Pan American Advanced Studies Institute
Program on Process Systems Engineering
Nonlinear Programming and Dynamic Optimization
Exam Questions

1. Consider the NLP:

$$\begin{aligned} & \textit{Min}\ (x_2)^2 \\ s.t.\quad & x_1 - x_2 + 1 \le 0 \\ & -x_1 - x_2 + 1 \le 0 \end{aligned}$$

   a) Write the KKT conditions for this problem and solve them.

KKT Conditions

$$u_1 - u_2 = 0$$
$$2x_2 - u_1 - u_2 = 0$$
$$u_1 \ge 0, u_2 \ge 0$$
$$x_1 - x_2 + 1 \le 0 \qquad -x_1 - x_2 + 1 \le 0$$
$$u_1(x_1 - x_2 + 1) = 0 \quad u_2(-x_1 - x_2 + 1) = 0$$

Adding the two constraints leads to $x_2 \ge 1$ and from first two equations we know that $u_1+u_2>0$ and $u_1 = u_2$. This means that both inequality constraints are active and we can solve for $x_1 = 0$, $x_2 = 1$, $u_1=u_2=1$.

   b) Identify the basic and nonbasic variables. How many superbasic variables are there? Are the sufficient second order KKT conditions satisfied?

If we added slack variables to the inequality constraints, these would be set to zero and they would be classified as nonbasic variables. Since x_1 and x_2 are solved by the equality constraints, they are basic variables. There are no superbasic variables, hence no constrained directions for the second order conditions. As a result, the sufficient second order conditions are vacuously satisfied.

   c) Solve this problem with a barrier method. Quantitatively describe the trajectory of $x(\mu)$ and $f(x(\mu))$ as $\mu \rightarrow 0$.

The barrier problem can be written as:

$$Min\ x_2^2 - \mu(\ln(x_2 - x_1 - 1) + \ln(x_1 + x_2 - 1))$$

Differentiating leads to the following equations:

$$\frac{\mu}{x_2 - x_1 - 1} - \frac{\mu}{x_2 + x_1 - 1} = \frac{2\mu x_1}{(x_2 + x_1 - 1)(x_2 - x_1 - 1)} = 0 \Rightarrow x_1 = 0$$

$$2x_2 - \frac{\mu}{x_2 - x_1 - 1} - \frac{\mu}{x_2 + x_1 - 1} = 2x_2 - \frac{2\mu}{(x_2 - 1)} = 0 \text{ (with } x_1 = 0)$$

Solving these equations gives

$$x_2^2 - x_2 - \mu = 0 \Rightarrow x_2 = 1/2(1 + (1 + 4\mu)^{1/2})$$

$$f(x) = x_2^2 = 1/2(1 + 2\mu + (1 + 4\mu)^{1/2})$$

2. Using the coordinate basis, apply range and null space decomposition and solve for the linear system:

$$\begin{bmatrix} W & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} d \\ \lambda \end{bmatrix} = -\begin{bmatrix} \nabla f \\ c \end{bmatrix} \quad with\ W = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad A = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \quad \nabla f = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad c = [2]$$

Solution:

$$Z = \begin{bmatrix} -C^{-1}N \\ I \end{bmatrix} = \begin{bmatrix} -2 \\ 1 \end{bmatrix},\ Y = \begin{bmatrix} 1 \\ 0 \end{bmatrix},\ A^T Y = 1,\ Z^T WZ = 3,\ Z^T WY = -2,\ Y^T WY = 1$$

$$A^T Y d_Y = -c \Rightarrow d_Y = -2$$

$$Z^T WY d_Y + Z^T WZ d_Z = -Z^T \nabla f = 4 + 3d_Z = 2 \Rightarrow d_Z = -2/3$$

$$Y^T WY d_Y + Y^T WZ d_Z + Y^T A\lambda = -Y^T \nabla f = -2 + 4/3 + \lambda = -1 \Rightarrow \lambda = -1/3$$

$$d = Zd_Z + Yd_Y = \begin{bmatrix} -2/3 \\ -2/3 \end{bmatrix}$$

3. Consider the reactor optimal control problem below. Assume that temperature is a function of time.

$$Max\ c_2(1.0)$$

s.t. $dc_1/dt = -\ k_1(T)\ c_1^2,\ c_1(0) = 1$

$dc_2/dt = k_1(T)\ c_1^2 - k_2(T)\ c_2,\ c_2(0) = 1$

where $k_1 = 4000 \exp(-2500/T)$, $k_2 = 62000 \exp(-5000/T)$ and $298 \le T(t) \le 398$.

a) Write the optimality conditions for this optimal control problem.

$$Define\ \ H = -\lambda_1 \mathrm{k}_1(\mathrm{T})\,\mathrm{c}_1^{\,2} + \lambda_2(\,\mathrm{k}_1(\mathrm{T})\,\mathrm{c}_1^{\,2}\ \text{-}\ \mathrm{k}_2(\mathrm{T})\,\mathrm{c}_2)$$

$$\frac{d\lambda_1}{dt} = 2k_1 c_1(\lambda_1 - \lambda_2),\ \lambda_1(1) = 0 \qquad \frac{d\lambda_2}{dt} = k_2\lambda_2,\ \lambda_2(1) = \text{-}1$$

$$(\lambda_2 - \lambda_1)k_1(T)\ c_1^{\,2}(2500/T^2)\ \text{-}\ \lambda_2 k_2(T)\ c_2(5000/T^2) = \alpha_- - \alpha_+$$

$$298 \le T \le 398, \quad \alpha_-(T-298) = 0, \quad \alpha_+(T-398) = 0, \quad \alpha_- \ge 0, \quad \alpha_+ \ge 0$$

$$dc_1/dt\ =\ \text{-}\ k_1(T)\ c_1^{\,2},\ c_1(0)\ =\ 1$$

$$dc_2/dt\ =\ k_1(T)\ c_1^{\,2}\ \text{-}\ k_2(T)\ c_2,\ c_2(0)\ =\ 1$$

b) Formulate this problem as an NLP using orthogonal collocation on finite elements. Choose two collocation points and 10 elements. Do not solve.

$Max\ c_{2f}$

$$\left.\begin{aligned} \sum_{j=0}^{2} c_{1,ij}\dot{\ell}_j(\tau_k)\ &=\ h(\text{-}\ k_1(T_{ik})\ c_{1,ik}^{\ \ 2}) \\ \sum_{j=0}^{2} c_{2,ij}\dot{\ell}_j(\tau_k)\ &=\ h(k_1(T_{ik})\ c_{1,ik}^{\ \ 2}\ \text{-}\ k_2(T_{ik})\ c_{2,ik}) \end{aligned}\right\} i = 1,...10; k = 1,...2, h = 0.1$$

$$\left.\sum_{j=0}^{2} c_{1,ij}\ell_j(1) = c_{1,i+1,0}, \quad \sum_{j=0}^{2} c_{2,ij}\ell_j(1) = c_{2,i+1,0}\right\} i = 1,...9$$

$$\sum_{j=0}^{2} c_{1,10j}\ell_j(1) = c_{1,f}, \quad \sum_{j=0}^{2} c_{2,10j}\ell_j(1) = c_{2,f}$$

$$c_{1,10}\ =\ 1, \quad c_{2,10}\ =\ 1, \quad \tau_0 = 0,\ \tau_1 = 0.2113, \tau_2 = 0.7887.$$

Part 1. Exam. Mixed-Integer Optimization

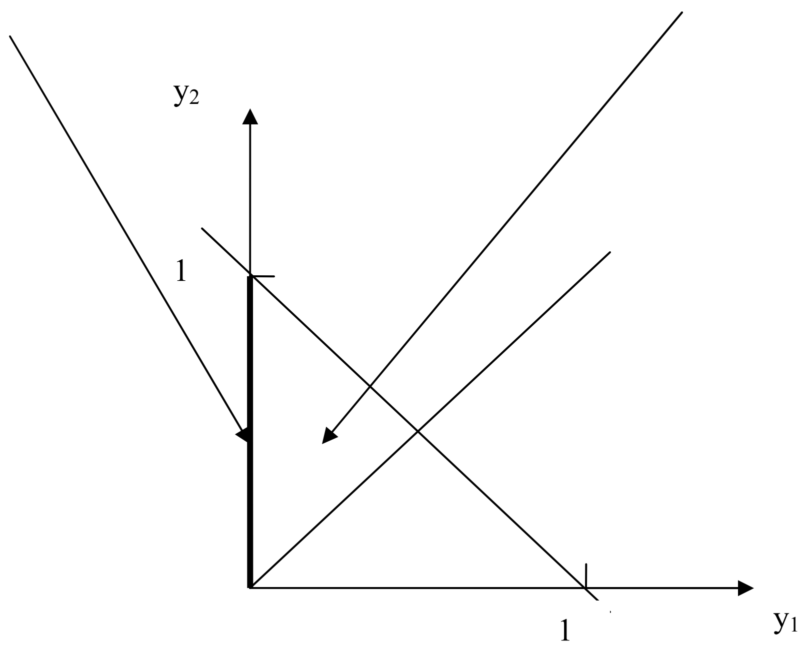
1. The logic condition $y_1 \Rightarrow y_2, \; \neg y_1 \vee \neg y_2$ can be represented with the constraints $y_1 = 0, y_2 = \delta, \delta = 0,1, \; 0 \le y_1, y_2 \le 1$. Is this a better, equal or worse model than using the following linear inequalities that are derived from CNF form,
$y_1 \le y_2, \; y_1 + y_2 \le 1, \; y_1, y_2 = 0,1$?

Assume the continuous relaxation of the CNF constraints, and that they are both active. That means, $y_1 = y_2, \; y_1 + y_2 = 1, \; \Rightarrow y_1 = y_2 = 0.5$

This in turn implies that this point $y_1 = y_2 = 0.5$ is infeasible for the relaxed logic condition $y_1 = 0, y_2 = \delta, \; 0 \le y_1, y_2, \; \delta \le 1$. This implies that the CNF constraints cannot be better than the original logic constraint.

To see how the feasible region of the relaxed logic constraint is included in the feasible region of the relaxation of the CNF constraints, plot the constraints in y_1, y_2 space.

$y_1 = 0, y_2 = \delta, \; 0 \le y_1, y_2, \; \delta \le 1$ $\qquad\qquad$ $y_1 \le y_2, \; y_1 + y_2 \le 1, \; 0 \le y_1, y_2 \le 1$



2. Formulate mixed-integer linear constraints for the following disjunction, using both big-M and convex-hull formulations:

Either $0 \le x \le 10$ or $20 \le x \le 30$

Solution:

a) Big-M

$0 \le x \le 10 + M(1-y_1)$

$-M(1-y_2) + 20 \le x \le 30$

$y_1 + y_2 = 1$

$y_1, y_2 = 0,1$

Note: Min value M = 20

b) Convex hull:

$x = u1 + u2$

$0 \le u1 \le 10y_1$

$20y_2 \le u2 \le 30y_2$

$y_1 + y_2 = 1$

$y_1, y_2 = 0,1$

3. Consider the mixed- integer linear programming problem

$$\begin{aligned} &\min Z = a^T x + b^T y \\ &s.t. \quad Ax + B y \leq d \\ &\quad\quad x \geq 0,\ y \in \{0,1\} \end{aligned}$$

Assume it is desired to solve this problem by Benders decomposition where the 0-1 variables are treated as "complicating" variables for the master problem. If the LP subproblems for fixed y^k, k=1, 2, . . . K are feasible with an optimal solution x^k and multipliers λ_k, show that the master problem can be formulated as follows:

$$\begin{aligned} &Z_L^K = \min \alpha \\ &st\ \ \alpha \geq b^T y + \lambda_k^T [By - d] \quad k = 1,2...K \\ &\quad \alpha \in R^1,\ \ y \in \{0,1\} \end{aligned}$$

<u>Solution:</u>

General form of Benders decomposition:

$$\begin{aligned} &\min \alpha \\ &st\ \ \alpha \geq c^T y + f(x^k) + (\lambda^k)^T [g(x^k) + By] \end{aligned} \quad (1)$$

For MILP problem, (1) leads to:

$$\begin{aligned} &\min \alpha \\ &st\ \ \alpha \geq b^T y + a^T x^k + (\lambda^k)^T [Ax^k + By - d] \end{aligned} \quad (2)$$

From KKT conditions for fixed y, defining Lagrangean,

$$L = b^T y + a^T x + (\lambda)^T [Ax + By - d]$$

It follows that applying stationary conditions,

$$a + A^T \lambda^k = 0 \Rightarrow a^T + (\lambda^k)^T A = 0 \Rightarrow [a^T + (\lambda^k)^T A] x^k = 0$$

Hence, (2) reduces to,

$$\begin{aligned} &Z_L^K = \min \alpha \\ &st\ \ \alpha \geq b^T y + \lambda_k^T [By - d] \quad k = 1,2...K \\ &\quad \alpha \in R^1,\ \ y \in \{0,1\} \end{aligned}$$

GLOBAL OPTIMIZATION EXAM SOLUTIONS FOR PASI COURSE

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Question 1. Find the generating sets for the convex and concave envelopes of the function $f = (x_1 x_2 + x_3 x_2)/y$ over $\{ 0 < x_i^L \le x_i \le x_i^U$ for $i = 1,\ldots,3,\ 0 < y^L \le y \le y^U \}$.

Solution

We will construct the generating set for the convex envelope. The construction of the generating set for the concave envelope follows similarly. Consider all variables fixed at some point between their bounds, except for variable x_k. Then *f* is linear, and therefore concave, in x_k. Hence, the interior of $[x_k^L, x_k^U]$ is irrelevant for the construction of the convex envelope of *f*. Now consider all *x* variables fixed at some combination of their bounds. Because *f* is then convex in y, the entire $[y^L, y^U]$ is needed to characterize the convex envelope of *f*. We conclude that the generating set of the convex envelope of *f* is:

$$G_f^{\text{epi}} = \{(x, y) \ \mid \ x_i \in \{x_i^L, x_i^U\}, i = 1,\ldots,3; \ \ y \in [y^L, y^U]\}.$$

Question 2. Find the generating sets for the convex and concave envelopes of the function $g = x/y + 3x + 4xy + 2xy^2$ over $\{ 0 < x^L \le x \le x^U,\ 0 < y^L \le y \le y^U \}$.

Solution

We will construct the generating set for the convex envelope. The construction of the generating set for the concave envelope follows with similar arguments. Let y be fixed in $[y^L, y^U]$. Then *g* is linear, and therefore concave, in x. Hence, the interior of $[x^L, x^U]$ is irrelevant for the construction of the convex envelope of *g*. Now consider x fixed at one of its bounds. Because *g* is then convex in y, the entire $[y^L, y^U]$ is needed to characterize the convex envelope of *g*. We conclude that the generating set of the convex envelope of *g* is $G_g^{\text{epi}} = \{(x, y) \ \mid \ x \in \{x^L, x^U\}, \ \ y \in [y^L, y^U]\}$.

Question 3. Consider the following pooling problem (Haverly, 1978):

$$\begin{aligned}
\min \quad & -9x_5 - 15x_9 + 6x_1 + 16x_2 + 10x_6 \\
\text{s.t.} \quad & x_1 + x_2 = x_3 + x_4 \\
& x_3 + x_7 = x_5 \\
& x_4 + x_8 = x_9 \\
& x_7 + x_8 = x_6 \\
& x_{10} x_3 + 2x_7 \le 2.5x_5 \\
& x_{10} x_4 + 2x_8 \le 1.5x_9 \\
& 3x_1 + x_2 = x_{10}(x_3 + x_4)
\end{aligned}$$

$$(0,0,0,0,0,0,0,0,0,1) \leq \mathbf{x} \leq (300,300,100,200,100,300,100,200,200,3)$$

(a) Solve this pooling problem by branch-and-bound manually:

- Disaggregate products and use the convex and concave envelopes of the bilinear terms to construct a relaxation.
- You may use GAMS/MINOS or GAMS/CPLEX or any other LP code to solve the relaxed problems.
- Use the best-bound node selection rule to select nodes.
- Use bisection of longest edge for branching but branch on the incumbent when possible.
- You may use GAMS/MINOS or your favorite local search every three branch-and-bound iterations using the corresponding relaxation point as the starting point.
- Terminate the search as soon as your lower and upper bounds are within 0.001.

(b) Solve the same model (after product disaggregation) with GAMS/BARON in two different ways:

1 Using default BARON settings.
2 Using BARON settings to apply the above algorithm (best-bound node selection, bisection of longest edge, branching on incumbent, local search every three branch-and-bound iterations, termination within an absolute gap of 0.001). *Hint:* If BARON outperforms your algorithm, it is because you need to change some of its default options.

Solution

(a) A GAMS file to solve the relaxations for part (a) is provided below. Using this relaxation, we obtain:

1 The root node lower bound is -500.
2 Local search at the root node gives -400 at point (0, 100, 0, 100, 0, 100, 0, 100, 200, 1).
3 Amongst the three nonconvex variables (x_3, x_4, and x_{10}), the longest edge rule selects x_4. Its range [0, 200] will be bisected to create two corresponding nodes. (Branching on the incumbent also branches at x_4=100.)
4 Both existing nodes have the same lower bound (-500). Arbitrarily, select the left child to solve. Its relaxation has an objective function value of -400. Thus, this node is fathomed.
5 The single remaining node is solved. Its relaxation also has an objective function value of -400. Thus, this node can also be eliminated.
6 The run terminates with a proof of global optimality of the incumbent.

```
variables x1, x2, x3, x4, x5, x6, x7, x8, x9, x10, intro_var1, intro_var2, relobj;

* intro_var1 = x10 * x3
* intro_var2 = x10 * x4
```

```
x1.lo = 0;
x2.lo = 0;
x3.lo = 0;
x4.lo = 0;
x5.lo = 0;
x6.lo = 0;
x7.lo = 0;
x8.lo = 0;
x9.lo = 0;
x10.lo = 1;

x1.up = 100;
x2.up = 150;
x3.up = 100;
x4.up = 200;
x5.up = 100;
x6.up = 250;
x7.up = 100;
x8.up = 150;
x9.up = 200;
x10.up = 3;

intro_var1.lo = x3.lo*x10.lo;
intro_var1.up = x3.up*x10.up;

intro_var2.lo = x4.lo*x10.lo;
intro_var2.up = x4.up*x10.up;

equations obj, e1, e2, e3, e4, e5, e6, e7, e8, e9, e10, e11, e12, e13, e14, e15;

obj .. relobj =e=  6*x1 + 16*x2 - 9*x5 + 10*x6 - 15*x9 ;

*linear problem constraints
e1 .. x1+x2 =e= x3+x4;
e2 .. x3+x7 =e= x5;
e3 .. x4+x8 =e= x9;
e4 .. x7+x8 =e= x6;

*linearized problem constraints
e5 .. intro_var1 + 2*x7 =l= 2.5*x5 ;
e6 .. intro_var2 + 2*x8 =l= 1.5*x9 ;
e7 .. 3*x1+x2 =e= intro_var1 + intro_var2 ;

*envelopes for x3*x10
e8 .. intro_var1 =g= x10.lo*x3 + x3.lo*x10 - x3.lo*x10.lo ;
```

```
e9 .. intro_var1 =g= x10.up*x3 + x3.up*x10 - x3.up*x10.up ;
e10 .. intro_var1 =l= x10.lo*x3 + x3.up*x10 - x3.up*x10.lo ;
e11 .. intro_var1 =l= x10.up*x3 + x3.lo*x10 - x3.lo*x10.up ;

*envelopes for x4*x10
e12 .. intro_var2 =g= x10.lo*x4 + x4.lo*x10 - x4.lo*x10.lo ;
e13 .. intro_var2 =g= x10.up*x4 + x4.up*x10 - x4.up*x10.up ;
e14 .. intro_var2 =l= x10.lo*x4 + x4.up*x10 - x4.up*x10.lo ;
e15 .. intro_var2 =l= x10.up*x4 + x4.lo*x10 - x4.lo*x10.up ;

model relaxation /all/;

solve relaxation minimizing relobj using lp;
```

(b) A GAMS/BARON options file for part (2) is provided below.

```
positive variables x1, x2, x3, x4, x5, x6, x7, x8, x9, x10;
variable f;

x10.lo = 1;

x1.up = 300;
x2.up = 300;
x3.up = 100;
x4.up = 200;
x5.up = 100;
x6.up = 300;
x7.up = 100;
x8.up = 200;
x9.up = 200;
x10.up = 3;

equations e1, e2, e3, e4, e5, e6, e7, obj;

obj .. f =e= -9*x5-15*x9+6*x1+16*x2+10*x6;

e1 .. x1+x2 =e= x3+x4;
e2 .. x3+x7 =e= x5;
e3 .. x4+x8 =e= x9;
e4 .. x7+x8 =e= x6;
e5 .. x10*x3+2*x7 =l= 2.5*x5;
e6 .. x10*x4+2*x8 =l= 1.5*x9;
e7 .. 3*x1+x2 =e= x10*x3+x10*x4;

model pool /all/;
```

```
solve pool minimizing f using nlp;
```

A BARON options file is provided below.

```
brvarstra 2
brptstra 2
numloc 0
dolocal -3
prelpdo 0
tdo 0
mdo 0
lbttdo 0
obttdo 0
pdo 0
optca 1e-3
optcr 1e-9
nodesel 1
```

PART 2. BILOGICAL PATHWAYS
Problem 1.i maximum biomass formation (supporting files in http://cepac.cheme.cmu.edu/pasilectures/costas.htm)

GAMS INPUT FILE
See Problem 1a in http://cepac.cheme.cmu.edu/pasilectures/costas.htm

SOLUTION

Objective = 1.016670
model status = 1
CPU for MIP:0.0150

v(1) =	10.00000	v(28) =	13.03787	v(54) =	1.43571
v(8) =	15.41904	v(30) =	0.00000	v(56) =	1.85451
v(11) =	16.58821	v(32) =	7.15333	v(58) =	1.85451
v(12) =	3.76168	v(33) =	7.97467	v(60) =	2.27331
v(14) =	1.82199	v(35) =	7.97467	v(69) =	2.52954
v(16) =	6.29122	v(36) =	7.97467	v(70) =	28.98356
v(18) =	6.29122	v(38) =	3.40378	v(71) =	30.83807
v(20) =	6.29122	v(40) =	4.57089	v(73) =	1.85451
v(22) =	14.56288	v(42) =	2.48878	v(75) =	39.88109
v(24) =	14.56288	v(44) =	2.48878	v(78) =	7.60000
v(26) =	13.03787	v(46) =	2.08211	v(79) =	1.01667
		v(48) =	2.97284	v(82) =	0.41880
		v(49) =	2.97284	v(83) =	0.41880
		v(51) =	2.55404		
		v(53) =	1.43571		

Problem1.ii Single reaction deletions
GAMS INPUT FILE
See Problem 1b in http://cepac.cheme.cmu.edu/pasilectures/costas.htm

SOLUTION

deletion(1)=	0.0539719553	deletion(27)=	1.0166696541
deletion(2)=	1.0166696541	deletion(28)=	0.0000000000
deletion(3)=	1.0166696540	deletion(29)=	1.0166696541
deletion(4)=	1.0166696540	deletion(30)=	1.0166696540
deletion(5)=	1.0166696540	deletion(31)=	1.0166696540
deletion(6)=	1.0166696540	deletion(32)=	1.0166696540
deletion(7)=	1.0166696540	deletion(33)=	0.9907312049
deletion(8)=	0.3176178660	deletion(34)=	1.0166696540
deletion(9)=	1.0166696540	deletion(35)=	0.9907312049
deletion(10)=	1.0166696540	deletion(36)=	0.9907312049
deletion(11)=	0.6348220683	deletion(37)=	1.0166696540
deletion(12)=	0.0000000000	deletion(38)=	0.0000000000
deletion(13)=	1.0166696540	deletion(39)=	1.0166696541
deletion(14)=	1.0119768191	deletion(40)=	0.9944865610
deletion(15)=	1.0166696540	deletion(41)=	1.0166696540
deletion(16)=	0.7042253521	deletion(42)=	0.9924346630
deletion(17)=	1.0166696540	deletion(43)=	1.0166696540
deletion(18)=	0.7042253521	deletion(44)=	0.9924346630
deletion(19)=	1.0166696540	deletion(45)=	1.0166696540
deletion(20)=	0.7042253521	deletion(46)=	0.9965469613
deletion(21)=	1.0166696540	deletion(47)=	1.0166696541
deletion(22)=	0.0000000000	deletion(48)=	0.0000000000
deletion(23)=	1.0166696541	deletion(49)=	0.0000000000
deletion(24)=	0.0000000000	deletion(50)=	1.0166696540
deletion(25)=	1.0166696541	deletion(51)=	0.0000000000
deletion(26)=	0.0000000000	deletion(52)=	1.0166696540

deletion(53)= 1.0148614610
deletion(54)= 1.0148614610
deletion(55)= 1.0166696540
deletion(56)= 0.9838783971
deletion(57)= 1.0166696540
deletion(58)= 0.9838783971
deletion(59)= 1.0166696540
deletion(60)= 0.9838783971
deletion(61)= 1.0166696540
deletion(62)= 1.0166696540
deletion(63)= 1.0166696540
deletion(64)= 1.0166696540
deletion(65)= 1.0166696540
deletion(66)= 1.0166696540
deletion(67)= 1.0166696540
deletion(68)= 1.0166696540
deletion(69)= 1.0000000000
deletion(70)= 0.9207092071
deletion(71)= 0.3176178660
deletion(72)= 1.0166696540
deletion(73)= 0.9838783971
deletion(74)= 1.0166696540
deletion(75)= 0.4919028340
deletion(76)= 1.0166696540
deletion(77)= 1.0166696540
deletion(78)= 7.6000000000
deletion(79)= 0.0000000000
deletion(80)= 1.0166696540
deletion(81)= 1.0166696540
deletion(82)= 1.0155263607
deletion(83)= 1.0155263607
deletion(84)= 1.0166696540
deletion(85)= 1.0166696540
deletion(86)= 1.0166696540
deletion(87)= 1.0166696540
deletion(88)= 1.0166696540
deletion(89)= 1.0166696540
deletion(90)= 1.0166696540
deletion(91)= 1.0166696540
deletion(92)= 1.0166696540

Problem 1.iii Maximum amount of ethanol

GAMS INPUT FILE

See Problem 1 c in http://cepac.cheme.cmu.edu/pasilectures/costas.htm

SOLUTION

ethanol production(1) = 0.0000000000
ethanol production(2) = 0.0000000000
ethanol production(3) = 0.0000000000
ethanol production(4) = 0.0000000000
ethanol production(5) = 0.0000000000
ethanol production(6) = 0.0000000000
ethanol production(7) = 0.0000000000
ethanol production(8) = 9.6691480562
ethanol production(9) = 0.0000000000
ethanol production(10) = 0.0000000000
ethanol production(11) = 0.0000000000
ethanol production(12) = 0.0000000000
ethanol production(13) = 0.0000000000
ethanol production(14) = 0.0000000000
ethanol production(15) = 0.0000000000
ethanol production(16) = 0.0000000000
ethanol production(17) = 0.0000000000
ethanol production(18) = 0.0000000000
ethanol production(19) = 0.0000000000
ethanol production(20) = 0.0000000000
ethanol production(21) = 0.0000000000
ethanol production(22) = 0.0000000000
ethanol production(23) = 0.0000000000
ethanol production(24) = 0.0000000000
ethanol production(25) = 0.0000000000
ethanol production(26) = 0.0000000000
ethanol production(27) = 0.0000000000
ethanol production(28) = 0.0000000000
ethanol production(29) = 0.0000000000
ethanol production(30) = 0.0000000000
ethanol production(31) = 0.0000000000
ethanol production(32) = 0.0000000000
ethanol production(33) = 0.0000000000
ethanol production(34) = 0.0000000000
ethanol production(35) = 0.0000000000
ethanol production(36) = 0.0000000000
ethanol production(37) = 0.0000000000
ethanol production(38) = 0.0000000000
ethanol production(39) = 0.0000000000
ethanol production(40) = 0.0000000000
ethanol production(41) = 0.0000000000
ethanol production(42) = 0.0000000000
ethanol production(43) = 0.0000000000
ethanol production(44) = 0.0000000000
ethanol production(45) = 0.0000000000
ethanol production(46) = 0.0000000000
ethanol production(47) = 0.0000000000
ethanol production(48) = 0.0000000000
ethanol production(49) = 0.0000000000
ethanol production(50) = 0.0000000000
ethanol production(51) = 2.5333333333
ethanol production(52) = 0.0000000000
ethanol production(53) = 0.0000000000
ethanol production(54) = 0.0000000000
ethanol production(55) = 0.0000000000
ethanol production(56) = 0.0000000000
ethanol production(57) = 0.0000000000
ethanol production(58) = 0.0000000000
ethanol production(59) = 0.0000000000

ethanol production(60) = 0.0000000000
ethanol production(61) = 0.0000000000
ethanol production(62) = 0.0000000000
ethanol production(63) = 0.0000000000
ethanol production(64) = 0.0000000000
ethanol production(65) = 0.0000000000
ethanol production(66) = 0.0000000000
ethanol production(67) = 0.0000000000
ethanol production(68) = 0.0000000000
ethanol production(69) = 0.0000000000
ethanol production(70) = 0.0000000000
ethanol production(71) = 9.6691480562
ethanol production(72) = 0.0000000000
ethanol production(73) = 0.0000000000
ethanol production(74) = 0.0000000000
ethanol production(75) = 0.0000000000
ethanol production(76) = 0.0000000000
ethanol production(77) = 0.0000000000
ethanol production(78) = 0.0000000000
ethanol production(79) = 0.0000000000
ethanol production(80) = 0.0000000000
ethanol production(81) = 0.0000000000
ethanol production(82) = 0.0000000000
ethanol production(83) = 0.0000000000
ethanol production(84) = 0.0000000000
ethanol production(85) = 0.0000000000
ethanol production(86) = 0.0000000000
ethanol production(87) = 0.0000000000
ethanol production(88) = 0.0000000000
ethanol production(89) = 0.0000000000
ethanol production(90) = 0.0000000000
ethanol production(91) = 0.0000000000
ethanol production(92) = 0.0000000000

Problem 2.
GAMS INPUT FILE
See Problem 2 in http://cepac.cheme.cmu.edu/pasilectures/costas.htm

SOLUTION
Single knock-out
Objective = 9.669148
model status = 1
CPU for MIP:0.0500

v(1) = 10.00000
v(5) = 4.58726
v(7) = 9.66915
v(11) = 2.14392
v(12) = 1.17519
v(14) = 7.22084
v(16) = 8.76658
v(18) = 8.76658
v(20) = 8.76658
v(22) = 18.22663
v(24) = 18.22663
v(26) = 17.75021
v(28) = 17.75021
v(30) = 6.67031
v(33) = 2.71563
v(35) = 2.71563
v(36) = 2.71563
v(38) = 1.13813
v(40) = 1.57750
v(42) = 0.85227
v(44) = 0.85227
v(46) = 0.72523
v(48) = 0.34938
v(49) = 0.34938
v(51) = 0.34938
v(62) = 9.66915
v(64) = 4.58726
v(66) = 4.58726
v(69) = 0.92109
v(78) = 7.60000
v(79) = 0.31762
v(84) = 15.78098
v(88) = 15.78098
y(71)= zero

Double knock-out
Objective = 11.179232
model status = 1
CPU for MIP:0.1800

v(1) = 10.00000
v(3) = 2.44918
v(7) = 11.17923
v(11) = 2.84108
v(12) = 0.88608
v(14) = 9.12914
v(16) = 9.47822
v(18) = 9.47822
v(20) = 9.47822
v(22) = 19.07110
v(24) = 19.07110
v(26) = 18.71188
v(28) = 18.71188
v(30) = 5.44846
v(33) = 0.82296
v(35) = 0.82296
v(36) = 0.82296
v(38) = 0.44994
v(40) = 0.37302
v(42) = 0.23441
v(44) = 0.23441
v(46) = 0.13862
v(48) = 2.71261
v(49) = 2.71261
v(51) = 2.71261
v(53) = 2.44918
v(54) = 2.44918
v(62) = 11.17923
v(69) = 3.14368
v(78) = 7.60000
v(79) = 0.23948
v(84) = 14.77792
v(88) = 14.77792
y(5)= zero
y(71)= zero

Problem 3.i

GAMS INPUT FILE

See Problem 3a in http://cepac.cheme.cmu.edu/pasilectures/costas.htm

SOLUTION

v(1)= 10.0000000000
v(2)= 0.0000000000
v(3)= 9.9238333333
v(4)= 0.0000000000
v(5)= 19.8476666667
v(6)= 0.0000000000
v(7)= 19.8422777778
v(8)= 50.0000000000
v(9)= 0.0000000000
v(10)= 0.0000000000
v(11)= 53.1986666667
v(12)= 3.7616777200
v(13)= 0.0000000000
v(14)= 100.0000000000
v(15)= 100.0000000000
v(16)= 100.0000000000
v(17)= 100.0000000000
v(18)= 100.0000000000
v(19)= 100.0000000000
v(20)= 100.0000000000
v(21)= 100.0000000000
v(22)= 100.0000000000
v(23)= 99.8750000000
v(24)= 100.0000000000
v(25)= 99.8750000000
v(26)= 100.0000000000
v(27)= 99.8900000000
v(28)= 100.0000000000
v(29)= 99.8900000000
v(30)= 100.0000000000
v(31)= 100.0000000000
v(32)= 36.5561666667
v(33)= 100.0000000000
v(34)= 100.0000000000
v(35)= 51.3680000000
v(36)= 100.0000000000
v(37)= 100.0000000000
v(38)= 100.0000000000
v(39)= 99.9926666667
v(40)= 100.0000000000
v(41)= 100.0000000000
v(42)= 100.0000000000
v(43)= 100.0000000000
v(44)= 100.0000000000
v(45)= 100.0000000000
v(46)= 100.0000000000
v(47)= 100.0000000000
v(48)= 19.8586666667
v(49)= 100.0000000000
v(50)= 99.9890000000
v(51)= 100.0000000000
v(52)= 99.9890000000
v(53)= 19.8476666667
v(54)= 100.0000000000
v(55)= 100.0000000000
v(56)= 100.0000000000
v(57)= 100.0000000000
v(58)= 100.0000000000
v(59)= 100.0000000000
v(60)= 100.0000000000
v(61)= 100.0000000000
v(62)= 100.0000000000

Problem 3.ii

GAMS INPUT FILE

See Problem 3b in http://cepac.cheme.cmu.edu/pasilectures/costas.htm

SOLUTION

acnA/pgk
Max Ratio = 800.000000
Min Ratio = 0.000110

acnA/pfkA
Max Ratio = 2702.702703
Min Ratio = 0.000110

acnA/gnd
Max Ratio = 20000.000000
Min Ratio = 0.000110

gnd/pfka
Max Ratio = 2702.702703
Min Ratio = 0.000000

gnd/pgk
Max Ratio = 800.000000
Min Ratio = 0.000000

pgk/pfka
Max Ratio = 9090.909091
Min Ratio = 0.001250

adhE/acnA
Max Ratio = 9090.909091
Min Ratio = 0.000000

adhE/gnd
Max Ratio = 20000.000000
Min Ratio = 0.000000

adhE/pgk
Max Ratio = 800.000000
Min Ratio = 0.000000

adhE/pfkA
Max Ratio = 2702.702703
Min Ratio = 0.000000

EXAM: MASS INTEGRATION AND POLLUTION PREVENTION

A pharmaceutical process uses a solvent (tetrahydrofuran THF) in two units: mixer and purification network as shown in Fig. 1. During solvent mixing with the feedstock, some amount of the solvent reacts with certain impurities in the feedstock to produce waste materials that are separated in the purification network. After the purification network, the mixture is fed to a reactor where the main product is generated. The product is processed in separation and drying systems leading to a dry powder which is palletized and sold. The offgases from the reactor and the separator/dryer are currently being flared. To reduce solvent consumption and improve the environmental performance of the process, it is desired to recover the solvent from the offgases.

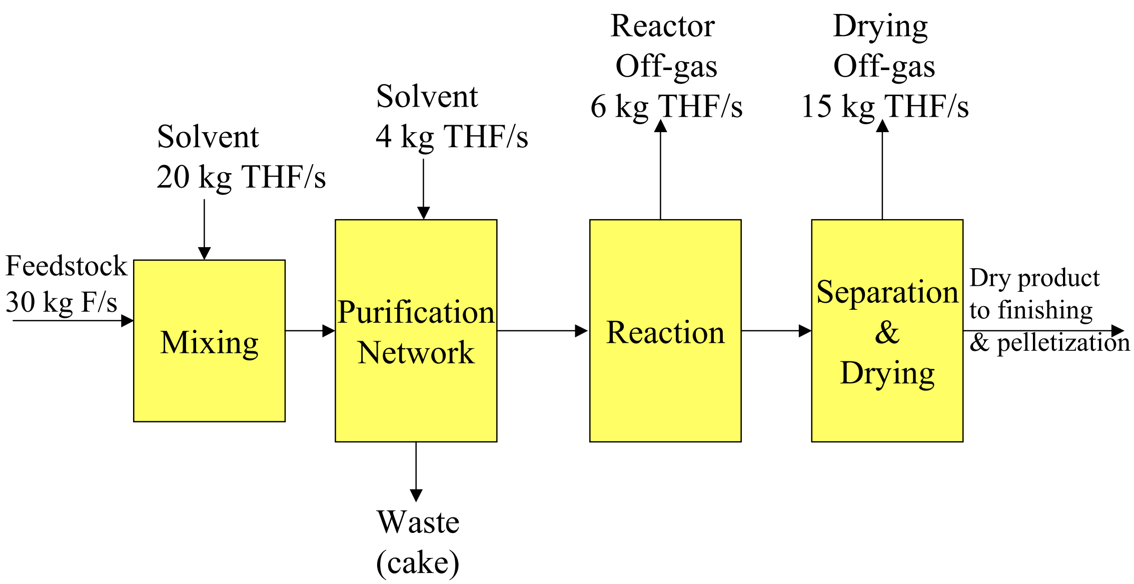


Fig. 1. Pharmaceutical Process

Problem 1. Using segregation, mixing, recycle, and interception, what is the target for minimum solvent consumption?

Problem 2. If no capital is available for new equipment, what is the target for minimum solvent consumption when direct recycle strategies (without new equipment) are used?

The relevant problem data are summarized in Tables 1 and 2. Assume that the only available fresh solvent is pure (100% THF).

Table 1. Sink Data for the Pharmaceutical Example

Sink	Flowrate kg/s	Maximum Inlet Mass Fraction of Impurities
Mixing	20.0	0.01
Purification Network	4.0	0.03

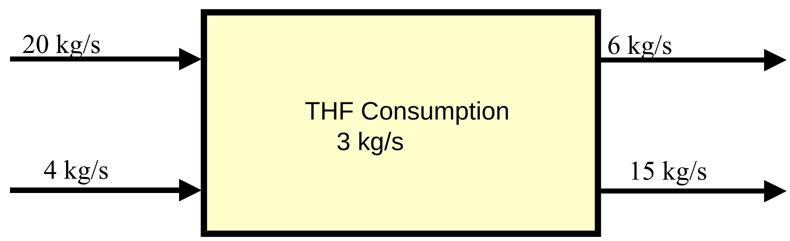
Table 2. Source Data for the Pharmaceutical Example

Source	Flowrate kg/s	Inlet Mass Fraction of Impurities
Reactor offgas	6.0	0.02
Drying offgas	15.0	0.05

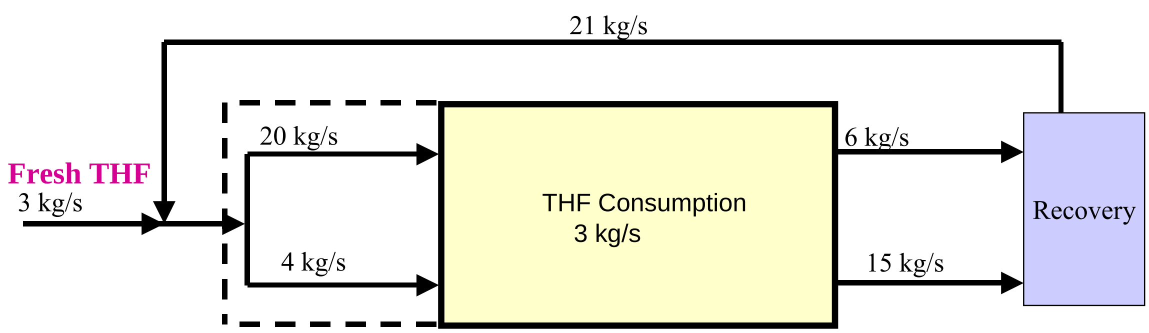
Problem 3. Problem 2 is revised by considering three fresh resources whose contents of impurities are 0.00, 0.01, and 0.06 (expressed as mass fractions). The costs of the three fresh resources are 3.0, 1.0, and 0.5 ($/kg solvent). What is the minimum cost of the fresh solvents when direct recycle strategies are used.

SOLUTION TO EXAM PROBLEMS

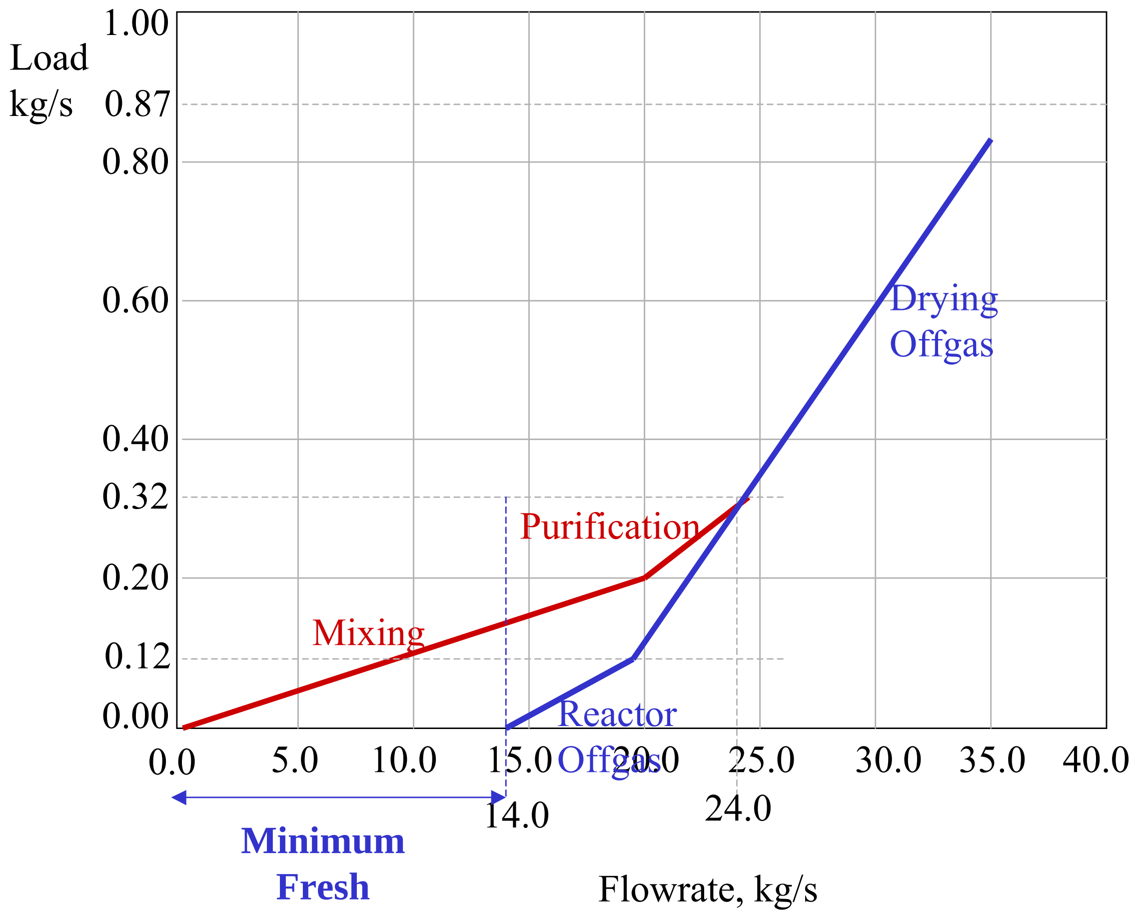
(1)



(a) Overall THF Balance Before Mass Integration

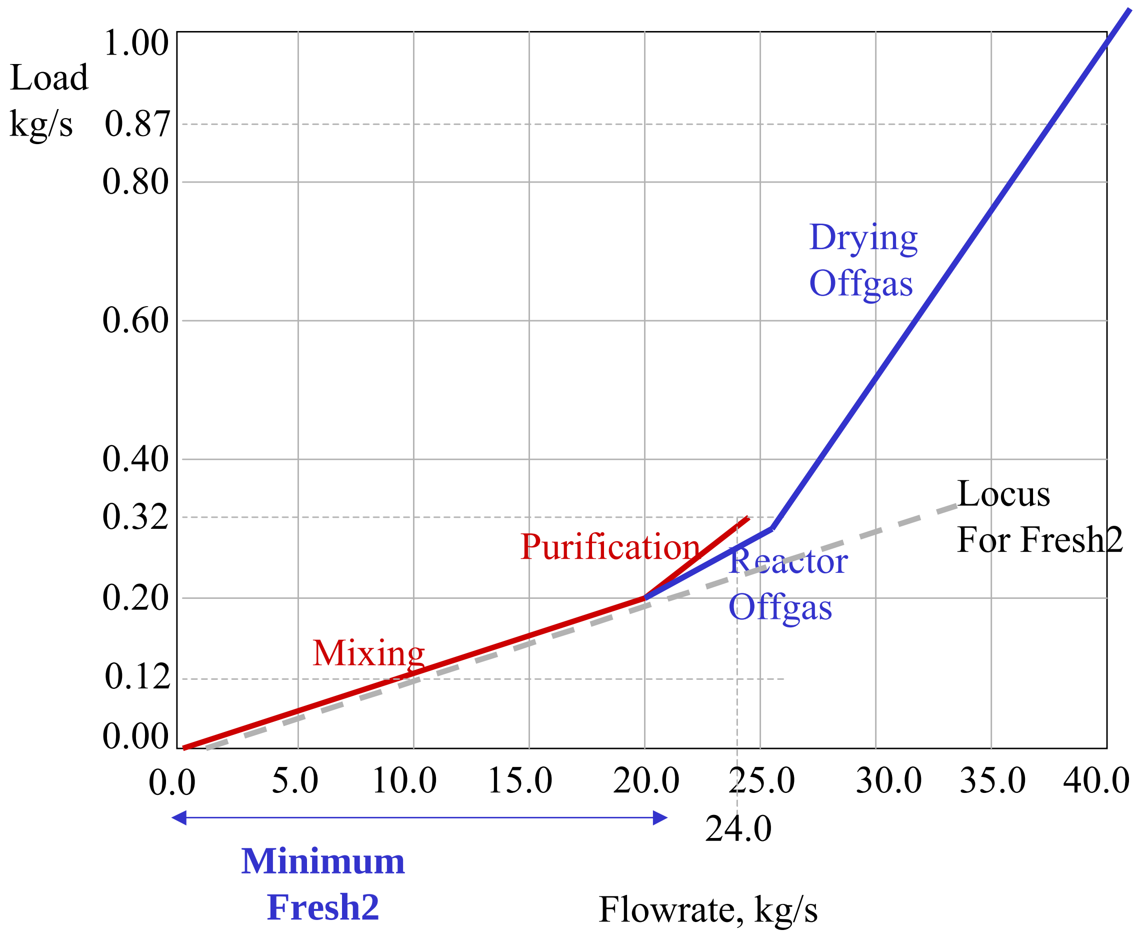


2.



Minimum fresh = 14 kg/s

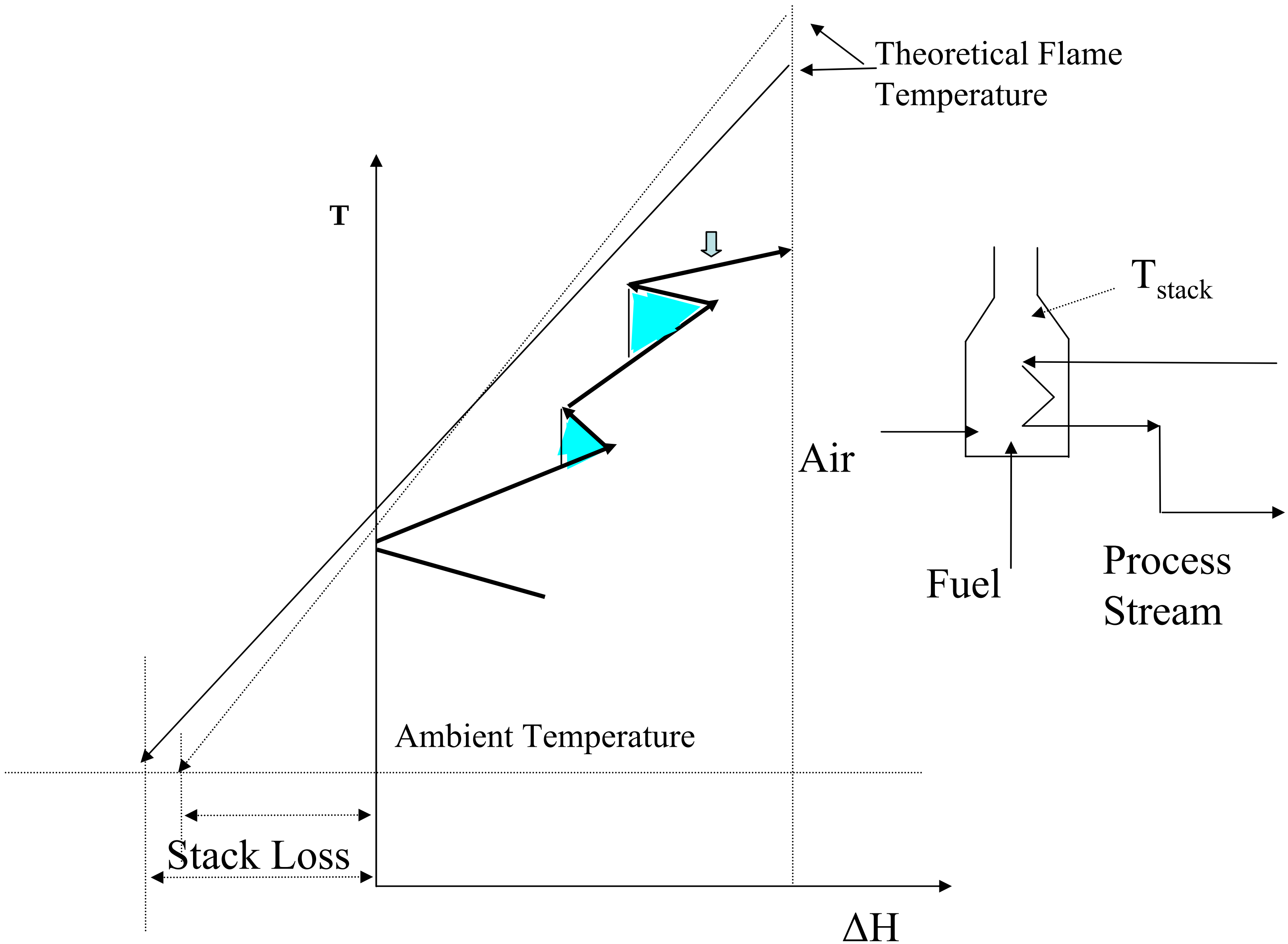
3. Fresh 3 will not be used since its composition exceeds that of the Drying Offgas (source prioritization rule). Compare fresh1 with fresh2 and evaluate flowrate* cost.



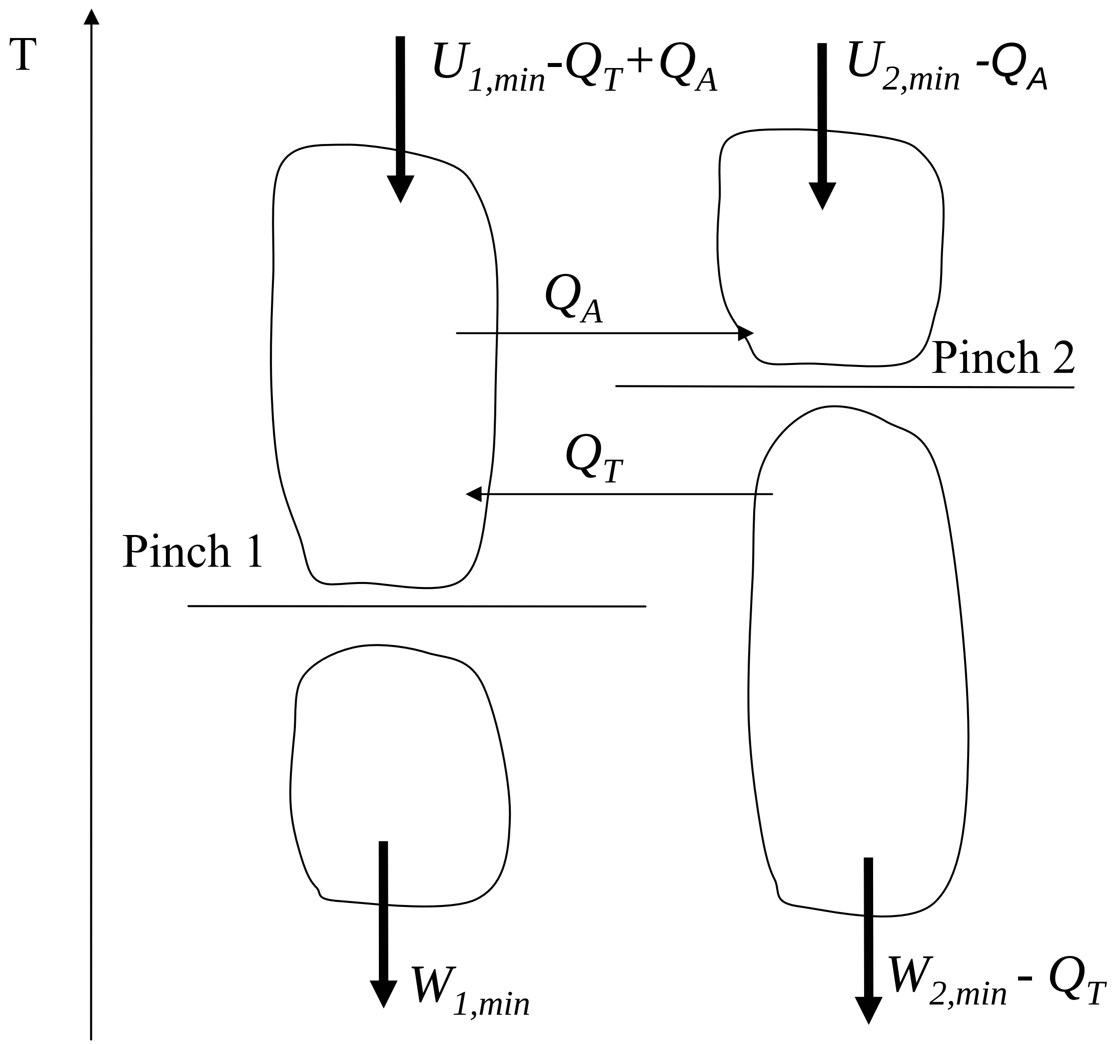
Minimum cost for fresh 1 = 14*3 = $42/s

Minimum cost for fresh 2 = 20*1 = $20/s ➔ Choose fresh 2.

ANSWER-Question 1



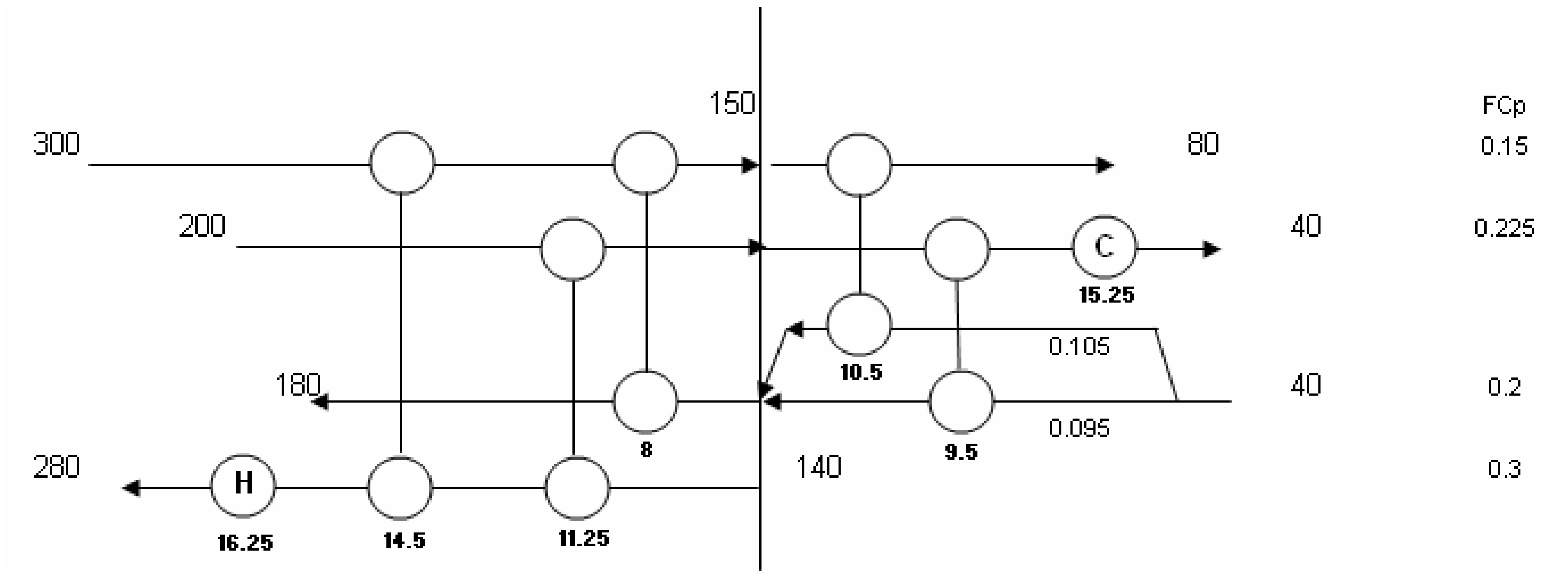
ANSWER-Question 2



This is called Assisted Heat and is transferred from Plant 1 to Plant 2 when Plant 1 has heat deficit at high temperature intervals and heat surplus at lower intervals. In such case there is a need to transfer the surplus to Plant 2 so that the surplus does not have to be cascaded down to plant 1 between pinches, allowing thus Q_T to be transferred fully.

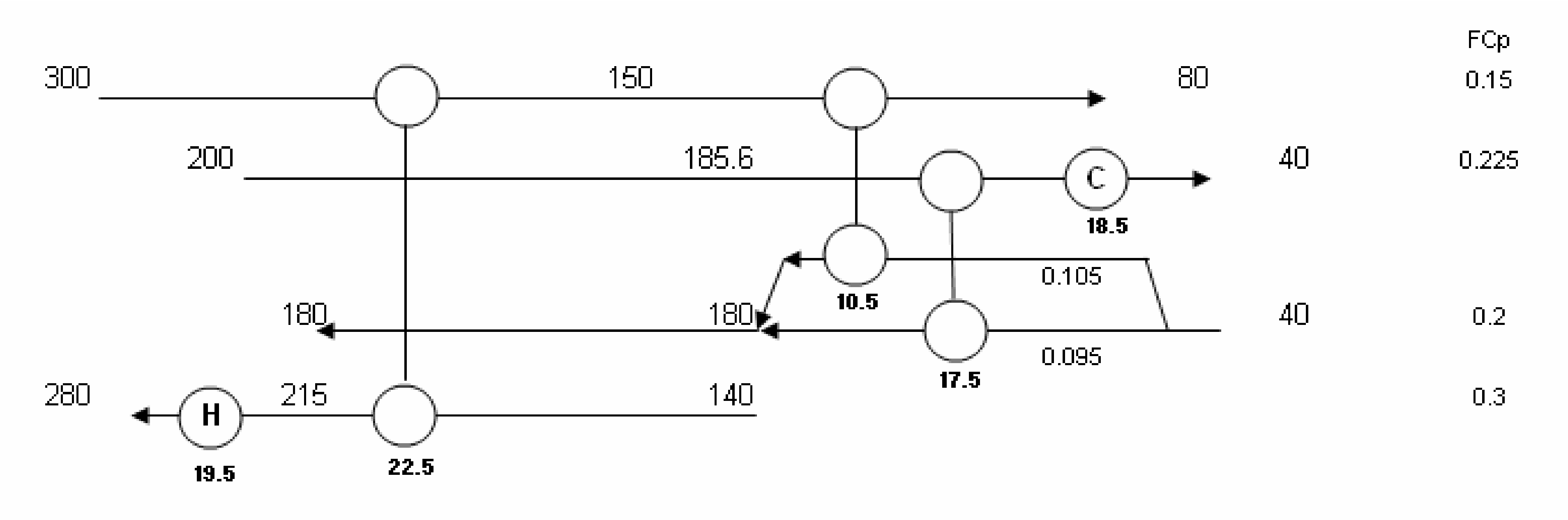
ANSWER Question 3a

Maximum energy recovery network.



ANSWER Question 3b

Energy Relaxed Network.



Exam

Pan American Advanced Studies Institute
Program on Process Systems Engineering
PASI-PSE 2005

Part 3. Batch Scheduling

Professor: Dr. Jaime Cerdá

Exercise 1. Solution

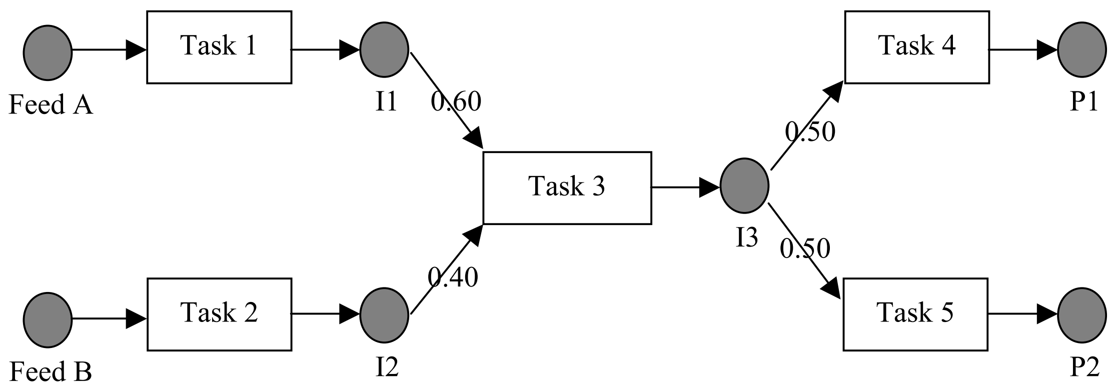


Fig. 1 - STN representation

(a.1) Discrete-Time Scheduling Formulation

```
Sets
i tasks /t1*t5/
s state /f1,f2,i1,i2,i3,p1,p2/
j equipment units   /e1*e3/
t time intervals /1*24/
;
Alias(i,ii);
Alias(t,tt);
Sets
A(i,j) assignment /(t1*t3).(e1,e2),(t4,t5).e3/
IN(s) limited inventory /i1,i2,i3/
isc(i,s) state consumed /t1.f1,t2.f2,t3.(i1,i2),(t4,t5).i3/
isp(i,s) state produced /t1.i1,t2.i2,t3.i3,t4.p1,t5.p2/
;
Parameters
cap(j) production capacity /e1 100,e2 200,e3 400/
io(s) initial inventory /f1 2000,f2 2000,i1 0,i2 0,i3 80,p1 50,p2 50/
ic(s) inventory capacity /i1 200,i2 200,i3 500/
pr(s) price /f1 -1,f2 -2,p1 8,p2 12/
dem(s) minimum demand /p1 250, p2 200/
;
```

```
Table
roc(i,s) consumption
         f1      f2      i1      i2      i3      p1      p2
t1       1       0       0       0       0       0       0
t2       0       1       0       0       0       0       0
t3       0       0       .6      .4      0       0       0
t4       0       0       0       0       .5       0       0
t5       0       0       0       0       .5       0       0
;
Table
rop(i,s) production
         f1      f2      i1      i2      i3      p1      p2
t1       0       0       1       0       0       0       0
t2       0       0       0       1       0       0       0
t3       0       0       0       0       1       0       0
t4       0       0       0       0       0       1       0
t5       0       0       0       0       0       0       1
;
Table
pt(i,j) processing times
         e1      e2      e3
t1       3       4       0
t2       5       5       0
t3       6       5       0
t4       0       0       3
t5       0       0       7
;

variables
w(i,j,t) batch initialization
b(i,j,t) batch size
il(s,t) inventory level
z  objective function;
positive variables
b,il;
binary variables
w;

equations
r1,r2,r3,r4,r5,r6,of;

r1(j,t).. sum(i$A(i,j),(sum(tt$((ord(tt) le ord(t))$(ord(tt) ge
(ord(t)-pt(i,j)+1))),
                 w(i,j,tt)))) =l= 1;
r2(i,j,t)$A(i,j)..b(i,j,t) =l= cap(j)*w(i,j,t);
r3(s,t).. il(s,t)=e=il(s,t-
1)+sum(i$isp(i,s),rop(i,s)*(sum(j$A(i,j),b(i,j,t-pt(i,j)))))-

sum(i$isc(i,s),roc(i,s)*(sum(j$A(i,j),b(i,j,t))))+io(s)$(ord(t) eq 1);
r4(s,t)$IN(s).. il(s,t) =l= ic(s);
r5(s)..sum((i,j,t)$(A(i,j)$isp(i,s)),b(i,j,t))=g=dem(s);
r6(i,j)$A(i,j)..sum(t$(ord(t) gt 24-pt(i,j)),w(i,j,t))=e=0;
of..z=e=sum(s,pr(s)*(sum((i,j,t)$(A(i,j)$isp(i,s)),b(i,j,t))+sum((i,j,
t)$(A(i,j)$isc(i,s)),b(i,j,t))));

model cerda /all/;
option limrow = 500;
solve cerda using mip maximizing z;
display  w.l,b.l,il.l,z.l;
```

Results

```
MODEL STATISTICS

BLOCKS OF EQUATIONS       7     SINGLE EQUATIONS      518
BLOCKS OF VARIABLES       4     SINGLE VARIABLES      553
NON ZERO ELEMENTS      2388     DISCRETE VARIABLES    192

       S O L V E      S U M M A R Y

     MODEL   cerda               OBJECTIVE  z
     TYPE    MIP                 DIRECTION  MAXIMIZE
     SOLVER  CPLEX               FROM LINE  86

**** SOLVER STATUS     1 NORMAL COMPLETION
**** MODEL STATUS      8 INTEGER SOLUTION
**** OBJECTIVE VALUE           10553.3333
 RESOURCE USAGE, LIMIT          0.359      1000.000
 ITERATION COUNT, LIMIT       927         10000
```

```
----     87 VARIABLE w.L  batch initialization
```

	1	4	6	7	10	11
t1.e1	1.000	1.000		1.000	1.000	
t2.e2	1.000					
t3.e2			1.000			1.000
t4.e3	1.000					
t5.e3		1.000				1.000

+	13	16	18	21
t1.e1	1.000			
t3.e2		1.000		
t4.e3			1.000	1.000

```
----     87 VARIABLE b.L  batch size
```

	1	4	6	11	13	16
t1.e1	100.000	100.000			100.000	
t2.e2	200.000					
t3.e2			166.667	166.667		166.667
t5.e3		160.000		333.333		

+	18	21
t4.e3	333.333	333.333

```
----     87 VARIABLE il.L  inventory level
```

	1	2	3	4	5	6
f1	1900.000	1900.000	1900.000	1800.000	1800.000	1800.000
f2	1800.000	1800.000	1800.000	1800.000	1800.000	1800.000
i1				100.000	100.000	
i2						133.333
i3	80.000	80.000	80.000			
p1	50.000	50.000	50.000	50.000	50.000	50.000
p2	50.000	50.000	50.000	50.000	50.000	50.000

+	7	8	9	10	11	12
f1	1800.000	1800.000	1800.000	1800.000	1800.000	1800.000
f2	1800.000	1800.000	1800.000	1800.000	1800.000	1800.000
i1	100.000	100.000	100.000	100.000		
i2	133.333	133.333	133.333	133.333	66.667	66.667
p1	50.000	50.000	50.000	50.000	50.000	50.000
p2	50.000	50.000	50.000	50.000	210.000	210.000

+	13	14	15	16	17	18
f1	1700.000	1700.000	1700.000	1700.000	1700.000	1700.000
f2	1800.000	1800.000	1800.000	1800.000	1800.000	1800.000
i2	66.667	66.667	66.667			
i3				166.667	166.667	

```
p1      50.000      50.000      50.000      50.000      50.000      50.000
p2     210.000     210.000     210.000     210.000     210.000     543.333

 +          19          20          21          22          23          24

f1    1700.000    1700.000    1700.000    1700.000    1700.000    1700.000
f2    1800.000    1800.000    1800.000    1800.000    1800.000    1800.000
p1      50.000      50.000     383.333     383.333     383.333     716.667
p2     543.333     543.333     543.333     543.333     543.333     543.333


----      87 VARIABLE z.L                    =     10553.333  objective function
```

Gantt Chart

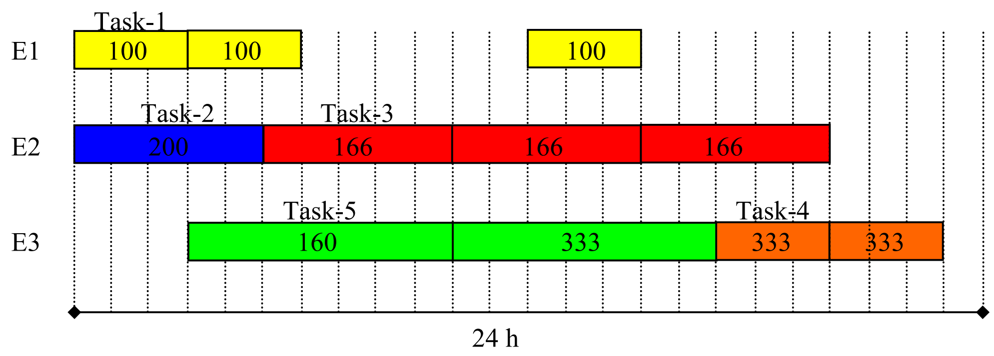


Fig. 2 – Optimal schedule with the discrete-time formulation

(a.2) Continuous-Time Scheduling Formulation

```
Sets
i tasks /t1*t5/
s state /f1,f2,i1,i2,i3,p1,p2/
j equipment units   /e1*e3/
n time points /1*6/               six time points
;
Alias(i,ii);
Alias(n,nn);
Sets
A(i,j) assignment /(t1*t3).(e1,e2),(t4,t5).e3/
IN(s) limited inventory /i1,i2,i3/
isc(i,s) state consumed /t1.f1,t2.f2,t3.(i1,i2),(t4,t5).i3/
isp(i,s) state produced /t1.i1,t2.i2,t3.i3,t4.p1,t5.p2/
;
Scalar
H horizon /24/;
parameters
cap(j) production capacity /e1 100,e2 200,e3 400/
io(s) initial inventory /f1 2000,f2 2000,i1 0,i2 0,i3 80,p1 50,p2 50/
ic(s) inventory capacity /i1 200,i2 200,i3 500/
pr(s) price /f1 -1,f2 -2,p1 8,p2 12/
dem(s) minimum demand /p1 250, p2 200/
;

Table
roc(i,s) consumption
         f1       f2       i1       i2       i3       p1       p2
t1       1        0        0        0        0        0        0
t2       0        1        0        0        0        0        0
t3       0        0        .6       .4       0        0        0
```

```
t4       0       0       0       0       .5      0       0
t5       0       0       0       0       .5      0       0
;
Table
rop(i,s) production
         f1      f2      i1      i2      i3      p1      p2
t1       0       0       1       0       0       0       0
t2       0       0       0       1       0       0       0
t3       0       0       0       0       1       0       0
t4       0       0       0       0       0       1       0
t5       0       0       0       0       0       0       1
;
Table
pt(i,j) processing times
         e1      e2      e3
t1       3       4       0
t2       5       5       0
t3       6       5       0
t4       0       0       3
t5       0       0       7
;

variables
ws(i,j,n) batch start
wf(i,j,n) batch finalization
bs(i,j,n) batch size (start)
bf(i,j,n) batch size (final)
bp(i,j,n) batch size (in process)
il(s,n) inventory level
t(n) time point location
ts(i,j,n) start time
tf(i,j,n) final time
z  objective function;

positive variables
bs,bf,bp,il,t,ts,tf;

binary variables
ws,wf;

t.up(n)=H;
tf.up(i,j,n)=H;

equations
r1,r1b,r2,r2b,r3,r3b,r4,r5,r6,r7,r8,r9,r10,r11,r12,r13,r14,ra,rb,rc,rd
,of;

r1(i,j,n)$A(i,j)..bs(i,j,n)=l=cap(j)*ws(i,j,n);
r2(i,j,n)$A(i,j)..bf(i,j,n)=l=cap(j)*wf(i,j,n);
r1b(i,j,n)$A(i,j)..bs(i,j,n)=g=ws(i,j,n);
r2b(i,j,n)$A(i,j)..bf(i,j,n)=g=wf(i,j,n);
r3(i,j,n)$A(i,j)..bp(i,j,n)=l=cap(j)*((sum(nn$(ord(nn) lt ord(n)),
ws(i,j,nn)) -
(sum(nn$(ord(nn) le ord(n)), wf(i,j,nn)))));
r3b(i,j,n)$A(i,j)..bp(i,j,n)=g=(sum(nn$(ord(nn) lt ord(n)),
ws(i,j,nn)) -
(sum(nn$(ord(nn) le ord(n)), wf(i,j,nn))));
r4(i,j,n)$(A(i,j)$(ord(n) gt 1))..bs(i,j,n-1)+bp(i,j,n-1) =e=
bf(i,j,n)+bp(i,j,n);
```

```
r5(s,n).. il(s,n)=e=il(s,n-
1)+sum(i$isp(i,s),rop(i,s)*(sum(j$A(i,j),bf(i,j,n))))-
sum(i$isc(i,s),roc(i,s)*(sum(j$A(i,j),bs(i,j,n))))+
io(s)$(ord(n) eq 1);

r6(s,n)$IN(s).. il(s,n) =l= ic(s);

r7(s)..sum((i,j,n)$(A(i,j)$isp(i,s)),bf(i,j,n))=g=dem(s);

r8(n)..t(n) =g= t(n-1);
r9(i,j,n)$A(i,j)..tf(i,j,n) =l= t(n) + pt(i,j)*ws(i,j,n) + H*(1-
ws(i,j,n));
r10(i,j,n)$A(i,j)..tf(i,j,n) =g= t(n) + pt(i,j)*ws(i,j,n) - H*(1-
ws(i,j,n));
r11(i,j,n)$(A(i,j)$(ord(n) gt 1))..tf(i,j,n-1) =l= t(n) + H*(1-
wf(i,j,n));
r12(i,j,n)$(A(i,j)$(ord(n) gt 1))..tf(i,j,n-1) =g= t(n) - H*(1-
wf(i,j,n));
r13(i,ii,j,n)$(A(ii,j)$(A(i,j)$(ord(n) gt 1)))..ts(ii,j,n) =g=
tf(i,j,n-1);
r14(i,j,n)$(A(i,j)$(ord(n) gt 1))..tf(i,j,n)-tf(i,j,n-1) =l=
H*ws(i,j,n);

ra(j,n)..sum(i$A(i,j), ws(i,j,n))=l=1;
rb(j,n)..sum(i$A(i,j), wf(i,j,n))=l=1;
rc(j,n)..sum(i$A(i,j),(sum(nn$(ord(nn) le ord(n)), ws(i,j,nn) -
wf(i,j,nn))))=l=1;
rd(i,j)$A(i,j)..sum(n, ws(i,j,n)) =e= sum(n, wf(i,j,n));

of..z=e=sum(s,pr(s)*(sum((i,j,n)$(A(i,j)$isp(i,s)),bf(i,j,n))+sum((i,j
,n)$(A(i,j)$isc(i,s)),bs(i,j,n))));

model cerda /all/;
option limrow = 500;
solve cerda using mip maximizing z;
display  ws.l,ts.l,tf.l,bf.l,il.l,z.l;
```

Results

```
MODEL STATISTICS

BLOCKS OF EQUATIONS      21     SINGLE EQUATIONS      748
BLOCKS OF VARIABLES      10     SINGLE VARIABLES      377
NON ZERO ELEMENTS      2791     DISCRETE VARIABLES     96


            S O L V E     S U M M A R Y

     MODEL   cerda               OBJECTIVE  z
     TYPE    MIP                 DIRECTION  MAXIMIZE
     SOLVER  CPLEX               FROM LINE  119

**** SOLVER STATUS     1 NORMAL COMPLETION
**** MODEL STATUS      8 INTEGER SOLUTION
**** OBJECTIVE VALUE             9360.0000

 RESOURCE USAGE, LIMIT          2.390      1000.000
 ITERATION COUNT, LIMIT     30656         10000

----    120 VARIABLE bf.L  batch size (final)

                2           3           4           5           6

t1.e1     100.000     100.000      40.000
t2.e2                 160.000
t3.e1                                         100.000
```

```
t3.e2                          200.000      100.000
t4.e3                                                    400.000
t5.e3                          160.000      400.000

----     120 VARIABLE il.L  inventory level

              1            2            3            4            5            6

f1     1900.000     1800.000     1760.000     1760.000     1760.000     1760.000
f2     1840.000     1840.000     1840.000     1840.000     1840.000     1840.000
i1                   100.000       80.000
i2                                 80.000
i3       80.000       80.000
p1       50.000       50.000       50.000       50.000       50.000      450.000
p2       50.000       50.000       50.000      210.000      610.000      610.000


----     120 VARIABLE z.L                    =     9360.000  objective function
```

Gantt Chart

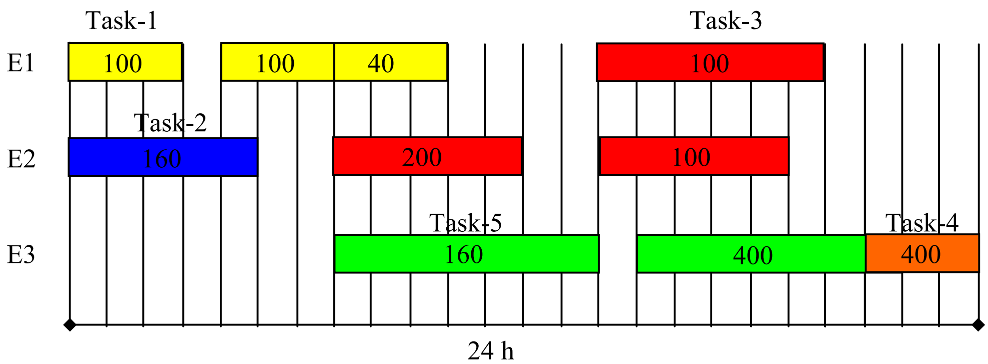


Fig. 3 – Optimal schedule with the continuous-time formulation

(b) Resource Constrained

New data added to model ***(a.1)***

```
Parameters
mu(i) fixed steam consumption /t1 5,t2 4/
nu(i) variable steam consumption /t1 0.2,t2 0.25/;

Positive variable
r(t) resource consumption;

r.up(t) = rup;

r7(t).. r(t) =e= sum((i,j)$A(i,j),(sum(tt$(ord(tt) le
pt(i,j)),mu(i)*w(i,j,t-(ord(tt)-1))+nu(i)*b(i,j,t-(ord(tt)-1)))));
```

Results

```
----      93 VARIABLE r.L

1  79.000,     2  79.000,     3  79.000,     4  79.000,     5  79.000,
6  25.000,     13 25.000,     14 25.000,     15 25.000;
```

*Note: If steam availability is above **79 units**, the optimal schedule remains inalterable.*

Exercise 2. Solution

A) No set up times
A.1) Slot-based Continuous Time Model

```
Sets
s stages /s1*s3/
p products /p1*p5/
e units /e1,e2,e4*e7/
n time slot /n1*n5/
;
Set A(s,e) /s1.(e1,e2),s2.(e4,e5),s3.(e6,e7)/;

Alias(p,pp);
Alias(e,ee);
Scalar
H horizon /300/;

Table
pt(p,s) processing times
         s1      s2      s3
p1       18      12      9
p2       16      13      11
p3       15      15      12
p4       10      12      15
p5       12      14      10
;

variables
tss(e,n) starting time slot
tfs(e,n) completion time slot
tsb(p,s) starting time batch
tfb(p,s) completion time batch
w(p,e,n,s) assignment
MS makespan
z  objective value;

positive variables
tfs,tss,tsb,tfb,MS;

binary variables
w;

equations
r1,r2,r3,r4,r5,r6,r7,r8,r9,of;

r1(s,p)..sum(e$A(s,e),sum(n,w(p,e,n,s))) =e= 1;
r2(e,n)..sum((p,s)$A(s,e),w(p,e,n,s)) =l= 1;;
r3(e,n)..tfs(e,n) =e= tss(e,n)+ sum((p,s)$A(s,e),w(p,e,n,s)*pt(p,s));
r4(p,s)..tfb(p,s) =e= tsb(p,s)+ sum((e,n)$A(s,e),w(p,e,n,s)*pt(p,s));
r5(e,n)..tfs(e,n-1) =l= tss(e,n);
r6(p,s)..tfb(p,s-1) =l= tsb(p,s);
r7(p,e,n,s)$A(s,e)..-H*(1-w(p,e,n,s))=l=tsb(p,s)-tss(e,n);
r8(p,e,n,s)$A(s,e)..H*(1-w(p,e,n,s))=g=tsb(p,s)-tss(e,n);
r9(p,s)..MS=g=tfb(p,s);
of..z=e=MS;
```

```
model cerda /all/;
option optcr=1e-4;
solve cerda using mip minimizing z;
display  w.l,tfb.l,tfs.l,z.l;
```

Results

```
               S O L V E      S U M M A R Y

     MODEL   cerda               OBJECTIVE  z
     TYPE    MIP                 DIRECTION  MINIMIZE
     SOLVER  CPLEX               FROM LINE  67

**** SOLVER STATUS     1 NORMAL COMPLETION
**** MODEL STATUS      8 INTEGER SOLUTION
**** OBJECTIVE VALUE               61.0000

 RESOURCE USAGE, LIMIT         34.406      1000.000
 ITERATION COUNT, LIMIT    321771         10000



----     68 VARIABLE w.L  assignment

INDEX 1 = p1

               s1          s2          s3

e1.n5       1.000
e5.n5                   1.000
e7.n4                               1.000

INDEX 1 = p2

               s1          s2          s3

e2.n2       1.000
e5.n4                   1.000
e7.n2                               1.000

INDEX 1 = p3

               s1          s2          s3

e2.n5       1.000
e4.n5                   1.000
e6.n5                               1.000

INDEX 1 = p4

               s1          s2          s3

e1.n4       1.000
e4.n3                   1.000
e6.n4                               1.000


INDEX 1 = p5

               s1          s2          s3

e1.n3       1.000
e5.n3                   1.000
e7.n1                               1.000
```

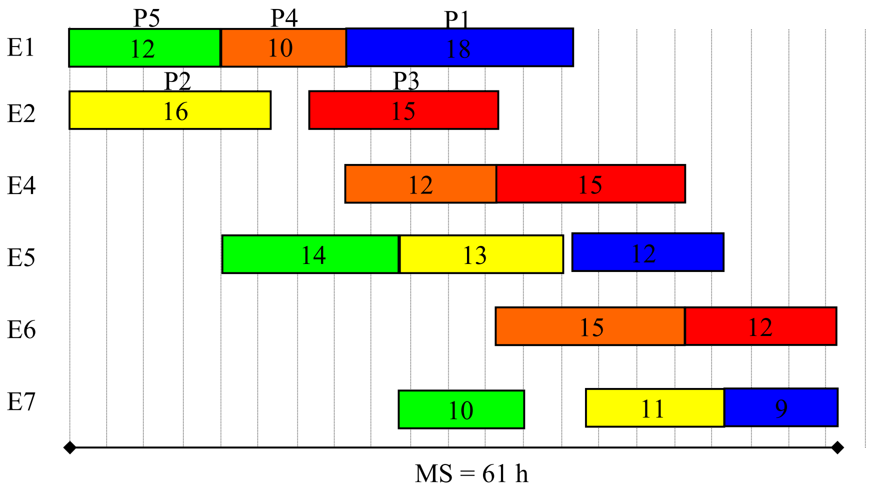
```
----     68 VARIABLE tfb.L  completion time batch

             s1          s2          s3

p1       40.000      52.000      61.000
p2       16.000      39.000      52.000
p3       34.000      49.000      61.000
p4       22.000      34.000      49.000
p5       12.000      26.000      36.000

----     68 VARIABLE z.L                   =       61.000  objective value
```

Gantt Chart



A.2) Global General Precedence Continuous Formulation

```
Sets
s stages /s1*s3/
p products /p1*p5/
e units /e1,e2,e4*e7/
;
Set A(s,e) /s1.(e1,e2),s2.(e4,e5),s3.(e6,e7)/;

Alias(p,pp);
Alias(e,ee);
Scalar
H horizon /300/;


Table
pt(p,s) processing times
         s1       s2       s3
p1       18       12       9
p2       16       13       11
p3       15       15       12
p4       10       12       15
p5       12       14       10
;

variables
c(p,e) completion time
y(p,e)
```

```
x(p,pp,e) sequencing
MS makespan
z  objective value;

positive variables
c,MS;

binary variables
x,y;

equations
r1,r2,r3,r4,r5,of;

r1(s,p)..sum(e$A(s,e),y(p,e)) =e= 1;
r2(p,pp,s,e)$(A(s,e)$(ord(pp) gt ord(p)))..c(pp,e)-pt(pp,s)=g=c(p,e)-
H*(2-y(p,e)-y(pp,e))-H*(1-x(p,pp,e));
r3(p,pp,s,e)$(A(s,e)$(ord(pp) gt ord(p)))..c(p,e)-pt(p,s)=g=c(pp,e)-
H*(2-y(p,e)-y(pp,e))-H*x(p,pp,e);
r4(e,ee,s,p)$A(s,e)..c(p,e)-pt(p,s)=g=c(p,ee)$(A(s-1,ee));
r5(p,e)$(A('s3',e)).. MS =g= c(p,e);
of..z=e=MS;

model cerda /all/;
option limrow = 500;
solve cerda using mip minimizing z;
display  c.l,x.l,z.l;
```

Results

```
      S O L V E     S U M M A R Y

     MODEL   cerda               OBJECTIVE  z
     TYPE    MIP                 DIRECTION  MINIMIZE
     SOLVER  CPLEX               FROM LINE  64

**** SOLVER STATUS     1 NORMAL COMPLETION
**** MODEL STATUS      1 OPTIMAL
**** OBJECTIVE VALUE               61.0000

 RESOURCE USAGE, LIMIT         67.375      1000.000
 ITERATION COUNT, LIMIT    718604         10000


----     66 VARIABLE c.L  completion time
```

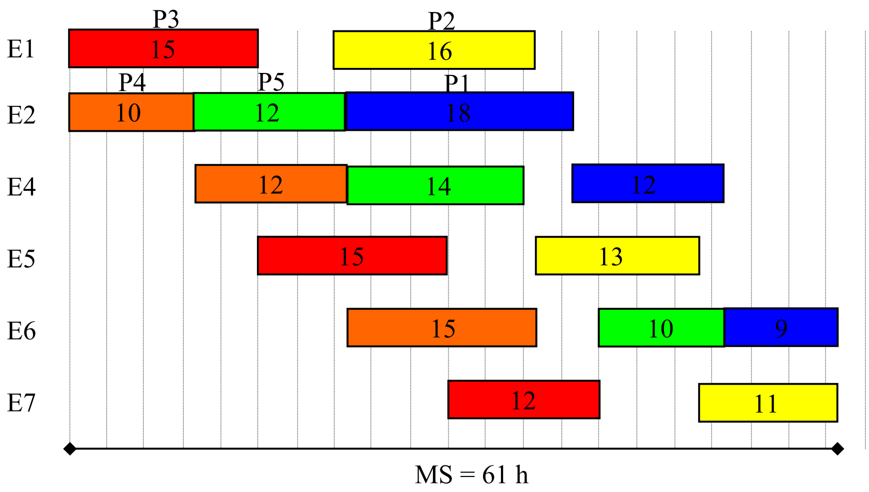
	e1	e2	e4	e5	e6	e7
p1		40.000	52.000		61.000	
p2	37.000			50.000		61.000
p3	15.000			30.000		42.000
p4		10.000	22.000		37.000	
p5		22.000	36.000		52.000	

```
----     66 VARIABLE y.L
```

	e1	e2	e4	e5	e6	e7
p1		1.000	1.000		1.000	
p2	1.000			1.000		1.000
p3	1.000			1.000		1.000
p4		1.000	1.000		1.000	
p5		1.000	1.000		1.000	

----   66 VARIABLE z.L   =   61.000 objective value

Gantt Chart



B) Sequence-Dependent Set up times

```
Sets
s stages /s1*s3/
p products /p1*p5/
e units /e1,e2,e4*e7/
;
Set A(s,e) /s1.(e1,e2),s2.(e4,e5),s3.(e6,e7)/;

Alias(p,pp);
Alias(e,ee);
Scalar
H horizon /300/;

Table
pt(p,s) processing times
         s1      s2      s3
p1       18      12      9
p2       16      13      11
p3       15      15      12
p4       10      12      15
p5       12      14      10
;

Table
tau(p,pp) processing times
         p1      p2      p3      p4      p5
p1       0       1.5     1       1.2     3
p2       1.3     0       .9      1.2     1.4
p3       .8      .9      0       .5      1
p4       1.1     2.5     .7      0       1.6
p5       1       1.4     .5      .6      0
;

variables
c(p,e) completion time
y(p,e)
x(p,pp,e) sequencing
MS makespan
z  objective value;

positive variables
```

```
c,MS;

binary variables
x,y;


equations
r1,r2,r3,r4,r5,of;

r1(s,p)..sum(e$A(s,e),y(p,e)) =e= 1;
r2(p,pp,s,e)$(A(s,e)$(ord(pp) gt ord(p)))..c(pp,e)-
pt(pp,s)=g=c(p,e)+tau(p,pp)-H*(2-y(p,e)-y(pp,e))-H*(1-x(p,pp,e));
r3(p,pp,s,e)$(A(s,e)$(ord(pp) gt ord(p)))..c(p,e)-
pt(p,s)=g=c(pp,e)+tau(pp,p)-H*(2-y(p,e)-y(pp,e))-H*x(p,pp,e);
r4(e,ee,s,p)$A(s,e)..c(p,e)-pt(p,s)=g=c(p,ee)$(A(s-1,ee));
r5(p,e)$(A('s3',e)).. MS =g= c(p,e);
of..z=e=MS;

model cerda /all/;
option optcr = 1e-4;
solve cerda using mip minimizing z;
display  c.l,x.l,z.l;
```

Results

```
               S O L V E      S U M M A R Y

     MODEL   cerda                OBJECTIVE  z
     TYPE    MIP                  DIRECTION  MINIMIZE
     SOLVER  CPLEX                FROM LINE  64

**** SOLVER STATUS     1 NORMAL COMPLETION
**** MODEL STATUS      1 OPTIMAL
**** OBJECTIVE VALUE               62.7000

 RESOURCE USAGE, LIMIT         47.968      1000.000
 ITERATION COUNT, LIMIT    377471         10000


----     65 VARIABLE c.L  completion time
```

	e1	e2	e4	e5	e6	e7
p1	41.700			53.700		62.700
p2		16.000		40.400		52.400
p3		31.900	50.700		62.700	
p4	22.600		34.600		50.000	
p5	12.000			26.000		40.000

----   65 VARIABLE z.L   =   62.700 objective value

SUPPLY CHAIN OPTIMIZATION

Problem 1

(A): Objective Function value: 219500.0000
Offices built: Denver

	LosAngeles	Tulsa	Denver	Seattle
Washington	0.00	0.00	40.00	0.00
Oregon	0.00	0.00	35.00	0.00
California	0.00	0.00	100.00	0.00
Idaho	0.00	0.00	25.00	0.00
Nevada	0.00	0.00	40.00	0.00
Montana	0.00	0.00	25.00	0.00
Wyoming	0.00	0.00	50.00	0.00
Utah	0.00	0.00	30.00	0.00
Arizona	0.00	0.00	50.00	0.00
Colorado	0.00	0.00	65.00	0.00
NewMexico	0.00	0.00	40.00	0.00
NorthDakot	0.00	0.00	30.00	0.00
SouthDakot	0.00	0.00	20.00	0.00
Nebraska	0.00	0.00	30.00	0.00
Kansas	0.00	0.00	40.00	0.00
Oklahoma	0.00	0.00	55.00	0.00

(B): Objective Function value: 478730.0000
Offices built: Tulsa Denver Seattle

	LosAngeles	Tulsa	Denver	Seattle
Washington	0.00	0.00	0.00	40.00
Oregon	0.00	0.00	0.00	35.00
California	0.00	0.00	0.00	100.00
Idaho	0.00	0.00	0.00	25.00
Nevada	0.00	0.00	15.00	25.00
Montana	0.00	0.00	0.00	25.00
Wyoming	0.00	0.00	50.00	0.00
Utah	0.00	0.00	30.00	0.00
Arizona	0.00	0.00	50.00	0.00
Colorado	0.00	0.00	65.00	0.00
NewMexico	0.00	30.00	10.00	0.00
NorthDakot	0.00	0.00	30.00	0.00
SouthDakot	0.00	20.00	0.00	0.00
Nebraska	0.00	30.00	0.00	0.00
Kansas	0.00	40.00	0.00	0.00
Oklahoma	0.00	55.00	0.00	0.00

(Item C): Objective Function value: 479855.0000

Offices built: Tulsa Denver Seattle

	LosAngeles	Tulsa	Denver	Seattle
Washington	0.00	0.00	0.00	40.00
Oregon	0.00	0.00	0.00	35.00
California	0.00	0.00	0.00	100.00
Idaho	0.00	0.00	0.00	25.00

Nevada	0.00	0.00	0.00	40.00
Montana	0.00	25.00	0.00	0.00
Wyoming	0.00	0.00	50.00	0.00
Utah	0.00	0.00	30.00	0.00
Arizona	0.00	0.00	50.00	0.00
Colorado	0.00	0.00	65.00	0.00
NewMexico	0.00	40.00	0.00	0.00
NorthDakot	0.00	0.00	30.00	0.00
SouthDakot	0.00	0.00	20.00	0.00
Nebraska	0.00	30.00	0.00	0.00
Kansas	0.00	40.00	0.00	0.00
Oklahoma	0.00	55.00	0.00	0.00

Problem 2

(A): Objective Function value: 7721816.0000

	NAmerica	SAmerica	Europe	Japan	Asia
USA	100.00	0.00	0.00	0.00	0.00
Germany	160.00	0.00	200.00	95.00	20.00
Japan	0.00	0.00	0.00	25.00	0.00
Brazil	10.00	190.00	0.00	0.00	0.00
India	0.00	0.00	0.00	0.00	80.00

(B): Objective Function value: 6425294.4000

	NAmerica	SAmerica	Europe	Japan	Asia
USA	0.00	0.00	0.00	0.00	0.00
Germany	0.00	0.00	0.00	0.00	0.00
Japan	0.00	0.00	0.00	0.00	0.00
Brazil	270.00	190.00	200.00	120.00	100.00
India	0.00	0.00	0.00	0.00	0.00

(C): Objective Function value with capacity improvement:
USA : 7721816.0000
Germany : 7706506.0000
Japan : 7721816.0000
Brazil : 7688519.8000
India : 7717226.0000

Problem 4

(A): Objective Function value: 3.6550000E+8
Option Chosen: OUTSOURCING Prob: 0.02
Option Chosen: CAPACITY INCREASE Prob: 0.08
Option Chosen: OUTSOURCING Prob: 0.08
Option Chosen: CAPACITY INCREASE Prob: 0.32
Option Chosen: OUTSOURCING Prob: 0.02
Option Chosen: CAPACITY INCREASE Prob: 0.08
Option Chosen: OUTSOURCING Prob: 0.08
Option Chosen: CAPACITY INCREASE Prob: 0.32

olutions to the fifth problem on Supply Chain Optimization

Problem 5

Objective Function value: 1053150.5689

Location of the new factory: x: 802.131 y: 969.810

Flow of units from suppliers to markets:

	Atlanta	Boston	Jacksonville	Philadelphia	NewYork
Buffalo	167.61	139.77	192.61	0.00	0.00
Memphis	0.00	0.00	0.00	0.00	0.00
StLouis	57.39	10.23	57.39	175.00	300.00

Advanced Process Dynamics and Control

Exam Solutions

1. What is the algebraic multiplicity a and the geometric multiplicity g of the eigenvalue $\lambda = -1$ of the matrix

$$\mathbf{A} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Solution to Problem 1.

Since $\det(\lambda\ s\mathbf{I} - \mathbf{A}) = (\lambda\ + 1)^3$ it is straightforward to conclude that the set of eigenvalues is $\{ -1, -1, -1 \}$. Hence, since the eigenvalue $\lambda = -1$ appears three times in the set, its algebraic multiplicity is

$$a = 3.$$

By inspection it can be readily determined that the following set is comprised of eigenvectors of **A**

$$\left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$$

which is clearly a linearly independent set. Since the set of eigenvectors is linearly independent it follows that the algebraic multiplicity of th eigenvalue $\lambda = -1$ is

$$g = 3.$$

2. Design a state feedback control law $\mathbf{u}(t) = -\mathbf{K}\ \mathbf{x}(t)$ that places the closed-loop eigenvalues at $\{ -1, -1 \}$ for an LTI system characterized by the matrices

$$\mathbf{A} = \begin{bmatrix} -1 & 0 \\ 1 & 2 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

Solution to Problem 2.

<u>Approach</u>: Use Ackermann's formula for placing the eigenvalues, using only the first input

Step 1: build the controllability matrix for the first input

$$\mathbf{b}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\mathbf{Ab}_1 = \begin{bmatrix} -1 & 0 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

$$\mathbf{Q}_c = \left[\mathbf{b}\ \mathbf{Ab}\right] = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix}$$

Since the 2x2 controllability matrix is invertible (its determinant is equal to 1), its rank is 2 = n, and it follows that the system is controllable.

Step 2: Specify the desired eigenvalue locations as {–1, –1}

Step 3: Find the coefficients of the desired closed-loop polynomial ($\lambda + 1$) ($\lambda + 1$) :

$$(\lambda + 1)\,(\lambda + 1) = \lambda^2 + 2\,\lambda + 1$$

Step 4: Find the polynomial matrix ***P***(***A***)

$$\mathbf{A}^2 = \begin{bmatrix} -1 & 0 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 1 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 4 \end{bmatrix}$$

$$P(\mathbf{A}) = \mathbf{A}^2 + 2\mathbf{A} + \mathbf{I} = \begin{bmatrix} 1 & 0 \\ 1 & 4 \end{bmatrix} + 2 \begin{bmatrix} -1 & 0 \\ 1 & 2 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 3 & 9 \end{bmatrix}$$

Step 5: Apply Ackermann's Formula

$$\mathbf{Q}_c^{-1} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$$

$$\mathbf{Q}_c^{-1}\ \mathbf{P}(\mathbf{A}) = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 3 & 9 \end{bmatrix} = \begin{bmatrix} 3 & 9 \\ 3 & 9 \end{bmatrix}$$

Ackermann's formula

$$\mathbf{k}^{\mathrm{T}} = \mathit{FirstRow}\left(\mathbf{Q}_c^{-1}\ \mathbf{P}(\mathbf{A})\right) = \mathit{FirstRow}\left(\begin{bmatrix} 3 & 9 \\ 3 & 9 \end{bmatrix}\right) = [\ 3 \quad 9\ ]$$

Setting $\mathbf{K} = \begin{bmatrix} \mathbf{k}^{\mathrm{T}} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} k_1 & k_2 \\ 0 & 0 \end{bmatrix}$ yields the desired state feedback matrix

$$\mathbf{K} = \begin{bmatrix} 3 & 9 \\ 0 & 0 \end{bmatrix}$$

3. Design a state feedback control law $\mathbf{u}(t) = -\mathbf{K}\,\mathbf{x}(t) - \mathbf{K_r}\,\mathbf{r}(t)$ that places the closed-loop eigenvalues at $\{ -1, -1 \}$ for the LTI system given in question 2

Solution to Problem 3. First set the state-feedback matrix as the solution to problem 2:

$$\mathbf{K} = \begin{bmatrix} 3 & 9 \\ 0 & 0 \end{bmatrix}$$

Then calculate a right-inverse matrix for **B** and calculate the matrix **A** – **BK**:

$$\mathbf{B}^{-\mathrm{R}} = \mathbf{B}^{-1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\mathbf{A} - \mathbf{BK} = \begin{bmatrix} -1 & 0 \\ 1 & 2 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 3 & 9 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 1 & 2 \end{bmatrix} - \begin{bmatrix} 3 & 9 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} -4 & -9 \\ 1 & 2 \end{bmatrix}$$

Hence, the feedforward matrix sought is

$$\mathbf{K_r} = \mathbf{B}^{\text{-R}}(\mathbf{A} - \mathbf{BK}) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} -4 & -9 \\ 1 & 2 \end{bmatrix} = \begin{bmatrix} -4 & -9 \\ 1 & 2 \end{bmatrix}$$

Exam Problems for Model Predictive Control

Prepared by Jay H. Lee

Pan American Advanced Studies Institute Program on Process Systems Engineering

1. Suppose the process has three inputs $u_1, \cdots, u_3$ and three outputs $y_1, \cdots, y_3$. y_1 and y_2 has the setpoints of 0.2 and 0.8 respectively. In addition, these two outputs must be kept below 0.25 and 0.85 and above 0.15 and 0.75, respectively, at all times (soft constraints). If these two outputs can be controlled at their setpoints, it is then desirable to drive y_3 to its maximum value of 2 (a secondary requirement). All three inputs must operate in the range of ± 0.5. Write down a reasonable *quadratic* objective to use for MPC. Use the prediction horizon of p and the control horizon of m.

   ANSWER:

$$\min_{\Delta u(k),\cdots,\Delta u(k+m-1)} \sum_{\ell=1}^{p} \left\{ \begin{bmatrix} y_1(k+\ell)-0.2 \\ y_2(k+\ell)-0.8 \\ y_3(k+\ell)-2 \end{bmatrix}^T \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \gamma_{small} \end{bmatrix} \begin{bmatrix} y_1(k+\ell)-0.2 \\ y_2(k+\ell)-0.8 \\ y_3(k+\ell)-2 \end{bmatrix} \right\}$$

$$+\sum_{i=0}^{m-1} \left\{ \begin{bmatrix} \Delta u_1(k+i) \\ \Delta u_2(k+i) \\ \Delta u_3(k+i) \end{bmatrix}^T \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix} \begin{bmatrix} \Delta u_1(k+i) \\ \Delta u_2(k+i) \\ \Delta u_3(k+i) \end{bmatrix} \right\}$$

$$+\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \end{bmatrix}^T \begin{bmatrix} \gamma_{large} & 0 \\ 0 & \gamma_{large} \end{bmatrix} \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \end{bmatrix}$$

   such that

$$\begin{aligned} 0.15-\epsilon_1 &\le y_1(k+\ell) \le 0.25+\epsilon_1 \\ 0.75-\epsilon_2 &\le y_2(k+\ell) \le 0.85+\epsilon_2 \\ -0.5 &\le u_1(k+i) \le 0.5 \\ -0.5 &\le u_2(k+i) \le 0.5 \\ -0.5 &\le u_3(k+i) \le 0.5 \end{aligned}$$

   Note that in the above, $\gamma_{small} \ll 1.0$ and $\gamma_{large} \gg 1.0$.

2. Consider the following SISO system.

$$\begin{aligned} \begin{bmatrix} x_1(k+1) \\ x_2(k+1) \end{bmatrix} &= \begin{bmatrix} 0.4 & 0.1 \\ 0 & 0.2 \end{bmatrix} \begin{bmatrix} x_1(k) \\ x_2(k) \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} u(k) \\ y(k) &= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} x_1(k) \\ x_2(k) \end{bmatrix} \end{aligned} \tag{1}$$

   (a) Calculate the impulse response and step response coefficients. What is the reasonable truncation point for this system?

   ANSWER: Impulse response: $H_i = CA^{i-1}B$ Step response: $S_i = H_1 + \cdots + H_i$ Truncate when $CA^{i-1}B$ becomes negligible.

(b) Write down the step response model that corresponds to the above state space system.
ANSWER: In the notes:

$$x(k+1) = M_1 x(k) + S\delta u(k)$$

where M_1 is a shift matrix and $S = \begin{bmatrix} S_1 \\ \vdots \\ S_n \end{bmatrix}$. n is the truncation point.

(c) Write down the prediction equation for the above system with $p = 2$ and $m = 2$.
ANSWER: From the notes,

$$\begin{bmatrix} y_{k+1|k} \\ y_{k+2|k} \end{bmatrix} = \begin{bmatrix} y_1(k) \\ y_2(k) \end{bmatrix} + \begin{bmatrix} S_1 & 0 \\ S_2 & S_1 \end{bmatrix} \begin{bmatrix} \Delta u(k) \\ \Delta u(k+1) \end{bmatrix} + \begin{bmatrix} S_1^d \\ S_2^d \end{bmatrix} \Delta d(k) + \begin{bmatrix} y_m(k) - y_0(k) \\ y_m(k) - y_0(k) \end{bmatrix}$$

(d) Derive the unconstrained control law for the above system with $\Lambda^y = 2$ and $\lambda^u = 0.5$.
ANSWER: The unconstrained solution is $\Delta U_m(k) = -\frac{1}{s} H^{-1} g(k)$ where H and $g(k)$ are as defined in the notes.

(e) How would you derive the unconstrained MPC law for $p = \infty$ and $m = 2$.
ANSWER: Use $p = m + n - 1$ and add a constraint that $y(m + n - 1|k) = 0$.

(f) How would the prediction equation change if the state space model is used directly?
ANSWER: From the notes,

$$\begin{bmatrix} y_{k+1|k} \\ y_{k+2|k} \end{bmatrix} = \begin{bmatrix} \Xi \\ \Xi\Phi \end{bmatrix} x(k) + \begin{bmatrix} S_1 & 0 \\ S_2 & S_1 \end{bmatrix} \begin{bmatrix} \Delta u(k) \\ \Delta u(k+1) \end{bmatrix} + \begin{bmatrix} S_1^d \\ S_2^d \end{bmatrix} \Delta d(k) + \begin{bmatrix} y_m(k) - y_0(k) \\ y_m(k) - y_0(k) \end{bmatrix}$$

3. Consider the following FIR system model:

$$y(k) = h_1 u(k-1) + h_2 u(k-2) + h_3 u(k-3) + \frac{1}{1 - q^{-1}} \varepsilon(k) \tag{2}$$

(a) Derive the expression for the one-step-ahead predictor and the prediction error.
ANSWER: From the notes

$$\begin{aligned} y(k|k-1) &= G(q)u(k) + (1 - H^{-1}(q))(y(k) - G(q)u(k)) \\ &= h_1 u(k-1) + h_2 u(k-2) + h_3 u(k-3) \\ &\quad + (y(k-1) - h_1 u(k-2) - h_2 u(k-3) - h_3 u(k-4)) \end{aligned}$$

$$\begin{aligned} e(k|k-1) &= H^{-1}(q)(y(k) - G(q)u(k)) \\ &= (y(k) - h_1 u(k-1) - h_2 u(k-2) - h_3 u(k-3)) \\ &\quad - (y(k-1) - h_1 u(k-2) - h_2 u(k-3) - h_3 u(k-4)) \end{aligned}$$

(b) Suppose you are given experimentally obtained time series data $y(1), \cdots, y(12)$ and $u(1), \cdots, u(12)$. Derive the formula for obtaining the parameters h_1, h_2, h_3 that minimize the prediction error for the given data.

ANSWER:

$$\begin{bmatrix} y(4) \\ y(5) \\ \vdots \\ y(12) \end{bmatrix} = \begin{bmatrix} u(3) & u(2) & u(1) \\ u(4) & u(3) & u(2) \\ \vdots & \ddots & \vdots \\ u(11) & u(10) & u(9) \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} + \begin{bmatrix} e(1) \\ e(2) \\ \vdots \\ e(12) \end{bmatrix}$$

Denoting the above as $Y = UH + E$, the least squares solution is $H^{LS} = (U^T U)^{-1} U^T Y$.

Process Control Design. Tom Marlin

Questions

1. The snow-ball effect was discussed during the class.

a. Describe the snow-ball effect in a recycle system.

b. An alternative design is proposed for the CSTR with recycle. It is given in the Figure 1. Discuss the behavior of this control system to the same disturbance considered in the class workshop, i.e., a feed impurity that reduces the reaction rate constant by 10%.

Specifically, does the snow-ball effect occur in this design for the specified disturbance? In your response, describe the qualitative dynamic behavior of key variables, including whether the final values are greater, less, or equal to their initial values.

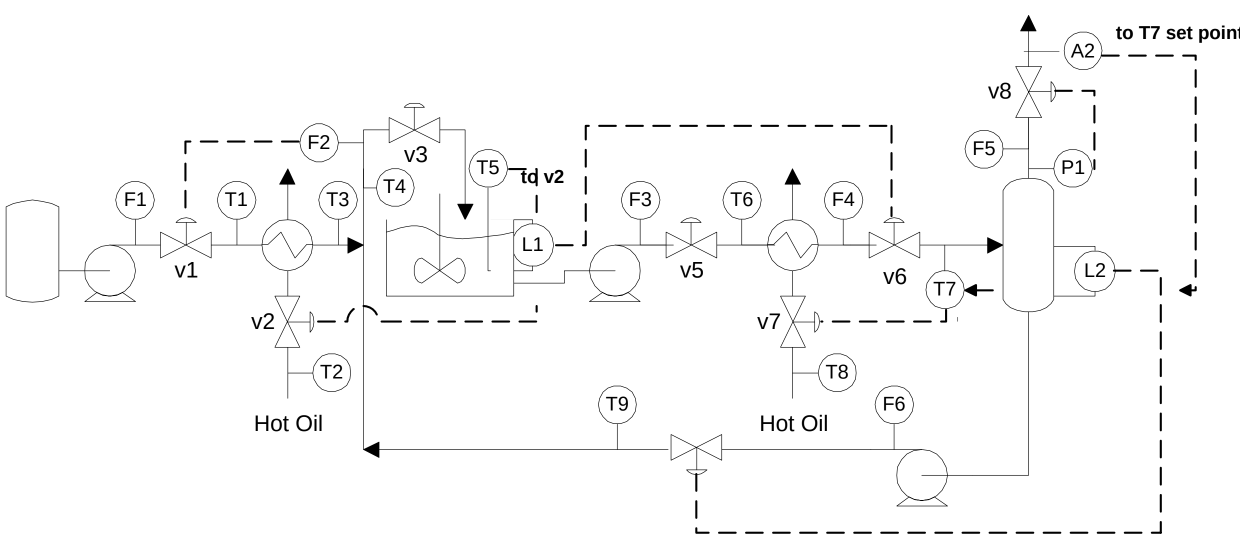


Figure 1

Notes:
1. The heat of reaction is 0.0.
2. The reaction is A $\rightarrow$ B with first order kinetics.
3. You may not add or modify controllers, sensors, valves or other process equipment.

2. You would like to design analyzer controls for the distillation tower in Figure 2. You decide to retain the pressure and level control; thus, you have a 2x2 control system to design. The transfer function model for the system is given in the following for the feedback process and a feed flow rate disturbance.

$$\begin{bmatrix} XD(s) \\ XB(s) \end{bmatrix} = \begin{bmatrix} \dfrac{12.8e^{-s}}{16.7s+1} & \dfrac{-18.9e^{-3s}}{21s+1} \\ \dfrac{6.6e^{-7s}}{10.9s+1} & \dfrac{-19.4e^{-3s}}{14.4s+1} \end{bmatrix} \begin{bmatrix} F_R(s) \\ F_V(s) \end{bmatrix} + \begin{bmatrix} \dfrac{3.8e^{-8.1s}}{14.9s+1} \\ \dfrac{4.9e^{-3.4s}}{13.2s+1} \end{bmatrix} F(s)$$

a. Evaluate whether the product purities are controllable in the steady-state.

b. Evaluate the integrity of all possible 2x2 multiloop control systems. Comment on the implications for the final design.

c. For all control systems with acceptable integrity, determine if the interaction is favorable for

   i. A set point change to the distillate controller.

   ii. The feed flow rate disturbance for which the model is given.

d. Would you recommend decoupling to improve the closed-loop feed-flow disturbance response?

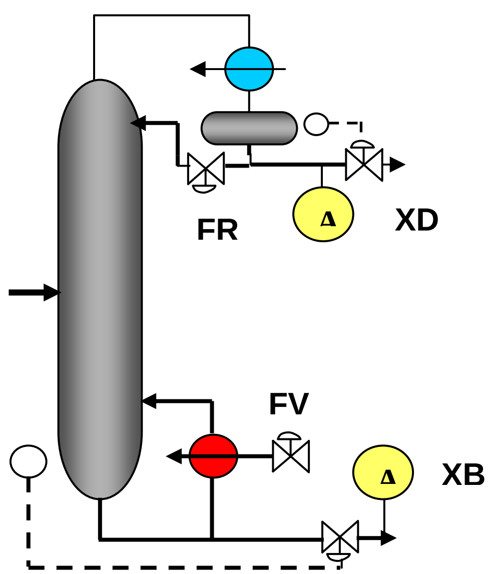


Figure 2.

3. The <u>mixing</u> process in Figure 3 involves a tank to mix components A and B. The effluent from the mixing tank in blended with a stream of component C. The flow of F6 stream is "wild", i.e. it changes to accommodate operations in another process and cannot be adjusted by this control strategy. Note that the flow to waste is to be <u>minimized</u>.

a. Using only the equipment shown in the figure, design a control system to tightly control the percentages of A, B, and C in the blended product. Can you achieve this and also control the total flow of blended product?

b. Improve your result in (a) by adding an on-stream analyzer that can measure all of the components in one stream. Decide the proper location and use it in the control system. Discuss why the analyzer would improve the performance.

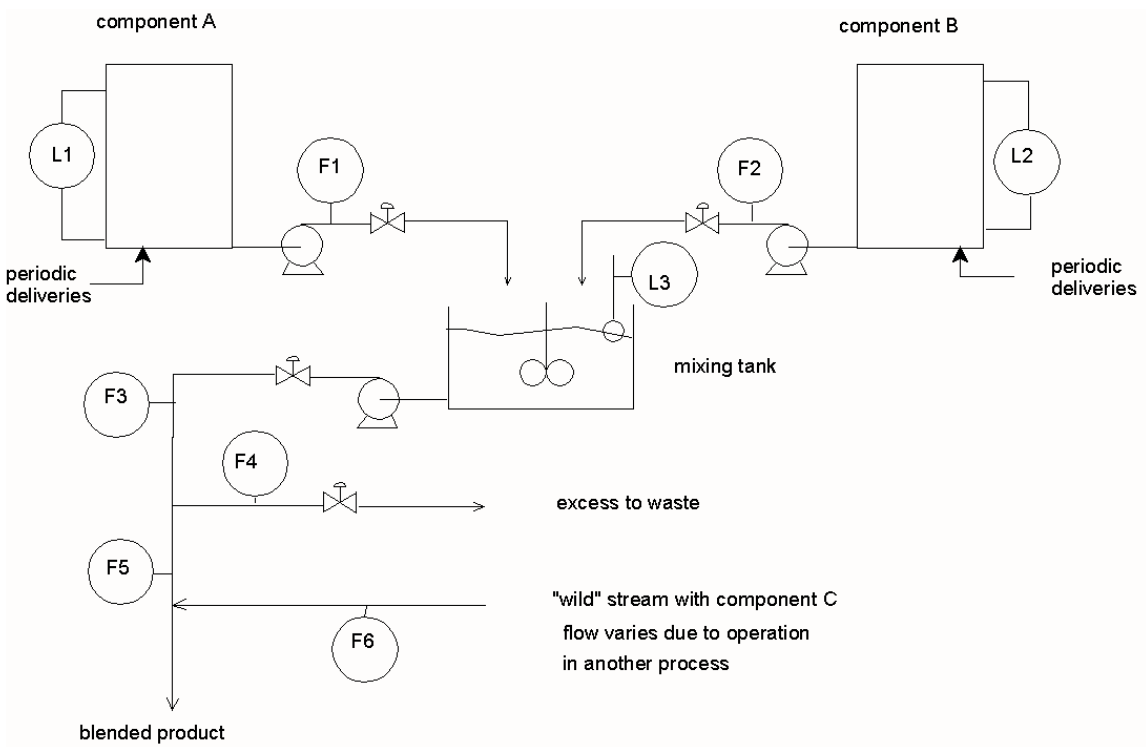


Figure 3.

Process Control Design
PASI 2005
SOLUTIONS

1. The snow-ball effect was discussed during the class.

a. Describe the snow-ball effect in a recycle system.

The snow-ball effect occurs when dynamic behavior of a variable (or variables) is strongly affected by recycle. Specifically, a variable has a very long time constant, and in the extreme, becomes unstable, i.e., an integrating variables.

In the class example of the reactor with recycle, the concentration of the reactant entered with the feed, was consumed in the reaction, and exited with the product in a fixed percentage of the product flow rate. Any disturbance affects this balance. For example, the case with a constant reactor temperature and a reduction in the rate constant, the consumption in the reactor decreased. The overall mass balance of reactant in the system indicated an accumulation. The fresh feed was constant and the effluent product changed very little, so that the recycle of unreacted reactant increased. A new steady state was achieved with the reactant concentration in the reactor much higher, so that the product of the reactant concentration and the rate constant returns to (approximately) its original value. However, the recycle flow increased substantially.

Similar behavior can occur with energy recycles as well. In the extreme, a system with "heat release" do to exothermic reaction can be unstable when recycle heat exchange is provided.

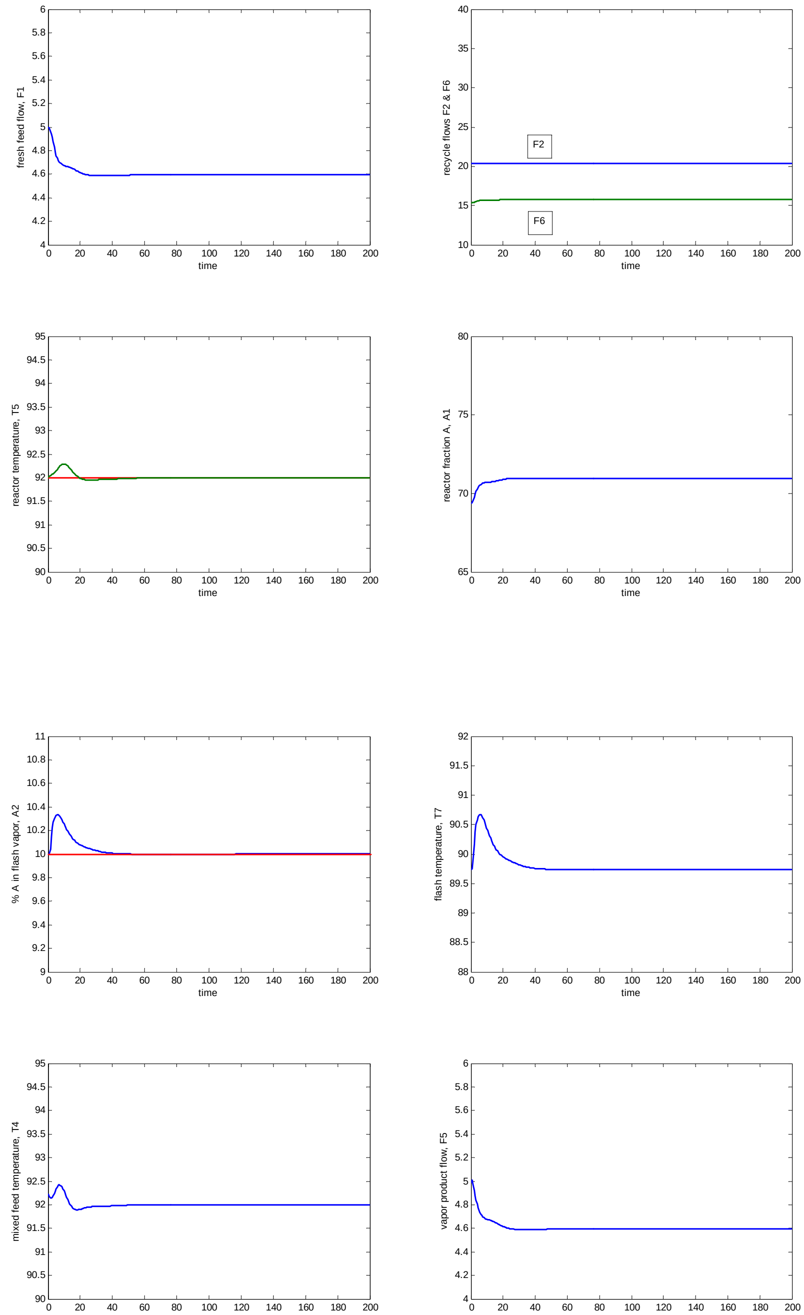
b. An alternative design is proposed for the CSTR with recycle. It is given in the Figure 1. Discuss the behavior of this control system to the same disturbance considered in the class workshop, i.e., a feed impurity that reduces the reaction rate constant by 10%. Specifically, does the snow-ball effect occur in this design?

The immediate effect of the disturbance is a reduction in the rate of reaction of A to products. We note that the composition of the product (% unreacted A) is controlled in the product stream. As a result of the increase in A and decrease in B in the reactor effluent, the product flow rate decreases and the recycle flow rate increases.

Importantly, we note that the total flow rate to the reactor (F2) is controlled. Therefore, when the recycle (F6) increases, the F2 controller immediately reduces the flow rate of fresh feed by partially closing valve v1. The reactor has essentially a constant feed flow rate and a lower (single-pass) conversion. At the new steady state, the product flow decreases, and the fresh feed flow decreases.

We note that the snow-ball effect does not occur with this design. The control system balances the reactant A by adjusting the fresh feed, to maintain the total feed to the reactor. This design eliminates the snow-ball effect without the expensive A1 analyzer.

A plot of the dynamic response with the proposed control design in given below.



We note that the variability of most measurement is lower and that the snow-ball effect does not occur. However, the feed and production rates have decreased, which might be a serious degradation of performance in some cases. If instantaneous control of production rate is not required, the rate could be returned slowly to its desired value by adjusting the set point to F2. However, this will result in the same final operation as the snow-ball effect.

2. You would like to design analyzer controls for the distillation tower in Figure 2. You decide to retain the pressure and level control; thus, you have a 2x2 control system to design. The transfer function model for the system is given in the following.

$$\begin{bmatrix} XD(s) \\ XB(s) \end{bmatrix} = \begin{bmatrix} \dfrac{12.8e^{-s}}{16.7s+1} & \dfrac{-18.9e^{-3s}}{21s+1} \\ \dfrac{6.6e^{-7s}}{10.9s+1} & \dfrac{-19.4e^{-3s}}{14.4s+1} \end{bmatrix} \begin{bmatrix} F_R(s) \\ F_V(s) \end{bmatrix} + \begin{bmatrix} \dfrac{3.8e^{-8.1s}}{14.9s+1} \\ \dfrac{4.9e^{-3.4s}}{13.2s+1} \end{bmatrix} X_F(s)$$

a. Evaluate whether the product purities are controllable in the steady state.

We determine the controllability of the steady state by evaluating the determinant of the gain matrix, which must not be zero; i.e., the square gain matrix must be non-singular.

$$\textbf{Det (K)} = 12.8(-19.4) - 6.6(-18.9) = -127 \neq 0$$

Therefore, the system is controllable, in the steady-state sense. We note that this result is for the specific operating point.

b. Evaluate the integrity of all possible 2x2 multiloop control systems. Comment on the implications for the final design.

To evaluate the integrity, we will look at the integral controllability with integrity. A necessary condition is that the multiloop design contains pairings on positive relative gain array elements. The relative gain is evaluated below.

$$\lambda_{11} = \frac{1}{1 - \dfrac{K_{12}K_{21}}{K_{11}K_{22}}} = \frac{1}{1 - \dfrac{(6.6)(-18.9)}{(12.8)(-19.4)}} = \frac{1}{1 - .489} = 2.0$$

	FR	FV
XD	2	−1
XB	−1	2

We observe that only one of the two possible pairings have positive values. We conclude that only the XD-FR and XB-FV pairings should be considered <u>if integrity is a high priority</u>.

c. For all control systems with acceptable integrity, determine if the interaction is favorable for

i. A set point change to the distillate controller.

We know that the RDG = RGA for a single set point change. Here, RDG = RGA = 2 >1. Therefore, we conclude that the interaction is <u>unfavorable</u>. The multiloop IAE for XD will be at least twice the value obtained with the single-loop control (with XB off).

ii. The feed flow rate disturbance for which the model is given.

For this case, we must calculate the RDG for XD.

$$RDG(1,1) = \left(\frac{1}{1 - \left(K_{12}K_{21} \big/ K_{11}K_{22} \right)} \right) \left(1 - \frac{K_{d2}K_{12}}{K_{d1}K_{22}} \right)$$

$$\mathbf{RDG}_{\mathbf{XD}} = \mathbf{(2.0)} \left[\mathbf{1 - \frac{(4.9)(-18.9)}{(3.8)(-19.4)}} \right] = -0.51$$

$$\mathbf{RDG}_{\mathbf{XB}} = \mathbf{(2.0)} \left[\mathbf{1 - \frac{(3.8)(6.6)}{(4.9)(12.8)}} \right] = 1.20$$

We observe that the absolute values for the RDG's for both controlled variables are close to 1.0. Therefore, we expect that the multiloop control performance will be similar to each single-loop performance. We conclude that interaction is <u>favorable</u>. We recall that +/- cancellation is possible, so that this conclusion is not rigorous.

d. Would you recommend decoupling to improve the closed-loop feed-flow disturbance response?

To answer this question, we refer to the following table.

$\|(RDG)(f_{tune})\|$	Interpretation	Decision
< 1	Favorable interaction	Do not decouple
≈ 1	No significant difference	Do not decouple
> 1	Unfavorable interaction	Decouple (Caution regarding robustness)

We note that the f_{tune} values are usually between 1.0 and 2.0. Therefore,

For XD, $|RDG*f_{tune}|$ is about equal to 1.0. Therefore, no decoupling for XD is required.

For XB, $|RDG*f_{tune}|$ could be equal to 2.0. Therefore, decoupling could improve dynamic performance.

3.

a.

The key insight in the solution is that the production should be on flow control. Then, the level must "pull" feed into the tank. With this done, the stream to waste can be set to zero.

Also, certain flow ratios must be maintained; these are the FY symbols, and the values for the ratios must be set by a person. Perfect composition control is not achieved because of inevitable errors in the flow sensors.

The excess flow to waste is to be minimized; therefore, a design with the waste valve permanently closed is developed. Since the ratio of flow from the tank to the "wild" flow of C is to be controlled tightly, the valve leaving the tank is adjusted to achieve the ratio. Tight control is ensured with a flow controller whose set point is maintained as a constant multiple of the measured wild flow rate. This decision eliminates the tank flow out from use in controlling the tank level. The tank level and the ratio of A to (A+B) are to be controlled by adjusting the flows of A and B. This can be achieved by the strategy shown in Figure a. The ratios in this design must be entered by a person.

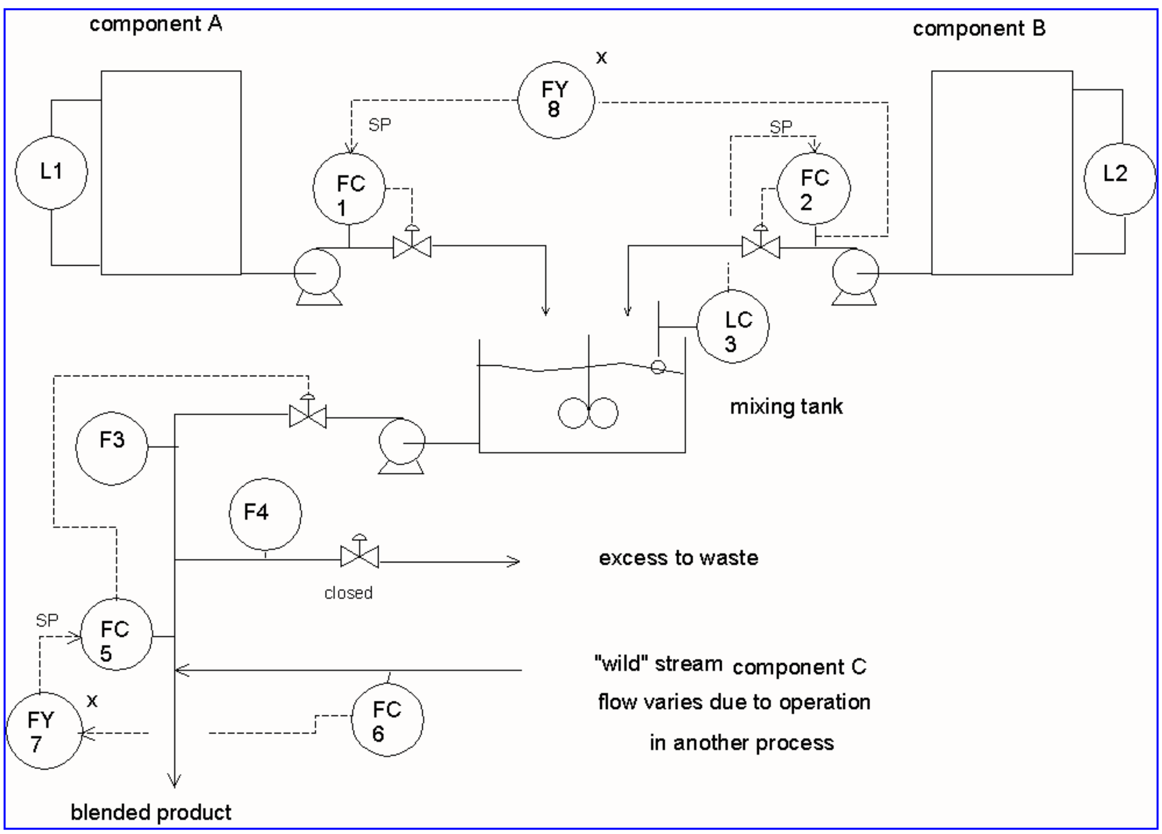


Figure 3.a.

3.

b.

If an analyzer can be added, it should be placed in the product where it can measure all components. The compositions can be used to control the ratios by manipulating the ratio values. Note that the control of appropriate ratios, C/(A+B+C) and A/(A+B), reduces interactions between the feedback controllers.

The main advantage for using the analyzers is to improve the feedback measurement for the compositions. While controlling the flow ratios could theoretically provide good performance, flow measurement errors and disturbances in the feed stream compositions would lead to sustained deviations from the desired product composition. Highly accurate onstream analysis would improve the composition performance.

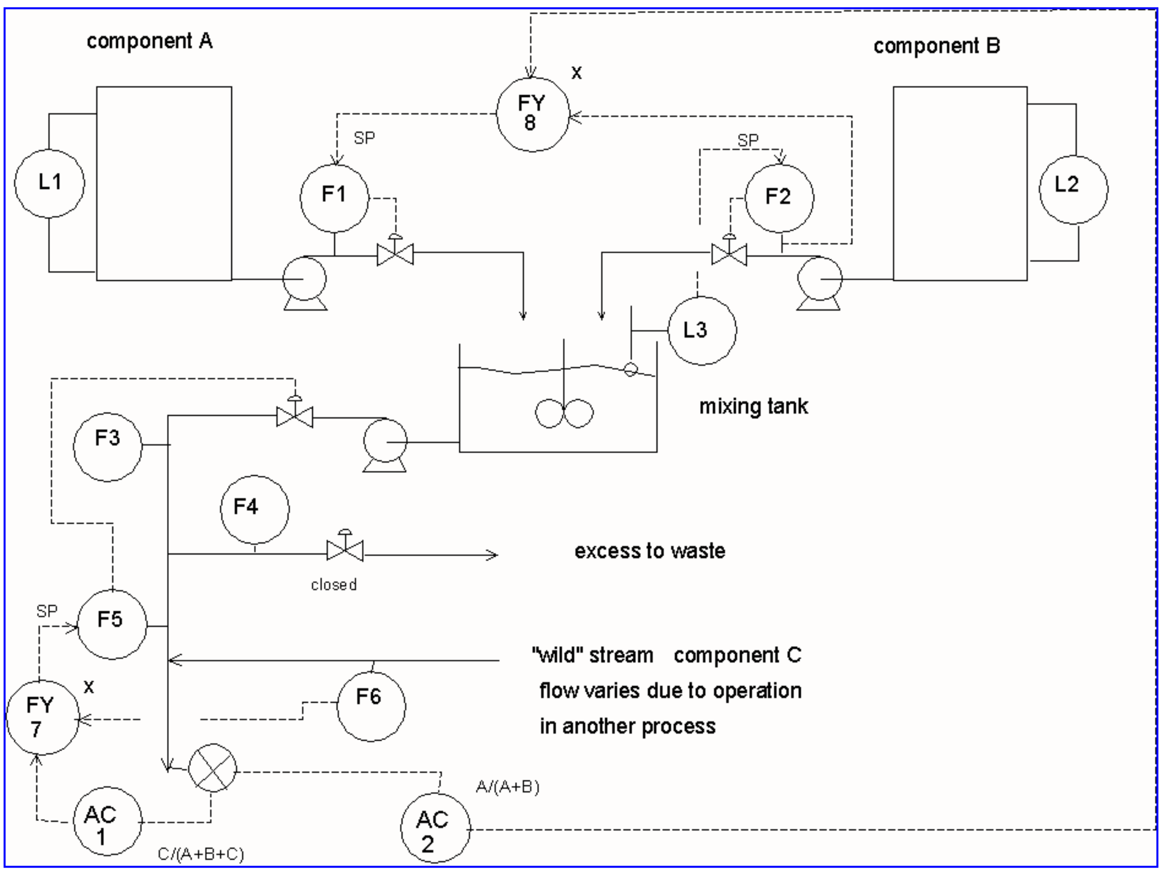


Figure 3.b.