1. Consider three common rules for the synthesis of distillation sequences.

$$P_1 \wedge \neg P_2 \implies \neg P_3$$
$$\neg P_1 \wedge P_4 \implies P_5$$
$$P_2 \implies P_3$$

where

P_1 = lowest concentration component

P_2 = most volatile component

P_3 = remove component from top of column

P_4 = easy component to separate

P_5 = remove component first

(a) Write these logical expressions as English sentences.

(b) Rewrite rules in conjunctive normal form and write as constraints with binary variables.

2. Using GAMS solve the following MINLP problem step by step with

   a) Generalized Benders decomposition
   b) Outer-approximation method
   c) Extended cutting plane

   Also verify your answer with GAMS/DICOPT.

   $$\min f = y_1 + 1.5y_2 + 0.5y_3 + x_1^2 + x_2^2$$

   s.t. $(x_1 - 2)^2 - x_2 \leq 0$

   $$x_1 - 2y_1 \geq 0$$

   $$x_1 - x_2 - 4(1-y_2) \leq 0$$

   $$x_1 - (1 - y_1) \geq 0$$

   $$x_2 - y_2 \geq 0$$

   $$x_1 + x_2 \geq 3y_3$$

   $$y_1 + y_2 + y_3 \geq 1$$

   $$0 \leq x_1 \leq 4. \quad 0 \leq x_2 \leq 4$$

   $$y_1, y_2, y_3 = 0. 1$$

   Starting point $y_1 = y_2 = y_3 = 1$

   $x_1 = x_2 = x_3 = 0$ for extended cutting plane.

3. For the Generalized Disjunctive Program given below.
   a) Reformulate it as an MINLP using the convex hull formulation for the disjunction
   b) Reformulate it as a big-M MINLP (M=50)
   c) Solve both reformulations and compare their relaxations.

$$\min Z = c + (x_1 - 3)^2 + (x_2 - 2)^2$$

st

$$\begin{bmatrix} Y_1 \\ x_1^2 + x_2^2 \leq 1 \\ c = 2 \end{bmatrix} \vee \begin{bmatrix} Y_2 \\ (x_1 - 4)^2 + (x_2 - 1)^2 \leq 1 \\ c = 1 \end{bmatrix} \vee \begin{bmatrix} Y_3 \\ (x_1 - 2)^2 + (x_2 - 4)^2 \leq 1 \\ c = 3 \end{bmatrix}$$

$$0 \leq x_1 \leq 8. \ 0 \leq x_2 \leq 8. \quad Y_j = true, false. \ j = 1.2.3$$

4. It is proposed to manufacture a chemical C with a process I that uses raw material B. B can either be purchased or manufactured with either of two processes. II or III, which use chemical A as a raw material. In order to decide the optimal selection of processes and levels of production that maximize profit formulate the MINLP problem and solve with the augmented penalty/outer-approximation/equality-relaxation algorithm in DICOPT++.

Data:

Conversion: Process I $C = 0.9B$
              Process II $B = \ln(1 + A)$ Maximum capacity: 5 ton prod/hr
              Process III $B = 1.2 \ln(1 + A)$
                            (A. B. C. in ton/hr)

Prices: A \$ 1.800/ton
          B \$ 7.000/ton
          C \$13.000/ton (maximum demand: 1 ton/hr)

Investment cost

	Fixed (10^3\$/hr)	Variable (10^3\$/ton product)
Process I	3.5	2
Process II	1	1
Process III	1.5	1.2

Note: Minimize negative of profit.

Solution - Hwk 6

1) Rules

$$P_1 \wedge \neg P_2 \implies \neg P_3$$
$$\neg P_1 \wedge P_4 \implies P_5$$
$$P_2 \implies P_3$$

a) i) If component in low concentration and not most volatile, do not remove from top.

ii) If component not in low concentration and easy to separate, then removes first.

iii) If most volatile, separate from top.

b) for i)
$$\neg (P_1 \wedge \neg P_2) \vee \neg P_3$$
$$(\neg P_1 \vee P_2) \vee \neg P_3$$
$$\neg P_1 \vee P_2 \vee \neg P_3 \qquad (1-y_1) + y_2 + (1-y_3$$

for ii) $\neg (P_1 \wedge P_4) \vee P_5$

$$\neg P_1 \vee \neg P_4 \vee P_5 \qquad (1-y_1) + (1-y_4)$$
$$+ y_5 \geq 1$$

for iii) $\neg P_2 \vee P_3$

$$(1-y_2) + y_3 \geq 1$$

2) 20 Point

a) Generalized Benders Decomposition:

<u>1st Iteration:</u>

$y_1 = 1 \quad y_2 = 1 \quad y_3 = 1$ NLP: $x_1 = 2 \quad x_2 = 2 \quad UB = 11 \quad \mu_1 = 8 \quad \mu_2 = 4$

                                   MILP: $y_1 = 0 \quad y_2 = 0 \quad y_3 = 1 \quad LB = -23.5$

<u>2nd Iteration:</u>

$y_1 = 0 \quad y_2 = 0 \quad y_3 = 1$ NLP: $x_1 = 1.5 \quad x_2 = 1.5 \quad UB = 5 \quad \mu_3 = 6$

                                     MILP: $y_1 = 1 \quad y_2 = 0 \quad y_3 = 0 \quad LB = -3.5$

<u>3rd Iteration:</u>

$y_1 = 1 \quad y_2 = 0 \quad y_3 = 0$ NLP: $x_1 = 2 \quad x_2 = 0 \quad UB = 5 \quad \mu_4 = 4$

                                     MILP: $y_1 = 0 \quad y_2 = 1 \quad y_3 = 0 \quad LB = -2.5$

<u>4th Iteration:</u>

$y_1 = 0 \quad y_2 = 1 \quad y_3 = 0$ NLP: $x_1 = 1 \quad x_2 = 1 \quad UB = 3.5 \quad \mu_5 = 1.333 \quad \mu_6 = 0.667$

                                     MILP: $y_1 = 0 \quad y_2 = 1 \quad y_3 = 0 \quad LB = 3.5$

b) Outer Approximation:

<u>1st Iteration:</u>

$y_1 = 1 \quad y_2 = 1 \quad y_3 = 1$ NLP: $x_1 = 2 \quad x_2 = 2 \quad UB = 11$

                                     MILP: $x_1 = 2 \quad x_2 = 0 \quad y_1 = 1 \quad y_2 = 0 \quad y_3 = 0 \quad LB = 1$

<u>2nd Iteration:</u>

$y_1 = 1 \quad y_2 = 0 \quad y_3 = 0$ NLP: $x_1 = 2 \quad x_2 = 0 \quad UB = 5$

                                     MILP: $x_1 = 1 \quad x_2 = 1 \quad y_1 = 0 \quad y_2 = 1 \quad y_3 = 0 \quad LB = 1.5$

<u>3rd Iteration:</u>

$y_1 = 0 \quad y_2 = 1 \quad y_3 = 0$ NLP: $x_1 = 1 \quad x_2 = 1 \quad UB = 3.5$

                                     MILP: $x_1 = 1 \quad x_2 = 1 \quad y_1 = 0 \quad y_2 = 1 \quad y_3 = 0 \quad LB = 3.5$

c) Extended Cutting Plane:

<u>1st Iteration:</u>

$y_1 = 0 \quad y_2 = 1 \quad y_3 = 1$
$x_1 = 1 \quad x_2 = 4 \quad Z = 0.5$

<u>2nd Iteration:</u>

$y_1 = 0 \quad y_2 = 0 \quad y_3 = 1$
$x_1 = 3 \quad x_2 = 0 \quad Z = 0.5$

<u>3rd Iteration:</u>

$y_1 = 0 \quad y_2 = 0 \quad y_3 = 1$
$x_1 = 1.5 \quad x_2 = 1.5 \quad Z = 0.5$

<u>4th Iteration:</u>

$y_1 = 0 \quad y_2 = 1 \quad y_3 = 0$
$x_1 = 1 \quad x_2 = 1 \quad Z = 3$

<u>5th Iteration:</u>

$y_1 = 0 \quad y_2 = 1 \quad y_3 = 0$
$x_1 = 1 \quad x_2 = 1 \quad Z = 3.5$

3)   20 Point

a) Convex Hull Reformulation:

$$x_1 = z_1 + z_2 + z_3$$
$$x_2 = w_1 + w_2 + w_3$$

$$\min \quad Z = (x_1 - 3)^2 + (x_2 - 2)^2 + 2y_1 + y_2 + 3y_3$$

$$\left[\left(\frac{z_1}{y_1 + \varepsilon}\right)^2 + \left(\frac{w_1}{y_1 + \varepsilon}\right)^2 - 1 - 1(y_1 - 1)\right](y_1 + \varepsilon) \le 0$$

$$\left[\left(\frac{z_2}{y_2 + \varepsilon} - 4\right)^2 + \left(\frac{w_2}{y_2 + \varepsilon} - 1\right)^2 - 1 + 16(y_2 - 1)\right](y_2 + \varepsilon) \le 0$$

$$\left[\left(\frac{z_3}{y_3 + \varepsilon} - 2\right)^2 + \left(\frac{w_3}{y_3 + \varepsilon} - 4\right)^2 - 1 + 19(y_3 - 1)\right](y_3 + \varepsilon) \le 0$$

$$y_1 + y_2 + y_3 = 1$$

$$0 \le z_1 \le 8y_1 \qquad\qquad 0 \le w_1 \le 8y_1$$
$$0 \le z_2 \le 8y_2 \qquad\qquad 0 \le w_2 \le 8y_2$$
$$0 \le z_3 \le 8y_3 \qquad\qquad 0 \le w_3 \le 8y_3$$

Note:
The convex hulls are formulated by using,

$$(\lambda + \varepsilon)\left[g\left(\frac{\gamma}{\lambda + \varepsilon}\right) + g(0)(\lambda - 1)\right] \le 0$$

b) Big-M Reformulation:

$$\min \quad Z = (x_1 - 3)^2 + (x_2 - 2)^2 + 2y_1 + y_2 + 3y_3$$
$$x_1^2 + x_2^2 \le 1 + M(1 - y_1)$$
$$(x_1 - 4)^2 + (x_2 - 1)^2 \le 1 + M(1 - y_2)$$
$$(x_1 - 2)^2 + (x_2 - 4)^2 \le 1 + M(1 - y_3)$$
$$y_1 + y_2 + y_3 = 1$$
$$y_1, y_2, y_3 \in \{0,1\}$$
$$0 \le x_1 \le 8$$
$$0 \le x_2 \le 8$$

c)

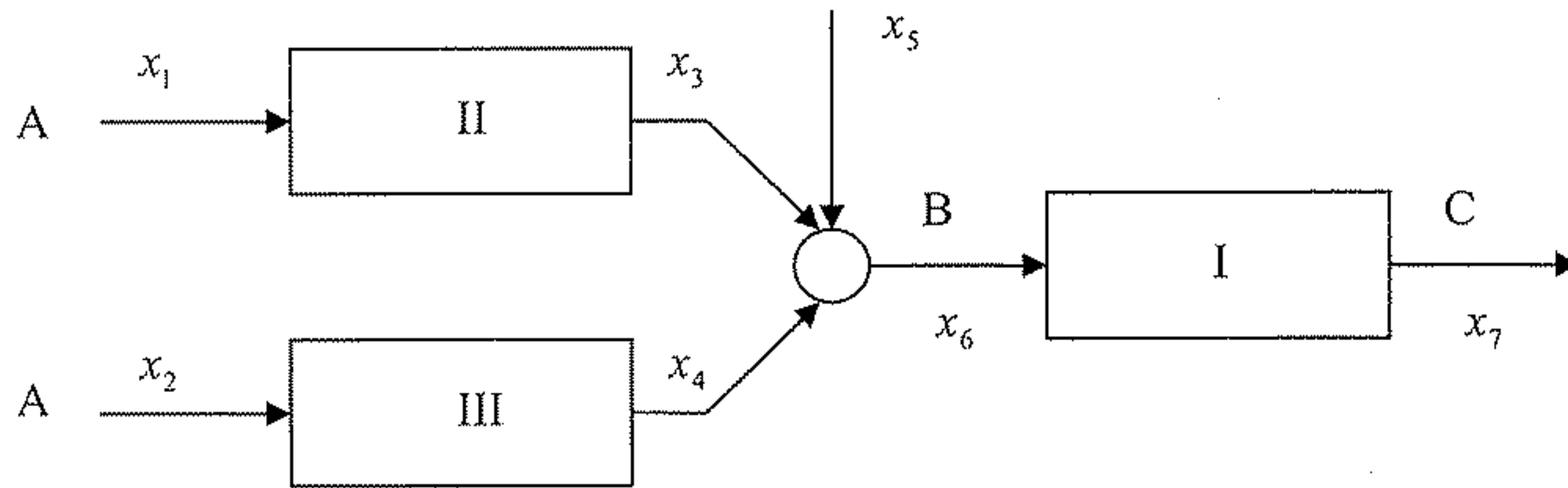|	
Optimal solution:	1.1716
	$y_2 = 1, x_1 = 3.293, x_2 = 1.707,$
Big-M relaxation (M=50):	1.0192
	$y_1 = 0.018, y_2 = 0, y_3 = 0.982, x_1 = 3.020, x_2 = 1.98$
Big-M relaxation (M=30):	1.0312
	$y_1 = 0.029, y_2 = 0.971, y_3 = 0, x_1 = 3.032, x_2 = 1.968$
Convex Hull relaxation:	1.1538
	$y_1 = 0.016, y_2 = 0.955, y_3 = 0.029, x_1 = 3.195, x_2 = 1.797$

Big-M relaxation is always worse than the convex hull relaxation.

4) 20 Point

A $\xrightarrow{x_1}$ [II] $\xrightarrow{x_3}$ $x_5 \downarrow$ $\bigcirc$ $\xrightarrow[x_6]{B}$ [I] $\xrightarrow[x_7]{C}$

A $\xrightarrow{x_2}$ [III] $\xrightarrow{x_4}$

$$Min \quad Z = -\left(-1800x_1 - 1800x_2 - 2000x_3 - 1000x_4 - 7000x_5 - 1200x_7 + 13000x_7 \right.$$
$$\left. - 3500y_1 - 1000y_2 - 1500y_3\right)$$

$s.t.$

$$x_7 \leq 1$$
$$x_7 = 0.9\, x_6$$
$$x_3 = \ln(1 + x_1)$$
$$x_4 = 1.2\ln(1 + x_2)$$
$$x_3 + x_4 + x_5 = x_6$$
$$x_7 \leq y_1$$
$$x_3 \leq 5y_2$$
$$x_4 \leq 10y_3$$

Solution:
$Z = \$1923 / hr$
$x_1 = 0$
$x_2 = 1.524$
$x_3 = 0$
$x_4 = 1.111$
$x_5 = 0$
$x_6 = 1.111$
$x_7 = 1.0$
$y_1 = 1$
$y_2 = 0$
$y_3 = 1$