pa/kmol°K |
| | = 8314 J/kmol°K |
| Air MW = 29.0 kg/kmol | Valve constant $C_L$ = 0.001 m³/Pa$^{1/2}$min |
| Outlet flow rate $F_2$ = 0.1 m³/min | Source pressure $P_1$ = $3.0 \times 10^5$ Pa |

(a) Assuming adiabatic expansion/compression due to the rise/fall of the liquid height, write down all the system-describing equations. Be sure to define all your variables which are unknown. Use the data given and simplify each equation as much as possible.

(b) Derive an ordinary differential equation that relates the liquid height as a function of time. Your final equation must contain Z as the only dependent variable.

(c) Solve the ODE in Part (b) using MATLAB and plot the liquid height Z as a function of time.

## 7. *Two Open Continuous Flow Tanks in Series*

Consider two tanks in series as shown where the flow out of the first tank enters the second tank. Our objective is to develop a model to describe how the height of liquid in tank 2 changes with time, given the input flowrate $F_0(t)$. Assume that the flow out of each tank is a linear function of the height of liquid in the tank (i.e. $F_1 = \beta_1 h_1$ and $F_2 = \beta_2 h_2$) and each tank has a constant cross-sectional area.
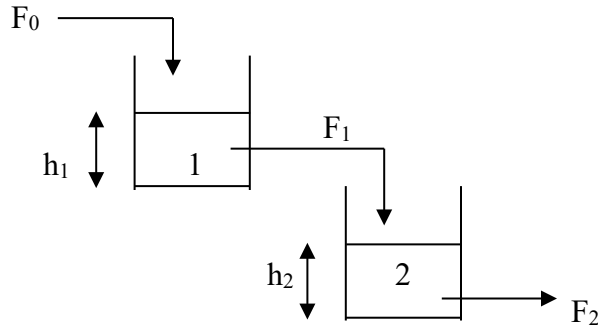
(a) Develop a system of equations to describe the liquid height of the two tanks as a function of time, assuming constant liquid density.  Be sure to define all your variables.

(b) Solve for $h_1$ and $h_2$ analytically if

$$A_1 = 10 \text{ ft}^2 \qquad A_2 = 20 \text{ ft}^2 \qquad F_0 = 2 \text{ ft}^3/\text{hr}$$
$$\beta_1 = \beta_2 = 1 \text{ ft}^2/\text{hr} \qquad \text{where } A_i \text{ is the cross-sectional area of tank i}$$

and tank 1 initially has a liquid height of 1 ft of while tank 2 is empty.  Plot the two liquid height profiles as a function of time from 0 hr to 5 hr.

(c) Suppose $F_0$ is no longer constant but equals to $2t + 1$ ft$^3$/hr.  Use MATLAB to solve for the liquid heights in both tanks.  Plot both profiles as a function time up to 5 hr.

8. *Liquid Height in a Spherical Tank*
   The following figure shows a spherical tank for storing water.  The tank is filled through a hole in the top and drained through a hole in the bottom.  If the tank's radius is $R$, one can
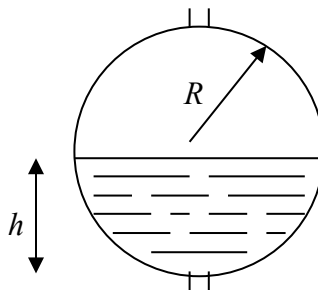


use integration to show that the volume of water in the tank as a function of its height $h$ is given by:

$$V(h) = \pi R h^2 - \frac{\pi h^3}{3}$$

Studies in fluid mechanics have identified the relation between the volume flow through the bottom hole and the liquid height as:

$$F = C_d A \sqrt{2gh}$$

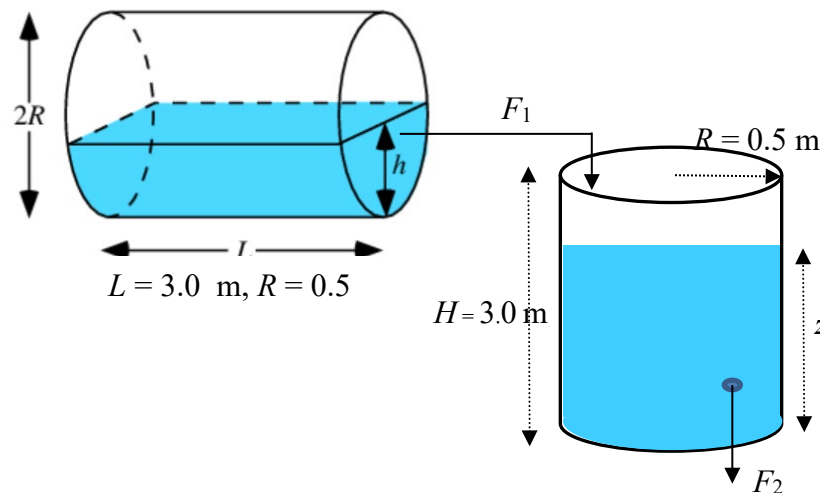where $A$ is the area of the hole, $g$ is the acceleration due to gravity (32.2 ft/sec$^2$), and $C_d$ is an experimentally determined value that depends partly on the type of fluid (for water, $C_d = 0.6$).

Suppose the initial height of water is 8 ft and the tank has a radius of 5 ft with a 1-inch diameter hole in the bottom. Use MATLAB to determine how long it will take for the tank to empty (i.e. drain completely), to the nearest second (i.e. no decimal places).

### 9. *Dynamics of Liquid Height in Two Vessels in Series*
A horizontal cylindrical vessel and a vertical cylindrical vessel with the given dimensions are connected in series as shown.



$$L = 3.0 \text{ m}, R = 0.5$$

Water flows out of the horizontal cylindrical vessel with $F_1 = 1.0$ m$^3$/min which then flows into the second vessel. There is a small spherical hole (radius = 2 cm or 0.02 m) at the bottom in the second vessel which drains the water based on gravity at a volumetric flow rate of:

$$F_2 = C_d A \sqrt{2gz}$$

where $A$ is the area of the hole, $g$ (9.81 m/s$^2$ or 35316 m/min$^2$) is the acceleration due to gravity, and $C_d$ is an experimentally determined value that depends partly on the type of fluid (for water, $C_d = 0.6$).

The following very complicated formula has been derived for the volume of a horizontal cylindrical vessel which is partially filled as a function of $L$, $R$ and $h$.

$$V(L, R, h) = L \left[ R^2 \cos^{-1} \left( \frac{R - h}{R} \right) - (R - h) \sqrt{2Rh - h^2} \right]$$

(a) At $t = 0$, the horizontal cylindrical vessel is three-quarter full. Calculate the height above the bottom of the horizontal cylindrical vessel at $t = 0$.

$h$ when the horizontal cylindrical vessel is three-quarter full = _____ meter

(b) Derive an ODE that expresses $h$ as a function of time in the horizontal cylindrical vessel. You must simplify the ODE as much as possible. Solve the ODE by *ode45* and plot the dynamics of the liquid height $h$ and determine the time it takes for the vessel to become completely empty. You will need the following formula:

$$\frac{d(\cos^{-1} x)}{dx} = -\frac{1}{\sqrt{1 - x^2}}$$

$t$ when the cylindrical vessel is empty = _____ minutes

(<u>Hint</u>: You could use simple volume calculations to verify your MATLAB answer.)

(c) Derive an analytical solution for the liquid height $z$ in the vertical cylindrical vessel as a function of time, given that at $t = 0$, the vertical vessel is one-half full.

$z$ at $t = 1$ minute = _____ meters

## 10. *Modeling Liquid Heights in a Two-Vessel System*

An open spherical vessel is connected to a closed rectangular tank through an open valve as shown in the figure below. Water flows continuously into the spherical vessel at a volumetric flow rate of $F_1$ with some of the water in the sphere also flowing into the rectangular tank at a rate of $F_2$. Water then flows out of the rectangular tank at a flow rate of $F_3$, and the temperature inside the tank is always maintained at 298.15 K. We wish to study the dynamics of the liquid heights in the two vessels using MATLAB.
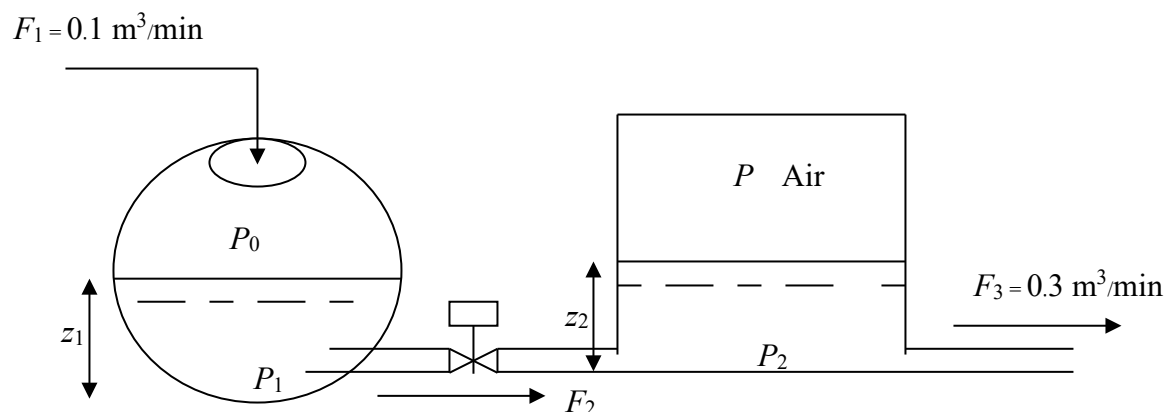
The following data are known about the system:

$C_V = 1 \times 10^{-5}$ m$^3$/Pa$^{1/2}$-min (characteristic valve constant)    $P_0 = 1.01325 \times 10^5$ Pascal
Cross-sectional area of rectangular tank $= 3$ m$^2$    Radius of sphere $R = 2$ m
Height of rectangular tank $= 10$ m
Initially at $t = 0$, $z_1 = 3$ m, $z_2 = 2$ m, $P = 1.01325 \times 10^5$ Pascal
Gravitational acceleration $g = 9.80665$ m/s$^2$    $\phi$ (water) $= 1000$ kg/m$^3$

Universal gas constant $R = 8314$ m$^3$-Pa/kmol-K $= 8314$ J/kmol-K
Liquid volume inside a sphere as a function of liquid height $z$ is given by:

$$V = \pi \ R \ z^2 - \frac{\pi \ z^3}{3}$$

Use MATLAB's *ode*45 to determine whether the liquid heights in the two vessels will ever be equal, i.e. $z_1 = z_2$. If so, report the time (accurate to one decimal place) at which this happens and the height.. If $z_1$ is never equal to $z_2$, determine when the two liquid heights are at the closest. Run your model for 20 minutes, which should be sufficient to answer the questions.

**Answer the following questions:**

Are the two liquid heights ever equal?    ☐ Yes    ☐ No

If yes, $z_1 = z_2 = $ _____ meters

Time at which the two liquid heights are equal or at the closest = _____ minutes

## 11. *Modeling Liquid Heights in a Two-Vessel System*
An open rectangular vessel is connected to a well-insulated (i.e. adiabatic) and closed spherical vessel shown in the figure below. Water from the rectangular vessel is drained through a hole (radius $= 4$ cm) at its bottom into the spherical vessel at a volumetric flow rate of:

$$F_1 = C_d A \sqrt{2 g z_1}$$

where $A$ is the area of the hole, $g$ is the acceleration due to gravity, and $C_d$ is an experimentally determined value that depends partly on the type of fluid (for water, $C_d = 0.6$). Water then flows out of the spherical vessel at a flow rate of $F_2$. We wish to study the dynamics of the liquid heights in the two vessels using MATLAB.
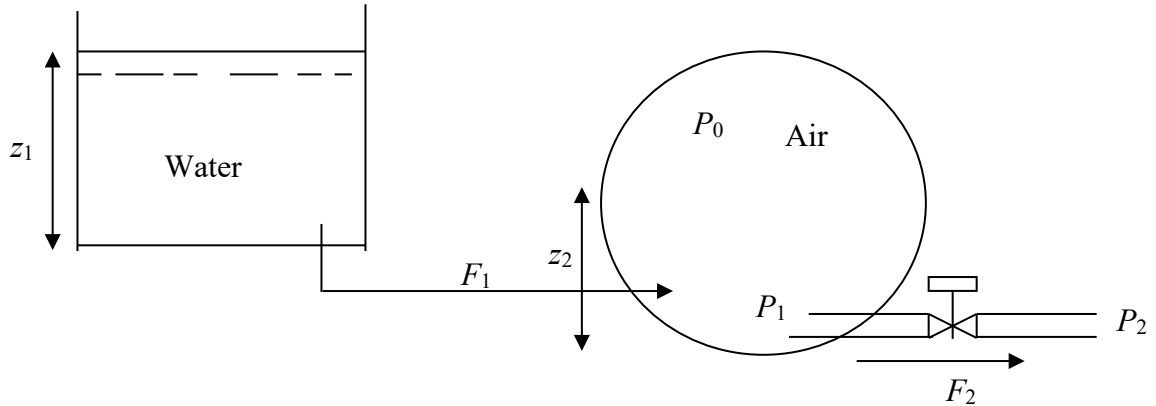
The following data are known about the system:

$C_{valve}$ = 1×10$^{-3}$ m$^3$/Pa$^{1/2}$-min (characteristic valve constant)
Cross-sectional area of the rectangular vessel = 4 m$^2$
Radius of sphere $R$ = 2 m          $P_2$ = 1.01325×10$^5$ Pascal          $\phi$ (water) = 1000 kg/m$^3$
$C_V$ (air heat capacity at constant volume) = 20850 J/kmol-K

Initially at $t$ = 0, $z_1$ = 6 m, $z_2$ = 2 m, $P_0$ = 1.01325×10$^5$ Pascal, $T_G$ = 303.15 K
Gravitational acceleration $g$ = 9.80665 m/s$^2$ = 35303.94 m/min$^2$

Universal gas constant $R$ = 8314 m$^3$-Pa/kmol-K = 8314 J/kmol-K
Conversion factors: 1 Pascal = 1 N/m$^2$ = 1 kg/m-s$^2$, 1 N = kg-m/s$^2$, 1 J = kg-m$^2$/s$^2$
Liquid volume inside a sphere as a function of liquid height $z$ is given by:

$$V = \pi\ R\ z^2 - \frac{\pi\ z^3}{3}$$

Derive an ODE for $z_2$ as a function of time (without $z_1$ in the ODE) and use MATLAB's *ode45* to simulate its dynamics until either the rectangular vessel dries up or the spherical vessel is full. You must simplify your final ODE as much as possible before using it in MATLAB. Note that *ode45* may result in solutions with imaginary parts. You can ignore them as long as the values are small which come from inherent problems in numerical integrations. **Hint:** Be very careful with your units and their conversions.

**Answer the following questions:**

Time at which the rectangular vessel dries up or the spherical vessel is full (whichever is

smaller) = _____ minutes

12. *Modeling Liquid Heights in a Two-Vessel System*
    Consider two tanks in series as shown where the water flow out of the first tank enters the second tank. The first tank is a cubic vessel with a width of 10 ft, a length of 10 ft, and a height of 10 ft, whereas the second tank is a cone-shaped vessel with a radius of 5 ft at the

top and a height of 20 ft. The first tank is filled with water at a volumetric flow rate $F_1$ and is drained through a hole (radius = 1 inch) at the bottom. Studies in fluid mechanics have identified the relation between the volume flow through the bottom hole and the liquid height as:

$$F_2 = C_d A \sqrt{2gz_1}$$

where $A$ is the area of the hole, $g$ is the acceleration due to gravity (32.2 ft/sec$^2$), and $C_d$ is an experimentally determined value that depends partly on the type of fluid (for water, $C_d$ = 0.6). Initially at $t = 0$, the cubic tank is filled with 2 ft of water and the cone-shaped tank is filled with 15 ft of water.

$F_1 = 15$ ft$^3$/min
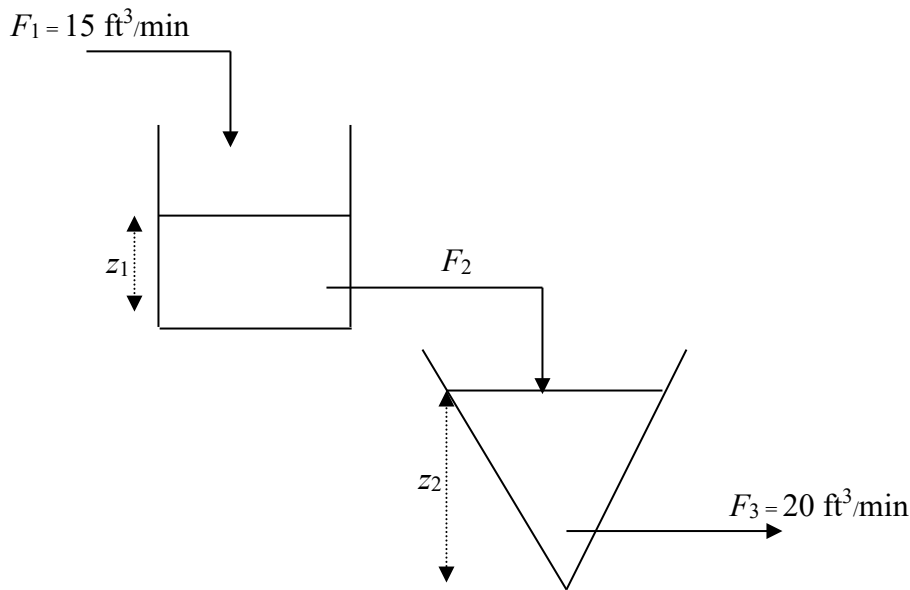


(a) Derive an analytical expression of liquid height $z_1$ of the cubic tank as a function of time. Does $z_1$ ever reach the steady-state, and if so, what is this value? Based on your analytical answer, also comment on whether $z_1$ reaches a maximum, reaches a minimum, overflows, or goes to zero and the time for that to happen. In your derivation, you are not allowed to use tables of integrals to perform the integration. Instead, use substitution and be careful with your unit conversions.

(b) Derive an ODE that describes the liquid height $z_2$ in the second tank. Together with the ODE for $z_1$ in Part (a), use MATLAB (ode45) to solve for $z_2$ as a function of time and plot both $z_1$ and $z_2$ as a function of time. Run the simulation for 20 minutes.

**Answer the following questions:**

$z_1$ ($t$ = 10 minutes) = _____ ft          $z_2$ ($t$ = 10 minutes) = _____ ft

### 13. *Dynamics of the Liquid Height in a Trapezoid Vessel*

An inverted trapezoid vessel shown in the diagram below consists the following dimensions: $b_1$, $b_2$, $L$, and $H$.
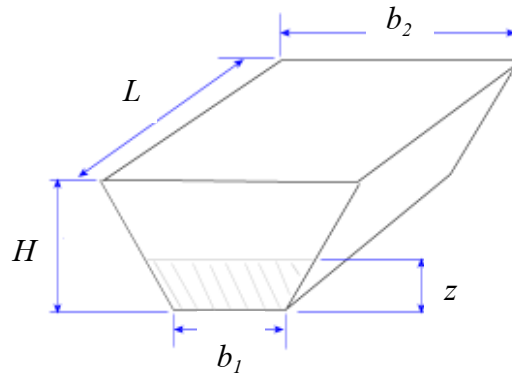


(a) (5 points) Prove mathematically using simple geometry to show that when the vessel is filled with a liquid at height $z$, the total volume of the liquid inside the vessel is given by:

$$V = \left(2b_1 + \frac{(b_2 - b_1)z}{H}\right)\left(\frac{zL}{2}\right)$$

(b) (10 points) A continuous stream of water flows into the vessel at a rate of $F_1 = 0.01$ m$^3$/min. Given that at $t = 0$, the vessel is empty and has the following dimension, derive an analytical expression of $z$ as a function of time.
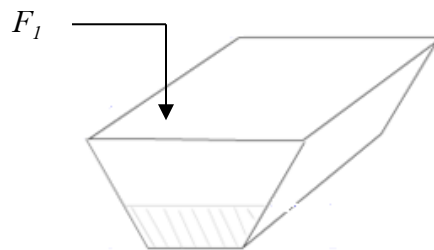


$L = 1.2$ m, $H = 0.4$ m, $b_1 = 0.2$ m, and $b_2 = 0.3$ m

Answers: $z$ ($t = 10$ mins) = _____ m

$t$ when the vessel is completely filled with water = _____ mins

(c) (20 points) Now, consider another scenario in which a continuous stream of water flows into the vessel with a rate of $F_1 = 0.01$ m$^3$/min just like in Part (b). However, a sophisticated control valve was installed that allows the liquid to flow out at a rate of $F_2 = 0.1z$ m$^3$/min. Given that at $t = 0$, the vessel is completely full, derive an analytical expression of $z$ as a function of time.

$$F_2 = 0.1z$$
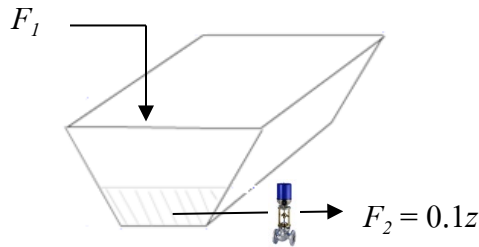
Answer: $z$ $(t = 2$ mins$)$ = _____ m

(d) (15 points) This scenario is the same as in Part (c), except the stream $F_2$ drains the water through a small hole at the bottom of the vessel based on gravity at a volumetric flow rate of:

$$F_2 = C_d A_H \sqrt{2gz}$$

where $A_H$ is the area of the hole with a radius of 2 cm or 0.02 m, $g$ (9.81 m/s² or 35316 m/min²) is the acceleration due to gravity, and $C_d$ is an experimentally determined value that depends partly on the type of fluid (for water, $C_d = 0.6$). An analytical solution for $z(t)$ is still possible in this case, but the math is very complicated. Instead, use *ode45* in MATLAB to obtain numerical solutions of $z$ as a function of time. Run the model for 3 minutes.

Answer: $z$ $(t = 1$ min$)$ = _____ m

## 14. *Simultaneous Mass and Energy Balance*

Consider the following heating tank problem. A dilute solution at 20 °C is added to a well-stirred tank at the rate of 180 kg/hr. A heating coil having an area of 0.9 m² is located in the tank and contains steam condensing at 150 °C. The heated liquid leaves at 120 kg/hr and at the temperature of the solution in the tank. There is 500 kg of solution at 40 °C in the tank at the start of the operation. The overall heat-transfer coefficient is 342 kcal/hr-m²-°C and the heat capacity of water is 1 kcal/kg-°C.



20 °C
180 kg/hr

120 kg/hr
T (Temperature)

150 °C
0.9 m²
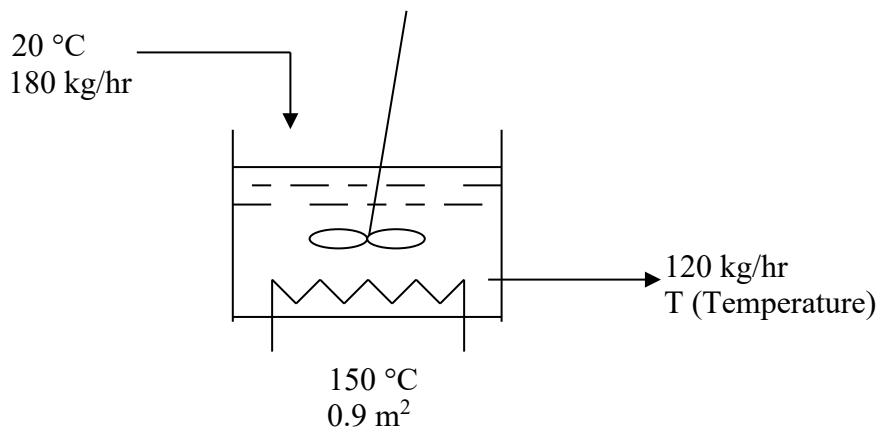
(a) Develop a system of mathematical equations to model this system. We are interested in determining the temperature of the solution in the tank at any given time.

(b) Solve for the temperature in the tank after 1 hour of heating. An analytical solution is possible for this particular system.

(c) Use MATLAB to solve for the temperature in the tank after 1 hour, and compare the answer with the exact solution in Part (b).


**15.** *Mass and Energy Balance of Two Vessels Connected in Series*

Consider two vessels connected in series, the first of which is heated as shown. Both vessels are initially filled with water, but some water in the first vessel flows into the second vessel at the rate of $F_1$ while some water leaves the second vessel at the rate of $F_2$. The first vessel is heated by steam inside a heating coil which is always submerged at the bottom of the first vessel (so the heat transfer area can be assumed to be constant).
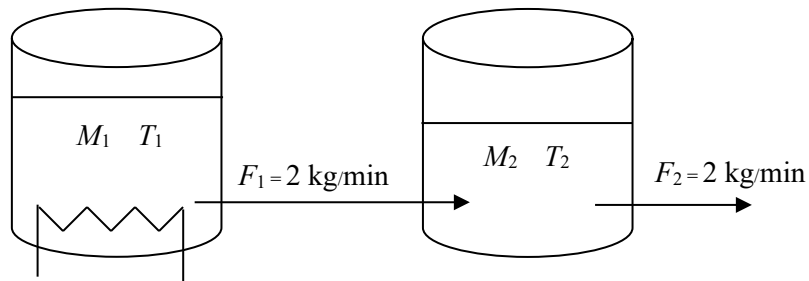


The following symbols are defined for all parameters and variables in this system. Data are also given for all symbols considered as parameters.

$$
\begin{aligned}
M_1 &= \text{Mass of water inside the first vessel (in kg)} = 200 \text{ kg at } t = 0 \\
M_2 &= \text{Mass of water inside the second vessel (in kg)} = 100 \text{ kg at } t = 0 \\
T_1 &= \text{Temperature of water inside the first vessel (in °C)} = 20 \text{ °C at } t = 0 \\
T_2 &= \text{Temperature of water inside the second vessel (in °C)} = 40 \text{ °C at } t = 0 \\
F_1 &= \text{Outflow rate from the first vessel to the second vessel} = 2.0 \text{ kg/min} \\
F_2 &= \text{Outflow rate from the second vessel} = 2.0 \text{ kg/min} \\
T_S &= \text{Steam temperature in the first vessel} = 100 \text{ °C} \\
U &= \text{Overall heat transfer coefficient of the heating coil} = 4.0 \text{ kcal/m}^2\text{-min-°C} \\
A &= \text{Heat transfer area of the heating coil (in m}^2) = 1.0 \text{ m}^2 \\
C_P &= \text{Heat capacity of water} = 1.0 \text{ kcal/kg-°C} \\
\phi &= \text{Mass density of water} = 1000 \text{ kg/m}^3
\end{aligned}
$$

(a) Derive an analytical expression of $T_1$ as a function of time. Answer the following question:

$T_1$ after 30 minutes = _____ °C

(b) Derive an explicit analytical expression of $T_2$ as a function of time. Simplify your final equation as much as possible, and answer the following questions:

$T_2$ after 30 minutes = _____ °C

$T_2$ when the first vessel becomes empty = _____ °C

(c) Solve for $T_1$ and $T_2$ again, this time numerically using *ode45* in MATLAB, if the first vessel has a radius of 0.5 m and is heated via a jacketed steam chamber ($T_s = 100$ °C). The heat transfer area consists of the bottom and the surface area around the vessel. As a result, this heat transfer area cannot be treated as constant. Answer the following questions:

$T_1$ after 30 minutes = _____ °C

$T_2$ after 30 minutes = _____ °C

## 16. *Energy Balance in a Two-Tank System*

Consider the following two-tank system in which water in the first tank flows into the second one with a flow rate of $F_1 = 2$ kg/min and vice versa with a flow rate $F_2 = 2$ kg/min. Water in both vessels is being heated with a heating coil with the same constant heat transfer area of $A = 0.5$ m² and the same heat transfer coefficient of $U = 4$ kcal/m²-min-°C. However, the temperature of the heating coil in Tank 1 (100 °C) is lower than that of the heating coil in Tank 2 (120 °C). We define $M_1$, $T_1$, $M_2$, and $T_2$ as the mass and the temperature of water in the first vessel and in the second vessel, respectively.
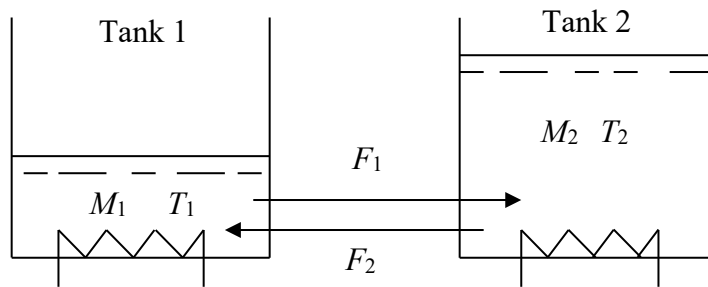


(a) Using the following data about the system, derive two ODEs that describe $T_1$ and $T_2$ as a function of time.

$C_P$ (water) = 1.0 kcal/kg-°C

Initially at $t = 0$: $M_1 = 50$ kg of water, $T_1 = 20$ °C, $M_2 = 100$ kg of water, $T_2 = 10$°C

(b) Solve the two ODEs in Part (a) and derive an analytical expression for $T_1$ and $T_2$ as a function of time.

(c) What is the domain of this system, i.e. the maximum time the derived model is valid for? Also, determine the time at which the temperatures in Tank 1 and Tank 2 are equal.

**Answer the following questions:**

Domain of this system = _____ minutes

$T_1 = T_2 =$ _____ °C when $t =$ _____ minutes

## 17. *Mass and Energy Balance in a Stirred Tank Heater*

Consider the following stirred tank heater shown below, where the tank inlet stream is received from another process unit. A heat transfer fluid is circulated through a jacket to heat the fluid in the tank. Assume that no change of phase occurs in either the tank liquid or the jacket liquid. The following symbols are used: $F_i$ = volumetric flowrate of stream $i$, and $T_i$ = temperature of stream $i$.
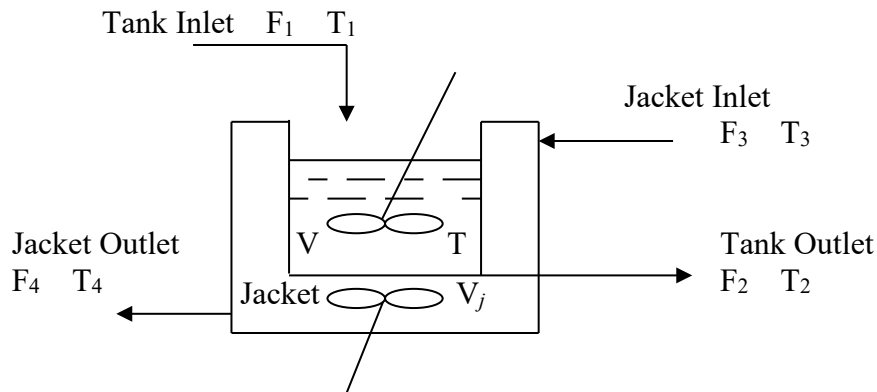


Additional assumptions are:
1. The liquid levels in both the tank and the jacket are constant.
2. There is perfect mixing in both the tank and the jacket.
3. The rate of heat transfer from the jacket to the tank is governed by the equation $Q = UA(T_4 - T_2)$, where U is the overall heat transfer coefficient and A is the area of heat exchange.

(a) Write the dynamic modeling equations (ODEs) to find the tank and jacket temperatures. Do not use any numerical values – leave these equations in terms of the process parameters and variables. Be sure to define any new symbols you introduce into the equations.

(b) Assume that both the tank fluid and the jacket fluid are water. The steady-state values of this system variables and some parameters are:

$F_1 = 1.0$ ft$^3$/min $\quad \rho C_P$ (in tank) $= \rho C_P$ (in jacket) $= 61.3$ Btu/°F-ft$^3$
$T_1 = 50$ °F $\qquad T_2 = 125$ °F $\qquad V = 10$ ft$^3$
$T_3 = 200$ °F $\quad T_4 = 150$ °F $\qquad V_j = 1$ ft$^3$

Solve for $F_3$ and UA (show units) at steady-state.

(c) If initially (t = 0), $T_2 = 50$ °F and $T_4 = 200$ °F, solve for $T_2$ and $T_4$ from the ODEs in Part (a) analytically as a function of time.

## 18. *Mass and Energy Balance in a Gas Surge Drum*

Consider a heated gas storage drum in which its gas is being drawn out at the rate of $F$ (in kmol/min). Assume ideal gas behavior in the drum and that heat is being added to the tank at the rate of $q$.
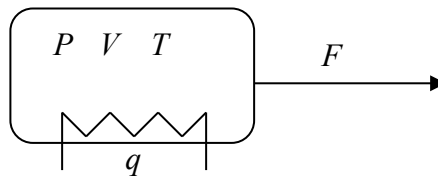


(a) Derive the modeling equations (ODEs) that describe how the temperature $T$ and pressure $P$ inside the drum vary with time. Note that for a gas, the accumulation term on the left-hand side of the energy balance equation is

$$\frac{dH}{dt} - \frac{d(PV)}{dt} = energy\,in \;-\; energy\,out$$

where $\quad \dfrac{dH}{dt} = \dfrac{d(\rho C_P VT)}{dt}$ , $\rho$ is the molar density of the gas, and $C_P$ is assumed constant.

For liquids, the $d(PV)/dt$ term is considered negligible (incompressible fluid and constant volume). But this is not true for gas so we cannot ignore the $PV$ derivative term in the energy balance. Your two ODEs must be in terms of the following symbols: $P$, $V$, $T$, $R$, $C_p$, $F$, and $q$. Hint: to obtain the right ODEs, you must be able to identify which symbols are constants and which are variables.

(b) Calculate the time at which the drum will become completely empty. Then solve the two ODEs in the Part (a) using MATLAB, running the model for 20 minutes (soon after which the drum will become empty). The data are:

$V = 100 \text{ m}^3$                                   $R = 0.08205 \text{ m}^3\text{-atm/kmol-K}$
                                                        $= 8.315 \text{ kJ/kmol-K}$
$C_P \text{ (gas)} = 125 \text{ kJ/kmol-K}$             $F = 0.2 \text{ kmol/min}$
$q = 1.5\text{x}10^4 \text{ kJ/min}$                    $T(t = 0) = 298.15 \text{ K} = 25 \text{ °C}$
$P(t = 0) = 1 \text{ atm}$

Notice that the gas constant $R$ is given in two different units. Both numbers must be used, depending on where in the ODEs which requires some dimensional analysis.

## Answer the following questions:

While it is obvious that the temperature profile in the drum will rise continuously, the pressure profile may go through a maximum, depending on the draw-out rate. Of course, $P$ inside the drum will eventually drop to zero, but it may rise for a brief moment because of the increasing temperature.

Time for the drum to become empty = _____ minutes

Does the pressure go through a maximum? Check one:  Yes _____    No _____

If yes, $P_{max}$ = _____ atm at $t$ = _____ minutes

| Time (min) | Pressure (atm) | Temp (Kelvin) |
|:----------:|:--------------:|:-------------:|
| 5 | | |
| 10 | | |
| 15 | | |
| 20 | | |

## 19. *Mass and Energy Balance in a 2-Tank System*

Consider the following 2 tanks (both cylindrical vessels) in series used to store a liquid solution. Tank 1 is heated while Tank 2 is not. Liquid is drawn from Tank 1 into Tank 2 at the rate of 10 kg/min. At the same time, a feed (40 °C) enters Tank 2 at the rate of 20 kg/min, and an outflow of 30 kg/min leaves the vessel. Initially (at t = 0), Tank 1 is charged with 300 kg of the solution at a temperature of 20 °C, while Tank 2 is charged with 100 kg at a temperature of 30 °C.

**Tank 1**       **Tank 2**       20 kg/min    40 °C

$T_1$     $T_2$    10 kg/min    30 kg/min
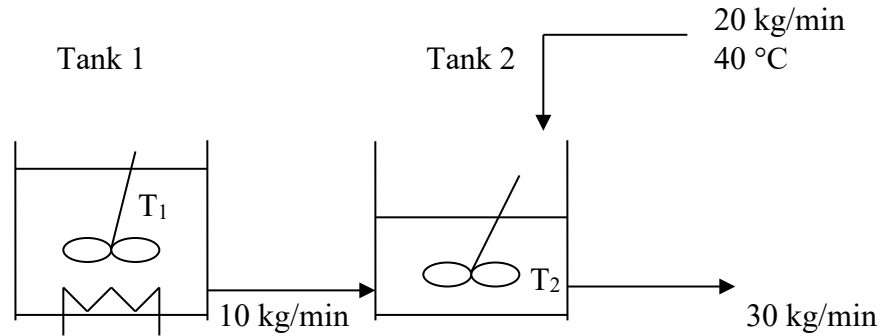
(a) Assuming that Tank 1 is being heated with a heating coil that remains submerged at all times (hence, the heat transfer area remains constant), derive an analytical expression for $T_2$, the temperature inside Tank 2 as a function of time. Also, compute $T_2$ at the time when Tank 1 is completely emptied. Use the following data:

$C_P$ = liquid heat capacity = 2.0 kJ/kg-°C        UA = 40 kJ/min-°C
$T_S$ = heating coil temperature = 200 °C

Assume there is no phase change in either tank (i.e. no boiling occurs).

(b) Consider again a similar 2-tank system in which Tank 1 is jacketed and is heated with steam at 200 °C as shown in the figure below. In this case, the heat transfer area is no longer constant and will vary with the liquid volume inside Tank 1.



20 kg/min    40 °C

$T_1$     $T_2$

Steam      10 kg/min    30 kg/min
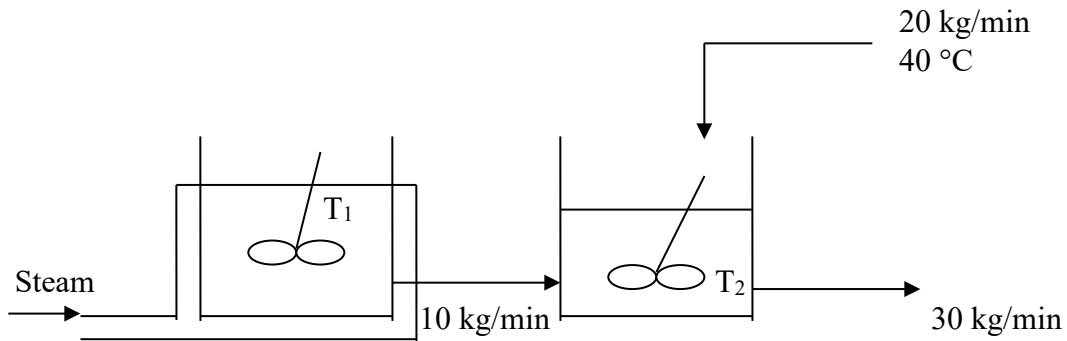
This liquid solution is known to boil at 150 °C. Determine the time it takes for the liquid in Tank 1 to boil off completely (including the time to heat the liquid to the boiling temperature). Use the following data:

$C_P$ = liquid heat capacity = 2.0 kJ/kg-°C
U = overall heat transfer coefficient = 25 kJ/m²-min-°C
$T_S$ = steam temperature = 200 °C
$\phi$ = liquid mass density = 1200 kg/m³
R = radius of both cylindrical vessels = 0.3 m
$\lambda$ = heat of vaporization at 150 °C = 1500 kJ/kg

Use the initial conditions given in Part (a)


## 20. *Boiling of Ethanol in a Cylindrical Vessel*

Consider the following cylindrical vessel which is initially filled with 100 kg of ethanol at the temperature of 20 °C.  The vessel is constantly being heated with a heating coil (assume constant heat transfer area) at $T = 100$ °C and $UA = 10$ kJ/min-°C.  The heating goes on until ethanol starts to boil at its normal boiling point of 78.55 °C.  While the heating is taking place and then later when boiling occurs as well, ethanol also flows out of the vessel at the rate of $F_1$.  Use the following additional data about ethanol to calculate the time it takes for ethanol to completely disappear from the cylindrical vessel.  Also, how much faster does the boiling help in emptying the vessel?



$v$   when boiling occurs

$F_1 = 2$ kg/min
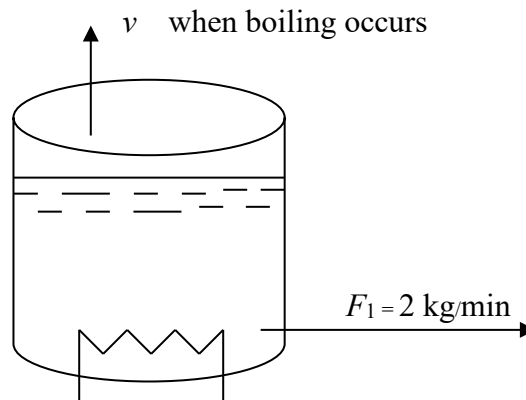
*MW* (molecular weight) = 46.07          $\lambda$ (heat of vaporization) = 38600 kJ/kmol
$C_P$ (heat capacity) = 78.28 kJ/kmol-°C

**Hint:** Watch the units and their conversions carefully in your calculations

**Answer the following question:**

Time when ethanol disappears completely from the vessel = _____ minutes

Time by which the boiling helps the vessel to empty faster = _____ minute


## 21. *Boiling and Draining of Ethanol in a Spherical Vessel*

Consider the boiling of pure ethanol in a jacketed spherical vessel with a radius $R = 1$ meter, as shown in the diagram.  The liquid is drained at the bottom of the vessel while some of it is boiled and escapes as vapor through the top of the vessel.
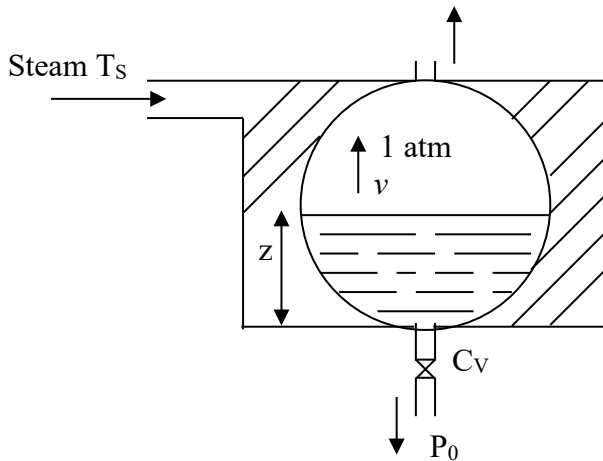
The following data are available:

$$MW = 46.07 \qquad \lambda(T_B) = 3.858 \times 10^7 \text{ J/kmol}$$

$$\rho = 16.575 \text{ kmol/m}^3 \qquad C_P = 1.4682 \times 10^5 \text{ J/kmol-°C}$$

$$\log_{10} P^{vap} = 8.04494 - \frac{1554.30}{T + 222.65} \qquad T \text{ in °C and } P^{vap} \text{ in mmHg}$$

$$C_V = 4.5 \text{ m}^3\text{-atm}^{-1/2}/\text{hr} = \text{valve constant}$$

$$T_S = 100 \text{ °C} \qquad U = 2.0 \times 10^6 \text{ J/hr-m}^2\text{-°C}$$

$$P_0 = 1 \text{ atm} \qquad z_0 = z(t{=}0) = 1 \text{ m}$$

(a) Model this operation and use MATLAB to determine the time it takes for the vessel to completely empty, assuming that initially the liquid is at its boiling point. Note that the heat transfer area $A_T$ is not constant.

(b) Repeat the calculations in Part (a), assuming that there is no draining of the liquid at the bottom (i.e. the liquid leaves the vessel only through boiling). Determine the solution analytically (an exact solution is possible in this case).

## Useful conversion factors and formulae:

g = gravitational constant = 9.807 m/s$^2$

1 atm = 1.01325 × 10$^5$ N/m$^2$ $\qquad\qquad$ 1 N = 1 kg-m/s$^2$

The volume of liquid V(z) in a spherical vessel as a function of its height z is given by

$$V(z) = \pi R z^2 - \frac{\pi z^3}{3}$$

while the surface area S(z) is given by

$$S(z) = 4\pi R z - \pi z$$

$$\int \frac{x}{a+bx} dx = \frac{\left[ a+bx - a\ln(a+bx) \right]}{b^2}$$

## 22. *Boiling and Heat/Mass Balance in an Open Inverted Cone-Shaped Vessel*

An inverted cone-shaped vessel ($R = 0.5$ m, $H = 2.0$ m) is initially filled with pure water at the height of 1.0 m as measured from the bottom of the vessel (see the figure). The liquid in the vessel flows out from bottom with a rate $F = 0.01$ m³/min.
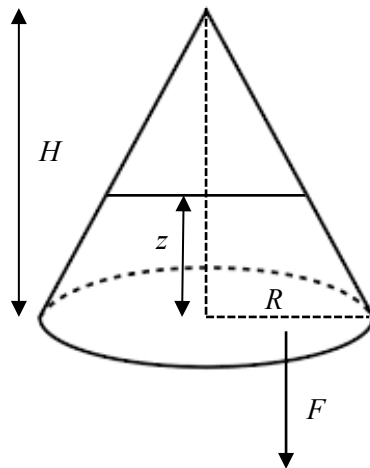


The following symbols are defined for all parameters and variables in this system. Data are also given for all symbols considered as parameters.

$V$ = Water volume inside the vessel (m³)
$\phi$ = Mass density of water = 1000 kg/m³
$z$ = Liquid height inside the vessel as measured from the bottom (in m)
$F$ = Outflow rate from the vessel = 0.01 m³/min
$C_P$ = Heat capacity of water = 1.0 kcal/kg-°C

The volume of a cone = $\frac{1}{3}\pi R^2 H$

Note that you can use this formula to derive the volume of the inverted cone at any given liquid height $z$. Be very careful with this derivation because the cone is inverted; otherwise all your subsequent answers will be wrong.

(a) Derive an analytical expression for $z$ as a function of time, and answer the following question:

*t* when the vessel becomes empty = _____ minutes

(b) Now, suppose the cone-shaped vessel is being heated via steam through the circular area at the bottom of the vessel (hence, the overall heat transfer area can be assumed to be constant). With the additional data given below, derive an analytical expression for *T* as a function of time (valid up till the boiling-point temperature of water at 100 °C). Then taking into account the vaporization of water, calculate the total time it takes for the vessel to become empty without using MATLAB. Hint: note that this total time must be less than the time calculated in Part (a).

$T$ = Temperature of water inside the vessel (in °C) = 20 °C at $t = 0$.
$\lambda$ = Heat of vaporization of water = 539.4 kcal/kg at 100 °C
$U$ = Overall heat transfer coefficient = 5.0 kcal/m$^2$-min-°C
$T_S$ = Steam temperature = 150 °C
$v$ = Vaporization or boiling rate of water from the vessel (in kg/min)

*t* when the temperature in the vessel reaches 100 °C = _____ minutes

Total *t* when the vessel becomes empty = _____ minutes

## 23. *Boiling of Acetone in a Cylindrical and a Spherical Vessels in Series*
Consider the boiling of pure acetone in a jacketed cylindrical vessel and a jacketed spherical vessel in series, as shown in the diagram. The cylinder has a radius of $R_1 = 1.0$ m and a height of H = 1.5 m, while the sphere has a radius of $R_2 = 1.0$ m. In addition to the liquid already in the vessel, pure acetone at its boiling point is added continuously at a rate $F_1 = 15$ m$^3$/hr. The cylinder also has a hole at the bottom, which allows acetone to flow out and into the sphere according to the relation

$$F_2 = C_d A (2gz_1)^{1/2} \qquad \text{(in m}^3\text{/hr)}$$

where $A$ is the area of the hole, $g$ is the acceleration due to gravity, and $C_d$ is an experimentally determined value.

$$F_1 = 15 \text{ m}^3/\text{hr at } 56.0 \text{ °C}$$
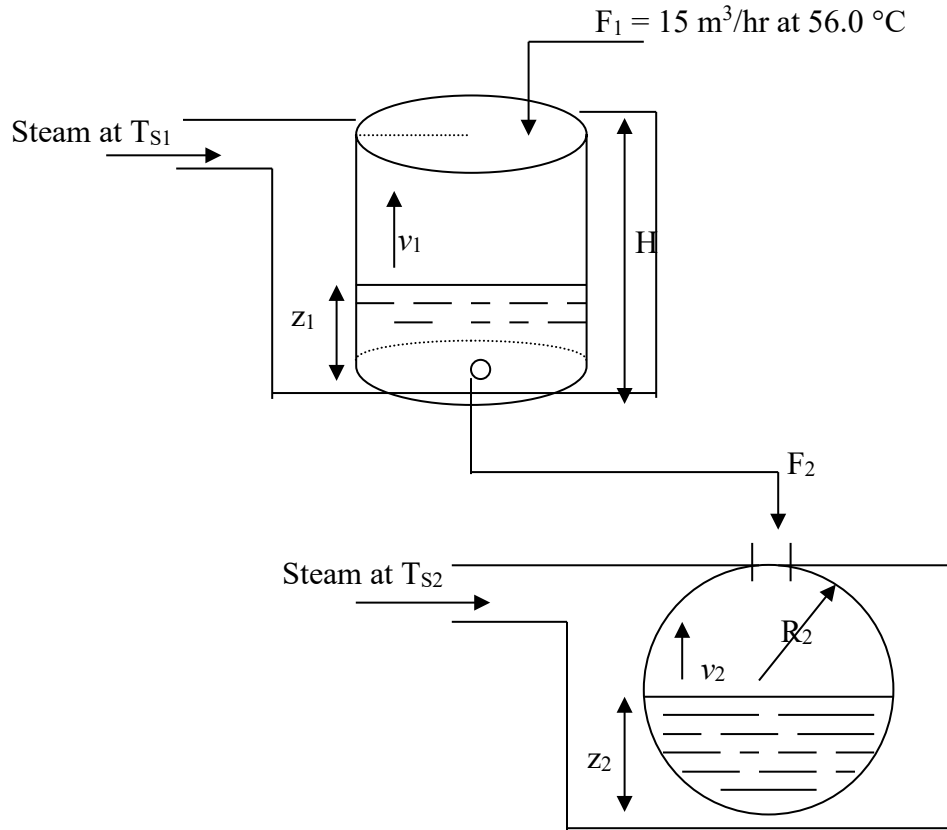


The following data are available:

MW = 58.08        $\rho = 13.62 \text{ kmol/m}^3$

$\lambda(T_B) = 3.02 \times 10^7 \text{ J/kmol}$        $T_B = 56.0 \text{ °C}$

$C_P = 1.30735 \times 10^5 \text{ J/kmol-°C}$        $U = 3.0 \times 10^6 \text{ J/hr-m}^2\text{-°C (for both vessels)}$

$T_{S1} = 150 \text{ °C}$        $T_{S2} = 100 \text{ °C}$

$C_d = 0.5$        $g = \text{gravitational constant} = 1.271 \times 10^8 \text{ m/hr}^2$

$r = \text{hole radius} = 0.01 \text{ m}$

$z_1(t=0) = 0.5 \text{ m}$        $z_2(t=0) = 1.5 \text{ m}$

(a) Model this operation and determine the time in hours (correct to 2 decimal places) at which the cylindrical vessel will either empty completely or overflow. Assume that the liquid in both vessels is already at its boiling point at t = 0.

(b) Determine the time in hours (correct to 2 decimal places) at which the liquid height $z_1$ in the cylinder is equal to the liquid height $z_2$ in the sphere.

## 24. *Semi-Batch Reactor with a Single 1$^{st}$-Order Reaction*

Consider the case where a batch reactor is being filled. Assume a single, first-order reaction (A → B) and a sinusoidal volumetric flowrate into the reactor $F = 4.0 + 2\sin(10t)$ with no flow out of the reactor.
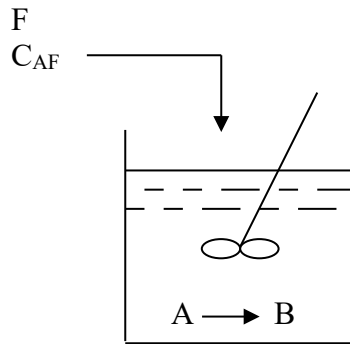
If $C_{AF}$ (feed concentration) = 5 mol/m³, k = 1 hr $^{-1}$, with V = 2.0 m³ and $C_A$ = 0 at t = 0, simulate the concentration of A as a function of time using MATLAB. Run the model for 10 hours and plot the concentration profile.

## 25. *Batch Reactor with a Series Reaction*

Consider the series reaction:

$$\begin{array}{cccc} k_1 & k_2 & k_3 \\ A \rightarrow B \rightarrow C \rightarrow D \end{array}$$
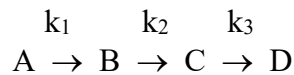
(a) Assuming that each of the reactions is first-order and constant volume, write down the modeling equations for $C_A$, $C_B$, and $C_C$, where $C_A$, $C_B$, and $C_C$ represent the concentrations (mol/volume) of components A, B, and C, respectively.

(b) Derive a third-order ODE for the concentration of C. That is, your ODE should look like

$$f\left( \frac{d^3C_C}{dt^3}, \frac{d^2C_C}{dt^2}, \frac{dC_C}{dt}, C_C, k_1, k_2, k_3 \right) = 0$$

(c) If $k_1$ = 1 hr $^{-1}$, $k_2$ = 2 hr $^{-1}$, $k_3$ = 3 hr $^{-1}$, and $C_{A0} = C_A(t=0)$ = 1 mol/liter, solve the ODE in Part (b) analytically for the concentration of C at any given time t.

## 26. *Batch Reactor with a Series Reaction*

Consider a batch reactor with a series reaction where component A reacts to form component B. Component B can also react reversibly to form component C. The reaction scheme can be characterized by:

$$A \xrightarrow{k_1} B \underset{k_{2r}}{\overset{k_{2f}}{\rightleftarrows}} C$$

Here $k_{2f}$ and $k_{2r}$ represent the kinetic rate constants for the forward and reverse reactions for the conversion of B to C, while $k_1$ represents the rate constant for the conversion of A to B.

(a) Assuming that each of the reactions is first-order and constant volume, write down the 3 modeling equations for $C_A$, $C_B$, and $C_C$, where $C_A$, $C_B$, and $C_C$ represent the concentrations (mol/volume) of components A, B, and C, respectively.

(b) Using the following definitions:

| | |
|---|---|
| Dimensionless time, | $\tau = k_1 t$ |
| Conversion of A, | $x_1 = (C_{A0} - C_A) / C_{A0}$ |
| Dimensionless concentration of B, | $x_2 = C_B / C_{A0}$ |
| Ratio of rate constants, | $\alpha = k_{2f} / k_1$ |
| Ratio of forward and reverse rate constants, | $\beta = k_{2r} / k_1$ |

Derive a second-order ODE for the dimensionless concentration of B. Your ODE must contain only dimensionless quantities ($x_2$, $\tau$, $\alpha$, and $\beta$).

(c) Solve the ODE in Part (b) analytically to find $x_2$ as a function of $\tau$, $\alpha$, and $\beta$.

(d) Using the following data:

$$k_1 = 1.0 \ \text{min}^{-1} \qquad k_{2f} = 1.5 \ \text{min}^{-1} \qquad k_{2r} = 2.0 \ \text{min}^{-1}$$
$$C_{A0} = C_A (t = 0) = 3.0 \ \text{mol/liter}$$
$$C_{B0} = C_B (t=0) = 0 \ \text{mol/liter}$$
$$C_{C0} = C_C (t=0) = 0 \ \text{mol/liter}$$

Solve for $C_B$ analytically as a function of time.

(e) Given the data in Part (d), find the maximum concentration of B and the reaction time at this concentration. If no such maximum exists, prove it mathematically. Repeat the above calculations for the case of $k_1 = 3 \ \text{min}^{-1}$, $k_{2f} = 1.5 \ \text{min}^{-1}$, $k_{2r} = 1 \ \text{min}^{-1}$ while the initial conditions remain the same.

(f) Validate your analytical solutions by solving the differential equations in Part (a) with MATLAB and plot the time profiles of components A, B, and C. Use both sets of rate constants (i.e. $k_1 = 1.0 \ \text{min}^{-1}$, $k_{2f} = 1.5 \ \text{min}^{-1}$, $k_{2r} = 2.0 \ \text{min}^{-1}$ and $k_1 = 3.0 \ \text{min}^{-1}$, $k_{2f} = 1.5 \ \text{min}^{-1}$, $k_{2r} = 1.0 \ \text{min}^{-1}$).

## 27. *Modeling Two Reactions in Series in a Batch Reactor*
Consider the following two reactions in series:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$
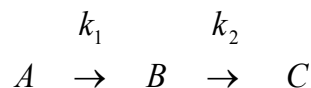
The orders of the two reactions do not follow the stoichiometry but instead can be described by the following modeling equations. i.e. the first reaction is $3^{rd}$-order while the second reaction is $0^{th}$-order:

$$\frac{dC_A}{dt} = -k_1 C_A^3 \qquad \frac{dC_B}{dt} = k_1 C_A^3 - k_2 \qquad \frac{dC_C}{dt} = k_2$$

(a) Derive an exact (analytical) expression of $C_A$ as a function of time in terms of $k_1$, given that at $t = 0$, $C_A = C_{A0}$, and $C_B = 0$. Then use the analytical solution to determine $C_A$ at $t = 1.0$ hour if $k_1 = 2.0$ (gmol/liter)$^{-2}$-hour$^{-1}$ and $C_{A0} = 2.0$ gmol/liter and $C_{B0} = 0$.

$C_A$ ($t = 1.0$ hour) = _____ gmol/liter

(b) Derive an exact (analytical) expression of $C_B$ as a function of time in terms of $k_1$ and $k_2$, given that at $t = 0$, $C_A = C_{A0}$, and $C_B = 0$. Simplify your final expression as much as possible. Then use the analytical solution to determine $C_B$ at $t = 1$ hour, given that $k_1 = 2.0$ (gmol/liter)$^{-2}$-hour$^{-1}$, $k_2 = 0.5$ gmol/liter-hour, $C_{A0} = 2.0$ gmol/liter, and $C_{B0} = 0$.

$C_B$ ($t = 1.0$ hour) = _____ gmol/liter

(c) Calculate $C_{B,max}$ and the time at which $C_B$ is at maximum based on the exact solution in Part (b).

$C_{B,max}$ ($t =$ _____ hour) = _____ gmol/liter

(d) Suppose the two reactions in series now follow the following modeling equations. Repeat Part (a).

$$\frac{dC_A}{dt} = -k_1 \sqrt{C_A} \qquad \frac{dC_B}{dt} = k_1 \sqrt{C_A} - k_2 C_B \qquad \frac{dC_C}{dt} = k_2 C_B$$

$C_A$ ($t = 1.0$ hour) = _____ gmol/liter

(e) Repeat Part (b) with the new modeling equations.

$C_B$ ($t = 1.0$ hour) = _____ gmol/liter

(f) Repeat Part (c) with the new modeling equations.

$C_{B,max}$ ($t =$ _____ hour) = _____ gmol/liter

### 28. *Isothermal Semi-Batch Reactor*

(a) Consider an isothermal semi-batch reactor where a single reaction takes place in a solvent S, which is inert. In this reaction, 2 moles of component A react with one mole of component B to form one mole of component C:   $2A + B \xrightarrow{k_1} C$.  The reaction rate does not conform to the stoichiometry but is $1^{st}$-order with respect to each reactant as follows: $r_A = -k_1 C_A C_B$

$F_A = 15$ liter/min    $F_B = 10$ liter/min
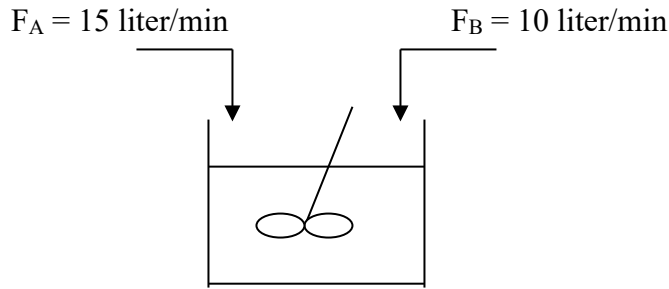
Initially ($t = 0$ min), the reactor contains 100 liters of solution and 300 moles of A. Assuming that all components have the same density of 60 mol/liter, derive 3 ODE equations needed to compute $C_A$, $C_B$, and $C_C$, the concentrations (moles/liter) of A, B, and C, respectively. Use *ode45* in MATLAB to solve for and plot (in a single graph) the concentrations of the 3 components. Run the model for 20 minutes with an increment of 0.5 minute.

The following experimental data have been obtained for this reaction when carried out in a batch reactor:

| Time(minute) | 0 | 5.0 | 7.5 | 12.0 | 15.5 | 25.0 | 32.0 | 40.0 |
|---|---|---|---|---|---|---|---|---|
| $C_A$(mol/liter) | 2.0 | 1.65 | 1.52 | 1.40 | 1.28 | 1.17 | 1.10 | 1.06 |
| $C_B$(mol/liter) | 0.5 | | | | | | | |

(b) At the end of 20 minutes, the 2 feeds to the reactor are suddenly shut off, and 4,500 moles of a new component called D (same density as components A, B, and C) are charged to the reactor. That is, the reactor now operates in a batch mode. Component D reacts with component C to form A and B, and the reaction now looks as follows:

$$2A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C + D$$
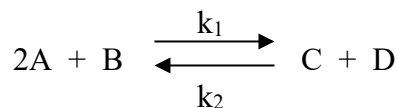
with a reaction rate of  $r_A = -k_1 C_A C_B + k_2 C_D$ ($2^{nd}$ -order forward and $1^{st}$-order reverse). The value of $k_2$ has been measured to be 1.0 min$^{-1}$.  Derive analytically the concentration of A as a function of time, and compute $C_A$ at steady state based on your

derived equation. Your final expression should be simplified as much as possible and should not contain any parameters except $t$ (time) and $C_A$.

**Useful Integrals:**
$$\int \frac{dx}{x(a+bx)} = -\left(\frac{1}{a}\right)\ln\left(\frac{a+bx}{x}\right)$$

$$\int \frac{dx}{B} = \begin{cases} +\dfrac{2}{\sqrt{\gamma}}\tan^{-1}\left(\dfrac{\omega}{\sqrt{\gamma}}\right) & \text{if } \gamma > 0 \\[2em] -\dfrac{2}{\omega} & \text{if } \gamma = 0 \\[2em] -\dfrac{2}{\sqrt{-\gamma}}\tanh^{-1}\left(\dfrac{\omega}{\sqrt{-\gamma}}\right) & \text{if } \gamma < 0 \end{cases}$$

where
$$B = a + bx + cx^2$$
$$\gamma = 4ac - b^2$$
$$\omega = b + 2cx$$

## 29. *Determination of Reaction Kinetics*

(a) The following laboratory data were obtained for the irreversible reaction under isothermal constant-volume conditions:

$$2A \rightarrow B + C$$
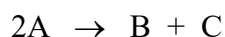
| Time (min) | 0 | 3.2 | 5.0 | 9.6 | 12.5 | 18.4 | 25.0 |
|---|---|---|---|---|---|---|---|
| [A] (mol/liter) | 0.1345 | 0.0772 | 0.0602 | 0.0352 | 0.0261 | 0.0168 | 0.0110 |

Determine the kinetics to explain these data (i.e. find the order of the reaction and its rate constant).

(b) The following laboratory data were obtained for the irreversible reaction under isothermal constant-volume conditions:

$$A + B \rightarrow C + D$$
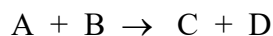
| Time (sec) | 0 | 2790 | 7690 | 9690 | 14000 | 19100 |
|---|---|---|---|---|---|---|
| [A] (mol/liter) | 0.1908 | 0.1833 | 0.1745 | 0.1719 | 0.1682 | 0.1650 |
| [B] (mol/liter) | 0.0313 | 0.0238 | 0.0150 | 0.0123 | 0.0086 | 0.0055 |

Determine the kinetics to explain these data.


## 30. *Isothermal Batch Reactor with a Series Reaction*

Consider an isothermal batch reactor with a series reaction where 2 moles of component A react to form one mole of component B. Component B also reacts to form component C. The reaction scheme can be characterized as follows:

$$2A \xrightarrow{\ k_1\ } B \xrightarrow{\ k_2\ } C$$

Initially ($t = 0$ hr), $C_A = C_{A0}$, $C_B = 0$, and $C_C = 0$, where $C_A$, $C_B$, and $C_C$ represent the concentrations (mol/liter) of components A, B, and C, respectively.

(a) Assume constant volume and that the first reaction $2A \rightarrow B$ is one-half order and the second reaction $B \rightarrow C$ is first-order, i.e.

$$dC_A/dt = -k_1 C_A^{1/2}$$

$$dC_B/dt = \frac{k_1}{2} C_A^{1/2} - k_2 C_B$$

Derive an analytical expression for $C_B$ as a function of time.

(b) The following experimental data were obtained for component $C_A$:

| Time(hr) | 0 | 0.05 | 0.15 | 0.35 | 0.60 | 0.85 | 1.0 |
|---|---|---|---|---|---|---|---|
| $C_A$(mol/liter) | 1.0 | 0.93 | 0.79 | 0.54 | 0.30 | 0.13 | 0.06 |

$C_B$ was also measured to be 0.11 mol/liter at $t = 1$ hr. Determine the values of $k_1$ and $k_2$ and the time $t_{max}$ at which $C_B$ is at its maximum. **Hint**: Use *Polyfit* function in MATLAB to help determine $k_1$ and $k_2$.

(c) Now, suppose the order of the above series reaction conforms to the stoichiometry, derive analytically a $1^{st}$-order ODE for $C_B$, i.e.

$$dC_B/dt + p(t)C_B = q(t)$$

but do not solve this ODE.

(d) When the reaction order conforms to the stoichiometry, the following experimental data were obtained for $C_A$:

| Time(hr) | 0 | 0.03 | 0.06 | 0.10 | 0.15 | 0.20 | 0.30 |
|---|---|---|---|---|---|---|---|
| $C_A$(mol/liter) | 1.0 | 0.76 | 0.63 | 0.51 | 0.39 | 0.33 | 0.25 |

It was also observed that $C_B$ reached a maximum of 0.14 mol/liter at $t = 0.1$ hr. Determine the values of $k_1$ and $k_2$.

## 31. *Maximizing Product Yield in an Isothermal Batch Reactor*
Consider an isothermal batch reactor with the following series of two reactions:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$
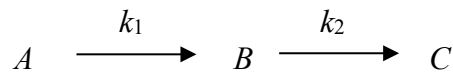
Chemical $B$ is the desirable product. The two reactions do not follow the stoichiometry. Instead, the first reaction is one-half$^{\text{th}}$-order while the second reaction is first-order with respect to the reactant, i.e.

$$\frac{dC_A}{dt} = -k_1 C_A^{1/2}$$

$$\frac{dC_B}{dt} = k_1 C_A^{1/2} - k_2 C_B$$

(a) Given that at $t = 0$, $C_A = C_{A0}$ and $C_B = 0$, derive analytically an expression of $C_B$ as a function of time. Note that your final equation for $C_B$ must be expressed in terms of $C_{A0}$, $k_1$, and $k_2$.

(b) It is obvious that the concentration of product $B$ will go through a maximum. Determine the time at which the concentration of $B$ is at the maximum if $C_{A0} = 1.0$ kmol/liter, $k_1 = 1.5$ kmol$^{1/2}$/liter$^{1/2}$-hour, and $k_2 = 2.0$ hour$^{-1}$. Also, calculate this maximum concentration.

### Answer the following questions:

$t_{max} =$ _____ hour          $C_{B,max} =$ _____ kmol/liter

## 32. *Modeling an Isothermal Reversible Reaction and Determining Rate Constants*

Consider an isothermal batch reactor with the following reversible reaction:

$$A \quad \underset{k_2}{\overset{k_1}{\rightleftarrows}} B$$
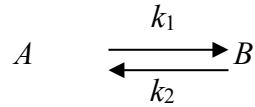
The reversible reaction does not follow the stoichiometry. Instead, the forward reaction is zero[th]-order while the backward reaction is second-order with respect to the reactant, i.e.

$$\frac{dC_A}{dt} = -k_1 + k_2 C_B^2$$

$$\frac{dC_B}{dt} = k_1 - k_2 C_B^2$$

(a) Given that at $t = 0$, $C_A = C_{A0}$ and $C_B = C_{B0}$, derive analytically an expression of $C_B$ as a function of time. Note that your final equation for $C_B$ must be expressed in terms of $C_{B0}$, $k_1$, and $k_2$.

(b) Based on the result in Part (a), derive now an analytical expression of $C_A$ as a function of time. Again, your final equation for $C_A$ must be expressed in terms of $C_{A0}$, $C_{B0}$, $k_1$, and $k_2$.

(c) The following data are available from experiments:

| $t$ (hour) | 0 | 0.05 | 0.15 | 0.30 | 0.40 | 0.55 | 0.70 |
|---|---|---|---|---|---|---|---|
| $C_B$ (mol/liter) | 6.0 | 4.40 | 3.10 | 2.36 | 2.20 | 2.08 | 2.03 |
| $C_A$ (mol/liter) | 6.0 | | | | | | |

Also, it was observed that at steady-state, $C_B = 2.0$ mol/lier. Determine the values of the two rate constants $k_1$ and $k_2$.

**Answer the following questions:**

$k_1 =$ _____ mol/hr          $k_2 =$ _____ liter$^2$/mol-hr

### 33. *Modeling Two Reversible Reactions in Series*

Consider the following reactions:

$$A \; \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \; B \; \underset{k_4}{\overset{k_3}{\rightleftharpoons}} \; C$$
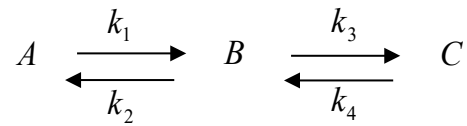
The reactions do not follow the stoichiometry but instead can be described by the following modeling equations:

$$\frac{dC_A}{dt} = -k_1 C_A + k_2 C_B \qquad\qquad \frac{dC_B}{dt} = k_1 C_A - k_2 C_B - k_3 + k_4 C_C$$

$$\frac{dC_C}{dt} = k_3 - k_4 C_C$$

(a) (10 points) Derive an exact (analytical) expression of $C_C$ as a function of time, assuming that $C_{C0} = 0$, which is the initial concentration of $C_C$ at $t = 0$. Note that your final equation for $C_C$ must be expressed in terms of $k_3$ and $k_4$.

(b) (30 points) Derive an exact (analytical) expression of $C_A$ as a function of time, assuming that $C_{B0} = 0$ and $C_{C0} = 0$. Note that your final equation for $C_A$ must be expressed in terms of $k_1$, $k_2$, $k_3$, and $k_4$, and $C_{A0}$, where $C_{A0}$, $C_{B0}$, and $C_{C0}$ are the initial concentrations of $C_A$, $C_B$, and $C_C$ at $t = 0$, respectively.

(c) (10 points) Component $B$ is the desired product whose concentration should be maximized. Given that $k_1 = 2.0 \text{ hr}^{-1}$, $k_2 = 1.0 \text{ hr}^{-1}$, $k_3 = 0.5$ gmol/liter-hr, $k_4 = 0.8 \text{ hr}^{-1}$, and $C_{A0} = 1.0$ gmol/liter, determine the maximum $C_B$ and the time at which this maximum occurs.

Answer the following questions (4 decimal places except for time):

$C_A(t = 2 \text{ hr}) = $ _____ gmol/liter $\qquad$ $C_B(t = 2 \text{ hr}) = $ _____ gmol/liter

$C_C(t = 2 \text{ hr}) = $ _____ gmol/liter

$C_{B, max} = $ _____ gmol/liter $\qquad\qquad$ $t_{max} = $ _____ hour (2 decimal places)

### 34. *Batch Distillation, I*

A liquid mixture containing 70.0 mole% n-pentane and 30.0 mole% n-hexane is distilled in a batch still, and is initially charged with 100 gmoles of the mixture.

V (gmoles/sec)

$y_i$

$x_i$    L (gmoles)
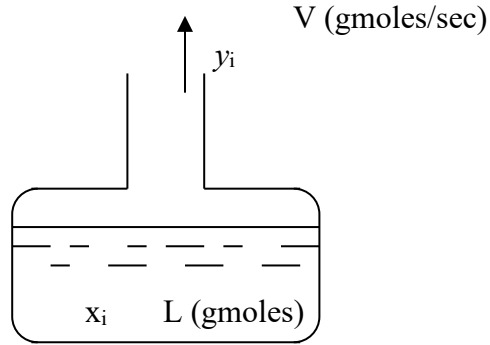
(a) The equilibrium relationship between the mole fraction $x$ of n-pentane in the liquid and that in the vapor $y$ is of the form

$$y_{C5} = x_{C5}\left(a + \frac{b}{1 + x_{C5}^2}\right)$$

Note that this equation is only valid for n-pentane, and not necessarily for n-hexane. Assuming ideal gas and ideal liquid and given

For n-pentane,    $\log_{10} P^{VAP} = 6.85221 - \dfrac{1064.630}{T + 232.00}$

For n-hexane,    $\log_{10} P^{VAP} = 6.87776 - \dfrac{1171.53}{T + 224.366}$

$P^{VAP}$ in mmHG
T in °C

Calculate the mole fraction of pentane in the vapor phase in equilibrium with the 70 mole% pentane-30 mole% hexane mixture at the initial system temperature of 46 °C.  Also, calculate the coefficients $a$ and $b$ in the n-pentane $x$-$y$ relationship.

(b) At any given instant, the vapor leaving the still may be considered to be in equilibrium with the remaining liquid.  Assuming that the values of $a$ and $b$ do not change with time and that vapor and liquid phases are constantly in equilibrium with each other, derive an analytical equation relating L, the amount of liquid left in the still, to x, the mole fraction of n-pentane in this liquid, i.e.

$$L = \text{function}(x_{C5})$$

## 35. *Batch Distillation, II*

A liquid mixture containing 60.0 mole% n-pentane and 40.0 mole% n-hexane is to be distilled in a batch still, and is initially charged with 100 gmoles of the mixture.  The equilibrium relationship between the mole fraction $x$ of n-pentane in the liquid and that in the vapor $y$ has been correlated to the following equation:

$$y = 1.8804\,x - 0.8804\,x^2$$

Note that this equation is only valid for n-pentane, and not necessarily for n-hexane.
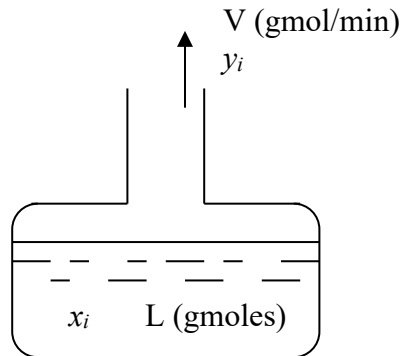


(a) Calculate the system temperature at which the above equilibrium relationship was established for the given liquid mixture (i.e. determine T in °C at which the above equation is valid). Also, compute the total system pressure P at the system temperature.

Assume ideal gas and ideal liquid, and the vapor pressures of the two components are:

For n-pentane, $\log_{10} P^{VAP} = 6.85221 - \dfrac{1064.630}{T + 232.00}$

For n-hexane, $\log_{10} P^{VAP} = 6.87776 - \dfrac{1171.53}{T + 224.366}$

$P^{VAP}$ in mmHG
T in °C

(b) Derive an analytical expression relating the amount of liquid left in the batch still L as a function of $x$ (mole fraction of n-pentane in the still) and compute the value of $x$ after 90% of liquid has been vaporized.


## 36. *Batch Distillation, III*

An equimolar liquid mixture of ethanol and water is to be distilled in a batch still at 1 atm and is initially charged with 100 gmoles of the mixture. Because water and ethanol forms a rather nonideal solution, Raoult's Law which fails to predict the azeotrope of the mixture cannot be used for vapor-liquid equilibrium calculations. Instead, the equilibrium relationship between the mole fraction $x$ of ethanol in the liquid and that in the vapor $y$ is correlated to the following empirical equation:

$$y = ax^3 + bx^2 + cx$$

where $a$, $b$, and $c$ are constants, which can be determined from experimental data. Note that the empirical equilibrium equation must and does satisfy the two end-points of the $x$-$y$ curve at $x = 0$ and $x = 1$. The following two pairs of data are known about the mixture: the azeotrope occurs at 89.43 mol% ethanol and when $x = 0.1661$, $y = 0.5089$.
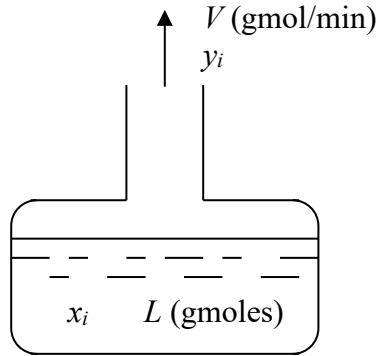
Derive an analytical expression relating the amount of liquid left in the batch still $L$ as a function of $x$ (mole fraction of ethanol in the still).

**Answer the following questions:**

(i) Compute the value of $x$ after 75% of liquid has been vaporized: $x =$ _____

(ii) How much liquid is left when $y = 0.70$? $L =$ _____ gmol

Carry four decimal places in your hand calculations. You may use MATLAB to solve any linear or nonlinear equations you encounter during your derivation of the analytical solution.

## 37. *Batch Distillation of a Water/Acetic-Acid System*

The following vapor-liquid equilibrium data (mole fractions) are available for the water/acetic-acid binary system at 25 °C.

| $x_{water}$ | $y_{water}$ | $x_{water}$ | $y_{water}$ |
|---|---|---|---|
| 0 | 0 | 0.6 | 0.6993 |
| 0.1 | 0.2329 | 0.7 | 0.7770 |
| 0.2 | 0.3558 | 0.8 | 0.8530 |
| 0.3 | 0.4517 | 0.9 | 0.9274 |
| 0.4 | 0.5379 | 1.0 | 1.0 |
| 0.5 | 0.6198 | | |

First, we will use the *Polyfit* function in MATLAB to fit the above data to a quadratic polynomial in the form of

$$y = ax^2 + bx + c$$

The water-acid system is distilled in a batch still as shown, which is initially charged with 100 gmoles of the mixture. The heating of the batch still is controlled such that it vaporizes 5 gmoles of the liquid every minute.



$V$ (gmol/min)
$y_i$

$x_i$     $L$ (gmoles)
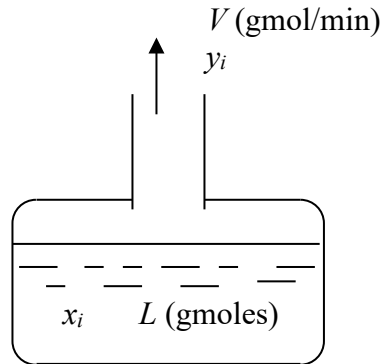
It has also been observed that it takes exactly 10 minutes to distill the mixture to reach 50 mole% water in the liquid. Without using the *ode* solver in MATLAB (although you may use it to verify your answer), compute analytically the initial composition of the liquid mixture.

**Answer the following question:**

Initial mole fraction of water in the liquid mixture = _____

# Part II


# Basic Principles of Process Optimization

1. *Solving Constrained Optimization Problems by Graphical Method, I*
Solve the following nonlinear constrained optimization problems by graphical method by finding their maxima and minima. After drawing your diagrams, you may need to use sophisticated algebra and calculus to determine the exact optima in each problem.

(a)     $f(x,y) = x^2 + 4y^2$
s.t.
$$y - x \geq 2$$
$$0 \leq x \leq 5$$
$$0 \leq y \leq 4$$

(b)     $f(x,y) = (x - 10)^2 + (y - 6)^2$
s.t.
$$y - 0.2x \leq 10$$
$$y - 0.1x^2 + 2x \geq 12$$

(c)     $f(x,y) = x + y$
s.t.
$$y \geq x^2$$
$$\frac{(y-2)^2}{36} + \frac{(x-1)^2}{9} \leq 1$$


2. *Solving Constrained Optimization Problems by Graphical Method, II*
Solve the following nonlinear constrained optimization problems by graphical method by finding their maxima and minima. After drawing your diagrams, you may need to use sophisticated algebra and calculus to determine the exact optima in each problem.

(a)     $f(x,y) = -x + 2y$
s.t.
$$x^2 + y^2 \leq 5$$
$$x - y \geq -1$$

(b)
$$f(x_1, x_2) = x_1$$
$$s.t. \quad (x_1 - 2)^2 + (x_2 - 2)^2 \leq 9$$
$$x_1 - x_2 \leq 2$$

(c)     $f(x_1, x_2) = x_1^2 + x_2^2$
s.t.
$$x_1 - (x_2 - 2)^2 \geq -1$$
$$2x_1 - x_2 \leq 2$$

### 3. *Solving Constrained Optimization Problems by Graphical Method, III*

Solve the following two optimization problems by graphical method. After drawing your diagrams, use sophisticated algebra and calculus to determine the exact optima in each problem.

(a) Find both the minimum and maximum of:

$$f(x,y) = y - x$$

$$s.t. \quad y - 3x \leq 2$$
$$y + x \leq 4$$
$$-y + 0.5x \leq 4$$
$$x \geq 0$$

(b) Find both the minimum and maximum of:

$$f(x,y) = y - x^2 + 2x$$

$$s.t. \quad y - x \leq 2$$
$$y + x \leq 8$$
$$y - 0.2x \geq -2$$

Calculate the optimal objective values in both problems as well.

**Instructions**: For Problems 4 through 21, classify each problem as either linear (LP), quadratic (QP), nonlinear (NLP), integer linear (ILP), or mixed integer linear (MILP) programming problem. If the problem is quadratic or nonlinear, state whether it is constrained. Some problems can be solved by calculus but some cannot. Do not solve each problem unless you are explicitly told to do so.

### 4. *Optimal Height and Diameter of an Absorption Tower*

An absorption tower containing wooden grids is to be used for absorbing $SO_2$ in a sodium sulfite solution. A mixture of air and $SO_2$ will enter the tower at a rate of 70,000 ft$^3$/min, temperature of 250°F, and pressure of 1.1 atm. The concentration of $SO_2$ in the entering gas is specified, and a given fraction of the entering $SO_2$ must be removed in the absorption tower. The molecular weight of the entering gas mixture may be assumed to be 29.1. Under the specified design conditions, the number of transfer units necessary varies with the superficial gas velocity as follows:

$$\text{Number of transfer units} = 0.32G_s^{0.18}$$

where $G_s$ is the entering gas velocity as lbm/(hr-ft$^2$) based on the cross-sectional area of the empty tower. The height of a transfer unit is constant at 15 ft. The cost for the installed tower is \$1 per cubic foot of inside volume, and annual fixed charges amount to 20 percent

of the initial cost.  Variable operating charges for the absorbent, blower power, and pumping power are represented by the following equation:

$$\text{Total variable operating cost as \$/hr} = 1.8 \times 10^{-8} G_s^2 + \frac{81}{G_s} + \frac{4.8}{G_s^{0.8}}$$

The unit is to operate 8,000 hr/year.  Formulate this problem as an optimization problem to minimize the annual cost and classify it.

You must simplify all your equations so that in the end the only variable(s) left in the formulation are the unknowns (decision variables).

## 5. *Formulation of a Manufacturing Optimization Problem*

A chemical manufacturing firm has discontinued production of a certain unprofitable product line.  This has created considerable excess production capacity on the three existing batch production facilities.  Management is considering devoting this excess capacity to one or more of three new products: call them products 1, 2, and 3.   The available capacity on the existing units which might limit output is summarized in the following table, and each of the three new products requires the following processing time for completion:

| Unit | Available Time, hours/week | Productivity, hours/batch | | |
|---|---|---|---|---|
| | | **Product 1** | **Product 2** | **Product 3** |
| A | 20 | 0.8 | 0.2 | 0.3 |
| B | 10 | 0.4 | 0.3 | ….. |
| C | 5 | 0.2 | ….. | 0.1 |

The sales department indicates that the sales potential for products 1 and 2 exceeds the maximum production rate and that the sales potential for product 3 is 20 batches per week. The profit per batch would be $20, $6, and $8, respectively, on products 1, 2, and 3.

Formulate this problem as an optimization problem and classify it.  Assume that the number of batches needs not be integer.   Propose three feasible solutions (for example, one solution may involve the production of just product 1 and no product 2 and 3).  Compare the objective function of your three feasible solutions.

## 6. *Maximizing Total Profit in Making Two Display Boxes*

A cabinet maker is asked by a jeweler to build two display boxes with <u>lids</u> made from a special shatter and break-proof transparent material. Only 8 square feet of the material are in stock at present and no more can be procured within the time available to build the boxes. For Box 1, the length has to be 1 foot whereas the width and height are to be equal to an unspecified size $x_1$. For Box 2, the height has to be 1 foot whereas the width and length are to be equal to unspecified size $x_2$.

The cost of the material and labor is $ 0.5 per square foot of the outside of each box (Hint: There are 6 sides to each box!). The cabinet maker charged the jeweler proportional to the sum of the three dimensions of the boxes, i.e., width + length + height at the rate of $ 2.00 for box 1 and $ 2.50 per foot for Box 2. The cabinet maker's problem is to determine nonnegative values of $x_1$ and $x_2$ which will satisfy the material constraint on the lids of the two boxes and at the same time maximize his total profit.
Formulate the cabinet maker's problem as an optimization problem and classify it.

## 7. *Formulation of a Manufacturing Optimization Problem*

A certain plant can manufacture 5 different products in any combination. Each product requires time on each of three machines in the following manner (all numbers are in minutes/unit):

| Product | Machine | | |
|---|---|---|---|
| | 1 | 2 | 3 |
| A | 12 | 8 | 5 |
| B | 7 | 9 | 10 |
| C | 8 | 4 | 7 |
| D | 10 | 0 | 3 |
| E | 7 | 11 | 2 |

Each machine is available 128 hours per week. Products $A$, $B$, and $C$ are purely competitive, and any amounts made may be sold at respective prices of $5, $4, and $5. The first 20 units of $D$ and $E$ produced per week can be sold at $4 each, but all made in excess of 20 can only be sold at $3 each. Variable labor costs are $4 per hour for machines 1 and 2 and $3 per hour for machine 3. Material costs are $2 for products $A$ and $C$, and $1 for products $B$, $D$, and $E$. You wish to maximize profit to the firm. Formulate this problem as an optimization problem and classify it.

## 8. *Optimization of a Refinery Production*

A refinery has four different crudes which are to be processed to yield four products: gasoline, heating oil, jet fuel, and lube oil. There are maximum limits both on product

demand (what can be sold) and crude availability.  A schematic of the processing operation is as follows:

**Crude Availability**
**bbl/wk = Barrels/week**

**Max. Product Demand**
**bbl/wk**
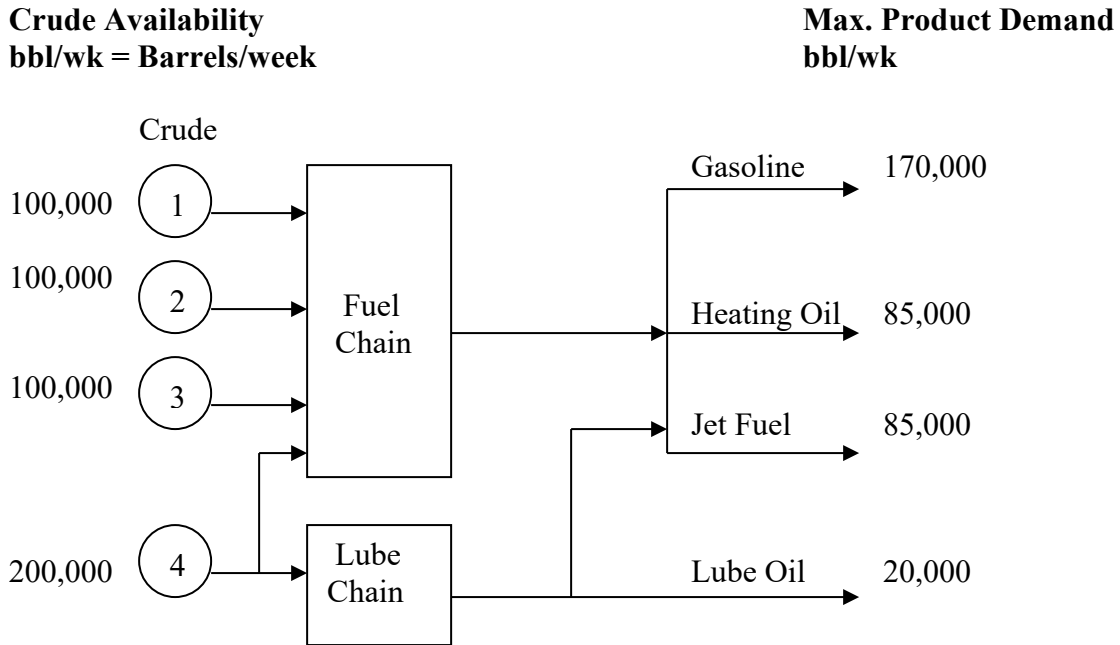


(a) Given the tabulated profits, costs, and yields in Table 1, formulate the problem as an optimization problem that maximizes the profit and classify it.

(b) Propose 3 feasible solutions (which are not necessarily optimal) to this problem.

**Table 1: Profits, Costs, and Yields Data**

| | | Crude Type | | | | | Product |
| | | 1 | 2 | 3 | 4 | | Value |
| | | | | | Fuel Process | Lube Process | $/bbl |
| **Yields** | Gasoline | 0.6 | 0.5 | 0.3 | 0.4 | 0.4 | 45.00 |
| (bbl product | Heating Oil | 0.2 | 0.2 | 0.3 | 0.3 | 0.1 | 30.00 |
| per bbl crude) | Jet Fuel | 0.1 | 0.2 | 0.3 | 0.2 | 0.2 | 15.00 |
| | Lube Oil | 0 | 0 | 0 | 0 | 0.2 | 60.00 |
| | Other* | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | |
| Crude cost $/bbl | | 15.00 | 15.00 | 15.00 | 25.00 | 25.00 | |
| Operating cost $/bbl | | 5.00 | 8.50 | 7.50 | 3.00 | 2.50 | |

* "Other" refers to losses in processing

## 9. *Finding the Shortest Length of a Ladder*

A rectangular box of height 2 meters and width 4 meters is placed adjacent to a wall (see figure below). Formulate this problem as an optimization and classify it. Find the length of the shortest ladder that can be made to lean against the wall.
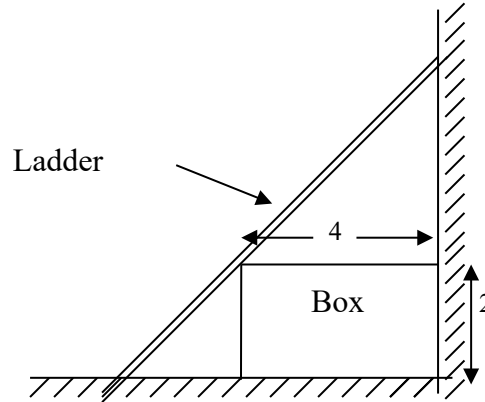


## 10. *Formulation and Minimization of a Heat Transfer Problem*

It is desired to cool a gas [$C_P = 0.3$ Btu/lbm-°F] from 195 to 90°F, using cooling water [$C_P = 1.0$ Btu/lbm-°F, $\rho = 62.4$ lbm/ft³] at 80°F in a counter-current heat exchanger. Water costs \$0.20/1000 ft³, and the annual fixed charges for the exchanger are \$0.50/ft² of heat transfer area. The heat transfer coefficient is $U = 8$ Btu/hr-ft²-°F for a gas rate of 3000 lbm/hr. The heat exchanger is operated 365 days/year (24 hours/day).

Formulate this heat exchange operation as an optimization problem to minimize the total annual cost and classify it.

**Hint:** $\Delta T_{\text{lm}} = $ log-mean $\Delta T = (\Delta T_2 - \Delta T_1)/\ln(\Delta T_2/\Delta T_1)$
where $\Delta T_2$ and $\Delta T_1$ are the terminal temperature differences of heat exchanger.

## 11. *Optimum Thickness of Insulation for a Furnace*

To reduce heat losses, the exterior flat wall of a furnace is to be insulated. To determine the optimum insulation thickness, it is necessary to consider and balance the costs of the insulation and the value of the energy saved by adding the insulation. The rate of heat transfer $Q$ through the wall is:

$$Q = UA \ (T_{\text{furnace}} - T_{\text{wall}})$$

where $T$ is in °F and $Q$ is in Btu/hr. The overall heat transfer coefficient $U$ is related to the outside convective heat transfer coefficient $h$ and the thermal conductivity of insulation $k$ by:

$$\frac{1}{U} = \frac{1}{h} + \frac{t}{12k}$$

where $t$ is the thickness in inches of the insulation.

We wish to maximize the savings in total operating cost, savings expressed as the difference between the dollar value of the heat conserved minus the cost of the insulation over a span of 5 years (after that, the insulation will have to be replaced). Formulate this problem as an optimization problem, classify it, and obtain the optimum value of $t$ (in inches) using the following data:

|  |  |
|---|---|
| Temperature inside the furnace | 500°F (constant) |
| Air temperature outside wall | Assume constant at 70°F |
| Heat transfer coefficients | |
|     Outside air film $h$ | 4.0 Btu/(hr)(ft$^2$)(°F) |
|     Conductivity of insulation $k$ | 0.03 Btu/(hr)(ft)(°F) |
| Total cost of insulation | $0.75/(ft$^2$)(per inch of thickness) |
|     (per unit area per inch of thickness) | |
| Values of energy saved | $0.60/10$^6$ Btu |
|     (i.e. the dollar difference between adding insulation and having no insulation for every 1 million Btu is $0.60.) | |
| Hours of operation | 8700 hours/year |

Prove that your optimum $t$ is a maximum. **Hint:** The heat transfer area $A$ is constant.

## 12. *An Airline Assignment Problem*

Large airlines tend to base their route structure around the hub concept. An airline will try to have a large number of flights arrive at the hub airport during a certain short interval of time, e.g. 9 A.M. to 10 A.M. and then have a large number of flights depart the hub shortly thereafter, e.g. 10 A.M. to 11 A.M. This allows customers of that airline to travel between a large combination of origin/destination cities with one stop and at most one change of planes. For example, United Airlines uses Chicago as a hub, Delta Airlines uses Atlanta, TWA uses St. Louis, and American uses Dallas/Fort Worth. A desirable goal in using a hub structure is to minimize the amount of changing of planes (and the resulting moving of baggage) at the hub. The following problem illustrates this airline assignment problem.

A certain airline has 6 flights arriving at O'Hare airport between 9 and 9:30 A.M. The same 6 airplanes depart on different flights between 9:40 and 10:20 A.M. The average numbers of people transferring between incoming and leaving flights appear in the table below:

|  | L01 | L02 | L03 | L04 | L05 | L06 |
|---|---|---|---|---|---|---|
| I01 | 20 | 15 | 16 | 5 | 4 | 7 |
| I02 | 17 | 15 | 33 | 12 | 8 | 6 |
| I03 | 9 | 12 | 18 | 16 | 30 | 13 |
| I04 | 12 | 8 | 11 | 27 | 19 | 14 |
| I05 | 0 | 7 | 10 | 21 | 10 | 32 |
| I06 | 0 | 0 | 0 | 6 | 11 | 13 |

**Flights I05 arrives too late to connect with L01. Similarly, I06 is too late for flights L01, L02, and L03.**

All the planes are identical. A decision problem is which incoming flight should be assigned to which outgoing flight. For example, if incoming flight 102 is assigned to

leaving flight L03, 33 people (and their baggage) will be to remain on their plane at the stop at O'Hare.  Formulate this assignment problem as an optimization and classify it.

### 13. *Toll-Way Staffing Problem*

The Northeast Tollway out of Chicago has a toll plaza with the following staffing demands during each 24-hour period:

| Hours | Collectors Needed |
|---|---|
| 12 a.m.  to   6 a.m. | 2 |
| 6 a.m.  to  10 a.m. | 8 |
| 10 a.m.  to  12 a.m. | 4 |
| 12 a.m.  to   4 p.m. | 3 |
| 4 p.m.  to   6 p.m. | 6 |
| 6 p.m.  to  10 p.m. | 5 |
| 10 p.m.  to 12 Midnight | 3 |

Each collector works 4 hours, is off one hour, and then works another 4-hours.  A collector can be started at any hour.  Assuming the objective is to minimize the number of collectors hired, formulate this problem as an optimization problem.

### 14. *Formulation of a Manufacturing Problem*

A chemical company manufactures four products (1, 2, 3, and 4) on two machines ($X$ and $Y$). The time (in minutes) to process one unit of each product on each machine is shown below:

|  |  | Machine | |
|---|---|---|---|
|  |  | $X$ | $Y$ |
| Product | 1 | 10 | 27 |
|  | 2 | 12 | 19 |
|  | 3 | 13 | 33 |
|  | 4 | 8 | 23 |

The profit per unit for each product (1, 2, 3, and 4) is $10, $12, $17, and $8 respectively. Each product can be produced on either machine.

The factory is very small and this means that floor space is very limited. Only one week's production is stored in 50 square meters of floor space where the floor space taken up by each product is 0.1, 0.15, 0.5, and 0.05 (square meters) for products 1, 2, 3, and 4 respectively.

Customer requirements mean that the amount of product 3 produced should be related to the amount of product 2 produced. Over a week, twice as many units of product 2 should be produced as product 3.

Machine $X$ is out of action (for maintenance/because of breakdown) 5% of the time and machine $Y$ 7% of the time.

Assuming a working week 35 hours long, formulate the problem of how to manufacture these products as a linear program so as to maximize the total weekly profit and classify it.

## 15. *Maximizing the Monetary Value of a Cargo Load*

A cargo load is to be prepared from five types of articles. The weight $w_i$, volume $v_i$, and monetary value $c_i$ of different types of articles are given below.

| Article Type | $w_i$ | $v_i$ | $c_i$ |
|---|---|---|---|
| 1 | 4 | 9 | 5 |
| 2 | 8 | 7 | 6 |
| 3 | 2 | 4 | 3 |
| 4 | 5 | 3 | 2 |
| 5 | 3 | 8 | 8 |

Formulate this optimization problem which will determine the number of articles $x_i$ selected from the $i^{th}$ type (i = 1, 2, 3, 4, 5), so that the total monetary value of the cargo load is maximized. The total weight and volume of the cargo cannot exceed the limits of 2000 and 2500 units, respectively. Classify the problem but <u>do not</u> solve for the optimum. Note that it is not possible to load a fraction of an article.

## 16. *Formulating and Solving a Vessel-Design Optimization Problem*

As a starting chemical engineer at Vessels Fabrication Co., Ltd., your first assignment is to design a cone-shaped vessel. Specifically, your job is to calculate the dimensions (radius $r$ and height $h$) of the cone with a maximum volume that can be inscribed (fit into) in a sphere of radius 2 meters. Formulate this assignment as an optimization problem, classify it, and solve it. Note that the volume of a cone is given by

$$V = \frac{1}{3} \pi r^2 h$$

Also, show that the volume found is indeed a maximum. A two-dimensional side view of the geometry is shown below.



two−
dimensional
side view
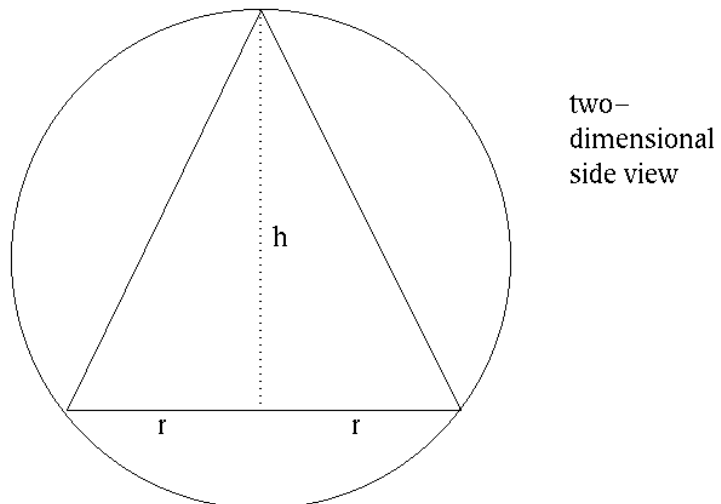
## 17. *Formulation of a Cargo Plane Optimization Problem*

A cargo plane has three compartments for storing cargo: front, center, and rear. These compartments have the following limits on both weight and space:

| Compartment | Weight capacity (tons) | Space capacity ($m^3$) |
|---|---|---|
| Front | 10 | 6800 |
| Center | 16 | 8700 |
| Rear | 8 | 5300 |

Furthermore, the weight of the cargo in the respective compartments must be the same proportion of that compartment's weight capacity to maintain the balance of the plane. The following four cargoes are available for shipment on the next flight:

| Cargo | Weight (tons) | Volume ($m^3$/ton) | Profit ($/ton) |
|---|---|---|---|
| C1 | 18 | 480 | 310 |
| C2 | 15 | 650 | 380 |
| C3 | 23 | 580 | 350 |
| C4 | 12 | 390 | 285 |

Any proportion of these cargoes can be accepted. The objective is to determine *how much* (if any) of each cargo C1, C2, C3 and C4 should be accepted and *how to distribute* each among the compartments so that the total profit for the flight is maximized. Formulate the above optimization problem and classify it, but do not solve it.

## 18. *Minimum Area under a Curve and Shortest Distances to the Curve*

The graph below shows the function $y = \exp(x)\cos(x)$ over the domain $[-2, 2]$.

(a) A shaded rectangle is enclosed under the curve between the curve, the vertical line $x = 0.5$, and the $x$-axis as shown. Calculate the maximum area of the shaded rectangle that is possible under the curve. Also, calculate the total unshaded area under the curve when the shaded rectangle has the maximum area.

Recall the formula for integration by parts: $\int u\,dv = uv - \int v\,du,$

The graph shows the curve $y = e^x \cos(x)$ with a vertical line at $x = 0.5$ and a shaded rectangle.
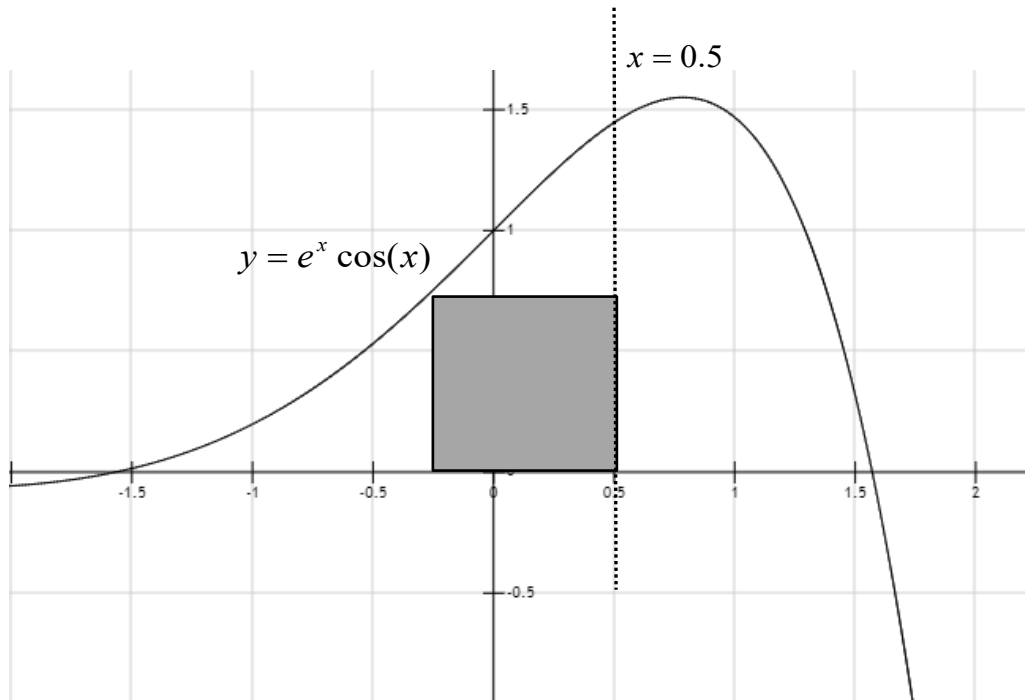
(b) Determine the point on the curve which has the shortest distance to the coordinate [0.5, 1.0].

## 19. *Solving Optimization Problems by Calculus*

As a chemical engineer, you have been called upon to solve the following optimization problems:

(a) You are asked to design a right inverted cone with a height $h$ and a radius $r$ at the base with a maximum volume that can be inscribed completely in a sphere with a radius of $R$.



(i) Derive the optimal value of $r$ in terms of $R$ that maximizes the volume of the cone.
(ii) Given that $R = 2$ ft, compute the maximum volume of the cone.
(iii) Prove that this volume is a maximum by showing that when $r = r_{opt} + \Delta$ and when $r = r_{opt} - \Delta$, the volumes of the cones at these two radii are smaller than the calculated maximum volume.
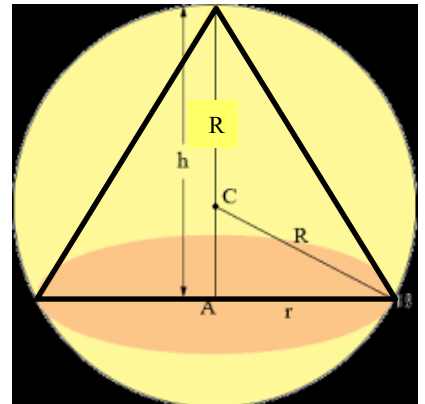
(b) You are asked to design a special piece of equipment which is a cone in which a cylinder is inscribed inside as shown in the figure. The cylinder inside has a radius $r$ and a height of $h$, while the outside cone has a radius $R$ and a height of $H$. The volume of the cylinder must be equal to 0.1 m$^3$.



    (i) We wish to minimize the volume of the cone which is given by $V_{cone} = \frac{1}{3}\pi R^2 H$. Find the optimal value of $R$ as a function of $r$ at this optimum. (Note that $R$ must be $> r$)

    (ii) Calculate the minimum volume of the cone if $r = 0.1$ m.

    (iii) Prove that the calculated volume is a minimum by showing that when $R = R_{opt} + \Delta$ and when $R = R_{opt} - \Delta$, the volumes of the cones at these two radii are larger than the calculated minimum volume.
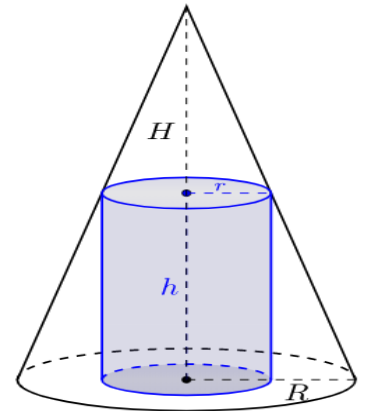
Formulas:

Volume (cone) $= \frac{1}{3}\pi r^2 h = \frac{1}{3}\pi R^2 H$, Volume (sphere) $= \frac{4}{3}\pi R^3$, Volume (cylinder) $= \pi r^2 h$

## 20. *Formulating a Compressor Storage Problem*

Acme Inc. engages in the business of building large and expensive compressors. The company operates 3 plants, called Plant *A*, *B*, and *C*, in different locations which have different manufacturing capacities (number of compressors built at the end of each production week). Because of their sizes, all the compressors built at each plant must be transported to a warehouse for storage at the end of each production week. The company owns three warehouses in different locations, which also have different storage capacities. The total cost associated with storing one compressor (e.g. transportation cost, space rental fee, etc.) at each warehouse is known and given in the table below.

As a chemical engineer working for Acme, you are asked to formulate this optimization problem and classify it. The objective is to minimize the total cost of storing all compressors manufactured at the end of a production week at the 3 warehouses.

### Cost of Storing a Compressor from a Plant at a Warehouse

|  | Warehouse 1 | Warehouse 2 | Warehouse 3 | Plant Capacity |
|---|---|---|---|---|
| **Plant *A*** | 15 | 20 | 50 | 30 |
| **Plant *B*** | 15 | 30 | 40 | 25 |
| **Plant *C*** | 30 | 10 | 10 | 40 |
| **Max. Storage Capacity** | 40 | 30 | 35 | |

## 21. *Minimizing the Piping Cost for an Offshore Oil Well*

An offshore oil well is located in the ocean at a point $W$, which is 5 miles from the closest shorepoint $A$ on a straight shoreline (see the figure below). The oil is to be piped to a shorepoint $B$ that is 8 miles from $A$ by piping it on a straight line under water from $W$ to some shorepoint $P$ between $A$ and $B$ and then on to $B$ via a pipe along the shoreline. If the cost of laying pipe is $100,000 per mile under water and $75,000 per mile over land, formulate this piping problem as an optimization problem to minimize the cost of laying the pipe, classify it as either unconstrained NLP, constrained NLP, LP, MILP, or MINLP, and determine analytically where the point $P$ should be located that gives the least possible cost? Compute this minimum cost as well.
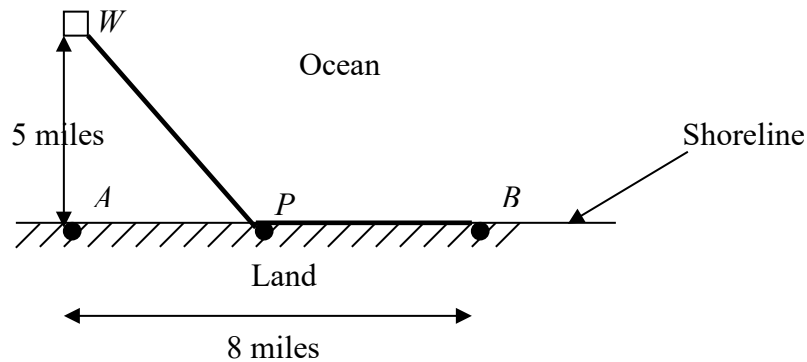


## 22. *Characterization of Stationary Points*

Identify and characterize (as local/global minimum, local/global maximum, or saddle point) the stationary points of the following functions. Compute the value of the function at each stationary point as well.

(a) $f(x) = x^4 + x^3 - 2x^2 - 2\exp(-x^2)$

(b) $f(x) = (x-1)^2 \exp[x(x+3)]$

(c) $f(x_1, x_2) = x_1^4 - 2x_1^3 - x_1^2 x_2 + x_2^2 - 2x_2$

(d) $f(x_1, x_2) = 2x_1^3 + 4x_1 x_2^2 - 10x_1 x_2 + x_2^2$

(e) $f(x_1, x_2, x_3) = x_1^2 + x_2^2 + 2x_3^2 - x_2^2 x_3 + \ln(x_3) - 4x_3 + 4$

(f) $f(x_1, x_2) = x_1^2 x_2 + x_1 x_2^2 + x_1^2 + x_2^2$

(g) $f(x_1, x_2) = x_1 x_2 - 4\sin(x_1) + \ln\left(\dfrac{x_1}{x_2}\right)$    $0 \le x_1, x_2 \le \pi$

(h) $f(x_1, x_2, x_3) = \exp(-x_1^2) + 2x_1^2 + x_2^2 + x_2 x_3 + x_3^3$

(i) $f(x_1, x_2) = x_1^3 + x_2^3 + 2x_1^2 + 4x_2^2 + 6$

(j) $f(x_1, x_2, x_3) = \dfrac{x_1}{(1 - x_2)} - \exp(x_2) + 2x_1^3 - 4x_1 + 2x_2 + x_1 x_2 x_3$

(k) $f(x, y) = x^2 y + xy^2 - 2x^2 - 2y^2$

(l) $f(x, y) = (x^2 + y^2)\exp(y^2 - x^2)$

(m) $f(x_1, x_2) = (x_1 - 2)\exp(x_1 + x_2^2) + x_2$

(n) $f(x_1, x_2) = 2x_1^2 + x_1^2 x_2 - x_1 x_2^2 + 2x_1 x_2 + 8x_1$


## 23. *Solving a Heat Transfer Minimization Problem*
Refer to Problem 10, which is a problem to minimize the total annual cost of a heat exchanger.

(a) Solve for the optimum analytically.

(b) Use the function *fminunc* in MATLAB to solve for the minimum annual cost. Briefly explain the application of this function.


## 24. *Optimization of a Solvent-Extraction Operation*
A solvent-extraction operation is carried out continuously in a plate column with gravity flow. The unit is operated 24 hr/day. A feed rate of 1500 ft³/day must be handled 300 days per year. The allowable velocity per square foot of cross-sectional tower area is 40 ft³ of combined solvent and charge per hour. The annual fixed costs for the installation can be predicted from the following equation:

$$C_F = 6{,}800 F^2_{SF} - 48{,}000 F_{SF} + 120{,}000 \quad \$/\text{year}$$

where $F_{SF}$ = cubic feet of solvent per cubic foot of feed. Operating and other variable costs depend on the amount of solvent that must be recovered, and those costs are $0.04 for each cubic foot of solvent passing through the tower.

(a) What tower diameter should be used for optimum conditions of minimum total cost per year?

(b) What is the answer in Part (a) if the annual fixed costs for the installation follow the equation below:

$$C_F = 400 F^4_{SF} - 1{,}800 F^3_{SF} - 12{,}000 F_{SF} + 120{,}000 \quad \$/\text{year}$$

Write a MATLAB program to implement the following methods to find the optimum diameter $D_{opt}$, correct to 3 decimal places, i.e. $|D_{opt,k+1}| - |D_{opt,k}| \geq 0.001$.
  (i)   Newton-Raphson method
  (ii)  Quasi-Newton method using a step size of $h = 0.1$
  (iii) Secant method


## 25. *Single-Variable Search Using 3 Different Techniques*
Carry out a single-variable search of the function

$$f(x) = x + 4/x \quad \text{on the interval } [1, 5]$$

using  (a) Newton-Raphson method
       (b) Quasi-Newton method using a step size of $h = 0.1$
       (c) Secant method

Carry out 5 iterations in each method using Excel. Also determine the true minimum of $f(x)$ analytically and compare the accuracy of the minima estimated by these three methods.


## 26. *Solving for the Optimal Height and Diameter of an Absorption Tower*
Refer to Problem 4 again. Recall that $G_s$, the superficial gas velocity, is the decision variable to be minimized in the cost function. Given that the optimal value of $G_s$ lies between 1000 and 2000 lbm/ft$^2$-hr, do the following:

(a) Use *fminbnd* function in MATLAB to solve for the optimal tower height, diameter, and minimum annual cost. What is the number of iterations, the number of function evaluations, and the algorithm used as reported by MATLAB?

(b) Write a MATLAB script file to implement Golden Section search to find the optimal $G_s$, accurate to 1 decimal place. What is the total number of iterations required?


## 27. *Solving for a Maximum Using Golden Section*
Find the maximum of the function $xe^{-x}$ over the interval $0 \leq x \leq 4$ by performing 6 function evaluations with the Golden Section search by hand. What is the accuracy of the result after 6 iterations? Confirm analytically that the solution is in fact a local maximum. Prove that it is a global maximum.


## 28. *Steepest Descent with Golden Section*
Consider a chemical process for which there are 2 design variables $x$ and $y$. After cost estimation and profitability analysis, it is determined that it is desirable to find the values of x and y that <u>minimizes</u> the cost function $C$:

$$C = 6.5x^{0.5} + \frac{3000}{xy} + 5y + 2x^2 + 60$$

The initial guess is $x^{(0)} = 2$ and $y^{(0)} = 7$.

In this problem you are asked to perform <u>one iteration</u> of the steepest descent method for solving this problem. That is, find $x^{(1)}$ and $y^{(1)}$, the next estimates of the optimum.

For the variable optimization with respect to the parameter $\lambda$ (line search, which indicates how far to move in the steepest descent direction), use the Golden Section method. Assume $C$ is unimodal with respect to $\lambda$, and that $0 \leq \lambda \leq 0.1$. You need to perform only <u>3 iterations</u> of the Golden Section method (so you will have to evaluate $C$ only 4 times). You must show all intermediate results in each iteration of Golden Section. Do not use Excel, MATLAB, or the programmable feature in your calculators and do not show your answers in the form of tables.

You should express your answer in terms of an interval. That is, determine what two numbers $x^{(1)}$ lies between and what two numbers $y^{(1)}$ lies between. Carry 4 decimal places in all your calculations.

## 29. *Unconstrained Optimization of a Two-Variable Problem*
Consider the following unconstrained minimization problem of two variables.

$$\text{Minimize } f(x_1, x_2) = 2x_1^2 + x_1^2 x_2 - x_1 x_2^2 + 2x_1 x_2 + 8x_1$$

Carry out one iteration of Steepest Descent Search and one iteration of Newton's method, starting at $x^{(0)} = [1.0 \ 1.0]^T$ in both cases. Carry 4 decimal places in all your calculations. Note that you must perform a line search in Steepest Descent Search using calculus. Compute the objective value after one iteration in both algorithms.

## 30. *Line Search with Golden Section in a 2-Variable Problem*
A one-dimensional search is to be carried out from the point $[0, 3]$ using $s = [1 \ 1]^T$; $s$ is the search direction on the function:

$$f(x) = (x_1 - 1)^2 + 4(x_2 - 2)^2$$

Use Golden Section method to find the minimum along this search direction (with respect to $\lambda$), with an accuracy of 4 decimal places. Also, find this optimum value analytically and show that it is $(-0.6, 2.4)$.

### 31. *Line Search with Golden Section in a 2-Variable Problem*

A one-dimensional search is to be carried out from the point $[1, 3]$ using $s = [1\ {-}2]^T$; $s$ is the search direction on the function:

$$f(x) = 2x_1^3 + 4x_1x_2^2 - 10x_1x_2 + x_2^2$$

Implement Golden Section method in MATLAB to find the minimum along this search direction (with respect to $\lambda$), with an accuracy of 4 decimal places. Also, use *fminbnd* to find the optimum value of the step size $\lambda$.

### 32. *Conjugate Search Directions for a Quadratic Function*

The general equation in matrix form for a quadratic function can be expressed as:

$$f(x) = a + b^T x + \tfrac{1}{2} x^T C x$$

where $b^T$ is a *1xn* matrix and C is an *nxn* symmetric matrix, and $n$ is the total number of variables.

(a) For the function

$$f(x) = 5x_1^2 + x_2^2 + 2x_3^2 + 2x_1x_2 - x_1x_3 - 4x_2 + 5x_3 + 8$$

show that the vectors $[1\ \ 0\ \ 0]^T$ and $[1\ \ 1\ \ 12]^T$ are conjugate directions with respect to the $C$ matrix.

(b) Compare the $C$ matrix with the Hessian matrix $H(x)$ of $f(x)$ and comment on their relationship.

(c) Is the function in Part (a) strictly convex, convex, strictly concave, concave, or none of the above?

### 33. *Combined Search Techniques in a Multivariable Minimization Problem*

Consider the following unconstrained minimization problem of two variables.

$$\text{Minimize}\ \ f(x_1, x_2) = x_1^2 - x_1x_2 + \ln(x_1 + x_2)$$

Carry out two iterations of Conjugate Direction Search, starting at $x^{(0)} = [1.0\ 1.0]^T$. In the first iteration, use the Steepest Descent as the search direction. In the second iteration, your search direction must be made conjugate to the search direction in the first iteration. Carry 4 decimal places in all your calculations. Note that you must perform a line search in both iterations using calculus. Compute the objective value of each iteration.

### 34. *Unconstrained Optimization of a Two-Variable Problem*

Consider the following unconstrained optimization problem of two variables. Carry out one iteration of each method below to minimize the given objective function.

$$Minimize \ f(x) = x_1^4 + 2x_1 x_2^2 - x_1 x_2$$

**Method 1:** Starting at $[x_1, x_2]^T = [1, 0]^T$, carry out one iteration of Steepest Descent search. Note that you must minimize $\lambda$, whose optimal value is less than 0.2, in the line search accurate to 4 decimal places. You may choose any line-search (one-variable) optimization technique but a fast convergence method is recommended. You must show all work instead of using your programmable calculator to give the final answer.

**Method 2:** Starting at $[x_1, x_2]^T = [1, 0]^T$, carry out one iteration of Conjugate Direction search. This search direction must be conjugate to the steepest descent search direction in Method 1. Fix the value of the second element of your conjugate vector to 1 and calculate its first element, i.e. $s = [s_1, 1]^T$. Once again, you must minimize $\lambda$, whose value is less than 0.2, in the line search accurate to 4 decimal places. You may choose any line-search (one-variable) optimization technique but a fast convergence method is recommended. You must show all work instead of using your programmable calculator to give the final answer.

**Method 3:** Starting at $[x_1, x_2]^T = [1, 0]^T$, carry out one iteration of Newton's method

Calculate $f(x)$ in each method after one iteration. What are the absolute relative percentage deviations of $x_1$, $x_2$, and $f(x)$ of the three methods when compared to the global minimum in this problem? Carry 4 decimal places in all your calculations.

<u>Formula</u>: The inverse of a square matrix $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ is $\dfrac{1}{\det(A)} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$

where $\det(A) = ad - bc$

### 35. *Using Steepest Descent to Solve a Multivariable Minimization Problem*

Consider an unconstrained optimization problem with two decision variables $x$ and $y$. It is desirable to find the values of $x$ and $y$ that <u>minimizes</u> the objective function $f(x, y)$:

$$f(x, y) = (y - x^2)^2 + (5 - x)^2$$

Carry out one iteration of the Steepest Descent method. Use an initial guess of $x = 2$ and $y = 5$. In your line search, carry out 5 iterations of Golden-Section Search.

### 36. *Conjugate-Gradient and Newton's Methods for a Multivariable Problem*
For the following quadratic function,

$$f(\mathbf{x}) = 4(x_1 - 5)^2 + (x_2 - 6)^2$$

starting at $\mathbf{x}^0 = [1 \quad 1]^T$.

(a) Use the Fletcher-Reeves (conjugate-gradient) search to find the minimum.

(b) Use Newton's method to find the minimum.


### 37. *Newton's Methods for Another Multivariable Problem*
Solve the following problem by Newton's method:

Minimize $f(\mathbf{x}) = 1 + x_1 + x_2 + x_3 + x_4 + x_1x_2 + x_1x_3 + x_1x_4 + x_2x_3 +$

$$x_2x_4 + x_3x_4 + x_1^2 + x_2^2 + x_3^2 + x_4^2$$

starting from $\mathbf{x}^0 = [-3 \quad -30 \quad -4 \quad -0.1]^T$.


### 38. *Steepest Descent and Conjugate Direction Methods*
Consider the maximization of

$$f(\mathbf{x}) = 12x_1 - 2x_1^2 - 2x_2^2 + 2x_1x_2 - 12$$

(a) Find the stationary point analytically, and prove that it is a local maximum.

(b) Carry out 3 iterations of steepest descent (with the line search) from the point $[1 \quad 1]^T$. What are the values of $x_1$, $x_2$, and $f(\mathbf{x})$ after 3 iterations?

(c) Determine the maximum using conjugate search directions. Since the number of variables is 2 and $f(\mathbf{x})$ is quadratic, it should take you only 2 iterations to find the maximum.


### 39. *Conjugate-Gradient Method, Newton's Method, and fminunc for a Multivariable Problem*
For the following optimization problem,

$$\text{Minimize } f(\mathbf{x}) = \exp(-x_1^2) + 2x_1^2 + x_2^2 + x_2x_3 + x_3^3$$

Write a MATLAB program to implement the following:

(a) 10 iterations of the Fletcher-Reeves (conjugate-gradient) search to find the minimum starting at $x^0 = [0\ -0.5\ 0.5]^T$. Do not perform the line search in each iteration. Instead, use a fixed step size of $\lambda = 0.1$.

(b) 5 iterations of Newton's method to find the minimum starting at $x^0 = [0\ -1\ 1]^T$.

(c) Use *fminunc* function to solve for the minimum at $x^0 = [1\ 1\ 1]^T$. Do not use the default algorithm of Quasi-Newton line search because it will not converge the problem at the given starting point. Instead, use the trust-region Newton algorithm.


## 40. *Sequential Simplex Method and MATLAB's fminsearch*

For the following function

$$f(x) = [\exp(x_1)][4x_1^2 + 2x_2^2 + 4x_1x_2 + 2x_2 + 1]$$

(a) Carry out 5 steps of sequential simplex method to find the minimum, using a simplex with a length of 0.2 and a starting point of $x^0 = [2\ -2]^T$.

(b) Use *fminsearch* in MATLAB to find the minimum starting at $x^0 = [2\ -2]^T$.


## 41. *Combined Search Techniques in a Multivariable Minimization Problem*

Consider a chemical process for which there are 2 design variables $x_1$ and $x_2$. After cost estimation and profitability analysis, it is determined that it is desirable to find the values of $x_1$ and $x_2$ that <u>minimizes</u> the cost function $f(x)$:

$$f(x_1, x_2) = x_1^2 + 2x_1x_2^2 - x_1x_2$$

In searching for the minimum, perform 3 iterations using the following combination of search techniques:

Iteration 1: use Steepest Descent search
Iteration 2: use a search direction which is conjugate to the search direction in Iteration 1
Iteration 3: use Newton's method

Use an initial guess of $x_1 = 2$ and $x_2 = 1$. In Iteration 1 and 2, you must carry out a line search (i.e. minimize the step size $\lambda$ completely), and in each iteration use the solution from the previous iteration as the starting point. Calculate and report the value of $f(x)$ in each iteration as well.


## 42. *Profit Maximization in a Chemical Process as an LP*

(a) A chemical company makes two products, Product A and Product B, which sell for a profit of $3,000 per unit and $3,200 per unit, respectively. It takes 32 minutes to produce Product A and 40 minutes to produce Product B. The total production time of each day

is 660 minutes. To stay in business, the company must produce at least 5 units of Product B but no more than 14 units per day. At the same time, the market demand dictates that the company should not produce more than a combined total of 20 units of Product A and Product B. Finally, the machinery used in producing Product A and Product B requires that both products must be produced in multiples of 5 units. Formulate this problem as an ILP (because the number of product units must be a whole number) and solve for the maximum profit per day by graphical method.

(b) A chemical company produces 2 kinds of product, namely Saccharin and Nutrasweet which are sugar substitutes because of their extreme sweetness. Saccharin generates a profit of $4100 per batch, requires 4 hours of production per batch in Plant 1 and 2 hours per batch in Plant 2. Nutrasweet has a profit contribution of $5900 per batch, requires 2 hours per batch in Plant 1 and 3 hours per batch in Plant 2 to produce. The available time in one production cycle in Plant 1 and Plant 2 are 160 hours and 180 hours, respectively. Each hour used in Plant 1 costs $90, while each hour spent in Plant 2 costs $60. Formulate the problem as an LP in order to maximize the profit in one production cycle. Solve the LP problem graphically. Solve the same problem again using the Simplex algorithm.

## 43. *Formulation of an LP Problem*

Anti-H5N1 Inc. is a pharmaceutical company specialized in producing an expensive vaccine to inoculate humans against the avian flu. The vaccines come in two varieties, one for immunization against Strain A (called AFVAX-A) and one against Strain B (called AFVAX-B). A facility is used to produce both AFVAX-A and AFVAX-B. Because of the high demands for its products, the company must produce a total of at least 14 batches in one production cycle, of which at least 3 batches must be AFVAX-A and at least 2 batches must be AFVAX-B. It takes 8.0 hours to produce one batch of the Strain-A vaccine and 6.25 hours to produce one batch of the Strain-B vaccine. A maximum of 100 operation hours is available at the facility in one production cycle. The net profit for the Strain-A vaccine is $25,000 per batch, while that of the Strain-B is $19,800 per batch.

Anti-H5N1 Inc. wants to know how much of AFVAX-A and AFVAX-B they must produce in one production cycle in order to achieve the highest possible profit.

(a) Formulate an LP model for this problem. Treat all variables as continuous and use the graphical method to solve this model.

(b) Now treat the model as an ILP problem, i.e. the number of batches must be an integer. Use the graphical method again to solve for the optimum. You must show all your work to get full credit.

## 44. *Optimal Manufacturing of Candies*

A confectioner manufactures 2 kinds of candy bars: Ergies (packed with energy for kiddies) and Nergies (the "low-calorie" nugget for weight watchers without will power). Ergies sell at a profit of 50 cents per box while Nergies have a profit of 60 cents per box. The candy is processed in 3 main operations: blending, cooking, and packaging. The following table records the average time in *minutes* required by each box of candy, for each of the three activities.

|          | Blending | Cooking | Packaging |
|----------|----------|---------|-----------|
| Ergies   | 1        | 5       | 3         |
| Nergies  | 2        | 4       | 1         |

During each production run, the blending equipment is available for a maximum of 14 machine hours, the cooking equipment for at most 40 machine hours, and the packaging equipment for at most 15 machine hours.

(a) If each machine can be allocated to the making of either type of candy at all times that it is available for production, determine how many boxes of each kind of candy the confectioner should make in order to realize the maximum profit. Formulate this optimization problem as a linear program and use a graphical technique to solve for the optimum. Also, compute the maximum profit in dollars (Note: 100 cents = 1 US dollar).

(b) The marketing department proposed that the confectioner add a third kind of candy bar named Munchies into the production line in order to try to make more profit. Munchies has a profit of 80 cents per box with the following operation times: blending time = 2 minutes, cooking time = 5 minutes, packing time = 2 minutes. Due to some adjustments in the production equipment required to accommodate the making of Munchies, the maximum hours available for the blending equipment is now reduced by 3 machine hours, the maximum for the cooking equipment is reduced by 2 machine hours, and the maximum for the packaging equipment is reduced by 2 machine hours.

As a ChEPS graduate working for the confectioner, do you agree with this proposal from marketing? Support the conclusion you make analytically (if you use linear programming to prove your answer, use the Simplex algorithm to solve the problem). There is no minimum number of boxes the confectioner is obligated to make for each kind of candy bars.

### 45. *Optimal Production of Two Chemicals as an LP Problem*

A chemical manufacturer plans to make two products $P$ and $Q$ by batch reaction. By varying reaction conditions and batch time, both products can be made from the same reactants $A$ and $B$ as follows:

<u>Reaction 1</u>:      0.5 kg $A$ + 0.6 kg $B$ → 1 kg $P$ + waste
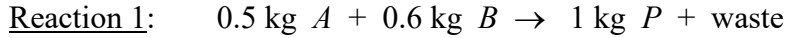
                     Required batch time (including time to charge and empty reactor) = 2.5 hours
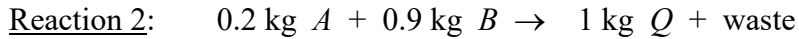
<u>Reaction 2</u>:      0.2 kg $A$ + 0.9 kg $B$ → 1 kg $Q$ + waste

                     Required batch time (including time to charge and empty reactor) = 5 hours

$P$ can be sold at a profit of $ 55/ton, and $Q$ at a profit of $ 80/ton. The company plans to use the same batch reactor to produce both products. So part of the time the reactor will be used to produce $P$ using reaction 1, and the remaining time the reactor will be used to produce $Q$ using reaction 2. In either case, each batch produces 0.5 ton of product $P$ or $Q$. The reactor operates 330 days/year for 24 hours/day. The company is able to purchase up to 600 tons/year of $A$ and up to 1000 tons/year of $B$. Additional supplies of $A$ and $B$ are not available.

(a) Assuming you want to maximize the total annual profit from selling $P$ and $Q$, formulate this problem as a linear programming (LP) problem.

(b) How much $P$ should you produce, and how much $Q$ should you produce? Use the Simplex algorithm to solve for the optimum.

### 46. *Formulation of an LP Problem*

A Thai shrimp company with a farming area of 10 rais wishes to optimize the growing of 3 kinds of shrimps, namely tiger shrimps, prawns, and rock shrimps. The company can sell tiger shrimps at 100 baht a kilogram, prawns at 160 baht a kilogram, and rock shrimps at 200 baht a kilogram. The average yield per rai is 1,500 kilograms of tiger shrimps, 1,000 kilograms of prawns, and 800 kilograms of rock shrimps. Labor required per rai during each harvest cycle is 3 man-days, 6 man-days, and 4 man-days for tiger shrimps, prawns, and rock shrimps, respectively. No more than 50 man-days are available during the harvest cycle, and each worker is paid 300 baht per man-day. Feed and other operating expenses cost 60 baht per kilogram, while feed requirements are: 300 kilograms per rai of tiger shrimps, 450 kilograms per rai of prawns, and 500 kilograms per rai of rock shrimps.

(a) Based on this information, formulate this problem as an LP model to determine the optimal usage of the farming area such that the profit in each harvest cycle is maximized.

(b) Carry out 1 iteration of Simplex to solve this LP model. Is the solution optimal after 1 iteration?

## 47. *Simplex Algorithm, I*

Consider the following LP minimization problem:

$$\text{Minimize} \quad f(x) = -2x_1 + x_2 - x_3$$

s.t.

$$
\begin{array}{lll}
x_1 + x_2 & \leq \quad 12 & (1) \\
-x_1 + 4x_2 - 2x_3 & \geq \quad -6 & (2) \\
2x_1 + x_2 - 2x_3 & = \quad 6 & (3) \\
x_1, x_2, x_3 \geq 0
\end{array}
$$

Solve the LP problem and find the minimum by starting Simplex with the feasible basic solution in which $x_2 = x_3 = 0$. You are <u>not</u> allowed to eliminate any variables and reduce the number of constraints when using Simplex.

## 48. *Simplex Algorithm, II*

Use the Simplex algorithm to solve for the optimum of the following LP:

$$\text{Minimize} \quad f(x) = x_1 + 2x_2 + 2x_3 - x_4$$

s.t.

$$
\begin{array}{lll}
x_1 + 2x_2 - 2x_3 & \geq \quad 0 & (1) \\
2x_1 - 4x_2 - x_3 + x_4 & \leq \quad 14 & (2) \\
-2x_1 + x_2 + 3x_3 - x_4 & \geq \quad -6 & (3) \\
x_1 + x_2 + x_3 + x_4 & = \quad 12 & (4)
\end{array}
$$

$$x_1, x_2, x_3, x_4 \geq 0$$

You are <u>not</u> allowed to eliminate any variables and thus reduce the number of constraints when using Simplex. A close inspection of the LP formulation shows that one feasible basic solution can be found by making $x_2$ and the slack/surplus variables of Constraint (1) and Constraint (3) non-basic variables. Start your Simplex with this basic solution.

## 49. *Simplex Algorithm, III*

Use the Simplex algorithm to solve for the optimum of the following LP:

$$\text{Maximize} \quad f(x) = x_1 - 2x_2 + 4x_3$$

s.t.

$$
\begin{array}{ll}
2x_1 + x_2 - x_3 & \geq \quad 6 \\
x_1 + x_2 + x_3 & \leq \quad 20 \\
x_2 + x_3 & \geq \quad 8
\end{array}
$$

$$x_1 \geq 0, x_2 \text{ is unrestricted}, x_3 \geq 0$$

You are <u>not</u> allowed to eliminate any constraint when using Simplex.

## 50. *Steel Blending Problem*

The Pittsburgh Steel (PS) Co. has been contracted to produce a new type of steel which has the following tight quality requirements:

| Content | At Least | Not More Than |
|---------|----------|---------------|
| Carbon | 3.00% | 3.50% |
| Chrome | 0.30% | 0.45% |
| Manganese | 1.35% | 1.65% |
| Silicon | 2.70% | 3.00% |

PS has the following materials available for mixing up a batch:

| | Cost/lb. | Percent Carbon | Percent Chrome | Percent Manganese | Percent Silicon | Amount Available |
|---|----------|----------------|----------------|-------------------|-----------------|------------------|
| Pig Iron 1 | 0.03 | 4.0 | 0 | 0.9 | 2.25 | Unlimited |
| Pig Iron 2 | 0.0645 | 0 | 10.0 | 4.5 | 15.0 | Unlimited |
| Ferro-Silicon 1 | 0.065 | 0 | 0 | 0 | 45.0 | Unlimited |
| Ferro-Silicon 2 | 0.061 | 0 | 0 | 0 | 42.0 | Unlimited |
| Alloy 1 | 0.10 | 0 | 0 | 60.0 | 18.0 | Unlimited |
| Alloy 2 | 0.13 | 0 | 20.0 | 9.0 | 30.0 | Unlimited |
| Alloy 3 | 0.119 | 0 | 8.0 | 33.0 | 25.0 | Unlimited |
| Carbide | 0.08 | 15.0 | 0 | 0 | 30.0 | Unlimited |
| Steel 1 | 0.021 | 0.4 | 0 | 0.9 | 0 | 200 lb. |
| Steel 2 | 0.02 | 0.1 | | 0 | 0.3 | 0  200 lb. |
| Steel 3 | 0.0195 | 0.1 | 0 | 0.3 | 0 | 200 lb. |

A one-ton (2000 lb.) batch must be blended which satisfies the quality requirements stated earlier. The problem now is what amounts of each of the eleven materials should be blended together so as to minimize the cost but satisfy the quality requirements. An experienced steel man claims that the least cost mix will not use more than nine of the eleven raw materials. Formulate this problem as an LP problem. To verify the steel man's claim, use LINDO to solve for the optimum. Is the steel man's claim correct or wrong?

### 51. *Reclaiming Solid Wastes*

The SAVE-IT COMPANY operates a reclamation center that collects four types of solid waste materials and treats them so that they can be amalgamated into a salable product (Treating and amalgamating are separate processes.) Three different grades of this product can be made (see the first column of Table 1), depending upon the mix of the materials used. Although there is some flexibility in the mix for each grade, quality standards may specify the minimum or maximum amount allowed for the proportion of a material in the product grade. (This proportion is the weight of the material expressed as a percentage of the total weight for the product grade.) For each of the two higher grades, a fixed percentage is specified for one of the materials. These specifications are given in Table 1 along with the cost of amalgamation and the selling price for each grade.

The reclamation center collects its solid waste materials from regular sources and so is normally able to maintain a steady rate for treating them. Table 2 gives the quantities available for collection and treatment each week, as well as the cost of treatment, for each type of material.

The Save-It Co. is solely owned by Green Earth, an organization devoted to dealing with environmental issues, so Save-It's profits are used to help support Green Earth's activities. Green Earth has raised contributions and grants, amounting to $30,000 per week, to be used exclusively to cover the entire treatment cost for the solid waste materials. The board of directors of Green Earth has instructed the management of Save-It to divide this money among the materials in such a way that *at least half* of the amount available of each material is actually collected and treated. These additional restrictions are listed in Table 2.

Within the restrictions specified in Tables 1 and 2, management wants to determine the *amount* of each product grade to produce *and* the exact *mix* of materials to be used for each grade. The objective is to maximize the net weekly profit (total sales income *minus* total amalgamation cost), exclusive of the fixed treatment cost of $30,000 per week that is being covered by gifts and grants. Formulate this problem as an LP and solve it using LINDO.

**Table 1: Product data for Save-It Co.**

| Grade | Specification<br>Cost per Pound ($) | Amalgamation<br>per Pound ($) | Selling Price |
|---|---|---|---|
| A | Material 1: Not more than 30% of total<br>Material 2: Not less than 40% of total<br>Material 3: Not more than 50% of total<br>Material 4: Exactly 20% of total | 3.00 | 8.50 |
| B | Material 1: Not more than 50% of total<br>Material 2: Not less than 10% of total<br>Material 4: Exactly 10% of total | 2.50 | 7.00 |
| C | Material 1: Not more than 70% of total | 2.00 | 5.50 |

**Table 2: Solid waste materials data for Save-It Co.**

| Material | Pounds per Week Available | Treatment Cost per Pound ($) | Additional Restrictions |
|---|---|---|---|
| 1 | 3,000 | 3.00 | 1. For each material, at least half of the |
| 2 | 2,000 | 6.00 | pounds per week available should be |
| 3 | 4,000 | 4.00 | collected and treated. |
| 4 | 1,000 | 5.00 | 2. $30,000 per week should be used to |
|   |   |   | treat these materials. |

## 52. *The Method of Lagrange Multipliers, I*

Use the method of Lagrange Multiplier to solve for <u>all</u> stationary points of the following constrained optimization problem:

$$f(x) = x_1^2 x_2 - x_1 x_2 + 3x_2$$

$$s.t. \quad x_1 x_2 \leq 10$$

$$x_1 + x_2 = 4$$

You need <u>not</u> characterize the stationary points, but do compute the objective function value of each stationary point and their Langrage multipliers.

## 53. *The Method of Lagrange Multipliers, II*

Consider the following nonlinear constrained optimization problem:

$$\text{Minimize} \quad f(x) = x_1^2 + 2x_1 x_2 + (x_2 - 1)^2$$

$$\text{subject to} \quad g(x) = x_1^2 + x_2^2 - 9 \quad \leq \quad 0$$
$$h(x) = x_1 + 2x_2^2 \quad = \quad 10$$

Use the Method of Lagrange Multipliers to find all the stationary points. For each stationary point you find, be sure to calculate the values of the Lagrange Multipliers as well as the values of $f(x)$. You do not need to classify each stationary point.

## 54. *The Method of Lagrange Multipliers, III*

Use the method of Lagrange Multiplier to solve for <u>all</u> stationary points of the following constrained optimization problem:

$$f(x) = x_1 x_2$$

$$s.t. \quad x_1 + 2x_2 \leq 2$$

$$2x_1^2 - x_2 = 6$$

You need <u>not</u> characterize the stationary points, but do compute the objective function value of each stationary point and their Langrage multipliers.

### 55. *Method of Lagrange Multipliers and fmincon, I*

(a) Find all the stationary points of the following constrained NLP by the method of Lagrange Multiplier. You must calculate the values of all variables in the Lagrangian $L$, including the values of the objective function and the multipliers. But do not classify each stationary point.

$$f(x_1, x_2) = x_1 x_2^2$$

$$\text{s.t.} \quad x_1 + 2x_2 = 10$$

$$x_1^2 + x_2^2 \leq 25$$

(b) Write down the MATLAB syntax (input commands and M-files) and use *fmincon* to solve the following constrained NLP problem:

$$\text{Maximize } f(x) = 3x_1 \exp(-0.1x_1 x_6) + 4x_2 + x_3^2 + 7x_4 + \frac{10}{x_5} + x_6$$

s.t.

| | |
|---|---|
| $x_2 x_6 = 5$ | (Constraint 1) |
| $x_1 + x_2 + x_3 + x_4 + x_5 + x_6 = 10$ | (Constraint 2) |
| $2x_1 + x_2 + x_3 + 3x_4 \geq 2$ | (Constraint 3) |
| $\dfrac{x_1}{x_2} + x_3^2 x_4^3 = 1$ | (Constraint 4) |
| $-8x_1 - 3x_2 - 4x_3 + x_4 - x_5 + x_6 \geq -10$ | (Constraint 5) |
| $-2x_1 - 6x_2 - x_3 - 3x_4 - x_6 \geq -13$ | (Constraint 6) |
| $-x_1 - 4x_2 - 5x_3 - 2x_4 \geq -18$ | (Constraint 7) |
| $\sqrt{x_5} + x_6 \leq 6$ | (Constraint 8) |
| $-20 \leq x_i \leq 20 \quad i = 1, \ldots, 6$ | |

Use an initial guess of $x_i = 1.0$, $i = 1, \ldots, 6$. The solution from MATLAB is $x_1 = 1.4158$, $x_2 = 1.5583$, $x_3 = -3.0346$, $x_4 = 0.2149$, $x_5 = 6.6369$, and $x_6 = 3.2087$ with $f(x) = 24.3585$. Which inequality constraint(s) is/are active (identify by constraint number)? Be sure to write neatly and pay attention to details such as semicolons, periods, etc., since the syntax must be precise.

### 56. *Method of Lagrange Multipliers and fmincon, II*

(a) Use the method of Lagrange multipliers to determine the stationary points of the following nonlinear constrained problem. There is no need to classify the calculated

stationary points as maximum, minimum, or saddle point, but you must calculate the values of the Lagrange multiplier and the objective function of each stationary point.

$$\text{Minimize} \quad f(x, y) = xy^2$$

$$\text{s.t.} \quad x^2 - y^2 \leq 16$$

$$x - y \quad = \quad 3$$

(b) Write down the MATLAB syntax (input commands and M-files) and use *fmincon* to solve the following constrained NLP problem:

$$\text{Maximize } f(x) = 3x_1 \exp(-0.1x_1x_6) + 4x_2 + x_3^2 + 7x_4 + \frac{10}{x_5} + x_6$$

s.t.

| | |
|---|---|
| $x_2 x_6 = 5$ | (Constraint 1) |
| $x_1 + x_2 + x_3 + x_4 + x_5 + x_6 = 10$ | (Constraint 2) |
| $2x_1 + x_2 + x_3 + 3x_4 \geq 2$ | (Constraint 3) |
| $\dfrac{x_1}{x_2} + x_3^2 x_4^3 = 1$ | (Constraint 4) |
| $-8x_1 - 3x_2 - 4x_3 + x_4 - x_5 + x_6 \geq -10$ | (Constraint 5) |
| $-2x_1 - 6x_2 - x_3 - 3x_4 - x_6 \geq -13$ | (Constraint 6) |
| $-x_1 - 4x_2 - 5x_3 - 2x_4 \geq -18$ | (Constraint 7) |
| $\sqrt{x_5} + x_6 \leq 6$ | (Constraint 8) |
| $-20 \leq x_i \leq 20 \quad i = 1, ...., 6$ | |

Use an initial guess of $x_i = 1.0$, $i = 1, ...., 6$. The solution from MATLAB is $x_1 = 1.4158$, $x_2 = 1.5583$, $x_3 = -3.0346$, $x_4 = 0.2149$, $x_5 = 6.6369$, and $x_6 = 3.2087$ with $f(x) = 24.3585$. Which inequality constraint(s) is/are active (identify by constraint number)? Be sure to write neatly and pay attention to details such as semicolons, periods, etc., since the syntax must be precise.

## 57. *Using fmincon to Solve 3 NLPs*
(a) Westerberg and Shah (1978) in Swaney (1990) studied the following NLP problem:

$$\text{Min} \quad 35x_1^{0.6} + 35x_2^{0.6}$$
$$\text{s.t.} \quad 600x_1 - 50x_3 - x_1x_3 + 5000 = 0$$
$$600x_2 + 50x_3 - 15000 = 0$$
$$(0, 0, 100) \leq x \leq (34, 17, 300)$$

in which one local optimum ($f(x) = 286.943$) and the global optimum ($f(x) = 189.311627$) were reported by Ryoo and Sahinidis (1995). Use *fmincon* to find both solutions.

(b) Stoecker (1971) in Liebman *et al.* (1986) studied the following insulated steel tank design NLP problem:

$$\text{Min} \quad 400x_1^{0.9} + 1000 + 22(x_2 - 14.7)^{1.2} + x_4$$
$$\text{s.t.} \quad x_2 = \exp[-3950/(x_3 + 460) + 11.86]$$
$$144(80 - x_3) = x_1 x_4$$
$$(0, 14.7, -459.67, 0) \leq \boldsymbol{x} \leq (15.1, 94.2, 80, \infty)$$

in which the global optimum ($f(x) = 5194.866243$) was reported by Ryoo and Sahinidis (1995). Use *fmincon* to find the global optimum.

(c) Stephanopoulos and Westerberg (1975) studied the following NLP problem of a design of three-stage process system with recycle.

$$\text{Min} \quad x_1^{0.6} + x_2^{0.6} + x_3^{0.4} - 4x_3 + 2x_4 + 5x_5 - x_6$$

$$\text{s.t.} \quad -3x_1 + x_2 - 3x_4 = 0$$
$$-2x_2 + x_3 - 2x_5 = 0$$
$$4x_4 - x_6 = 0$$
$$x_1 + 2x_4 \leq 4$$
$$x_2 + x_5 \leq 4$$
$$x_3 + x_6 \leq 6$$
$$(0, 0, 0, 0, 0, 0) \leq x \leq (3, 4, 4, 2, 2, 6)$$

in which the global optimum ($f(x) = -13.401904$) was reported by Ryoo and Sahinidis (1995). Use both the interior-reflective Newton method and the SQP method in *fmincon* to find the global optimum.
**Hint**: You may need to try different starting points to find the solutions.


## 58. *Using fmincon in MATLAB, II*
Write down the MATLAB syntax (input commands and M-files) using *fmincon* to solve the following constrained NLP problem:

$$\text{Maximize} \;\; f(\boldsymbol{x}) = x_3 \sin(x_1 x_2) - x_3 x_4 + x_4^3 + \frac{4}{x_1} - 2\ln(x_1 x_4)$$

s.t.

| | |
|---|---|
| $2x_1 - 2x_2 + x_3 - 4x_4 = -10$ | (Constraint 1) |
| $\sqrt{2x_1} - \dfrac{x_3}{x_2} + \exp(-x_4) \geq 2$ | (Constraint 2) |
| $x_1 + 2x_2 - x_4 \geq 0$ | (Constraint 3) |

$$\frac{x_1}{x_2} + 8.28 \times 10^{-4} x_3 + x_4 = 3 \qquad \text{(Constraint 4)}$$

$$2x_1 + 8x_2 + x_3 + 4x_4 \leq 100 \qquad \text{(Constraint 5)}$$

$$x_2 + 0.0693 \exp\left(\frac{x_2 x_4}{x_3}\right) = -14 \qquad \text{(Constraint 6)}$$

$$x_1 x_2 x_4 - 30 x_3 \leq 40 \qquad \text{(Constraint 7)}$$

$$3x_1 + x_3 + 6x_4 = 50 \qquad \text{(Constraint 8)}$$

$$-100 \leq x_i \leq 100 \qquad i = 1, \ldots, 4$$

Use an initial guess of $x_i = 2$, $i = 1, \ldots, 4$. The solution from MATLAB is $x_1 = 33.8022$, $x_2 = -14.1737$, $x_3 = -84.1338$, and $x_4 = 5.4545$ with $f(x) = 695.0049$. Which inequality constraint(s) is/are active (identify by constraint number)? Be sure to write neatly and pay attention to details such as semicolons, periods, etc., since the syntax must be precise.

### 59. *Formulation and Solving an ILP Problem*

Three high-value chemical products, $A$, $B$, and $C$ are to be produced from two raw materials, namely RawMat 1 and RawMat 2. The production of 1 batch of $A$ requires 4 kg of RawMat 1 and 2.5 kg RawMat 2 and 3.5 hours of labor. On the other hand, the production of 1 batch of $B$ requires 1 kg of RawMat 1 and 3.5 kg of RawMat 2 and 2 hours of labor. Finally, the production of 1 batch of $C$ requires 8.5 kg of RawMat 1 and 4 kg of RawMat 2 and 5 hours of labor.

In terms of resource capacities for one week of production, 1,000 kg of RawMat 1 and 1,200 kg of RawMat 2 are available, while 20 employees each working 40 hours are used.

The following marketing data are available:

|  | Profit/batch (\$) | Demand/week |
|---|---|---|
| Product $A$ | 10.00 | 40 batches |
| Product $B$ | 5.00 | 100 batches |
| Product $C$ | 15.00 | 30 batches |

(a) Formulate this optimization problem in which the goal is to determine the number of batches products $A$, $B$, and $C$ are to be produced in a week so as to maximize the total profit. Also, classify the problem. Note that a partial batch cannot be produced.

(b) Solve the ILP problem using LINDO.

## 60. *Integer Linear Programming*
Solve the following problems via the branch and bound method. You may use LINDO to solve each LP sub-problem (node).

(a)      Maximize $f(x) = 75x_1 + 6x_2 + 3x_3 + 33x_4$

Subject to   $774x_1 + 76x_2 + 22x_3 + 42x_4 \leq 875$
$67x_1 + 27x_2 + 794x_3 + 53x_4 \leq 875$
$x_1, x_2, x_3, x_4$ either 0 or 1

(b)      Maximize $f(x) = 2x_1 + x_2$

Subject to   $x_1 + x_2 \leq 5$
$x_1 - x_2 \geq 0$
$6x_1 + 2x_2 \leq 21$
$x_1, x_2 \geq 0$ and integer

## 61. *Using LINDO to Solve Scheduling Problems*
Consider the following 8-product, 3-unit multistage scheduling problem with unlimited intermediate storage:

| | | | | Processing Times (in minutes) | | | | |
|---|---|---|---|---|---|---|---|---|
| **Product** | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| **Unit 1** | 20 | 12 | 30 | 45 | 60 | 20 | 15 | 25 |
| **Unit 2** | 55 | 30 | 50 | 40 | 30 | 20 | 25 | 32 |
| **Unit 3** | 15 | 20 | 38 | 25 | 51 | 14 | 26 | 33 |

Use LINDO to solve for the optimal schedule with the shortest makespan.

## 62. *Completion Time Calculations and UIS Makespan Minimization*
Consider a 4-stage multiproduct plant with 4 products. The processing time matrix (in minutes) is given below.

| | | Products | | |
|---|---|---|---|---|
| Units | 1 | 2 | 3 | 4 |
| 1 | 5 | 1 | 2 | 2 |
| 2 | 10 | 3 | 18 | 2 |
| 3 | 10 | 3 | 10 | 25 |
| 4 | 32 | 10 | 5 | 15 |

(a) Assuming the production sequence to be 1-2-3-4 on all four processing units, use Gantt charts to calculate a complete schedule and the makespan for the following cases:

i) UIS policy
ii) NIS policy
iii) ZW policy
iv) MIS policy with ZW between units 1 and 2, NIS between units 2-3, and FIS with one storage unit between units 3 and 4.

 (b) For the UIS policy, formulate the problem as an MILP, and use LINDO to solve for an optimal schedule that minimizes the makespan.

### 63. *UIS Scheduling with Makespan Minimization*
Consider the makespan minimization of a 5-product, 3-unit UIS multiproduct plant with unlimited intermediate storage and the following processing time matrix (in minutes):

| Units | Products | | | | |
|---|---|---|---|---|---|
|  | 1 | 2 | 3 | 4 | 5 |
| 1 | 15 | 10 | 10 | 5 | 8 |
| 2 | 8 | 20 | 15 | 15 | 14 |
| 3 | 5 | 12 | 16 | 9 | 18 |

(a) Write a MATLAB code to use brute force (i.e. examine every possible solution) to find a schedule that minimizes the makespan.

(b) Formulate the problem as an MILP, and use LINDO to solve for an optimal schedule in Part (a)

### 64. *Optimal Scheduling of Products in a Serial Batch Process*
An important optimization problem that arises in a batch chemical plant (or non-continuous processes) is the scheduling problem. Short-term scheduling involves sequencing and scheduling the production of $N$ products across $M$ processing units to optimize a suitable performance or cost-based criterion (Ku *et al.* 1987).

Consider the following serial batch process which consists of 2 batch reactors followed by a centrifuge and a tray dryer. The process is to



Products
*A*, *B*, *C*, *D*,
*E*, and *F*

Reactor    Reactor    Centrifuge    Tray Dryer
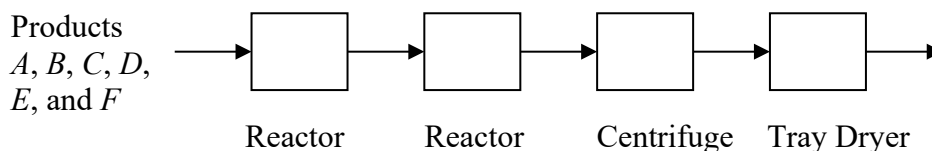
manufacture 6 products, namely *A*, *B*, *C*, *D*, *E*, and *F*. All products must follow the same production sequence, i.e. they must first pass through the first reactor, followed by the second, then onto the centrifuge and finally the tray dryer. The processing time of each product required in each processing unit is given in the table below. Each product also has a delivery due date after which a penalty would be incurred.

An effective heuristic (method yielding an approximate and not necessarily optimal solution) called Duedate-Over-Penalty or DOP algorithm [Ku, H.M., and Karimi, I.A., "Scheduling in Serial Multiproduct Batch Processes with Due Date Penalties", **Ind. Eng. Chem. Res., 29**, 4, 580, (1990)] has been proposed to solve the due-date scheduling problem as follows:

1. Compute $d_i/p_i$, $i = 1, N$.

2. Sequence products in the ascending order of $d_i/p_i$.

3. Compute the completion times and the total penalty cost $P$ for the above sequence.

Solve the problem using the DOP algorithm, and compare the solution you obtain with the brute force approach (i.e. examining every possible solution) using MATLAB. Assume that there is unlimited intermediate storage (UIS policy) available to store intermediate products between every 2 stages.

| Batch Unit | Processing Times (Hours) | | | | | |
|---|---|---|---|---|---|---|
| | *A* | *B* | *C* | *D* | *E* | *F* |
| Reactor 1 | 5 | 35 | 10 | 40 | 25 | 45 |
| Reactor 2 | 15 | 20 | 30 | 18 | 32 | 7 |
| Centrifuge | 10 | 15 | 30 | 12 | 16 | 22 |
| Tray Dryer | 8 | 10 | 20 | 10 | 28 | 38 |
| Due Date, $d_i$ (Days) | 1.5 | 4.0 | 2.5 | 5.0 | 3.0 | 6.0 |
| Penalty, $p_i$ ($/Hour) | 500 | 400 | 600 | 800 | 300 | 200 |

## 65. *Optimal Scheduling of Products in a Serial Batch Process with FIS Policy*

Now, consider another batch process with only 2 processing stages as shown:

Products
*P*1, *P*2, *P*3,
*P*4, and *P*5

Reactor    Storage    Stripper
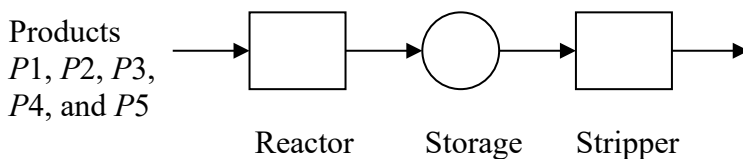
This 2-unit serial system operates under the Finite Intermediate Storage policy (FIS) with one storage vessel, and is used to produce 5 products, namely *P*1, *P*2, *P*3, *P*4, and *P*5. The processing time matrix for this system is given below.

| Batch Unit | Processing Times (Minutes) | | | | |
|---|---|---|---|---|---|
| | *P*1 | *P*2 | *P*3 | *P*4 | *P*5 |
| Reactor | 10 | 6 | 2 | 4 | 15 |
| Stripper | 9 | 5 | 14 | 8 | 20 |

For the FIS policy, the following recurrence relations were developed by Ku (1984) to compute the completion time of each product on each processing unit for a given production sequence: $k_1$ - $k_2$ - $k_3$ - … - $k_N$   where product $k_i$ is in the ith position in the production sequence:

$$C_{ij} \quad = \quad \text{Max} \left[ \, C_{(i-1)j} \, , \, C_{i(j-1)} \, , \, C_{(i-1-z)(j+1)} - t_{kj} \, \right] \, + \, t_{kj} \qquad \begin{array}{l} i = 1, \, …, \, N \\ j = 1, \, …, \, M \end{array}$$

$$C_{ij} \quad = \quad 0 \quad \text{if } \; i \leq 0 \; \text{ or } \; j \leq 0$$

where   $C_{ij}$   = completion time of the ith product on the jth processing unit
         = the time at which the ith product leaves unit $j$
$t_{kj}$   = processing time of product $k_i$ on unit $j$
$z_j$   = number of storage units available in the FIS policy between unit $j$ and unit ($j$+1)

Formulate this FIS scheduling problem as an MILP model and determine an optimal production sequence that minimizes the makespan in the production of the 5 products. Also, use MATLAB to implement the brute force approach by examining every possible solution in order to find the same optimal schedule solved in the MILP model.


## 66. *A Two-Machine Scheduling Problem under UIS and FIS Storage Policies*

Consider a two-machine scheduling problem of 6 products as shown with the following processing time matrix:
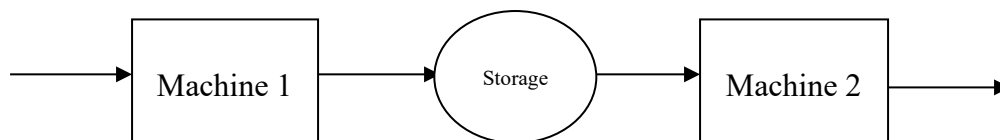
|  |  | Processing Times $t_{ij}$ Machine | |
|  |  | 1 | 2 |
| --- | --- | --- | --- |
| Product | A | 50 | 10 |
|  | B | 10 | 15 |
|  | C | 15 | 30 |
|  | D | 26 | 5 |
|  | E | 6 | 20 |
|  | F | 8 | 26 |

(a) A simple optimization algorithm called Johnson's Rule (March, 1954) exists that gives an optimal sequence with the minimum makespan when there is unlimited intermediate storage (UIS operating policy). The Rule can be stated as follows:

1. Create a list $P$ containing products whose $t_{i1} \leq t_{i2}$ and are arranged in the increasing value of their $t_{i1}$.
2. Create a second list $Q$ containing products whose $t_{i1} > t_{i2}$ and are arranged in the decreasing value of their $t_{i2}$.
3. Concatenate $P$ and $Q$, i.e. combine them so that the optimal sequence is $P \cup Q$.

Use Johnson's Rule to determine the sequence with the minimum makespan in this scheduling problem. Also, calculate this minimum makespan.

(b) Write out the complete formulation for this UIS scheduling problem. In your formulation, you must first define all the variables, and then state the objective function and all the constraints term by term. Do not use any summation sign to show your objective function or constraints. Processing times should also be written down as numbers, not as symbols, in the formulation. Finally, use LINDO to obtain the optimal schedule which should give the same answer as in Part (a).

(c) When the storage operating policy is FIS (finite intermediate storage), the completion time of a product in position $i$ from machine $j$ is given as (Ku and Karimi, 1988):

$$C_{ij} = \max(C_{(i-1)j}, C_{i(j-1)}, C_{(i-z-1)(j+1)} - t_{ij}) + t_{ij}$$

where $z$ = the number of storage vessels, e.g $z = 0$ if there is no storage and $z = \infty$ if there is unlimited intermediate storage. Using the optimal sequence under UIS obtained in Part (a), calculate its makespan when $z = 1$. Note that this sequence is not necessarily an optimal one under the FIS policy.