Appendix A

Problem A.1

(a) $$\boldsymbol{A}\ \boldsymbol{B} = \begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix}\begin{bmatrix} 0 & 4 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 7 \\ 1 & 11 \end{bmatrix}$$

$$\boldsymbol{B}\ \boldsymbol{A} = \begin{bmatrix} 0 & 4 \\ 1 & 3 \end{bmatrix}\begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 8 & 4 \\ 7 & 4 \end{bmatrix}$$

$$\boldsymbol{A}\ \boldsymbol{B} \neq \boldsymbol{B}\ \boldsymbol{A}$$

(b) $$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{B} = \begin{bmatrix} 1 & 2 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} 0 & 4 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 2 & 10 \\ 1 & 7 \end{bmatrix}$$

(c) $$\boldsymbol{A}+\boldsymbol{B} = \begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 4 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 5 \\ 3 & 4 \end{bmatrix}$$

(d) $$\boldsymbol{A}-\boldsymbol{B} = \begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 4 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 1 & -3 \\ 1 & -2 \end{bmatrix}$$

(e) $$\det \boldsymbol{A} = (1)(1)-(1)(2) = 1$$
$$\det \boldsymbol{B} = (0)(3)-(1)(4) = -4$$

(f) $$\operatorname{adj} \boldsymbol{A} = \begin{bmatrix} 1 & -1 \\ -2 & 1 \end{bmatrix} \qquad \operatorname{adj} \boldsymbol{B} = \begin{bmatrix} 3 & -4 \\ -1 & 0 \end{bmatrix}$$

(g) $$\boldsymbol{A}^{-1} = \frac{\operatorname{adj} \boldsymbol{A}}{\det \boldsymbol{A}} = \begin{bmatrix} -1 & 1 \\ 2 & -1 \end{bmatrix} \qquad \boldsymbol{B}^{-1} = \frac{\operatorname{adj} \boldsymbol{B}}{\det \boldsymbol{B}} = \begin{bmatrix} -3/4 & 1 \\ 1/4 & 0 \end{bmatrix}$$

Verify: $$\boldsymbol{A}^{-1}\boldsymbol{A} = \begin{bmatrix} -1 & 1 \\ 2 & -1 \end{bmatrix}\begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\boldsymbol{B}^{-1}\boldsymbol{B} = \begin{bmatrix} -3/4 & 1 \\ 1/4 & 0 \end{bmatrix}\begin{bmatrix} 0 & 4 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Problem A.2

(a) $\boldsymbol{A} = \begin{bmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \\ 1 & 0 & 1 \end{bmatrix} \quad \boldsymbol{b} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \quad \det \boldsymbol{A} = -8$

$$\boldsymbol{D} = [\boldsymbol{A} \vdots \boldsymbol{b}] = \begin{bmatrix} 1 & 2 & 3 & 1 \\ 3 & 2 & 1 & 2 \\ 1 & 0 & 1 & 1 \end{bmatrix}$$

subtract row 1 from row 3

$$\boldsymbol{D} = \begin{bmatrix} 1 & 2 & 3 & 1 \\ 3 & 2 & 1 & 2 \\ 0 & -2 & -2 & 0 \end{bmatrix} \quad \det \boldsymbol{A} = -8$$

multiply row 1 by 3 and subtract from row 2

$$\boldsymbol{D} = \begin{bmatrix} 1 & 2 & 3 & 1 \\ 0 & -4 & -8 & -1 \\ 0 & -2 & -2 & 0 \end{bmatrix} \quad \det \boldsymbol{A} = -8$$

multiply row 2 by ½ and subtract from row 3

$$\boldsymbol{D} = \begin{bmatrix} 1 & 2 & 3 & 1 \\ 0 & -4 & -8 & -1 \\ 0 & 0 & 2 & 1/2 \end{bmatrix} \quad \det \boldsymbol{A} = -8$$

Thus,

$$\begin{bmatrix} 1 & 2 & 3 \\ 0 & -4 & -8 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ 1/2 \end{bmatrix}$$

$$2x_3 = \tfrac{1}{2} \Rightarrow x_3 = \tfrac{1}{4}$$
$$-4x_2 - 8x_3 = -4x_2 - 8(1/4) = -1 \Rightarrow x_2 = -1/4$$
$$x_1 + 2x_2 + 3x_3 = x_1 + 2(-1/4) + 3(1/4) = 1$$

$$\Rightarrow x_1 = 3/4$$

$$\boldsymbol{x} = \begin{bmatrix} 3/4 & -1/4 & 1/4 \end{bmatrix}^{\mathrm{T}}$$

(b) $\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$

$$\boldsymbol{A}^{-1} = \frac{\text{adj}\,\boldsymbol{A}}{\det\boldsymbol{A}} = \frac{\begin{bmatrix} 2 & -2 & -2 \\ -2 & -2 & 2 \\ -4 & 8 & -4 \end{bmatrix}^{\mathrm{T}}}{-8} \qquad = \begin{bmatrix} -1/4 & 1/4 & 1/2 \\ 1/4 & 1/4 & -1 \\ 1/4 & -1/4 & 1/2 \end{bmatrix}$$

$$\boldsymbol{x} = \begin{bmatrix} -1/4 & 1/4 & 1/2 \\ 1/4 & 1/4 & -1 \\ 1/4 & -1/4 & 1/2 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 3/4 \\ -1/4 \\ 1/4 \end{bmatrix}$$

(c)

$$x_1 = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 2 & 1 \\ 1 & 0 & 1 \end{bmatrix} \div \det\boldsymbol{A} = \frac{-6}{-8} = 3/4$$

$$x_2 = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 2 & 1 \\ 1 & 1 & 1 \end{bmatrix} \div \det\boldsymbol{A} = \frac{2}{-8} = -1/4$$

$$x_3 = \begin{bmatrix} 1 & 2 & 1 \\ 3 & 2 & 2 \\ 1 & 0 & 1 \end{bmatrix} \div \det\boldsymbol{A} = \frac{-2}{-8} = 1/4$$

Problem A.3

$$z_1 = 3x_1 + x_3$$

$$z_2 = x_1 + x_2 + x_3 \quad \text{or } \boldsymbol{z} = \boldsymbol{A}\boldsymbol{x} \quad , \boldsymbol{A} = \begin{bmatrix} 3 & 0 & 1 \\ 1 & 1 & 1 \\ 0 & 2 & 1 \end{bmatrix}$$

$$z_3 = 2x_2 + x_3$$

Solve $x_3 = z_1 - 3x_1$

$$z_2 = x_1 + x_2 + z_1 - 3x_1 = x_2 - 2x_1 + z_1$$

$$x_2 = \frac{1}{2} z_3 - \frac{1}{2} x_3 = \frac{1}{2} z_3 - \frac{1}{2} z_1 + \frac{3}{2} x_1$$

Then $\quad z_2 = \frac{1}{2} z_3 - \frac{1}{2} z_1 + \frac{3}{2} x_1 - 2x_1 + z_1$

$$x_1 = z_1 - 2z_2 + z_3$$

Now $\quad x_3 = z_1 - 3x_1 = z_1 - 3(z_1 - 2z_2 + z_3)$

$$x_3 = -2z_1 + 6z_2 - 3z_3$$

and, $\quad x_2 = \frac{1}{2} z_3 - \frac{1}{2} x_3$

$$x_2 = z_1 - 3z_2 + 2z_3$$

or, $\quad \boldsymbol{x} = \begin{bmatrix} 1 & -2 & 1 \\ 1 & -3 & 2 \\ 2 & 6 & -3 \end{bmatrix} \boldsymbol{z}$

Also, $\quad \boldsymbol{x} = \boldsymbol{A}^{-1} \boldsymbol{z}$

$$\boldsymbol{A}^{-1} = \left[\frac{\text{adj}\,\boldsymbol{A}}{\det \boldsymbol{A}} \right] = \frac{\begin{bmatrix} -1 & -1 & 2 \\ 2 & 3 & -6 \\ -1 & -2 & 3 \end{bmatrix}^{\mathrm{T}}}{-1} = \begin{bmatrix} 1 & -2 & 1 \\ 1 & -3 & 2 \\ -2 & 6 & -3 \end{bmatrix}$$

This checks with the result obtained using algebraic manipulation.

Problem A.4

$$\|\boldsymbol{x}\| = \left(\boldsymbol{x}^{\mathrm{T}} \boldsymbol{x} \right)^{1/2}$$

$$\|\boldsymbol{x}_1\| = \left(1^2 + 1^2 + 2^2 \right)^{1/2} = \sqrt{6} = 2.45$$

$$\|\boldsymbol{x}_2\| = \left(1^2 + 0^2 + 2^2 \right)^{1/2} = \sqrt{5} = 2.24$$

$$\boldsymbol{x}_1^{\mathrm{T}} \boldsymbol{x}_2 = [1\ 1\ 2] \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix} = 5$$

$$\boldsymbol{x}_1\boldsymbol{x}_2^T = \begin{bmatrix}1\\1\\2\end{bmatrix}\begin{bmatrix}1 & 0 & 2\end{bmatrix} = \begin{bmatrix}1 & 0 & 2\\1 & 0 & 2\\2 & 0 & 4\end{bmatrix}$$

$$\boldsymbol{x}_1^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x}_1 = \begin{bmatrix}1 & 1 & 2\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\0 & 2 & 0\\0 & 0 & 4\end{bmatrix}\begin{bmatrix}1\\1\\2\end{bmatrix} = \begin{bmatrix}1 & 2 & 8\end{bmatrix}\begin{bmatrix}1\\1\\2\end{bmatrix} = 19$$

Let $\boldsymbol{x}_3 = \begin{bmatrix}x_3^1 & x_3^2 & x_3^3\end{bmatrix}^{\mathrm{T}}$. Then $\boldsymbol{x}_1^{\mathrm{T}}\boldsymbol{x}_3 = x_3^1 + x_3^2 + 2x_3^3$

Let $\boldsymbol{x}_3^1 = \boldsymbol{x}_3^2 = 1$. Then $\boldsymbol{x}_1^{\mathrm{T}}\boldsymbol{x}_3 = 0 \Rightarrow \boldsymbol{x}_3^3 = -1$

$\boldsymbol{x}_3 = \begin{bmatrix}1 & 1 & -1\end{bmatrix}^{\mathrm{T}}$ is orthogonal to $\boldsymbol{x}_1$.

$$\det\begin{bmatrix}\boldsymbol{x}_1 \vdots \boldsymbol{x}_2 \vdots \boldsymbol{x}_3\end{bmatrix} = \det\begin{bmatrix}1 & 1 & 1\\1 & 0 & 1\\2 & 2 & -1\end{bmatrix} = 3 \quad (\neq 0)$$

$\boldsymbol{x}_1$, $\boldsymbol{x}_2$ and $\boldsymbol{x}_3$ are linearly independent.

Problem A.5

$$\boldsymbol{A} = \begin{bmatrix}1 & 1 & 2\\-1 & 0 & 1\\-2 & -3 & 1\end{bmatrix}$$

Using minors of the second row,

$$\det\boldsymbol{A} = (-1)(-1)^{1+2}\begin{vmatrix}1 & 2\\-3 & 1\end{vmatrix} + (0)(-1)^{2+2}\begin{vmatrix}1 & 2\\-2 & 1\end{vmatrix}$$

$$+(1)(-1)^{3+2}\begin{vmatrix}1 & 1\\-2 & -3\end{vmatrix}$$

$$= 1(1+6) + 0 + (-1)(-3+2) = 8$$

Using minors of the third column,

$$\det \boldsymbol{A} = (2)(-1)^{1+3}\begin{vmatrix} -1 & 0 \\ -2 & -3 \end{vmatrix} + (1)(-1)^{2+3}\begin{vmatrix} 1 & 1 \\ -2 & -3 \end{vmatrix}$$

$$+(1)(-1)^{3+3}\begin{vmatrix} 1 & 1 \\ -1 & 0 \end{vmatrix}$$

$$= 2(3+0) + (-1)(-3+2) + (1)(0+1) = 8$$

Problem A.6

(a) $\boldsymbol{A} = \begin{bmatrix} 0 & 1 \\ 1 & 4 \end{bmatrix} \quad \boldsymbol{A} - \lambda \boldsymbol{I} = \begin{bmatrix} -\lambda & 1 \\ 1 & 4-\lambda \end{bmatrix}$

$\det(\boldsymbol{A} - \lambda \boldsymbol{I}) = -\lambda(4-\lambda) - 1 = \lambda^2 - 4\lambda - 1 = 0$

Eigenvalues are $\lambda_1 = 2 + \sqrt{5}$ and $\lambda_2 = 2 - \sqrt{5}$.

The eigenvector $\boldsymbol{v}_1 = \begin{bmatrix} v_1^1 & v_1^2 \end{bmatrix}^{\mathrm{T}}$ corresponding to λ_1 is given by

$$\begin{bmatrix} 0 & 1 \\ 1 & 4 \end{bmatrix}\begin{bmatrix} v_1^1 \\ v_1^2 \end{bmatrix} = \left(2+\sqrt{5}\right)\begin{bmatrix} v_1^1 \\ v_1^2 \end{bmatrix} \qquad \begin{matrix} \text{Let } \; v_1^1 = 1 \\ \Rightarrow v_1^2 = 2+\sqrt{5} \end{matrix} \qquad \boldsymbol{v}_1 = \begin{bmatrix} 1 \\ 2+\sqrt{5} \end{bmatrix}$$

The eigenvector $\boldsymbol{v}_2 = \begin{bmatrix} v_2^1 & v_2^2 \end{bmatrix}^{\mathrm{T}}$ corresponding to λ_2 is

$$\begin{bmatrix} 0 & 1 \\ 1 & 4 \end{bmatrix}\begin{bmatrix} v_2^1 \\ v_2^2 \end{bmatrix} = \left(2-\sqrt{5}\right)\begin{bmatrix} v_2^1 \\ v_2^2 \end{bmatrix} \qquad \begin{matrix} \text{Let } \; v_2^1 = 1 \\ \Rightarrow v_2^2 = 2-\sqrt{5} \end{matrix} \qquad \boldsymbol{v}_2 = \begin{bmatrix} 1 \\ 2-\sqrt{5} \end{bmatrix}$$

(b) $\boldsymbol{A} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{bmatrix} \quad \det(\boldsymbol{A} - \lambda I) = (2-\lambda)(3-\lambda)(2-\lambda) = 0$

$\Rightarrow$ eigenvalues are $\lambda_1 = 2, \lambda_2 = 3$ and $\lambda_3 = 2$.

The eigenvector $\boldsymbol{v}_1$ corresponding to $\lambda_1 = 2$ is

$$\begin{bmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} v_1^1 \\ v_1^2 \\ v_1^3 \end{bmatrix} = 2 \begin{bmatrix} v_1^1 \\ v_1^2 \\ v_1^3 \end{bmatrix} \Rightarrow \begin{matrix} 2v_1^1 = 2v_1^1 \Rightarrow v_1^1 = \text{arbitrary} \\ 3v_1^2 = 2v_1^2 \Rightarrow v_1^2 = 0 \\ 2v_1^3 = 2v_1^3 \Rightarrow v_1^3 = \text{arbitrary} \end{matrix}$$

Say $\boldsymbol{v}_1 = [1\ 0\ 1]^{\mathrm{T}}$

The eigenvector v_2 corresponding to $\lambda_2 = 3$ is

$$\begin{bmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} v_2^1 \\ v_2^2 \\ v_2^3 \end{bmatrix} = 3 \begin{bmatrix} v_2^1 \\ v_2^2 \\ v_2^3 \end{bmatrix} \Rightarrow \begin{matrix} 2v_2^1 = 3v_2^1 \Rightarrow v_2^1 = 0 \\ 3v_2^2 = 3v_2^2 \Rightarrow v_2^2 = \text{arbitrary} \\ 2v_2^3 = 3v_2^3 \Rightarrow v_2^3 = 0 \end{matrix}$$

Say $\boldsymbol{v}_2 = [0\ 1\ 0]^{\mathrm{T}}$

The eigenvector $\boldsymbol{v}_3$ corresponding to $\lambda_3 = 2$ is (by comparison with $\boldsymbol{v}_1$), v_3^1, v_3^3 arbitrary, and $v_3^2 = 0$. Say $\boldsymbol{v}_3 = [1\ 0\ 1]^{\mathrm{T}}$.

Problem A.7

A 2x2 symmetric matrix has the form $\begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix}$

The eigenvalues are the roots of the equation

$$(\lambda - a_{11})(\lambda - a_{22}) - a_{12}{}^2 = 0, \text{ or}$$
$$\lambda^2 - (a_{11} + a_{22})\lambda + a_{11}a_{22} - a_{12}{}^2 = 0$$

The discriminant of this quadratic equation is

$$\text{D} = (a_{11} + a_{22})^2 - 4(a_{11}a_{22} - a_{12}^2) = (a_{11} - a_{22})^2 + a_{12}^2$$

Since D is the sum of the squares of two real numbers, it cannot be negative. Therefore the eigenvalues are real. Consider the asymmetric matrix $\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$

Its eigenvalues are the roots of the equation

$$(\lambda - a_{11})(\lambda - a_{22}) - a_{12}a_{21} = 0, \text{ or}$$

$$\lambda^2 - (a_{11} + a_{22})\lambda + a_{11}a_{22} - a_{12}a_{21} = 0$$

The discriminant of this quadratic equation is

$$\begin{aligned} \mathrm{D} &= (a_{11} + a_{22})^2 - 4(a_{11}a_{22} - a_{21}a_{12}) \\ &= (a_{11} - a_{22})^2 + 4a_{12}a_{21} \end{aligned}$$

For the eigenvalues to be complex, we must have D < 0. Thus an asymmetric matrix whose elements satisfy the condition

$$(a_{11} - a_{22})^2 + 4a_{12}a_{21} < 0$$

has complex eigenvalues.

Problem A.8

The LU decomposition algorithm used here is from B.A. Finlayson, "Nonlinear Analysis in chemical Engineering," McGraw Hill, NY, 1980.

$$\boldsymbol{A} = \begin{bmatrix} 1 & 1 & 0 \\ 2 & 3 & 1 \\ 1 & 0 & 1 \end{bmatrix}$$

Multiply row 1 by –2 and add to row 2, and multiply row 1 by –1 and add to row 3. Then,

$$\boldsymbol{A}^{(1)} = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & -1 & 1 \end{bmatrix}$$

Multiply row 2 by 1 and add to row 3. Then,

$$\boldsymbol{A}^{(2)} = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{bmatrix}$$

Now,

$$\boldsymbol{U} = \boldsymbol{A}^{(2)} = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{bmatrix}, \text{ and } L = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1 & -1 & 1 \end{bmatrix}$$

$$\boldsymbol{L}^{-1} = \frac{\text{adj } \boldsymbol{L}}{\det \boldsymbol{L}} = \frac{\begin{bmatrix} 1 & -2 & -3 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}^{\mathrm{T}}}{1} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -3 & 1 & 1 \end{bmatrix}$$

$$\hat{\boldsymbol{b}} = \boldsymbol{L}^{-1}\boldsymbol{b} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -3 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$$

$$\boldsymbol{Ux} = \hat{\boldsymbol{b}} \Rightarrow \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$$

From row 3, $2x_3 = 0 \Rightarrow x_3 = 0$
From row 2, $x_2 + x_3 = -1 \Rightarrow x_2 = -1$
From row 1, $x_1 + x_2 = 1 \Rightarrow x_1 = 2$

$$\boldsymbol{x} = [2 \quad -1 \quad 0]^{\mathrm{T}}$$

Problem A.9

$$g_1 = x_1^2 + x_2^2 - 8, \qquad g_2 = x_1 x_2 - 4$$

$$\boldsymbol{J} = \begin{bmatrix} \partial g_1 / \partial x_1 & \partial g_1 / \partial x_2 \\ \partial g_2 / \partial x_1 & \partial g_2 / \partial x_2 \end{bmatrix} = \begin{bmatrix} 2x_1 & 2x_2 \\ x_2 & x_1 \end{bmatrix}$$

Starting point $x^1 = [0 \ 1]^{\mathrm{T}}$. Note: superscript denotes iteration number.

Iteration 1:

$$g_1^1 = -7 \qquad J^1 = \begin{bmatrix} 0 & 2 \\ 1 & 0 \end{bmatrix} \qquad J^1 \Delta x^1 = -\begin{bmatrix} g_1^1 \\ g_2^1 \end{bmatrix}$$
$$g_2^1 = -4$$

$$\Rightarrow \Delta x_1^1 = 4, \quad \Delta x_2^1 = 3.5$$

$$\Delta x_1^2 = x_1^1 + \Delta x_1^1 = 4 \quad , x_2^2 = x_2^1 + \Delta x_2^1 = 4.5$$

Iteration 2:

$$g_1^2 = 28.25 \qquad \boldsymbol{J}^2 = \begin{bmatrix} 8 & 9 \\ 4.5 & 4 \end{bmatrix} \qquad \boldsymbol{J}^2 \boldsymbol{\Delta x}^2 = -\begin{bmatrix} g_1^2 \\ g_2^2 \end{bmatrix}$$
$$g_1^2 = 14$$

$$\Rightarrow \Delta x_1^2 = -26/17, \quad \Delta x_2^2 = -30.25/17$$
$$x_1^3 = x_1^2 + \Delta x_1^2 = 2.47059 x_2^3 = x_2^2 + \Delta x_2^2 = 2.72059$$

Iteration 3:

$$g_1^3 = 5.50541 \qquad \boldsymbol{J}^3 = \begin{bmatrix} 4.94118 & 5.44118 \\ 2.72059 & 2.47059 \end{bmatrix}$$
$$g_2^3 = 2.72145$$

$$\Delta x_1^3 = -0.46475, \quad \Delta x_2^3 = -0.58976$$
$$x_1^4 = 2.00584, \quad x_2^4 = 2.13083$$

Iteration 4:

$$g_1^4 = 0.56383 \qquad \boldsymbol{J}^4 = \begin{bmatrix} 4.01168 & 4.26166 \\ 2.13083 & 2.00584 \end{bmatrix}$$
$$g_2^4 = 0.27410$$

$$\Delta x_1^4 = -0.03594, \quad \Delta x_2^4 = -0.09847$$
$$x_1^5 = 1.96990, \quad x_2^5 = 2.03236$$

Iteration 5:

$$g_1^5 = 0.01099$$
$$g_2^5 = 0.00355$$

We stop now because g_1^5 and g_2^5 are "small enough". The solution is $\boldsymbol{x} = [1.96990 \;\; 2.03236]^{\mathrm{T}}$. The exact solution is $[2 \;\; 2]^{\mathrm{T}}$.

If $\boldsymbol{x}^1 = \left[4\ 4\right]^{\mathrm{T}}$ is the starting point, then

$\boldsymbol{J}^1 = \begin{bmatrix} 8 & 8 \\ 4 & 4 \end{bmatrix}$. In this case Δx_1^1 and Δx_2^1

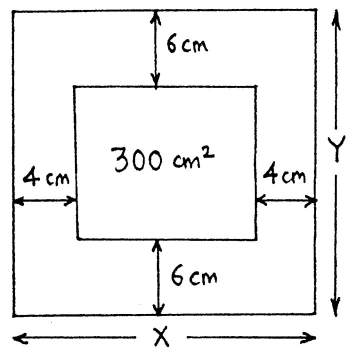
cannot be uniquely determined. Thus, $\left[4\ 4\right]^{\mathrm{T}}$ cannot be used as a starting point for the Newton-Raphson method.

SOLUTIONS MANUAL

CHAPTER 1

Problem 1.1

Minimize: $f(\mathrm{x},y) = xy$
Subject to: $(x\text{-}8)\ (y\text{-}12) = 300$
Total no. of variables = 2
No. of equality constraints = 1
No. of degrees of freedom =1
Independent variable: y



Solution:

Eliminate x using the equality constraint

$$xy - 12x - 8y + 96 = 300$$

$$x = \frac{204 + 8y}{y - 12}$$

$$f(x, y) = \frac{8y^2 + 204y}{y - 12}$$

$$\frac{\partial f}{\partial y} = \frac{(16y + 204)(y - 12) - (8y^2 + 204y)}{(y - 12)^2} = 0$$

$$(16y + 204)(y - 12) - (8y^2 + 204y) = 0$$

$$8y^2 - 192y - 2448 = 0$$

$$y = 33.21 \text{ cm}, -9.21 \text{ cm}$$

Neglecting the physically unrealizable negative value,

$$y^* = 33.21 \text{ cm}$$

$$x^* = \frac{204 - 8(33.21)}{33.21 - 12}$$

$$x^* = 22.14 \text{ cm}$$

Alternative Solution:

Minimize: area = $(w + 8)\ (z + 12)$

St. $wz = 300$

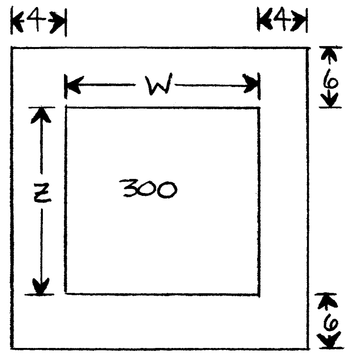
area $= wz + 8z + (2w + 96)$

$= 300 + 8z\ 12\left(\dfrac{300}{z}\right) + 96$

$\text{d(area)} = 0 = 8 + 3600\left(\dfrac{-1}{z}\right) = 0$

$z^2 = 450$
$z^* = +\ 21.21$
$w^* = 14.14$

$x^* = 8 + 14.14 = 22.14$
$y^* = 12 + 21.21 = 33.21$

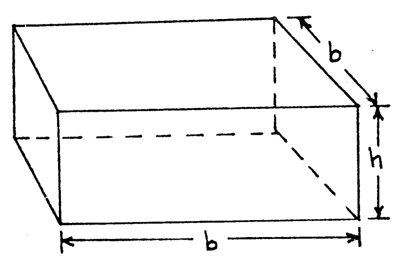


Problem 1.2

Since thickness is uniform, we just need to minimize the surface area of the inside of the box.

Minimize: $f = b^2 + 4bh$
Subject to: $b^2h = 1000$

Total no. of variables = 2
No. of equality constraints = 1
No. of degrees of freedom = 1
Independent variable = b



b > 0
h > 0

Solution:

Eliminate h using the equality constraint

$$h = \frac{1000}{b^2}$$

$$f = b^2 + \frac{4000}{b}$$

$$\frac{df}{db} = 2b = \frac{4000}{b^2} = 0$$

$$2b^3 - 4000 = 0$$

$$b = 12.6\ cm$$

$$\left\{ \frac{d^2 f}{db^2} = 2 + 8000/b^3 > 0 \text{ at } b = 12.6 \right\} \text{(not reqd.)} \Rightarrow \text{minimum.}$$

$$b^* = 12.6 \text{ cm}$$

$$h^* = \frac{1000}{(12.6)^2}$$

$$h^* = 6.3 \text{ cm}$$

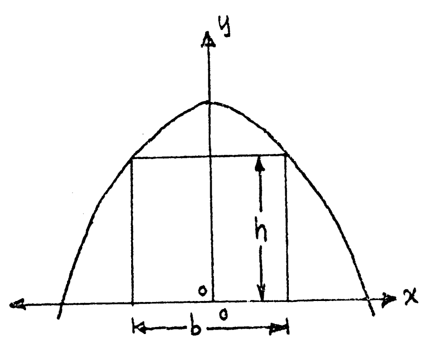
Note: Another viewpoint. Let Δt = thickness of material. If by material, the volume is used, then the volume of a side is (b) (Δt) (h) and of the bottom is (b) (Δt) (b) so that the objective function would be $\frac{f}{\Delta t}$.

Problem 1.3

Maximize: $A = bh$

Subject to: $h = 10\text{-}(b/2)^2$ and $\left(-\frac{b}{2}\right)^2$

Total no. of variables = 2
No. of equality constraints = 1
No. of degrees of freedom = 1
Independent variable: b



Solution:

$$A = b(10 - (b/2)^2) = 10b - b^3/4$$

$$\mathrm{d}A/\mathrm{d}b = 10 - 3b^2/4 = 0$$

$$b^* = 3.65$$

$$\left\{ \mathrm{d}^2 A/\mathrm{d}b^2 = -6b/4 < 0 \ at\ b^* = 3.65 \right\} \text{(not reqd.)} \Rightarrow \text{maximum}$$

$$h^* = 10 - (3.65/2)^2 = 6.67$$

$$A^* = (3.65)(6.67) = 24.35$$

Note: It is easier to maximize ½ of the rectangle as it is symmetric, and $b>0$, $h > 0$.

Problem 1.4

Let $x_1 = x_0 + h, \quad x_2 = x_0 + 2h$

Let $f = B_0 + B_1(x - x_0) + B_2(x - x_0)(x - x_1)$

$$f(x_0) = f_0 = B_0 + B_1(x_0 - x_0) + B_2(x_0 - x_0)(x_0 - x_1)$$

$$B_0 = f_0$$

$$f(x_1) = B_0 + B_1(x_1 - x_0) + B_2(x_1 - x_0)(x_1 - x_1) = f_1$$

$$B_1 = \frac{f_1 - B_0}{x_1 - x_0} = \frac{f_1 - f_0}{h}$$

$$f(x_2) = B_0 + B_1(x_2 - x_0) + B_2(x_2 - x_0)(x_2 - x_1) = f_2$$

$$B_2 = \frac{f_2 - B_0 - B_1(x_2 - x_0)}{(x_2 - x_0)(x_2 - x_1)} = \frac{f_2 - 2f_1 + f_0}{2h^2}$$

Problem 1.5

Minimize $\quad d = \sqrt{x^2 + y^2}$

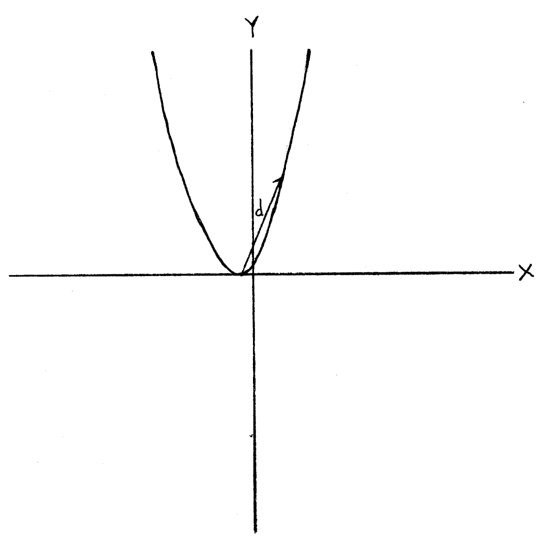
Subject to $\quad y = 2x^2 + 3x + 1$

Total no. of variables = 2

No. of equality constraints = 1

No. of degrees of freedom = 1

Independent variable: *x*



To avoid using the square root, minimizing *d* is the same as minimizing

$$D = d^2 = x^2 + y^2 = x^2 + (2x^2 + 3x + 1)^2$$
$$= 4x^4 + 12x^3 + 14x^2 + 6x + 1$$

$$\mathrm{d}D / \mathrm{d}x = 16x^3 + 36x^2 + 28x + 6 = 0$$
$$8x^3 + 18x^2 + 14x + 3 = 0$$

You need solutions of a cubic equation (Ref: R.H. Perry and C.H. Anilton, "Chemical Engineers Handbook", 5th ed., p.2-9, or use a computer code.

A cubic equation has the form $x^3 + a_1 x^2 + a_2 x + a_3 = 0$

Let $p = (3a_2 - a_1^{\ 2})/3,\ \ q = (27a_3 - 9a_1 a_2 + 2a_1^{\ 3})27$

and $R = (p/3)^3 + (q/2)^2$. If R>0, then the cubic equation has one real root and two complex conjugate roots. The real root is $x_1 = A + B - a_1/3$ where

$$A = \sqrt[3]{(-q/2) + \sqrt{R}}$$

$$B = \sqrt[3]{(-q/2) + \sqrt{R}}$$

For our problem, $a_1 = 18/8 = 2.25$,
$a_2 = 14/8 = 1.75,\ \ a_3 = 3/8 = 0.375$
$p = 0.0625,\ q = -0.09375,\ R = 2.2063\,x10^{-3}$

Since R > 0, there is one real root.
A = 0.4544355 , B = -0.0458311.
$x^* = -0.341$ and $y^* = 0.209$
$\mathrm{d}^2 D/\mathrm{d}x^2 = 48x^2 + 72x + 28 = 9.03$ at $x = -0.341 \Rightarrow$ minimum.

(-0.341, 0.209) is closest to the origin.

Note: You can use a least squares method too. If we have $f = C_0 + C_1 x + C_2 x^2$, this is equivalent to

$$C_0 = B_0 - B_1 x_0 + B_2 x_0 x_1$$
$$C_1 = B_1 - B_2 (x_0 + x_1)$$
$$C_2 = B_2$$

$\mathrm{d}f/\mathrm{d}x = B_1 + B_2\left[(x - x_0) + (x - x_1)\right] = 0$
Total no. of variables = 1
No equality constraints
No. of degrees of freedom = 1

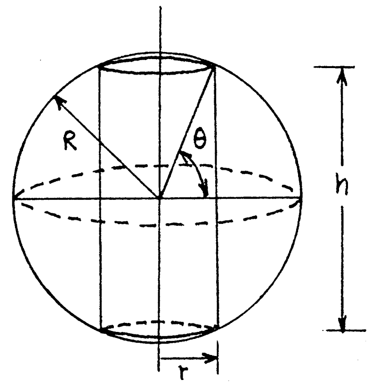
$$x^* = \frac{(x_0 + x_1)B_2 - B_1}{2B_2} = \frac{x_0 + x_1}{2} - h\left(\frac{f_1 - f_0}{f_2 - 2f_1 \ \_\ f_0}\right)$$

$d^2 f / dx^2 = 2B_2$.

f has a maximum at x^* *if* $B_2 < 0$; f has a minimum at x^* *if* $B_2 > 0$.

Problem 1.6

Maximize: $V = \Pi r^2 h$



Subject to:

$r = R \cos\ \theta$

$h = 2R \sin\ \theta$

$0 \leq \theta \leq \Pi / 2$

Total no. of variables = 3
No. of equality constraints = 2
No. of degrees of freedom = 1
Independent variable = θ

Solution:

Eliminate r and h using the equality constraints.

$V = 2\Pi R^3 \cos^2\theta \sin\theta$

$$dv / dB = 2\Pi R^3 \left[2\cos\theta \sin\theta(-\sin\theta) + \cos^3\theta \right] = 0$$

$$-2\cos\theta \sin^2\theta + \cos^3\theta = 0$$

$$-2\cos\theta(1 - \cos^2\theta) + \cos^3\theta = 0$$

$$\cos\theta(-2 + 3\cos^2\theta) = 0$$

$\cos\theta = 0$ and $\sin\ \theta = 1$, or

$\cos\theta = \sqrt{2/3}$ and $\sin\theta = \sqrt{1/3}$

$d^2V / d\theta^2 = 2\Pi R^3 (2\sin^3\theta - 7\cos^2\theta \sin\theta)$

At $\cos\theta = 0, \sin\theta = 1,$

$d^2V / d\theta^2 = 4\Pi R^3 > 0 \Rightarrow$ minimum

At $\cos\theta = \sqrt{2/3}, \sin\theta = \sqrt{1/3},$

$d^2V / d\theta^2 = -8\Pi R^3 / \sqrt{3} < 0 \Rightarrow$ maximum

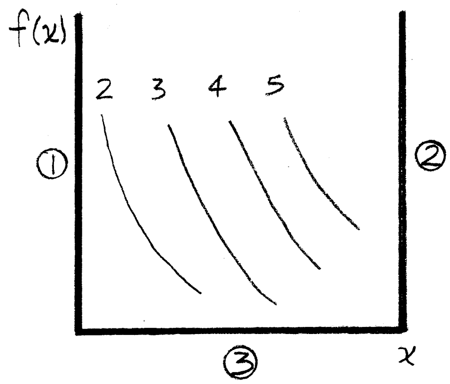
$$V^* = 2\Pi R^3 \left(\frac{2}{3}\right)\left(\sqrt{\frac{1}{3}}\right)$$

$$V^* = \frac{4}{3\sqrt{3}} \Pi R^3$$

Problem 1.7

$0 < x \leq 1$

$f(x) \geq 0$



Problem 1.8

Let n_A = no. of trucks of type *A*
n_B= no. of trucks of type *B*
n_C = no. of trucks of type *C*

Objective function

Minimize $f = 2100n_A + 3600n_B + 3780n_C$ (ton-mile/day)

Constraints

1. $10{,}000\ n_A + 20{,}000\ n_B + 23{,}000\ n_C \leq 600{,}000$ ($)

2. $n_A + 2n_B + 2n_C \leq 145$ (drivers)

3. $n_A + n_B + n_C \leq 30$ (trucks)

4. $n_A \geq 20 \quad n_B \geq 0 \quad n_C \geq 0$ (physical requirement)

Problem 1.9

Minimize

$f(x) = 19.4x_1^{-1.47} + 16.8x_2^{-1.66} + 91.5x_3^{-0.30}$

Constraints

$0 \le x_3 \le 0.05$ $\qquad$ $x_0 > x_1 > x_2 > x_3$

$x_2 \ge 0$

$x_1 \ge 0$

Problem 1.10

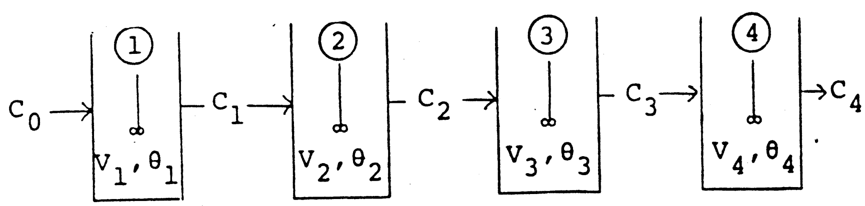
Minimize: $\quad f(x) = 4x_1 - x_2^2 - 12$

Subject to:
$$25 - x_1^2 - x_2^2 = 0$$
$$10x_1 - x_1^2 + 10x_2 - x_2^2 - 34 \ge 0$$
$$(x_1 - 3)^2 + (x_2 - 1)^2 \ge 0$$
$$x_1, x_2 \ge 0$$

No. variables: 2 $\qquad$ x_1 and x_2

One equation reduces the number of independent variables to 1, say x_1 (or x_2).

Problem 1.11



1. Objective function. Maximize C_4

2. Variables C_1, C_2, C_3 (dependent) $\quad$ C_4 is in the objective function
   $\theta_1, \theta_2, \theta_3, \theta_4$ (independent)

3. Equality constraints
   $\sum V_i = 20$ so that $\sum \theta_i = \dfrac{\sum Vi}{q} = \dfrac{20}{71}$
   Material balances

$$C_1 = C_2 + \theta_2 k C_1^{\ n}$$
$$C_2 = C_3 + \theta_3 k C_2^{\ n}$$
$$C_3 = C_4 + \theta_4 k C_3^{\ n}$$

4. Inequality constraints

$\theta_i \geq 0 \quad C_i \geq$ possibly

Problem 1.12

1. Objective function

Minimize $F = p^{*1.40} + (350 - T)^{1.9}$

Variables p^*, T $\quad$ $p = p^*$ since water condenses

Constraints:

$$\frac{p^*}{p_T} = \frac{n^*}{n_T} \leq 0.01 \quad \text{and} \quad \begin{matrix} p^* \geq 0 \\ T^* \geq 0 \end{matrix} \quad \text{inequality}$$

$$\log_{10} p^* = 8.10765 - \frac{1750.286}{235.0 + T + 273.15} \quad \text{equality}$$

Let p_T = 14.7 psia

1. One technique of solution would be to apply NLP to the above statement.
2. Another technique would be to assume p^* is at its bound so that p^* = 0.01(14.7) psia. Introduce this value into the Antoine eq., solve for T, and then calculate F. (This procedure implies 2 equality constraints exist as the problem has no degrees of freedom).

Problem 1.13

(a) The independent variable is not time but temperature (via the k's). Think of the solution of the two ODE's -- t is fixed.

(b) The dependent variables are A and B.

(c) Equality constraints are the 4 equations (including initial conditions).

(d) The inequality constraint is $T \leq 282°F$.

Also implicit are $T \geq 0$
$A \geq 0$
$B \geq 0$
$t \geq 0$

(e) Any answer is ok, as for example:

- get analytical solution of A and B vs T and minimize
- convert ODE's to difference equations (constraints) and minimize
- approximate solution via collocation (constraints) and minimize
- introducing the following transformations:

$$y_1 = \frac{A}{A_0} \quad y_2 = \frac{B}{A_0} \quad u = k_1 \ , \ \frac{u^2}{2} = k_2$$

simplifies the optimization problem to:

Maximize: $y_2(1.0)$

Subject to:
$$\dot{y}_1 = -(u + u^2/2)y_1$$
$$\dot{y}_2 = uy_1$$
$$y_1(0) = 1 \ , y_2(0) = 0$$
$$0 \leq u \leq 5$$

Note that the control variable $u(t)$ is the rate constant k_1, and directly corresponds to temperature. This insight eliminates the exponential terms and simplifies the structure of the problem.

Problem 1.14

(a) The problem consists of (at constant T and p)

Minimize: $G = \sum_i (\mu_i^o + RT \ln p + RT \ln x_i) n_i$

$$= \underset{\text{constant}}{\text{RT ln p}} + \left[\sum_i \mu_i^o + RT \sum_i \ln x_i \right] (n_i)$$

$$\uparrow \qquad \uparrow$$

$$\sum \text{RT ln K}_x \qquad \frac{n_i}{n} = \frac{n_i}{\sum n_i}$$

subject to the element balances:

$$\sum_i a_{ik} n_i = b_k \quad \text{for each of the elements } k = 1 \ldots M$$

and inequality constraints

$n_i \geq 0$

with $n_i = x_i n.$ For $C + D \rightarrow A + B$ $K_x = \dfrac{\dfrac{n_A}{n_T} \dfrac{n_B}{n_T}}{\dfrac{n_C}{n_T} \dfrac{n_D}{n_T}}$

(b) The element balances are based on

	At start (b_k)			At equilibrium		
	C	H	O	C	H	O
CO	1		1	n^*_{CO}	-	n^*_{CO}
H_2O	-	2	1	-	$2n^*_{H_2O}$	$n^*_{H_2O}$
CO_2	-	-	-	$n^*_{CO_2}$	-	$2n^*_{CO_2}$
H_2	-	-	-	-	$2n^*_{H_2}$	0

Total moles = 2

Total moles n^* = $n^*_{CO} + n^*_{H2O} + n^*_{H_2} + n^*_{CO_2}$

As variables use x_i or n_i (either are ok)

C balance: $1 = n_{CO_2} + n_{CO}$

O balance: $2 = 2n_{CO_2} + n_{CO} + n_{H_2O}$

H balance: $2 = 2n_{H_2} + n_{H_2O}$

$$K_x = \frac{x_{CO_2} x_{H_2}}{x_{CO} x_{H_2O}} = \frac{n_{CO_2} N_{H_2}}{n_{CO} N_{H_2O}}$$

$x_i = \dfrac{ni}{nT}$ so that nT cancels

Problem 1.15

$$W = \frac{kP_1V_1}{k-1}\left[\left(\frac{P_2}{P_1}\right)^{\frac{k-1}{k}} - 2 + \left(\frac{P_3}{P_2}\right)^{\frac{k-1}{k}}\right]$$

$$\frac{\mathrm{d}W}{\mathrm{d}P_2} = \frac{kP_1V_1}{k-1}\left[\frac{k-1}{k}\left(\frac{p_2}{p_1}\right)^{-\frac{1}{k}}\left(\frac{1}{p_1}\right) + \frac{k-1}{k}\left(\frac{p_3}{p_2}\right)^{-\frac{1}{k}}\left(-\frac{p_3}{p_2^2}\right)\right] = 0$$

$$\left(\frac{p_2}{p_1}\right)^{-\frac{1}{k}}\left(\frac{1}{p_1}\right) - \left(\frac{p_3}{p_2}\right)^{-\frac{1}{k}}\left(\frac{p_3}{p_2^2}\right) = 0$$

$$p_2^{-1/k} p_1^{\frac{1}{k}-1} - p_3^{1-\frac{1}{k}} p_2^{\frac{1}{k}-2} = 0$$

$$\left(p_2^{\,2}\right)^{\frac{1}{k}-1} = \left(p_1 p_3\right)^{\frac{1}{k}-1}$$

$$p_2^{\,2} = p_1 p_3$$

$$p_2 = \sqrt{p_1 p_3} = \sqrt{(1)(4)} = 2 \text{ atm}$$

Problem 1.16

(a) $C = 50 + 0.1P + \dfrac{9000}{P}$ (\$/bbl)

$$\frac{\mathrm{d}C}{\mathrm{d}P} = 0.1 - \frac{9000}{P^2} = 0$$

$$P^* = 300 \text{ bbl/day}$$

(b) $$f = 300 - 50 - 0.1P - \frac{9000}{P} \quad (\$/\text{bbl})$$

$$f = \left(300 - 50 - 0.1P - \frac{9000}{P}\right)\frac{\$}{\text{bbl}}\left(\frac{P\text{bbl}}{\text{day}}\right)$$

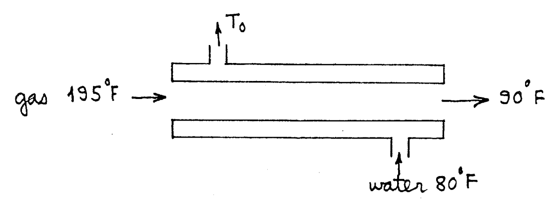
(c) $$\frac{\mathrm{d}f}{\mathrm{d}p} = 300 - 50 - 0.2P - 0 = 0$$

$$P^* = \frac{250}{0.2} = 1250 \text{ bbl/day}$$

(d) They are different because you can sell more

Problem 1.17

Basis: 1 hr



Heat balance for the gas:

$q = \quad m \quad C_p \quad \Delta T$

$q = (3000)\ (0.3)\ (195 - 90) = 9.45 \text{ x}10^4 \text{ Btu/hr}$

Heat balance for cooling water

$q = m(1)\ (T_o - 80) = m(T_o - 80) \text{ Btu/hr}$ so $m = \dfrac{q}{70 - 80}$

For the heat exchanger

$$q = UA\Delta T_{\text{LM}} \quad = 8A\Delta T_{\text{LM}} \text{ Btu/hr}$$

where so $A = \dfrac{q}{8\Delta T_{LM}}$

$$\Delta T_{\text{LM}} = \frac{(195 - T_o) - (90 - 80)}{\ln\left(\dfrac{195 - T_o}{90 - 80}\right)} \text{ in } {}^0\text{F}$$

Basis: 1 yr.

Annual cooling water cost (\$)

$$= \left(\frac{9.45x10^4}{T_o - 80}\right)\left(\frac{1}{62.4}\right)\left(\frac{0.2}{1000}\right)(24 \text{ x } 365)$$

$$= \frac{2.6533 \text{ x}10^3}{T_o - 80}$$

Annual fixed charges for the exchanger ($)

$$= \left(\frac{9.45\text{x}10^4}{8\Delta T_{\text{LM}}}\right)(0.5) = \quad \frac{5.9063\text{x}10^3}{\Delta T_{\text{LM}}}$$

$$\frac{\mathrm{d}c}{\mathrm{d}D} = 1.5C_1 D^{0.5} L - 0.081 C_2 m^3 \rho^{-2} L D^{-6} = 0$$

$$D^{opt} = 0.638\left(\frac{C_2}{C_1}\right)^{0.1538} m^{0.4615} \rho^{-0.3077}$$

For $\mu = 1cP(2.42 \text{ lb/ft hr})$, $p = 60 \text{ lb/ft}^3$,

$D^{opt} = 0.366\text{ft.}$

Problem 1.18

(a) $C = C_1 D^{1.5} L + C_2 m \Delta P / \rho$

where

$$\Delta P = 2\rho V^2 L / Df$$

$$f = \frac{0.046\mu^{0.2}}{D^{0.2} V^{0.2} \rho^{0.2}}$$

$$V = 4m / \Pi \rho D^2$$

Substituting the expression for f and V into that for ΔP, we get

$$\Delta P = 0.1421\rho^{-1} m^{1.8} \mu^{0.2} D^{-4.8} L$$

The cost function in terms of D is now

$$C = C_1 D^{1.5} L + 0.1421 C_2 \rho^{-2} m^{2.8} \mu^{0.2} D^{-4.8} L$$

$$\frac{\mathrm{d}c}{\mathrm{d}D} = 1.5C_1 D^{0.5} L - 0.682 C_2 \rho^{-2} m^{2.8} \mu^{0.2} D^{-5.8} L = 0$$

Solving this equation for *D*, we get

$$D^{opt} = 0.882\left(\frac{C_2}{C_1}\right)^{0.1587} \rho^{-0.317} m^{0.444} \mu^{0.0317}$$

From this,

$$V^{opt} = 1.6367\left(\frac{C_1}{C_2}\right)^{0.3174} \rho^{-0.366} m^{0.112} \mu^{-0.0634}$$

$$C^{opt} = 0.828 C_1^{\ 0.8413} C_2^{\ 0.1587} \rho^{-0.4755} m^{0.666} \mu^{-0.0476} + 0.2596 C_1^{\ 0.7618} C_2^{\ 0.2382} \rho^{-04784} m^{0.6688} \mu^{0.0478} L$$

(b)
$$\left.\begin{aligned} C_1 &= 1.42363\ x10^{-3}\ \$/\text{hr ft}^{2.5} \\ C_2 &= 2.7097\ x10^{-13}\ \$\text{hr}^2/\text{ft}^2\text{lb} \end{aligned}\right\} \text{for } C \text{ in \$/hr}$$

For $\mu = 1cP(2.42\ \text{lb/ft hr}), \rho = 60\ \text{lb/ft}^3$

$$D^{opt} = 0.384\text{ft}, \quad V^{opt} = 1151.5\text{ft/hr}$$

For $\mu = 0.2cP(0.484\ \text{lb/ft hr}), \rho = 50\ \text{lb/ft}^3$

$$D^{opt} = 0.387\text{ft}, \quad V^{opt} = 1363.2\text{ft/hr}$$

For $\mu = 10cP(24.2\ \text{lb / ft hr}), \rho = 80\ \text{lb/ft}^3$

$$D^{opt} = 0.377\text{ft}, \quad V^{opt} = 895.6\text{ft/hr}$$

Problem 1.19

$$D^{opt} = 0.882\left(\frac{C_2}{C_1}\right)^{0.1587} \rho^{-0.317} m^{0.444} \mu^{0.0317}$$

$$S_\rho^{Dopt} = \left(\frac{\text{dln D}^{\text{opt}}}{\text{dln p}}\right)_{\mu,m,C_2} = -0.317$$

$$S_\mu^{Dopt} = \left(\frac{\text{d}\ln\ D^{opt}}{\text{d}\ln\mu}\right)_{\rho,m,C_2} = 0.317$$

$$S_m^{Dopt} = \left(\frac{\text{dln } D^{opt}}{\text{dln } m}\right)_{\mu,\rho,C_2} = 0.444$$

$$S_{C_2}^{Dopt} = \left(\frac{\text{dln } D^{opt}}{\text{dln } C_2}\right)_{\rho,\mu,m} = 0.1587$$

$$C^{opt} = 0.828 C_1^{0.8413} C_2^{0.1587} \rho^{-0.4755} m^{0.666} \mu^{0.0476} L \\ + 0.2596 C_1^{0.7618} C_2^{0.2382} \rho^{-0.4784} m^{0.6688} \mu^{0.0478} L$$

$$S_\rho^{Copt} = \left(\frac{\partial \ln C^{opt}}{\partial p}\right)_{\mu,m,C_2} = \frac{1}{C^{opt}}(-0.4755 T_1 - 0.4784 T_2)$$

$$S_\mu^{Copt} = \left(\frac{\partial \ln C^{opt}}{\partial \ln \mu}\right)_{\rho,m,C_2} = \frac{1}{C^{opt}}(0.476 T_1 + 0.0478 T_2)$$

$$S_m^{Copt} = \left(\frac{\partial \ln C^{opt}}{\partial \ln m}\right)_{\rho,\mu,C_2} = \frac{1}{C^{opt}}(0.666 T_1 + 0.6688 T_2)$$

$$S_{C_2}^{Copt} = \left(\frac{\partial \ln C^{opt}}{\partial \ln C_2}\right)_{\rho,\mu,m} = \frac{1}{C^{opt}}(0.1587 T_1 + 0.2382 T_2)$$

where $T_1 = 0.828 C_1^{0.8413} C_2^{0.1587} \rho^{-0.4755} \mu^{0.0476} m^{0.666}$

and $T_2 = 0.2596 C_1^{0.7618} C_2^{0.2382} \rho^{-0.4784} \mu^{0.0478} m^{0.6688} L$

For $\rho = 60 \text{lb/ft}^3$ and $\mu = 1 \text{cp} (2.42 \text{ lb/ft hr})$

$$S_\rho^{C^{opt}} = -0.476$$

$$S_\mu^{C^{opt}} = 0.476$$

$$S_m^{C^{opt}} = 0.666$$

$$S_{C_2}^{C^{opt}} = 0.163$$

Problem 1.20

The variables selected could be times, but the selection below is easier to use.

Let X_{ij} be the number of batches of product i (i = 1, 2, 3) produced per week on unit j ($j = A,B,C$). We want to maximize the weekly profit.

Objective function: *Units:* (\$/batch) (batch/week) = \$/week:

Maximize: $f(\boldsymbol{X}) = 20(X_{1A} + X_{1B} + X_{1C}) + 6(X_{2A} + X_{2B} + X_{2C}) + 8(X_{3A} + X_{3B} + X_{3C})$

Subject to: Sales limits. *Units*: batch/week

$X_{3A} + X_{3B} + X_{3C} \le 20$ (none on 1 and 2)

Hours available on each unit

$$\left(\frac{0.8\text{hr}}{\text{batch}}\right)\left(\frac{\text{X batch}}{\text{week}}\right)$$

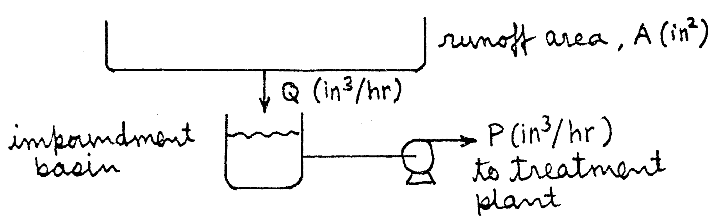
$$\begin{array}{lll} \text{Unit A} & 0.8X_{1A} + 0.2X_{2A} + 0.3X_{3A} & \le 20 \text{ hr week} \\ & 0.4X_{1B} + 0.3X_{2B} & \le 10 \\ & 0.2X_{1C} \qquad\qquad + 0.1X_{3C} & \le 5 \end{array}$$

and non-negativity constraints

$x_{ij} > 0$, $i = 1, 2, 3$, $j = A, B, C$

Problem 1.21

We have to minimize the pumping rate subject to the constraint that the basin cannot overflow.



Let rain fall for T hours at a stretch (T should be specified). The volume of rain during this period is

$$A(a + bT^2) \ \text{in}^3$$

The maximum amount of water that can be treated during a time period T is

$$P_{\max}T \quad \text{in}^3$$

Thus,

$$A(a+bT^2)-P_{\max}T \quad \le V$$

The minimum $P_{\max}$ is therefore given by

$$A(a+bT^2)-P_{\max}T \quad = V$$

or $$P_{\max} = \frac{1}{T}\left\{A(a+bT^2)-V\right\}$$

Of course, we must have $P_{\max} \ge 0$

Problem 1.22

Assume: (*i*) first order reactive, (ii) flat velocity profile

Objective function:

$$\text{maximize} \quad \int_0^1 rx(r,L,\theta)dr$$

Equality constraints:

$$\frac{\partial x}{\partial t}-\frac{D_{\text{AB}}}{R^2}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial x}{\partial r}\right)+V\frac{\partial x}{\partial z}-k_f(1-x)+k_r x=0$$

$\partial x/\partial r = 0$ at $r=0$, all z,t (symmetry)
$\partial x/\partial r = 0$ at $r=1$, all z,t (impenetrable wall)
$x = x_0$ at $z = 0$, all r,t (feed conversion)
$x = x_{\text{i}}(r,z) = 0$ (initial conversion profile)

$$C_p\frac{\partial T}{\partial t}+VG\frac{\partial T}{\partial z}-\frac{k}{R^2}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)-(\Delta H)\left[k_f(1-x)-k_r x\right]$$

$\partial T/dr = 0$ at $r=0$, all z,t (symmetry)
$-k\partial T/\partial r - U(T-T_o)=0$ at $r=1$, all z,t (heat transfer to jacket)
$T-T_{\text{in}}=0$ at $z=0$, all r,t (feed temperature)
$T=T_i(r,z)$ at $t=0$ (initial temp. profile)

Inequality constraints:

$x \geq 0$ all r, z, t
$T \geq 0$ all r, z, t

$T_{\max} - T \geq 0$ at all r, z, t
$T_o \geq T_{o\min}$
$T_o \leq T_{o\max}$

Problem 1.23

$$C = C_1 D^{1.5} L + C_2 m \Delta P / \rho$$

where

$$\Delta P = (2 \rho V^2 L / D) f$$
$$f = 0.005$$
$$V = 4m / \Pi \rho D^2$$

Substituting the expressions for ΔP, f and V into the cost function, we obtain C in terms of D:

$$C = C_1 D^{1.5} L + 0.016 C_2 m^3 \rho^{-2} D^{-5} L$$

$$\frac{\mathrm{d}C}{\mathrm{d}D} = 1.5 C_1 D^{0.5} L - 0.081 C_2 m^3 \rho^{-2} L D^{-6} = 0$$

$$D^{opt} = 0.638 \left(\frac{C_2}{C_1} \right)^{0.1538} m^{0.4615} \rho^{-0.3077}$$

For $\mu = 1cP(2.42 \text{ lb/ft hr})$, $\rho = 60$ lb/ft^3,

$D^{opt} = 0.366$ *ft*.

Problem 1.24

$C = 7000 + 2500^{2.5} L + 200\, DL$

(a) $\dfrac{\partial C}{\partial D} = 250L(2.5)D^{1.5} + 200L$ is the absolute sensitivity

$$\frac{\frac{\partial C}{C}}{\frac{\partial D}{D}} = 250L(2.5)D^{1.5} + 200L\left(\frac{D}{2000 + 250D^{2.5} + 200DL}\right)$$ is the relative sensitivity

(b) The relations for sensitivity are the same; the constraints limit the feasible region of application.

Problem 1.25

$$\ln C = a_0 + a_1 \ln S + a_2(\ln S)^2 \qquad \text{(a)}$$

$$\text{dln } C = \frac{dC}{C} = a_1 \frac{dS}{S} + a_2(2)(\ln S)\frac{dS}{S}$$

$$\frac{\text{d}C}{\text{d}S} = 0 = a_1 \frac{C}{S} + 2a_2 \frac{C}{S}(\ln S) \qquad \text{(b)}$$

or $\quad a_1 = -2a_2 \ln S \quad$ or $\quad \frac{a_1}{2a_2} = \ln \frac{1}{S}\quad$ or $\quad S = e^{-a_1/2a_2}$

$$\frac{\text{d}C/C}{\text{d}S/S} = a_1 + 2a_2 \ln S$$

Problem 1.26

Refer to Section 1.7 of the text.

CHAPTER 2

Problem 2.1

(a) The model is linear if the ratios $h_1 / S_1\rho_1 Cp_1$ and $h_1 / \rho_2 Cp_2 S_2$ plus V are independent of temperature. If they are not, then the model is nonlinear.
(b) If D is independent of concentration, then the model is linear. Else, it is nonlinear.

Problem 2.2

(a) Nonlinear
(b) Linear if v_x is independent of v_y; otherwise, nonlinear

---

Problem 2.3

2.1 (a) Unsteady state
(b) Unsteady state
2.2 (a) Steady state
(b) Steady state

Problem 2.4

2.1 (a) Distributed
(b) Distributed
2.2 (a) Lumped
(b) Distributed

Problem 2.5

(a) A distributed parameter model would be best. A plug flow mode is also possible.

(b) Steady state (except on start up and shut down)

(c) Linear

Problem 2.6

Total variables (2 streams + Q): 2(C+2)+1 = 2C+5

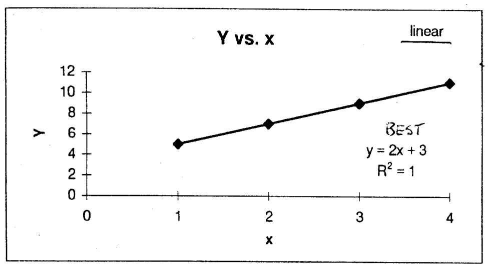
Constraints:

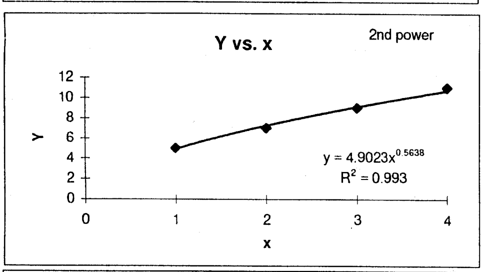
independent material balances: C
energy balance : 1
no. of degrees of freedom = 2C+5-(C+1) = C + 4

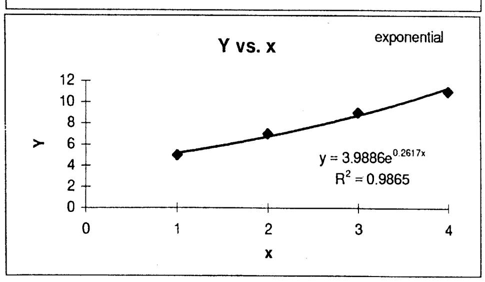
Conventional specifications are the variables in the entering stream (C+2) and the temperature and pressure of the exit stream. In some instances, *Q* may be specified rather than the temperature of the exit stream.

Problem 2.7

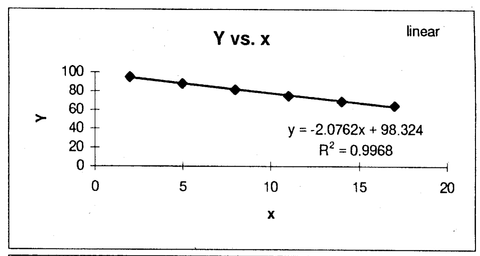
x	Y
1	5
2	7
3	9
4	11

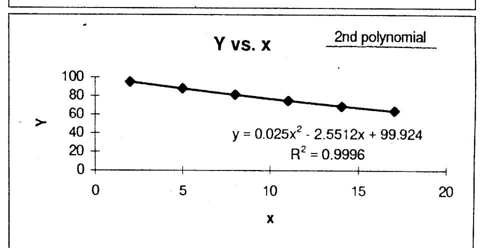


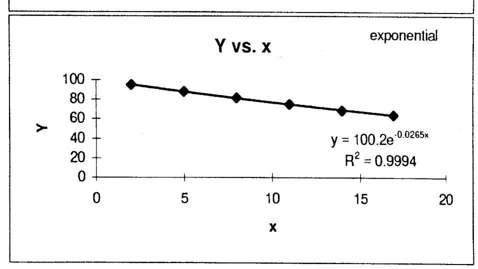




x	Y
2	94.8
5	87.9
8	81.3
11	74.9
14	68.7
17	64.0







Alternative Analysis

(a)

x	y	$\Delta y/\Delta x$
1	5	-
2	7	2
3	9	2
4	11	2

Since $\Delta y/\Delta x$ is a constant, a linear fit is best:

$$y = ax + b$$

(b)

x	y	$\Delta \log y/\Delta x$
2	94.8	-
5	87.9	-0.0109
8	81.3	-0.0113
11	74.9	-0.0115
14	68.7	-0.0125
17	64.0	-0.0102

Since $\Delta \log y/\Delta x$ is nearly constant, a good functional relation is

$$y= a\, b^x$$

(c)

x	y	$\Delta \log x/\Delta \log y$
2	0.0245	-
4	0.0370	1.68
8	0.0570	1.60
16	0.0855	1.71
32	0.1295	1.67
64	0.2000	1.59
128	0.3035	1.66

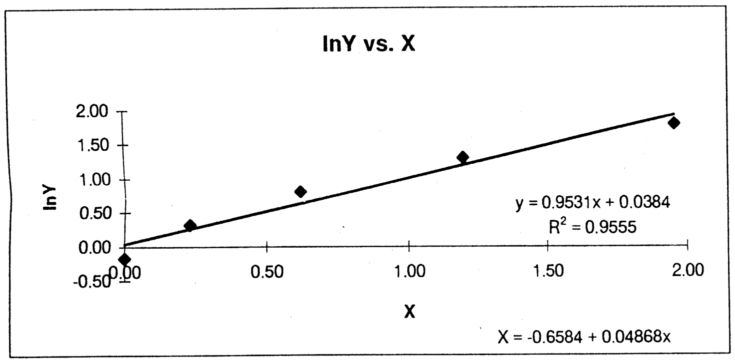
Since $\Delta \log x/\Delta \log y$ is nearly constant,

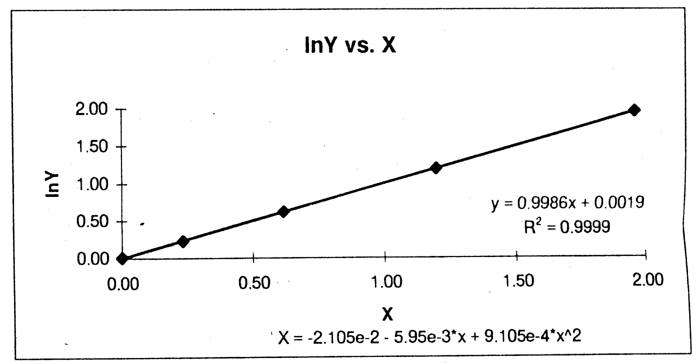
$$y = a\, x^b$$

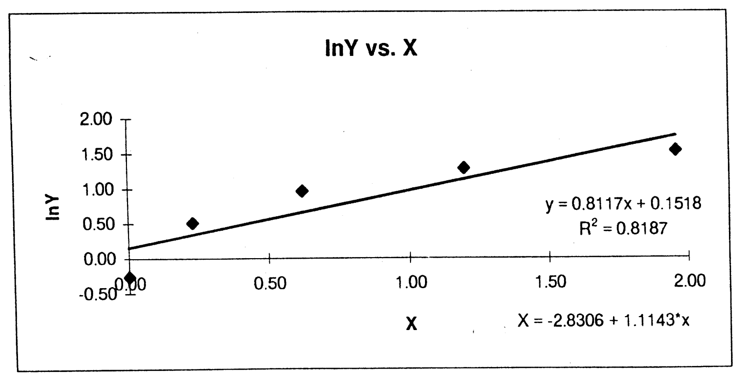
is a good functional relationship.

Problem 2.8

	x	Y	lnY	x*lnY	x^2	X1	x^3	x^4	x^2*lnY	X2	ln(x)	ln (x)^2	ln(x)*ln(Y)	X3
	10	1.00	0.00	0.00	100	-0.17	1000	10000	0.00	0.01	2.30	5.30	0.00	-0.26
	20	1.26	0.23	4.62	400	0.32	8000	160000	92.44	0.22	3.00	8.97	0.69	0.51
	30	1.86	0.62	18.62	900	0.80	27000	810000	558.52	0.62	3.40	11.57	2.11	0.96
	40	3.31	1.20	47.88	1600	1.29	64000	2560000	1915.12	1.20	3.69	13.61	4.42	1.28
	50	7.08	1.96	97.86	2500	1.78	125000	6250000	4893.18	1.96	3.91	15.30	7.66	1.53
Sum	150	14.51	4.01	168.98	5500	4.01	225000	9790000	7459.27	4.01	16.30	54.76	14.88	15.33

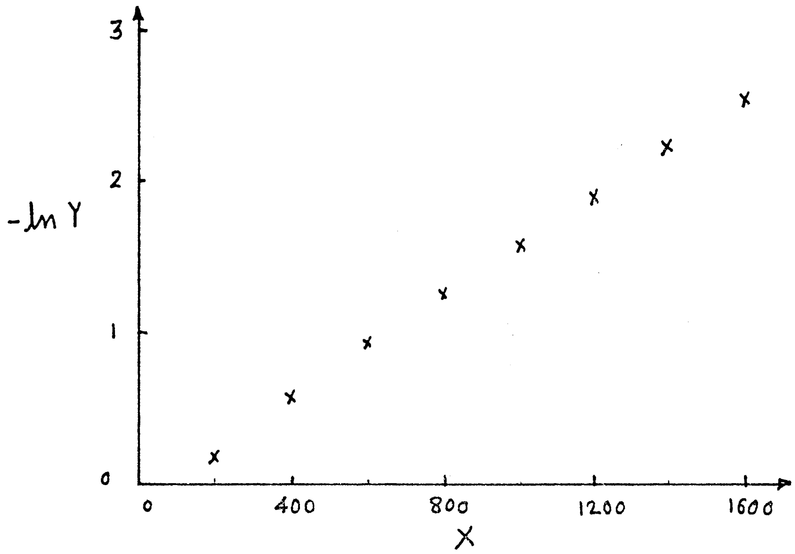






Problem 2.9

A plot of the date looks like:



Since the data seems to lie on a straight line after the transformation, a good model is

$$\ln Y = \alpha + \beta x$$
$$\text{or } Y = e^{\alpha + \beta x}$$

$$E = \sum (\alpha + \beta x_i - \ln Y_i)^2$$

$$\partial E / \partial \alpha = 2 \sum (\alpha + \beta x_i - \ln Y_i) = 0$$
$$\partial E / \partial \beta = 2 \sum x_i (\alpha + \beta x_i - \ln Y_i) = 0$$

$$\begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \sum \ln Y_i \\ \sum x_i \ln Y_i \end{bmatrix}$$
$$\begin{bmatrix} 8 & 7200 \\ 7200 & 8160000 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} -11.074 \\ -12777.698 \end{bmatrix}$$
$$\alpha = 0.1217, \quad \beta = -0.001673$$
$$Y = \exp\ (0.1217 - 0.001673x)$$

Problem 2.10

(a) To find C_o, C_1 and C_2

$$E = \sum_{i=1}^{4}(C_0 + C_1 e^{3x_i} + C_2 e^{-3x_i} - y_i)^2$$

$$\partial E/\partial C_0 = 2\sum_{i=1}^{4}(C_0 + C_1 e^{3x_i} + C_2 e^{-3x_i} - y_i) = 0$$

$$\partial E/\partial C_1 = 2\sum_{i=1}^{4} e^{3x_i}(C_0 + C_1 e^{3x_i} + C_2 e^{-3x_i} - y_i) = 0$$

$$\partial E/\partial C_2 = -2\sum_{i=1}^{4} e^{-3x_i}(C_0 + C_1 e^{3x_i} + C_2 e^{-3x_i} - y_i) = 0$$

$$\begin{bmatrix} n & \sum e^{3x_i} & \sum e^{-3x_i} \\ \sum e^{3x_i} & \sum e^{6x_i} & n \\ \sum e^{-3x_i} & n & \sum e^{-6x_i} \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum e^{3x_i} y_i \\ \sum e^{-3x_i} y_i \end{bmatrix}$$

$n = 4$
$\sum e^{3x_i} = 8527.6$
$\sum e^{6x_i} = 65823128$
$\sum e^{-3x_i} = 1.0524$
$\sum e^{-6x_i} = 1.00248$
$\sum y_i = 6$
$\sum e^{3x_i} y_i = 8951.11$
$\sum e^{-3x_i} y_i = 1.10466$

Solution of the set of 3 linear equations gives

$C_0 = 2.0552$
$C_1 = -1.302 \text{ x}10^{-4}$
C_2 - -1.0551

If C_0 is set equal to zero, then

$$E = \sum(C_1 e^{3x_i} + C_2 e^{-3x_i} - y_i)^2$$

$$\partial E/\partial C_1 = 2\sum e^{3x_i}(C_1 e^{3x_i} + C_2 e^{-3x_i} - y_i) = 0$$

$$\partial E/\partial C_2 = 2\sum e^{-3x_i}(C_1 e^{3x_i} + C_2 e^{-3x_i} - y_i) = 0$$

$$\begin{bmatrix} \sum e^{6x_i} & n \\ n & \sum e^{-6x_i} \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = \begin{bmatrix} \sum e^{3x_i} & y_i \\ \sum e^{-3x_i} & y_i \end{bmatrix}$$

Solution of this set of equations gives

C_1 = 1.3592 x10^{-4}
C_2 = 1.101385

(b) If $y_i = a_1 x_i e^{-a_2 x_i}$, then

$\ln y_i = \ln a_1 + \ln x_i - a_2 x_i$

Let $\ln a_1 = b_1$. Then

E = $\sum (b_1 + \ln x_i - a_2 x_i - \ln y_i)^2$

$\partial E / \partial b_1 = 2\sum (b_1 + \ln x_i - a_2 x_i - \ln y_i) = 0$

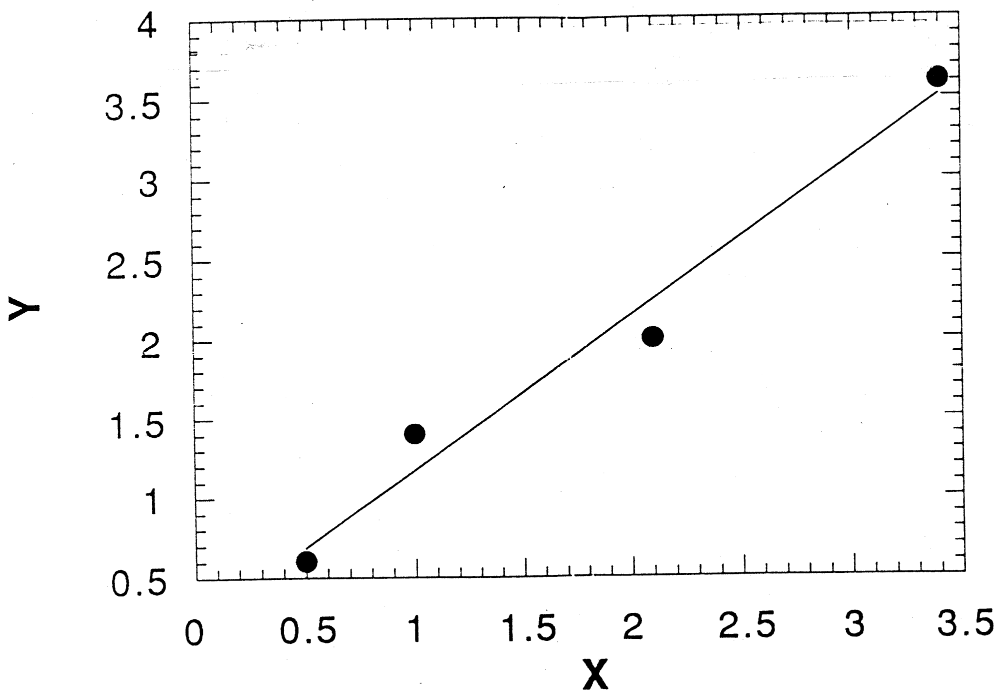
$\partial E / \partial a_2 = -2\sum xi(b_1 + \ln x_i - a_2 x_i - \ln y_i) = 0$

$$\begin{bmatrix} n & -\sum x_i \\ \sum x_i & -\sum x_i^2 \end{bmatrix} \begin{bmatrix} b_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum \ln y_i - \sum \ln x_i \\ \sum x_i \ln y_i - \sum x_i \ln x_i \end{bmatrix}$$

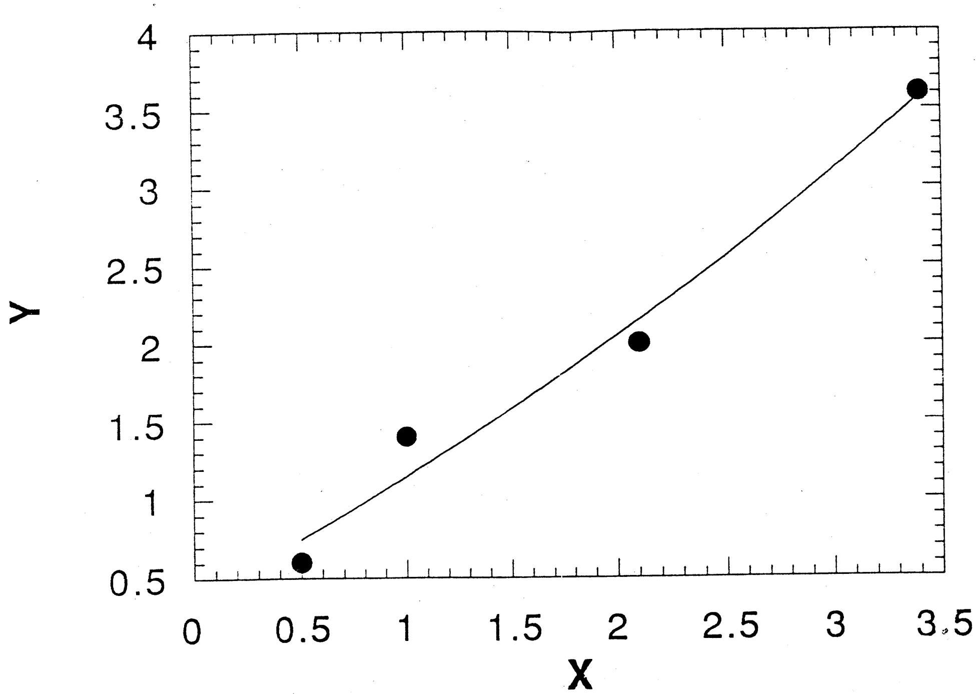
$$\begin{bmatrix} 4 & -6 \\ 6 & -14 \end{bmatrix} \begin{bmatrix} b_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 13.41005 \\ -2.6026759 \end{bmatrix}$$

b_1 = 10.167834 $\Rightarrow a_1$ = 26051.595
a_2 = 4.5435487

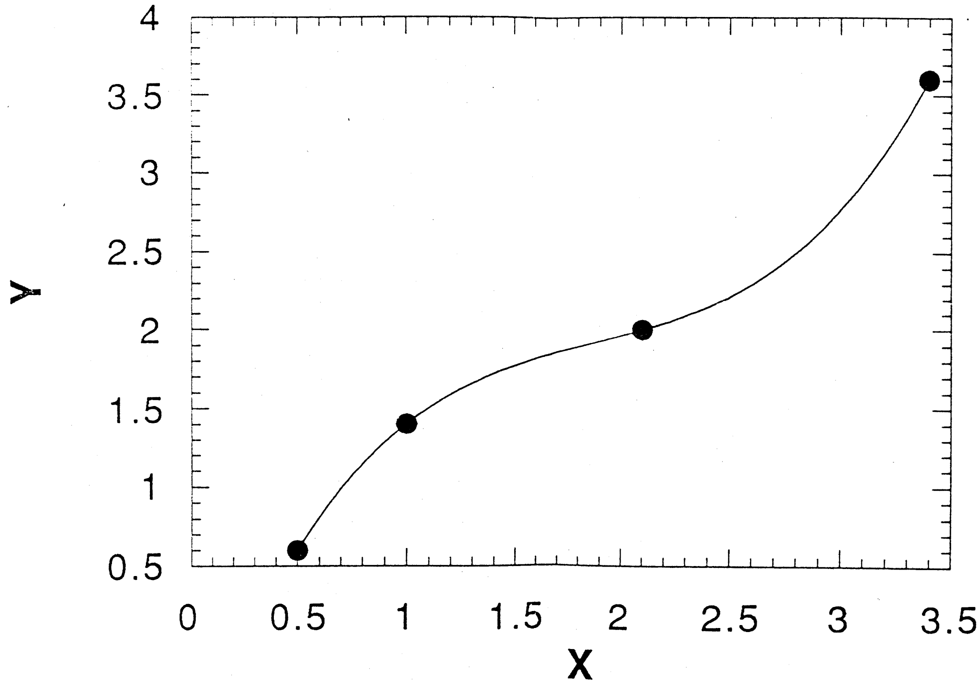
Problem 2.11



Problem 2.12



$$Y = 0.384431 + 0.686198x + 0.0731065\, x^2$$



$Y = 0.87157 + 3.77758x - 1.83175\, x^2 + 0.325737x^3$

Problem 2.13

Apply least squares as the objective function

Minimize $\sum (y_{\exp} - b_0 - b_1 e^{-cx_i})^2$

Subject to $x \geq 0$

1. Form the objective function
2. Apply a NLP code

Problem 2.14

$F = \sum (\rho_i - \alpha - 1.33c_i)^2$

$\dfrac{dF}{d\alpha} = 2\sum(\rho_i - \alpha - 1.33C_i)(-1) = 0$ solve to get

$$\text{optimal value of } \alpha = \frac{\sum \rho_i - 1.33\sum c_i}{5} = \frac{29.94 - 1.33(15.04)}{5} = 1.98$$

or introduce the data into the equation and sum 5 linear equations squared, and then differentiate, set the derivative = 0, and solve the same equation for α; α = 1.98

Problem 2.15

$$x^T x b = x^T x$$
$$b = (x^T x)^{-1} x^T y$$

$$x^T x = \begin{bmatrix} P & \sum x & \sum x^2 \\ \sum x & \sum x^2 & \sum x^3 \\ \sum x^2 & \sum x^3 & \sum x^4 \end{bmatrix} = \begin{bmatrix} 11 & 31 & 111 \\ 31 & 111 & 451 \\ 111 & 451 & 1959 \end{bmatrix}$$

$$x^T y = \begin{bmatrix} \sum y \\ \sum xy \\ \sum x^2 y \end{bmatrix} = \begin{bmatrix} 105.6 \\ 3601 \\ 1460 \end{bmatrix}$$

$$b = \begin{bmatrix} 8.24 \\ -2.93 \\ 0.95 \end{bmatrix}$$

$$y = 0.95\, x^2 - 2.93\, x + 8.24$$

Is the Design Orthogonal?

No, the design is not orthogonal. You need two independent variables to even obtain an orthogonal design. Our problem has only one (x).

Problem 2.16

$$b = (x^T x)^{-1} x^T Y$$

$$b = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} \quad x = \begin{bmatrix} \mathrm{x}_0 & \mathrm{x}_1 & \mathrm{x}_2 \\ 1 & 160 & 1 \\ 1 & 160 & 1 \\ 1 & 160 & 7 \\ 1 & 160 & 7 \\ 1 & 200 & 1 \\ 1 & 200 & 1 \\ 1 & 200 & 7 \\ 1 & 200 & 7 \end{bmatrix} \quad Y = \begin{bmatrix} 4 \\ 5 \\ 10 \\ 11 \\ 24 \\ 26 \\ 35 \\ 38 \end{bmatrix}$$

Use a computer to get

$$b = \begin{bmatrix} -91.33 \\ 0.5813 \\ 1.4588 \end{bmatrix}$$

Problem 2.17

$$E = \sum_{i=1}^{n} (\alpha + \beta x_i - y_i)^2$$

$$\frac{\partial E}{\partial \alpha} = 2\sum_{i=1}^{n} (\alpha + \beta x_i - y_i) = 0$$

$$n\alpha + \beta \sum_{i=1}^{n} x_i - \sum_{i=1}^{n} y_i = 0$$

$$\alpha = \frac{1}{n}\left[\sum_{i=1}^{n} y_i - \beta \sum_{i=1}^{n} x_i \right]$$

Problem 2.18

Let $p_1 = \dfrac{x_1 - 3}{2}$ and $p_2 = \dfrac{x_2 - 260}{20}$

When the *Y* values for a given (p_1, p_2) are averaged, we get

p_1	p_2	Y
-1	-1	24
1	-1	44
-1	1	4
1	1	20

For $y = \beta_0 + \beta_1 p_1 + \beta_2 p_2$, we have

$$\begin{bmatrix} n & \Sigma p_1 & \Sigma p_2 \\ \Sigma p_1 & \Sigma p_1^2 & \Sigma p_1 p_2 \\ \Sigma p_2 & \Sigma p_1 p_2 & \Sigma p_2^2 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} \Sigma Y \\ \Sigma p_1 Y \\ \Sigma P_2 Y \end{bmatrix}$$

$$\begin{bmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 92 \\ 36 \\ -44 \end{bmatrix}$$

$\beta_0 = 23,\ \beta_1 = 9,\ \beta_2 = -11$

$Y = 23 + 9p_1 - 11p_2$

$Y = 152.5 + 4.5x_1 - 0.55x_2$

Problem 2.19

y	x_1	x_2	x
96.0	1	0	1
78.7	0.5	0.866	1
76.7	-0.5	0.866	1
54.6	-1	0	1
64.8	-0.5	-0866	1
78.9	0.5	-0.866	1
91.8	0	0	4

The last point has a weight of 4 because it is the average of 4 data points.

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2 + \beta_5 x_1 x_2$$

Then,

$$\text{Min E} = \sum_{i=1}^{7} w_i(\beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{1i}^2 + \beta_4 x_{2i}^2$$

$$+\beta_5 x_{1i} x_{2i} - Y_i)^2$$

The answer is

$$\beta_0 = 91.8$$
$$\beta_1 = 16.483$$
$$\beta_2 = 3.378$$
$$\beta_3 = -16.5$$
$$\beta_4 = -17.2$$
$$\beta_5 = -6.986$$
$$E = 106.68$$

Problem 2.20

(a) $\text{E} = \sum(C_0 + C_1 x_A + C_2 s - Y_p)^2$

$$\begin{bmatrix} n & \sum x_A & \sum s \\ \sum x_A & \sum x_A{}^2 & \sum x_A s \\ \sum s & \sum s x_A & \sum s^2 \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \end{bmatrix} = \begin{bmatrix} \sum Y_p \\ \sum x_A Y_p \\ \sum s Y_p \end{bmatrix}$$

$$\begin{bmatrix} 3 & 0.3 & 90 \\ 0.3 & 0.09 & 0 \\ 90 & 0 & 4500 \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \end{bmatrix} = \begin{bmatrix} 1.0 \\ 0.06 \\ 39 \end{bmatrix}$$

$$C_0 = 0.1,\ C_2 = 0.3333,\ C_3 = 0.00667$$

In this case, one can also solve three equations in the three unknowns, without a least-squares fit.

(b) If $Y_p = 0$ for $x_A = s = 0,$ then $C_0 = 0$.

$$E = \sum(C_1 x_A + C_2 s - Y)^2$$

$$\partial E / \partial C_1 = 2\sum x_A (C_1 x_A + C_2 s - Y) = 0$$
$$\partial E / \partial C_2 = 2\sum s (C_1 x_A + C_2 s - Y) = 0$$

$$\begin{bmatrix} \sum x_A^2 & \sum x_A s \\ \sum x_A s & \sum s^2 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = \begin{bmatrix} \sum x_A Y \\ \sum sY \end{bmatrix}$$

$$\begin{bmatrix} 0.09 & 0 \\ 0 & 4500 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = \begin{bmatrix} 0.06 \\ 39 \end{bmatrix}$$

$$C_1 = 0.667, \ C_2 = 0.008667$$

Problem 2.21

Assume that the feed is a single phase stream, and not the same as any of the other streams. Total variables (5 streams + Q) : 5 (C+2)+1
= 5 C+11

Constraints:

independent material balances	:	C
energy balance	:	1
equilibrium relationships	:	C
T same in each phase	:	1
P same in each phase	:	1
		2c+3

No. of degrees of freedom = (5c+11) – (2c+3)
= 3c + 8

Problem 2.22

There are six components. Therefore, the total number of variables is (3 streams + Q): 3(C+2) + 1 = 25

Constraints:

(1)	matl. balances (C, H, O, N)	:	4
(2)	energy balance	:	1
(3)	fixed O_2/N_2 ratio in air	:	1
(4)	zero concentration of components in		
	fuel	:	4
	air	:	4

	flue gas	:	1
(5)	specification of % excess air	:	1
(6)	specification of % N_2 in fuel	:	1
(7)	specification of three temperatures	:	3
			20

No. of degrees of freedom = 25-20 = 5.
Three pressures must be specified, and one extensive variable – either feed, air or flue gas flowrate. The last variable would be the CO/CO_2 ratio.

Problem 2.23

Total no. of variables for 7 streams: 7(C+2) = 35

Constraints:

(1)	3 independent material balances for each piece of equipment	:	12
(2)	one energy balance for each piece of equipment	:	4
(3)	specification of $F_0, w_{A_0}, W_{A_0}, W_{A_4}$ and F_5/F_4	:	5
(4)	*P-V-T* relationship for each stream	:	7
			28

No. of degrees of freedom = 35-28 = 7.

Problem 2.24

Objective function:

Minimize total cost per year

$$C_{tot} = (C_s + C_t)r + C_{op}$$

or minimize present value of total costs

$$C_{tot} = C_s + C_t + \left(\sum_{i=1}^{N} C_{op}\right)F$$

where r = capital recovery factor
F = discount factor

Subject to:

$$C_s = 2.5W_s$$

$$W_s = \Pi D z L_s \rho_s$$

$D = P(n_p + 1)$dia. of shell for triangular pitch

$P = 1.25d_0$ pitch

$$n_p = \left(\frac{4n-1}{3}\right)^{1/2}$$

$$C_{t=}150A_0$$

$$A_0 = \Pi d_0 nL$$

$$C_{op} = \left\{W_g \Delta P_g / (102\eta\rho_g)(3600)\right\}(8400\frac{\text{hr}}{\text{yr}}(0.06\frac{\$}{kwh})$$

$W_g = 25000$ kg/hr

$$\Delta P_g = \frac{1.5V^2\rho g}{2g} + \frac{fL_s V^2 \rho g}{2gd_i}$$

f = 0.023

$$Y = 4Wg/(3600\rho_g \Pi d_i^{\,2} n)$$

$$Pg = 273MW/\left[22.4(273 + Tg)\right]$$

$$Q = U_0 A_0 \Delta T_{in}$$

$$Q = W_g Cp(T_2 - T_1)$$

$$U_0 = 0.95h_{io}$$

$$h_{io} = h_i(d_i / d_o)$$

$$h_i d_i / k = 0.023(3600\rho_g V d_i / \mu)^{0.8}(C_p \mu / k)^{0.4}$$

$C_p = 0.24$ kcal/kg^{o}C

$\mu = 0.14$ kg m/h

$k = 0.053$ kcal/(m)(hr)(^{o}C)

$$\Delta T_{\ell n} = \frac{(T_0 - T_1) - T_0 - T_2)}{\ell n\left(\frac{T_0 - T_1}{T_0 - T_2}\right)}$$

$$T_1 = 1200^{O}C$$

$$T_2 = 350^{O}C$$

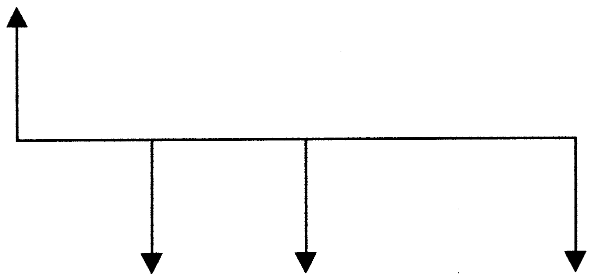
CHAPTER 3

Problem 3.1

P = 100,000 and the present value of the sum of future payments must equal 100,000

$$\left[\frac{i(1+i)^n}{(1+i)^n-1}\right]P=\left[\frac{0.1(1.1)^{10}}{(1.1)^{10}-1}\right](100000)$$

= \$16274.54 for each payment each year



or use $P=100,000=\frac{F_1}{(1+i)^1}+\frac{F_2}{(1+i)^2}+\cdots+\frac{F_{10}}{(1+i)^{10}}$

The schedule of interest and payments is:

Year	Amount Paid annually (\$)	Year ending principal balance (\$)	Interest (\$)
1	16274.54	100000.00	10000.00
2	16274.54	93725.46	9372.55
3	16274.54	86823.47	8682.35
4	16274.54	79231.28	7923.13
5	16274.54	70879.87	7087.99
6	16274.54	61693.32	6169.33
7	16274.54	51588.11	5158.81
8	16274.54	40472.38	4047.24
9	16274.54	28245.08	2824.51
10	16274.54	14795.05	1479.51

Problem 3.2

I_o = \$10000 , i = 12%

Year	(a)	(b)
1	-1000	-800
2	-1000	-1400
3	-1000	-1200
4	-1000	-1000
5	-1000	-1000
6	-1000	-1000
7	-1000	-900
8	-1000	-900
9	-1000	-900
10	-1000	-900
NPV =	-5650	-5779

Problem 3.3

$$10{,}000 - 5{,}000\,(1+i)^8 = 0$$

which yields $i = 9.05\%$

Problem 3.4

Split the problem into three parts: the present value of \$550,000 received at the end of 5 years, the expense of \$25,000 at the end of year 2 (a negative amount), and 5 dividends each of \$15,000 received at the end of each year for 5 years.

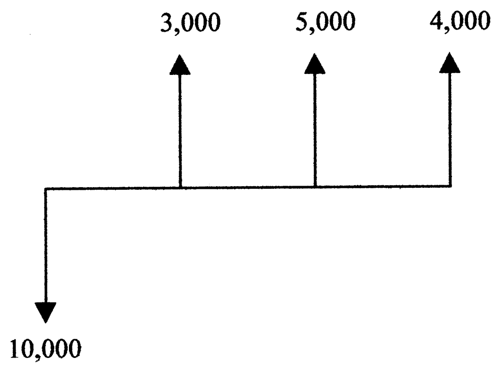
$$P = \frac{15{,}000}{1.15} + \frac{15{,}000}{(1.15)^2} - \frac{25{,}000}{(1.15)^2} + \frac{15{,}000}{(1.15)^3} + \frac{15{,}000}{(1.15)^4}$$

$$+\frac{15{,}000}{(1.15)^5} + \frac{550{,}000}{(1.15)^5} = \$304{,}825.94$$

or $P = 15{,}000 \dfrac{(1.15)^5 - 1}{0.15(1.15)^5} - \dfrac{25{,}000}{(1.15)^2} + \dfrac{550{,}000}{(1.15)^5} = \$304{,}825.94$

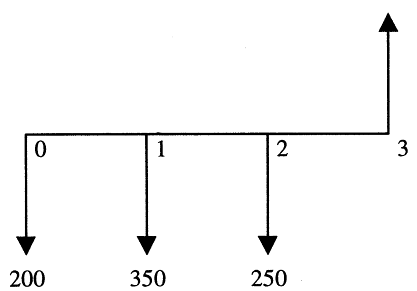
Problem 3.5

The time line is



Answer -$980.52. The improvement should not be implemented.

Problem 3.6



F = ?

$i = 0.06$

$$\frac{i}{12} = 0.005$$

$$F_0 = 200(1+0.005)^{36} = 200(1.1967) = 239.34$$
$$F_1 = 350(1+0.005)^{24} = 350(1.127) = 394.50$$
$$F_2 = 250(1+0.005)^{12} = 250(1.0617) = 265.42$$

Answer: $899.27

Problem 3.7

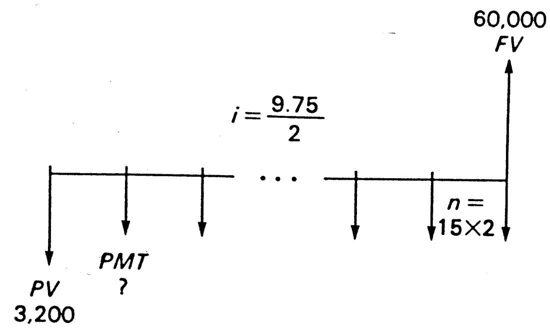
This is a problem in which the payments are not uniform

$$F = \sum_{k=1}^{n} F_k (1+i)^{n-k+1} \quad \text{applies}$$

An iterative solution is needed. The interest is charged and the payments made 24 times a year. The answer given is 58 payments (29 months). You can split the problem into one initial payment of $775 and a subsequent series of equal payments of $50, and add the two parts to get the answer.

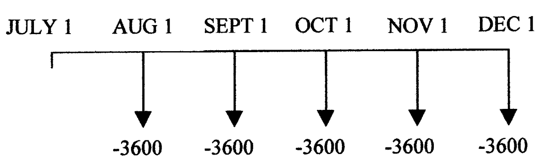
Problem 3.8

The time line is



Answer: $717.44

Problem 3.9



i = 14.0%

		Payments	
Date	Payment	Interest	Principal
Aug	$3600	$1400.00	$2200.00
Sep	↓	1374.33	2225.67
Oct		1348.37	2251.63
Nov		1322.10	2277.90
Dec		1295.52	2304.48
		$6740.32	

40% of the interest paid is a benefit, but the benefit is received at end of the year only
$6740.32 (.40) = 2696.13

$$P = \frac{F}{(1+i)^n} = \frac{\$2696.13}{(1.0117)^5} = \$2544.21$$

Problem 3.10

The statement is true for the same interest rates. For example:

(a) For a \$1000 mortgage at 10% paid over 30 years (F is the annual payment)

$$1000 = F_{30}\left(\frac{1.10^{30}-1}{0.10(1.10)^{30}}\right) \qquad F_{30} = 106.04$$

(b) For 15 years

$$1000 = F_{15}\left(\frac{1.10^{15}-1}{0.10(1.10)^{15}}\right) \qquad F_{15} = 131.41$$

From the values of F you can split each payment into interest and principal, and find that the sum of the interest payments over the 30 years is higher than that over 15 years.

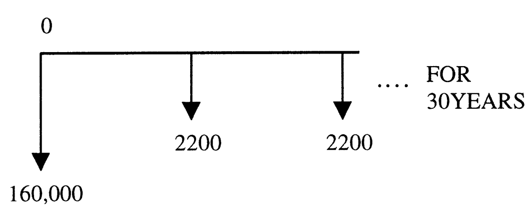
Problem 3.11

You borrow \$300,000 for 4 years at an interest rate of 10% per year. You plan to pay in equal annual end-of-year installments. Fill in the following table.

Year	Balance Due at Beginning of Year, \$	Principal Payment \$	Interest Payment \$	Total Payment \$
1	\$300,000	\$64,641	\$30,000	\$94,641
2	\$235,359	\$71,105	\$23,536	\$94,641
3	\$164,253	\$78,216	\$16,425	\$94,641
4	\$86,037	\$86,037	\$8,604	\$94,641

Problem 3.12

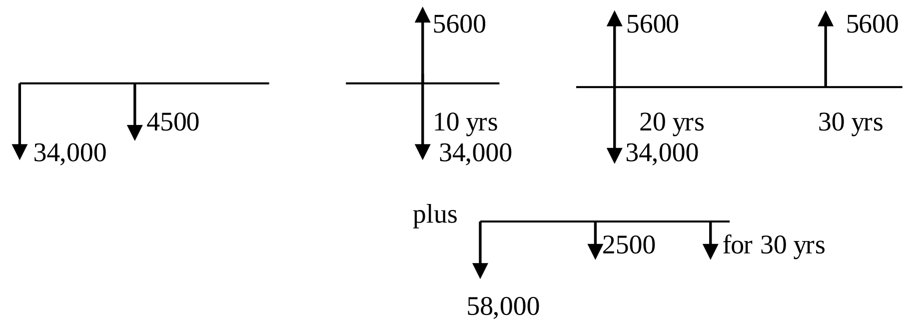
Plan A:



$$\sum_{1}^{30}\frac{1}{(1+i)^n} = \frac{(1+i)^n-1}{i(1+i)^n} = \frac{(1.12)^{30}-1}{0.12(1.12)^{30}}$$

NPV of 30 year costs = -160000 + $\sum_{j=1}^{30}\frac{-2200}{(1.12)^j}$ = \$-177,721

Plan B:



NPV of 30 year costs =

$$-34000+\frac{-34000}{(1.12)^{10}}+\frac{-34000}{(1.12)^{20}} \qquad \text{(capital costs)}$$

$$+\sum_{j=1}^{10}\frac{-4500}{(1.12)^{j}}+\sum_{j=11}^{20}\frac{-4500}{(1.12)^{j}}+\sum_{j=21}^{30}\frac{-4500}{(1.12)^{j}} \qquad \text{(operating costs)}$$

$$+\frac{+5600}{(1.12)^{10}}+\frac{+5600}{(1.12)^{20}}+\frac{+5600}{(1.12)^{30}} \qquad \text{(salvage value)}$$

$$+(-58000)+\sum_{j=1}^{30}\frac{-2500}{(1.12)^{j}} \qquad \text{(ditch costs)}$$

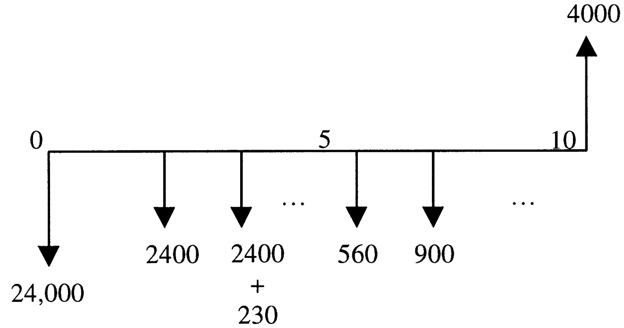
= \$-160,288

Plan *B* is favored because its *NPV* of costs is higher (less negative) than that for plan *A*

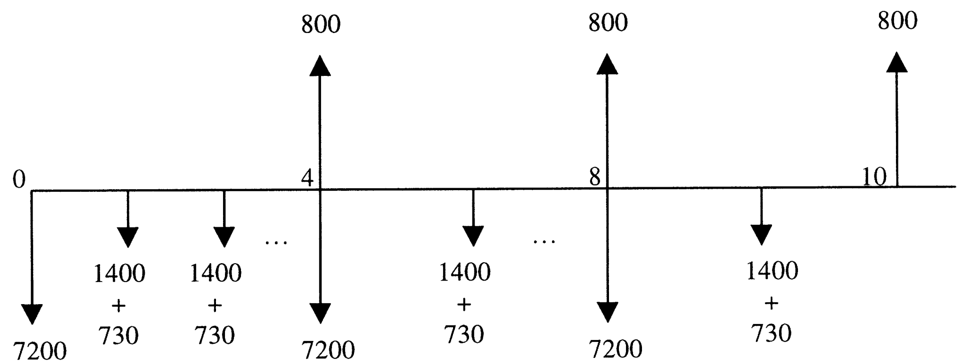
Problem 3.13

The total annual cash flows for each reactor, and the present values of the cash flows and total costs are tabulated below:

GLASS LINED



CAST IRON



Glass-lined reactor: (all flows in \$) Note: -2400 + 1700 = -700

Year	Operating costs	*PV* (*i* = 0.1)	*PV* (*i* = 0.2)
1	-700	-636	-583
2	-930	-769	-646
3	-700	-526	-405
4	-700	-478	-338
5	-1260	-782	-506
6	-1600	-903	-536
7	-1600	-821	-447
8	-1600	-746	-372
9	-1600	-679	-310
10	+2400 (including salvage value)	+925	+388
		-5415	-3755

With the installed cost included, the value of all costs at the initial time is

$$\left.\begin{array}{ll}\text{for } i=0.1, & -5415-24000= \quad \$-29415 \\ \text{for } i=0.2, & -3755-24000= \quad \$-27755\end{array}\right\} \begin{array}{c} PV \\ \text{for 10 years}\end{array}$$

Cast iron reactor: (all flows in $) Note: -1440-730=-2170; -2170 + 800 = -1370

year	Operating costs	*PV* (*i* = 0.1)	*PV* (*i* = 0.2)
1	-2170	-1973	-1808
2	-2170	-1793	-1507
3	-2170	-1630	-1256
4	-1370	-936	-661
		-6332	-5232

With the installed cost included, the value of all costs at the initial time is

$$\left.\begin{array}{ll}\text{for } i=0.1, & -6332-7200= \quad \$-13532 \\ \text{for } i=0.2, & -5232-7200= \quad \$-12432\end{array}\right\} \text{for 4 years}$$

You have to calculate operating costs for another 4 year period followed by a 2 year period for a total of 10 years, but you can see that adding roughly (1.5) (6000) = 9000 to 13,500 gives a value smaller than that for the gas lined reactor.

The cast iron reactor is favored for either interest rate.

Problem 3.14

Project A has the largest rate of return, because most of the cash flow is returned early in the life of the project, and is discounted less.

Problem 3.15

For after tax profits of $10,000 per year,

$$\sum_{j=1}^{20} \frac{10000}{(1+i)^j} - 100000 = 0 \qquad \Rightarrow i = 7.75\%$$

For after tax profits of $12,000 per year,

$$\sum_{j=1}^{20} \frac{12000}{(1+i)^j} - 100000 = 0 \qquad \Rightarrow i = 10.39\%$$

For after tax profits of $8,000 per year,

$$\sum_{j=1}^{20} \frac{8000}{(1+i)^j} - 100000 = 0 \qquad \Rightarrow i = 4.98\%$$

Relative sensitivity = $\dfrac{\Delta i / i}{\Delta s / s}$

For a + 20% error,

$$RS = \frac{(10.39 - 7.75)/7.75}{12000 - 10000)/10000} = 1.70$$

Problem 3.16

Installed capital cost = $200/hp
Operating cost = $0.04 / kwhr
η = 70%
i = 10%
Basis: 8000 hr/yr operation
Assume life = 5 years
Then, r = 0.264
Basis: 1 hp
Installed capital cost = $200

Assume the pump efficiency corrects the $0.04 to actual cost.

Operating cost

$0.04	8000 hr	5 yr	0.746 kw	1 actual power		
Kwh	yr		1 hp	0.7 theo. power	.264	= $6460

$$\frac{PV \text{ of capital cost}}{PV \text{ of operating cost}} = \frac{200}{6460} = 0.031$$

Operating costs are more substantial.

Problem 3.17

The ratio is $R = \dfrac{I}{\displaystyle\sum_{j=n+1}^{n+m+1} \frac{C}{(1+i)^j}}$

where I = initial investment
C = annual cash flow
n = no. of years to build the facility
m = life of facility (years)

$$R = 1 = \frac{10^6}{\displaystyle\sum_{j=2}^{17} \frac{150000}{(1+i)^j}} \qquad i = 11.0\%$$

For n = 2,

$$R = 1 = \frac{10^6}{\displaystyle\sum_{j=3}^{18} \frac{150000}{(1+i)^j}} \qquad i = 9.6\%$$

For n = 3,

$$R = 1 = \frac{10^6}{\displaystyle\sum_{j=4}^{19} \frac{150000}{(1+i)^j}} \qquad i = 8.5\%$$

Problem 3.18

Let n be the payback period.

PV of initial investment = \$10,000

PV of maintenance costs = $\displaystyle\sum_{j=1}^{n} \frac{\$300(1.08)^j}{(1.15)^j}$

PV of savings = $\displaystyle\sum_{j=1}^{n} \frac{\$3760(1.08)^j}{(1.15)^j}$

To find the payback period, we solve the following equation for n:

$$10000+\sum_{j=1}^{n}\frac{300(1.08)^j}{(1.15)^j}-\sum_{j=1}^{n}\frac{3760(1.08)^j}{(1.15)^j}=0$$

$$10000-\sum_{j=1}^{n}\frac{3460}{(1.0648)^j}=0$$

$$10000-3460\left[\frac{(1.0648)^n-1}{(0.0648)(1.0648)^n}\right]=0$$

$$10000-54925.715\left[1-\frac{1}{(1.0648)^n}\right]=0$$

n = 3.2 years.

Problem 3.19

Objective function:

$$\textbf{Basis: 100 ft}^2$$

C = Annual cost = -Energy savings + Capital Costs (in \$/yr)
(b) (a)

Installation cost

$$\frac{\$0.75}{(\text{ft}^2)\ (\text{in})}\ \Big|\ 100\ \text{ft}^2\ \Big|\ t\ \text{in.} = 75\ t$$

(a) *Capital cost per year*. $(75t)\ (0.30) = 21.5\ t\ \dfrac{\$}{\text{yr}}$

Heat loss savings are Q without insulation minus Q with insulation

$$\Delta Q = \frac{\Delta U\ \text{Btu}}{(\text{hr})\ (\text{ft}^2)(\ °\text{F})}\ \Big|\ 100\ \text{ft}^2\ \Big|\ (500\text{-}70)°\text{F} = 43{,}000\ \Delta U\frac{\text{Btu}}{\text{hr}}$$

Overall heat transfer coefficient change gives ΔQ

with: $\frac{1}{U} = \frac{1}{4} + \frac{t}{(12)(0.30)} = 0.25 + 0.278t$

without: $\frac{1}{U} = \frac{1}{4} = 0.25$

$$\Delta U = \left(\frac{1}{0.25} - \frac{1}{0.25 + 0.278t} \right)$$

Heat savings per year

$$\frac{\$0.60}{10^6\,\text{Btu}} \bigg| \frac{(8700)(43{,}000)}{} \left(\frac{1.11t}{(0.25 + 0.278t)} \right) \frac{\text{Btu}}{\text{yr}}$$

(b) $$= \frac{\$249.2t}{0.25 + 0.278t} \frac{\$}{\text{yr}}$$

Constraints

$t \geq 0 \quad C \geq 0$

To get optimal t, minimize C so set $\frac{dC}{dt} = 0$

$$\frac{-69.28t}{(0.25 + 0.278t)^2} + \frac{249.2}{(0.25 + 278t)} - 21.5 = 0$$

$$t = 7.02\text{in}$$

Problem 3.20

(a) In this problem recognize that an exchanger of infinitely large area will maximize the energy recovery in the stream but at an exorbitant cost. Hence we expect there to be a trade-off between capital cost and energy savings. The variables to be optimized include T_2 and A as well as the amount of steam generated, w_{steam}. First determine if any equality constraints exist in the problem. The energy balance for the steam generator is

$$w_{oil} C_{p_{oil}} (400 - T_2) = \frac{UA(400 - T_2)}{\ln[150/(T_2 - 250)]} \qquad \text{(a)}$$

or

$$w_{oil}C_{p_{oil}} = \frac{UA}{\ln[150/(T_2 - 250)]} \qquad \text{(b)}$$

The water converted to steam is obtained from

$$w_{oil}C_{p_{oil}}(400 - T_2) = \Delta H_v w_{steam} \qquad \text{(c)}$$

where ΔH_v = 950 Btu/lb and w_{steam} = lb/h. Recognize that Eq. (*b*) relates the variables T_2 and A, hence they are not independent. In addition, Eq. (*c*) relates T_2 and w_{steam}. Therefore we can express all costs in terms of T_2 and with the aid of Eqs. (*b*) and (*c*). The capital cost is (dropping the "oil" subscript):

$$I_o = (25)(A) = \frac{25wC_p}{100}\ln\left(\frac{150}{T_2 - 250}\right) \qquad \text{(d)}$$

The annual credit for the value of the steam is

$$F = \left\{2\text{x}10^{-6}\left[\frac{\$}{Btu}\right]\right\}\left\{wC_p(400 - T_2)\left[\frac{\text{Btu}}{h}\right]\right\}\left\{8000\frac{\text{h}}{\text{year}}\right\}$$

$$F = [0.016]\left[wC_p(400 - T_2)\frac{\$}{\text{year}}\right] \qquad \text{(e)}$$

Note that wC_p for the oil appears in the expressions for both F and I_o and thus cancels. The profitability ratio is therefore

$$\text{ROI} = \frac{F}{I_o} = \frac{0.064(400 - T_2)}{\ln[150/(T_2 - 250)]} \qquad \text{(f)}$$

The maximum value of ROI must be found numerically because of the complicated expressions appearing on the right-hand side of (f). The optimum is at T_2 = 400°F, which is the same temperature as at the inlet, corresponding to $A \rightarrow 0$. At the optimum an extremely high rate of return occurs (r = 9.6), which can be found by applying L'Hopital's rule to the above expression for ROI when T_2 = 400°F. This outcome, of course, is an unrealistic answer, since it suggests the optimum return consists of an exchanger with infinitesimal area! Why does this result occur? The difficulty with using ROI as an objective function is that nothing in Eq. (f) constrains the area to be above a minimum size; in fact, as $T_2 \rightarrow 400°$, the investment I_o is decreasing faster than is the numerator, leading to a maximum value at T_2 = 400°. If T_2 > 400°, the rate of return becomes negative.

From the above example, you can see that the ratio of F/I_o may yield unrealistic results for an optimum. This occurs here because $I_o \rightarrow 0$ for $T_2 \rightarrow 400$. Consider reformulating the problem using the net present value (NPV) of before-tax profits as an alternative objective function. Use of NPV means that a rate of return on the capital is specified.

$$\text{NPV} = \left\{ \frac{(1+i)^n - 1}{i(1+i)^n} \right\} F - I_o$$

or

$$\text{NPV} = \frac{F}{r} - I_o$$

Since r is fixed by the assumptions about i and n, an equivalent criterion is

$$r \cdot \text{NPV} = F - rI_\text{o}$$

Note that this modified objective function $(r \cdot \text{NPV})$ is equivalent to the use of the annualization factor (repayment multiplier) to obtain the capitalization charge. In problems in which you seek to minimize only costs rather than maximizing profit because there is no stated income, then F is negative. An example arises in optimizing pipe size to minimize pump operating costs and pipe investment costs. Instead of maximizing $r \cdot \text{NPV}$, you can minimize $(-r \cdot \text{NPV})$.

(b) Let us use the net present value analysis to determine the optimum value of T_2. Assume an interest rate for capital of 15 percent and a period of 10 years. The objective function for net present value (to be maximized with respect to T_2) is

$$\begin{aligned} f &= F - rI_\text{o} \\ &= 2\text{x}10^{-6} wC_p (400 - T_2)(8000) - r \cdot 25 \cdot A (\$/\text{year}) \end{aligned} \qquad \text{(j)}$$

By elimination of A in terms of T_2, Eq. (b) gives:

$$f = (0.016) wC_p (400 - T_2) - 25r \frac{wC_p}{U} \ln \frac{150}{T_2 - 250} \qquad \text{(k)}$$

Note that wC_p is a common factor of the two terms and will not be involved in calculating T_2. We can differentiate Eq. (k) and set $\text{d}f/\text{d}T_2 = 0$:

$$\frac{\text{d}f}{\text{d}T} = 0 = \frac{25r}{100} \quad \frac{1}{T_2 - 250} - 0.016 \qquad \text{(l)}$$

$$T_2 = 250 + 15.62r \qquad \text{(m)}$$

If $r = 0.2$ ($n = 10$, $i = 15$ percent in Table 3.1), then $T_2 = 253.1$°F, a 3.1° approach (somewhat lower than the normal approach temperatures of 5 to 10°F recommended in design manuals). The optimal approach temperature, according to the analysis in this example, depends on U, r, and the ratio of the value of steam to the cost-per-unit area for the heat exchanger.

To calculate the annual profit before taxes, we compute the value of $F = (2 \times 10^6)(wC_p)(400 - T_2)(8000)$, which would be \$176,280. The optimum value of A is 2905 ft^2, so the original investment is \$72,625. The payout is, therefore, less than one year. Remember that while higher values of ROI can be obtained by selecting T_2 closer to 250°F, maximization of ROI leads to the meaningless solution obtained previously.

While the rate of return on investment (F/I_o) did not lead to meaningful results, there are some conditions under which this criterion can be employed effectively to obtain a reasonable value for the optimum. For example, if the heat transfer area costs were assumed to be $I_o = I'_o + 25$ A (I'_o is the fixed installation cost for the exchanger), then maximizing F/I_o would yield a more realistic result for T_2. Note that at $T_2 = 400$°F, ROI = 0.0, rather than 9.6 obtained earlier for Eq. (f). Another case which gives a meaningful answer for ROI occurs when several projects are considered simultaneously with a constraint on total capital expenditure. If \$100 million is to be invested among three projects, then an overall rate of return for the three projects, defined as $(F^1 + F^2 + F^3)/(I^1 + I^2 + I^3)$, can be formulated. The optimum, when calculated, should be meaningful because it is guaranteed that \$100 million will be committed to plant investment. In fact, $I^1 + I^2 + I^3$ in this case is a constant value (\$100 million), hence we simply optimize $F^1 + F^2 + F^3$.

Decisions made on the basis of the internal rate of return often favor investment in smaller facilities rather than large plants because the ratio of profit to investment is optimized.

Problem 3.21

The last sentence is not clear, but in general the statement is correct.

Problem 3.22

Refer to P3.5. Set $P = 0$. The answer is 10.13%.

Problem 3.23

The payback period is calculated as follows:

$$\text{PBP} = \frac{\text{cost of investment}}{\text{cash flow per period}}$$

$$\frac{\$30,000}{\$1000} = 30 \text{ months}$$

Problem 3.24

The return on investment in percent is calculated as follows:

$$\text{ROI} = \frac{\text{net income (after taxes)}}{\text{cost of investment}} 100$$

$$\frac{\$5000}{\$50,000}(100) = 10\%$$

Problem 3.25

Since all alternatives have acceptable individual IRR's, start with the one with the lowest-investment (A) and look at the incremental return on incremental investment in going to the next-larger investment alternative (B). This would be $12,000 investment with annual return of $3,100. The incremental IRR of this is 22.4%. This calculation can be done either with sequential cash flow entry or by trial-and-error solving the equation NPW = $12,000 + $3,100(*P/A,i*%,10) = 0. Because 22.4%>18%, B becomes the preferred case. You then calculate the IRR of the incremental investment of $5,000 going from B to C; this is 42.7% so C becomes the preferred case. Going from C to D costs $5,000 but the return of $500 per year is insufficient to justify that investment; C remains the preferred case. Going from C to E involves an investment of $15,000 that generates $2,900 per year. The IRR of this is 14.2%, which you reject because it is less than 18%. Thus C is the preferred alternative.

Problem 3.26

All of the outflows are negatives. Choose Alternative D3 because it has the lowest negative PV.

Problem 3.27

(a) Return an investment (ROI) = $\frac{\text{net savings}}{\text{investment}} = \frac{\$162,000}{\$1,000,000} = \begin{matrix} 0.162 \\ \text{or } 16.2\% \end{matrix}$

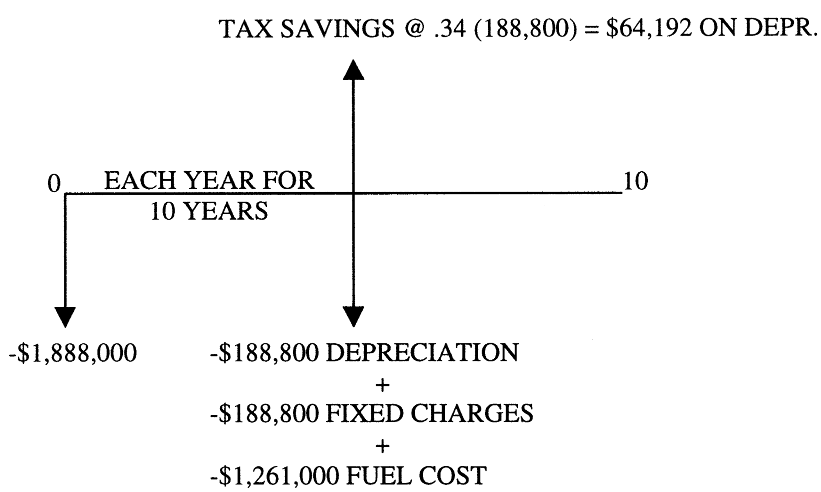
(b) IRR: $\sum_{k=1}^{10} \frac{162,000}{(1+i)^k} = 10^6 = \text{PV}$ $\qquad i = \frac{F}{I_o} - \frac{i}{(1+i)^n - 1}$

$$\frac{162,000}{10^6} = \frac{i(1+i)^{10}}{(1+i)^{10} - 1} = r = .162 \text{ so } i \cong 10\% \text{ from Table 3.1}$$

Problem 3.28

Find the present value of each option (use cost as the criterion). For depreciation use the MACR table or just 10% per year. Interest is .15 per year under one assumption:

Oil



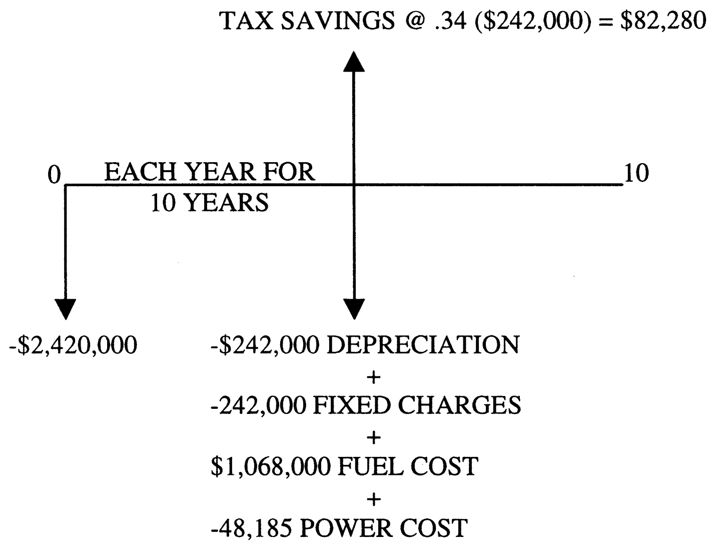
$$\text{PV}_1 = 1,888,000 + 1,574,000 \sum_{k=1}^{10} \frac{1}{(1+i)^k} \qquad i = .15$$

of costs

From Table 3.1 $\quad r \cong 0.200$ so $\frac{1}{r} = \sum \frac{1}{(1+i)^k} = 5.00$

$\text{PV}_1 = \$9,758,000$ (cost)

Rotary Air



$$\text{PV} = 2,420,000 + 1,517,000 \sum_{k=1}^{10} \frac{1}{(1+i)^k} \quad i = .15 \quad \frac{1}{r} = 5.00$$

$$\text{PV}_{2=} \$10,000,000$$

Too close to choose

Alternate Solution

Assume return on investment means ROI as in text

$$\text{ROI} = \frac{\text{net income after taxes (\$/yr)-assumed constant}}{\text{initial investment (\$)}}$$

$$\frac{\text{NI}}{I_0} = \frac{\text{net income}}{\text{initial investment}} = \frac{\text{sales}}{\text{initial invesment}} - \frac{\text{costs}}{\text{initial investment}}$$

If sales are fixed, the smallest costs/initial investment will have the biggest ROI

Oil

$$\frac{\text{NI}}{I_o} = \frac{\$1,570,000}{\$1,888,000} = 0.83$$

Rotary Air

$$\frac{\text{NI}}{I_o} = \frac{\$1,517,000}{\$2,420,000} = 0.63 \quad \text{smallest}$$

ROI may be < 15% depending on sales.

Another solution: Calculate the interest rate given present value and payments.

Problem 3.29

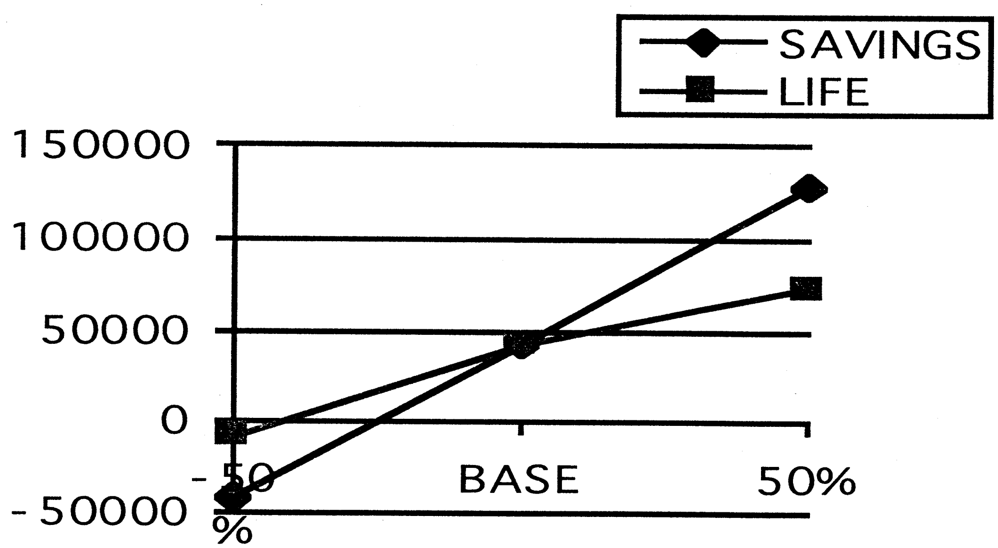
(a) What is the PV of your base case? $43,087.

PV = -$140,000 + $40,000 + $25,000 = -$140,000 + $12,745 + $170,342

(b) You calculate the PV of –50% annual savings to be -$42,084 and the PV for +50% annual savings to be $128,257. The PV at –50% life is -$8,539. What is the PV at +50% life? $72,229.

PV = -$140,000 + $40,000 + $25,000 = -$140,000 + $7,194 + $205,035

(c) Sketch the PV sensitivity diagram for these two variables below. To which of the two variables is the decision most sensitive? Savings.



CHAPTER 4

Problem 4.1

(a) continuous over $-\infty < x < \infty$

(b) discrete

(c) continuous over $0 \le x_S \le 1$ and $0 \le x_D \le 1$ if x_S and x_D are mole fractions.

Problem 4.2

In all cases, *i* is a continuous variable, and *n* is a discreet variable.

Problem 4.3

n may be treated as a continuous variable when small changes in *n* do not affect the average unit cost significantly. This happens when:

(i) *n* is very large, so that average unit cost $\approx V$ (limit $n \to \infty$)

(ii) *F* is very small (limit $F \to 0$).

Problem 4.4

$$R = 100(1-t)\frac{\left[S-(V+F/n)\right]}{I/n} = 100(1-t)\frac{\left[Sn-(Vn+F)\right]}{I}$$

$$\frac{dR}{dn} = \frac{100(1-t)(S-V)}{I} \quad \ne \text{function of } n$$

Thus, *R* increases linearly with *n* and there is no stationary maximum. The same is true when *n* is discreet.

Problem 4.5

(a) Minimize: $f(\boldsymbol{x}) = [3\ 2\ 1]\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$ or $f(\boldsymbol{x}) = \boldsymbol{a}^{\mathrm{T}}\boldsymbol{x}$

Subject to:

$$\boldsymbol{g}(x) = \begin{bmatrix} 2 & 3 & 1 \\ 1 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \geq \begin{bmatrix} 1\,0 \\ 1\,5 \end{bmatrix} \quad \text{or } \boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{Dx} \geq \boldsymbol{c}$$

(b) Maximize: $f(\boldsymbol{x}) = [5\ 10\ 12] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$ or $f(\boldsymbol{x}) = \boldsymbol{a}^{\mathrm{T}} \boldsymbol{x}$

Subject to:

$$\boldsymbol{g}(\boldsymbol{x}) = \begin{bmatrix} -15 & -10 & -10 \\ 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \geq \begin{bmatrix} -200 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\boldsymbol{h}(\boldsymbol{x}) = [10 \quad 25 \quad 20] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = 300$$

or
$$\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{Dx} \geq \boldsymbol{c}$$
$$\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{Ex} = \boldsymbol{d}$$

Problem 4.6

The function has the form

$$f(\boldsymbol{x}) = \boldsymbol{a} + \boldsymbol{x}^{\mathrm{T}} \boldsymbol{b} + \boldsymbol{x}^{\mathrm{T}} \boldsymbol{cx}$$

Let $\boldsymbol{a} = 3$

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \boldsymbol{b} = \begin{bmatrix} 2 \\ 3 \end{bmatrix} \quad \boldsymbol{c} = \begin{bmatrix} 2 & 1 \\ 1 & 6 \end{bmatrix}$$

$$[x_1 x_2] \begin{bmatrix} 2 & 1 \\ 1 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = [(2x_1 + x_2)(x_1 + 3x_1)] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

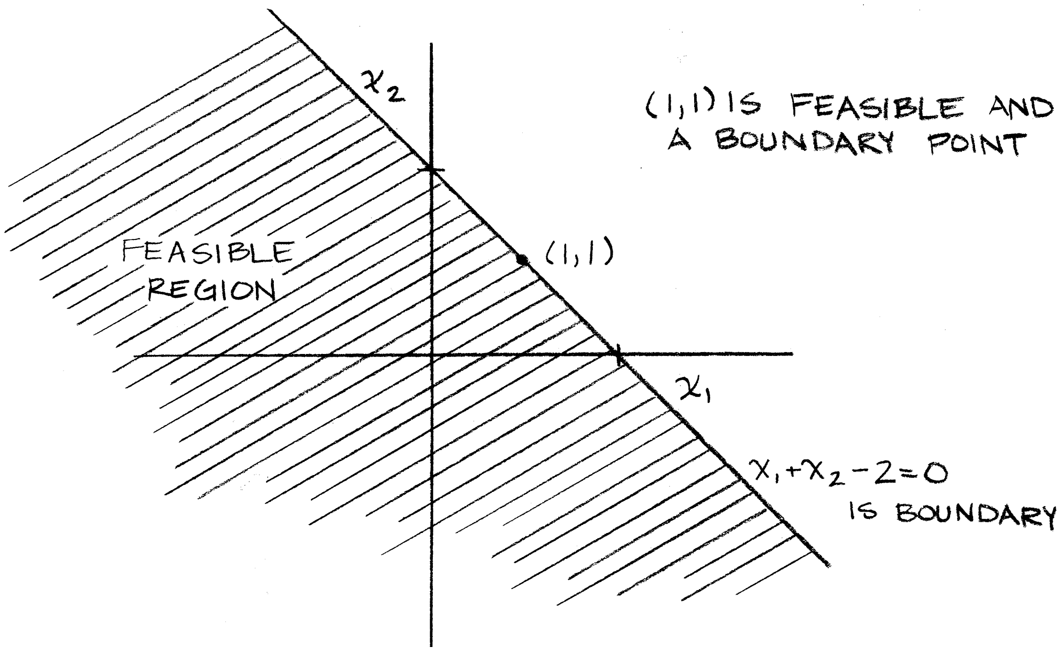
$$= 2x_1^{\ 2} + x_1x_2 + x_1x_2 + 6x_2^{\ 2}$$

or

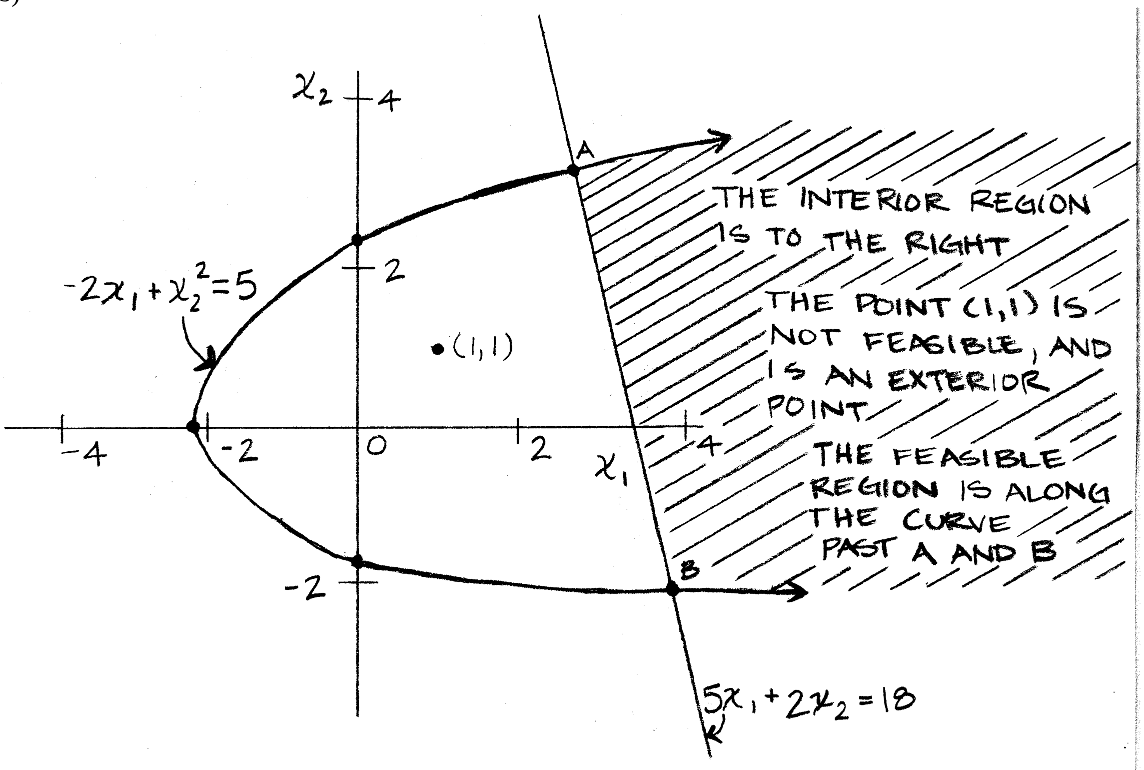
$$f(\mathbf{x}) = [1\ x_1\ x_2]\begin{bmatrix} 3 & 1 & 3/2 \\ 1 & 2 & 1 \\ 3/2 & 1 & 6 \end{bmatrix}\begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix}$$

Problem 4.7

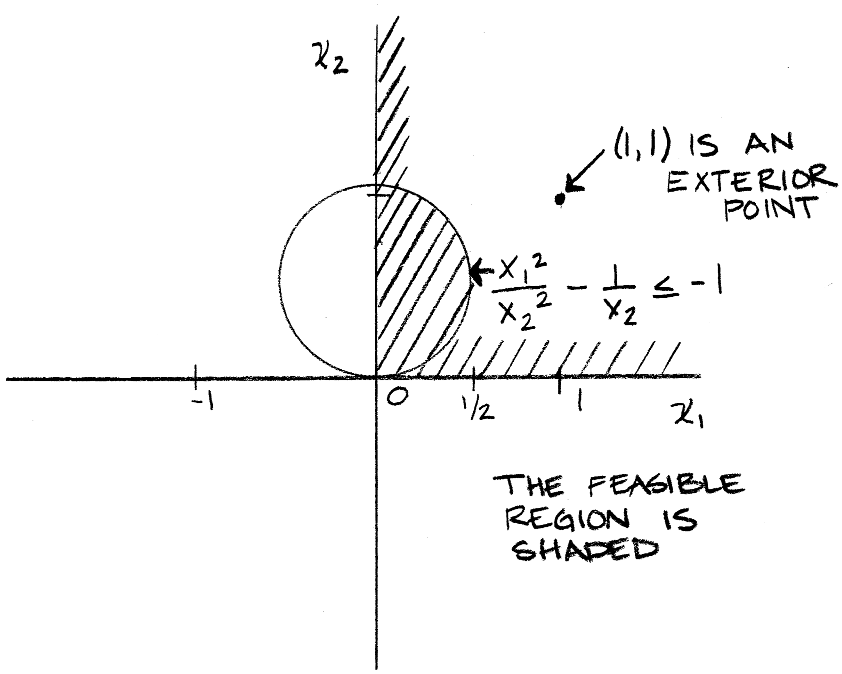
(a)



(b)


x_2
4
2
-2
-4
-2
0
2
4
x_1
$-2x_1+x_2^2=5$
$\bullet(1,1)$
A
B
$5x_1+2x_2=18$
THE INTERIOR REGION IS TO THE RIGHT
THE POINT (1,1) IS NOT FEASIBLE, AND IS AN EXTERIOR POINT
THE FEASIBLE REGION IS ALONG THE CURVE PAST A AND B

(c)


x_2
(1,1) IS AN EXTERIOR POINT
$\frac{x_1^2}{x_2^2} - \frac{1}{x_2} \le -1$
-1
0
1/2
1
x_1
THE FEASIBLE REGION IS SHADED

Problem 4.8

$$f(\boldsymbol{x}) = 2x_1^3 + x_2^2 + x_1^2 x_2^2 + 4x_1 x_2 + 3$$

$$\frac{\partial f(\boldsymbol{x})}{\partial x_1} = 6x_1^2 + 2x_1 x_2^2 + 4x_2 = 0 \qquad (1)$$

$$\frac{\partial f(\boldsymbol{x})}{\partial x_2} = 2x_2 + 2x_1^2 x_2 + 4x_1 = 0 \qquad (2)$$

(2) $$x_2 = -\frac{2x_1}{x_1^2 + 1}$$

(3) $$3x_1^2 + x_1\left(\frac{2x_1}{1+x_1^2}\right)^2 - 2\left(\frac{2x_1}{1+x_1^2}\right) = 0$$

$$x_1\left(3x_1^5 + 6x_1^4 + 3x_1^2 + 4x_1^3 - 4x_1 - 4x_1^3\right) = 0$$

$$x_1\left(3x_1^5 + 6x_1^3 + 3x_1 - 4\right) = 0$$

$x_1 = 0 \quad x_2 = 0$ is one solution

(4) $$3x_1^5 + 6x_1^3 + 3x_1 = 4$$

Only one other solution exists. The Newton-Raphson method was used to check the roots of the Equation (4) from different starting points (0.01,05,1. They all go to $x_1 =$ 0.65405 100)

Values of x_1	right hand side of equation
0.6541	4.000632
0.65405	3.99996
0.654053	4.0000003

x_2 = -0.9161783

Thus, $\boldsymbol{x}_1^* = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ and $\boldsymbol{x}_2^* = \begin{bmatrix} 0.654053 \\ -0.9161783 \end{bmatrix}$

Next, check the Hessian matrix.

For $\boldsymbol{x}^* = 0$

$$\boldsymbol{H} = \begin{bmatrix} 12x_1 + 2x_2^{\ 2} & 4x_1x_2 + 4 \\ 4x_1x_2 + 4 & 2x^2 + 2 \end{bmatrix}$$

$= \begin{bmatrix} 0 & 4 \\ 4 & 2 \end{bmatrix}$ is not positive or negative define, hence $\boldsymbol{x}$ is a *saddle* point.

The eigenvalues are

$$(0-\lambda)(2-\lambda)-16=0$$
$$\lambda^2 - 2\lambda - 16 = 0$$
$$\lambda = \frac{4 \pm \sqrt{4+4(16)}}{2} = 2 \pm \sqrt{1+16}$$

one is positive and one is negative.

For $\boldsymbol{x}^* = \begin{bmatrix} 0.654053 \\ -0.916173 \end{bmatrix}$

$$\boldsymbol{H} = \begin{bmatrix} .5274 & 1.60308 \\ 1.60308 & 2.85557 \end{bmatrix}$$ is positive definite

hence this $\boldsymbol{x}$ is a local minimum that is the global minimum

An alternate solution is to plot $f(\boldsymbol{x})$ vs. x_1 and x_2, and use the graph to reach a conclusion. The contours in the x_1=x_2 plane will yield the results calculated above.

Problem 4.9

(1) $\boldsymbol{x} = [5 \ \ 2 \ \ 10]^T$

g_2 to g_4 satisfied

5(15) + 10(2) + 10(10) = 195 ≤ 200 g_1 satisfied

10(5) + 25(2) + 20(10) = 300 h_1 is satisfied

(a) is a feasible point
(b) is an interior point

(2) $\boldsymbol{x}$ = [10 2 7.5)^T

g_2 to g_4 satisfied

$15(10) + 10(2) + 10(7.5) = 245 > 200$, g_1 is not satisfied

(a) hence not a feasible point
(b) is an exterior point

(3) $\boldsymbol{x} = [\,0\ \ 0\ 0]^T$

g_2 to g_4 satisfied (boundary points)

(a) h_1 is not satisfied, hence not a feasible point
(b) $g_1 = 0$ hence is a boundary point, not an interior or exterior point

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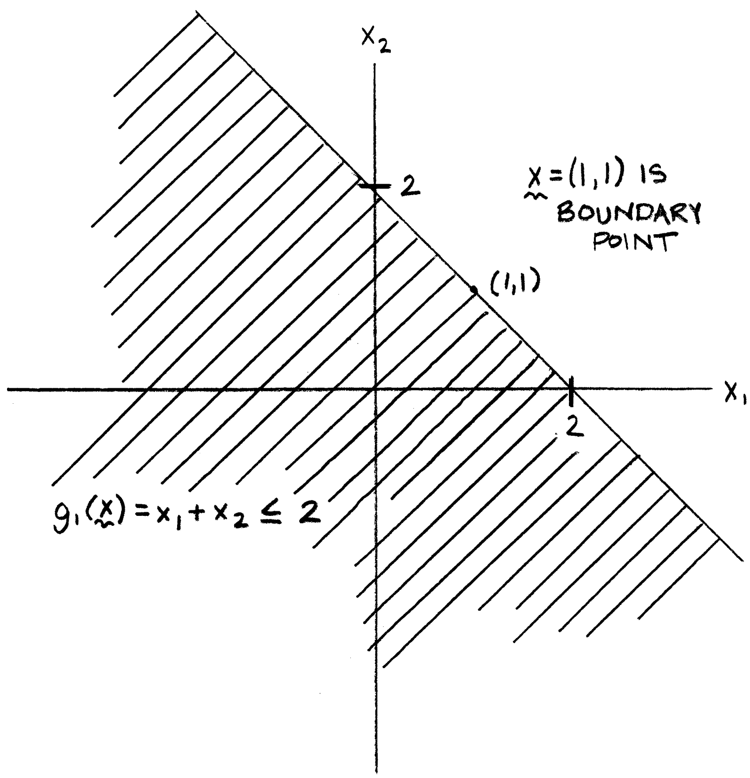
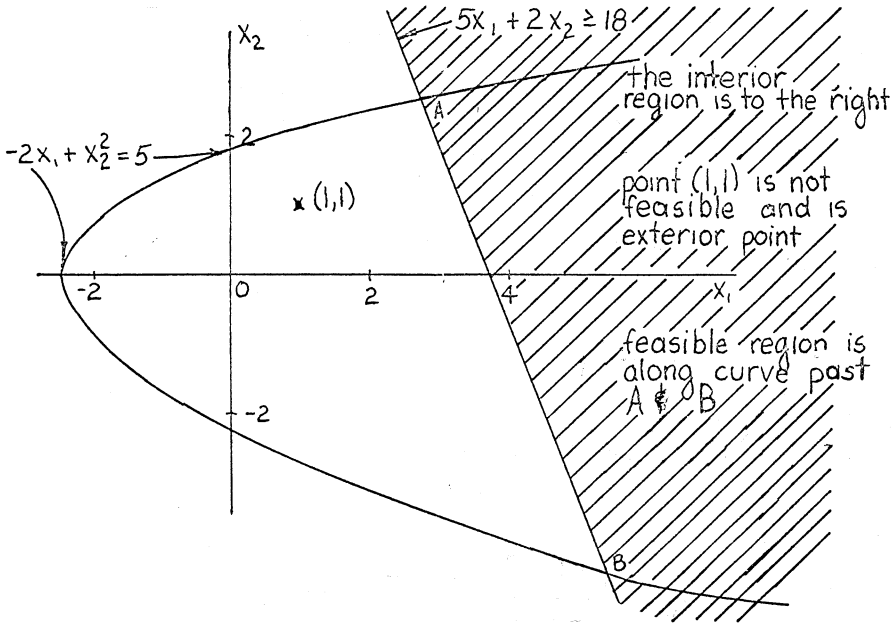
Problem 4.10

(a)

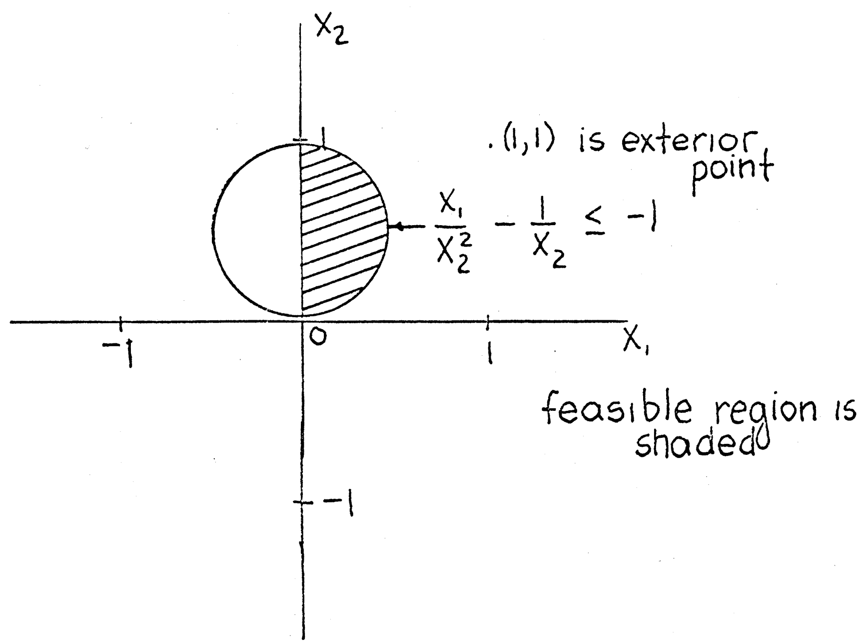


(b)



$5x_1 + 2x_2 \geq 18$
the interior region is to the right
$-2x_1 + x_2^2 = 5$
x (1,1)
point (1,1) is not feasible and is exterior point
feasible region is along curve past A & B
A
B
x_2
x_1
-2
0
2
4
2
-2

(c)

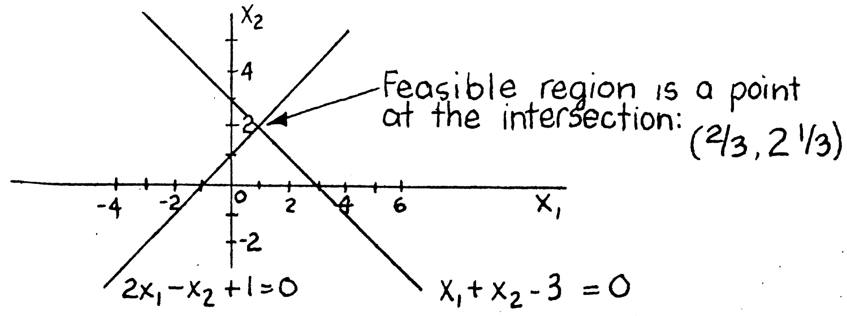


x_2
x_1
. (1,1) is exterior point
$\frac{x_1}{x_2^2} - \frac{1}{x_2} \leq -1$
feasible region is shaded
-1
0
1
1
-1

Problem 4.11

(a)

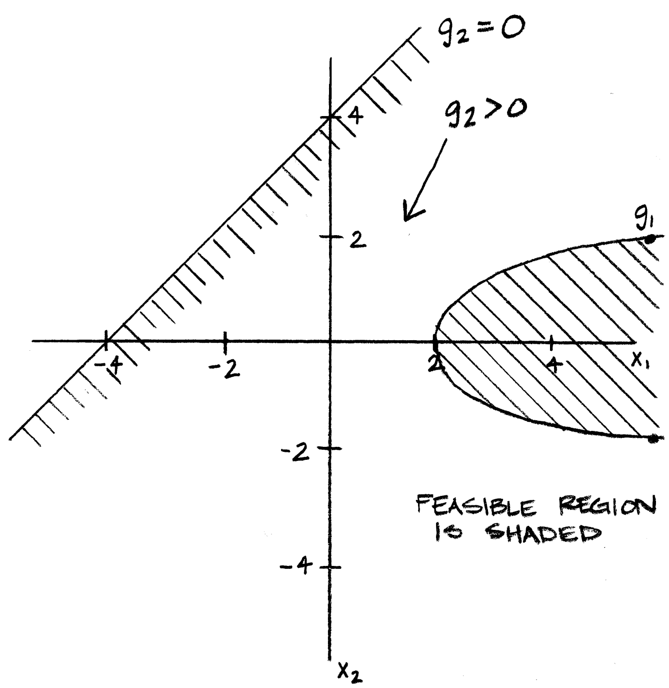
$$h_1(\tilde{x}) = x_1 + x_2 - 3 = 0$$
$$h_2(\tilde{x}) = 2x_1 - x_2 + 1 = 0$$



(b)
$$h_1(x) = x_1^2 + x_2^2 + x_3^2 = 0$$
$$h_2(x) = x_1 + x_2 + x_3 = 0$$

Feasible region is the origin

(c)
$$g_1(x) = x_1 - x_2^2 - 2 \geq 0$$
$$g_2(x) = x_1 - x_2 + 4 \geq 0$$

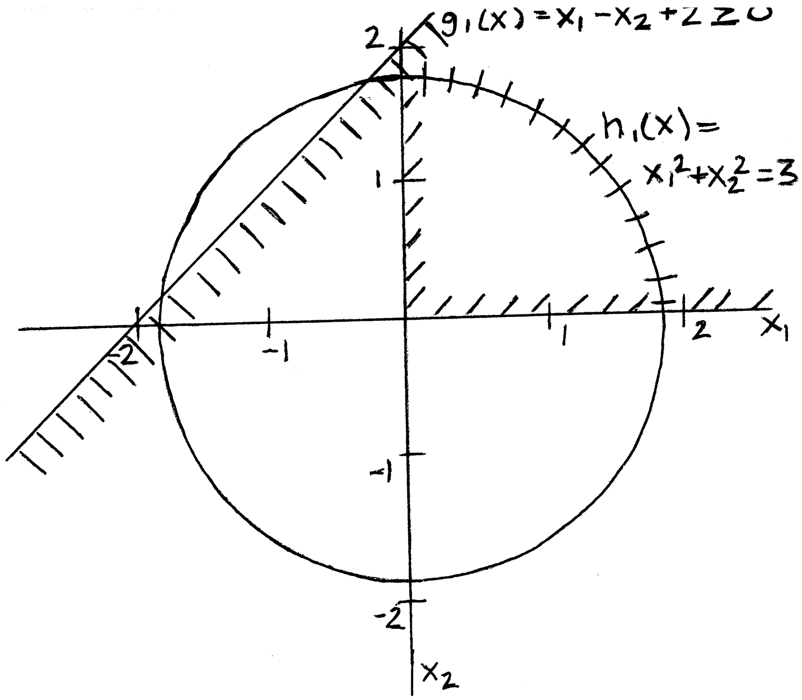


(d) $h_1(x) = x_1^{\,2} + x_2^{\,2} = 3$

$g_1(x) = x_1 - x_2 + 2 \geq 0$

$g_2(x) = x_1 \geq 0$

$g_3(x) = x_2 \geq 0$



Problem 4.12

For the first constraint:

$h_1(\boldsymbol{x}^1) = (0.947)^2 + 2(0.207)^2 + 3(-0.0772)^2 - 1 = 0\,?$ max

$= 3.9\text{x}10^{-4}$ ok

$h_1(\boldsymbol{x}^2) = (0.534)^2 + 2(0.535)^2 + 3(-0.219)^2 - 1 = 0?$ min

$=1.5\text{x}10^{-3}$ probably ok

For the second constraint:

$h_2(\boldsymbol{x}^1) = 5(0.947) + 5(0.207) - 3(-0.0772) - 6 = 0?$ max

$=1.6\text{x}10^{-3}$ ok

$h_2(\boldsymbol{x}^2) = 5(0.534) + 5(0.535) - 3(-0.219) - 6 = 0?$ min

$= 2 \times 10^{-3}$ probably ok

Problem 4.13

The point (1, 1) can be proven to be a local minimum by the methods described in Chapter 8. The question is: how can it be shown to be the global minimum for the problem? Some ways are:

(1) Start a numerical search from several starting points.

(2) Plot the contours of $f(\boldsymbol{x})$, an ellipse, in the x_1-x_2 plane along with the function $g(\boldsymbol{x}) = x_1^2 + x_2^2$, a circle, and locate the local minimum at $\boldsymbol{x}^* = [1\ 1]^T$. Then ascertain if any other minimum exists by examining the graph.

Problem 4.14

If the problem is a convex programming problem, that is if

$f(\boldsymbol{x})$ is convex

$g(\boldsymbol{x})$ are concave (form a convex set)

Another possibility is if $f(\boldsymbol{x})$ is unimodal in the feasible region.

Problem 4.15

$$f = 2x_1^2 + 2x_1x_2 + 3x_2^2 + 7x_1 + 8x_2 + 25$$

(a) $$\nabla f = \begin{bmatrix} 4x_1 + 2x_2 + 7 \\ 2x_1 + 6x_2 + 8 \end{bmatrix} \quad \boldsymbol{H} = \begin{bmatrix} 4 & 2 \\ 2 & 6 \end{bmatrix}$$

6 and 4 are $> 0, \begin{vmatrix} 4 & 2 \\ 2 & 6 \end{vmatrix} = 20 > 0 \Rightarrow \boldsymbol{H}$ is positive definite

Thus, f is both convex and strictly convex.

$\boldsymbol{x}^* = [-1.3 \quad -0.9]^T$ (not required)

(b) $f = e^{5x}, \nabla f = 5e^{5x}, \nabla^2 f = 25e^{5x}$

$\nabla^2 f > 0$ for $-\infty < x < \infty$

f is both convex and strictly convex.

Problem 4.16

(a) $f = (x_1 - x_2)^2 + x_2^{\ 2}$

$$\boldsymbol{\nabla} f = \begin{bmatrix} 2(x_1 - x_2) \\ -2(x_1 - x_2) + 2x_2 \end{bmatrix} \quad \boldsymbol{\nabla}^2 f = \begin{bmatrix} 2 & -2 \\ -2 & 4 \end{bmatrix}$$ is pos. def.

strictly convex

(b) $f = x_1^{\ 2} + x_2^{\ 2} + x_3^{\ 2}$

$$\boldsymbol{\nabla} f = \begin{bmatrix} 2x_1 \\ 2x_2 \\ 2x_3 \end{bmatrix} \quad \boldsymbol{\nabla}^2 f = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$ is pos. def.

strictly convex

(c) $f = e^{x_1} + e^{x_2}$

$$\boldsymbol{\nabla} f = \begin{bmatrix} e^{x_1} \\ e^{x_2} \end{bmatrix} \quad \boldsymbol{\nabla}^2 f = \begin{bmatrix} e^{x_1} & 0 \\ 0 & e^{x_2} \end{bmatrix}$$ is pos. def. in the finite plane

strictly convex in the finite plane

Problem 4.17

$f = e^{x_1} + e^{x_2}$

$$\boldsymbol{\nabla} f = \begin{bmatrix} e^{x_1} \\ e^{x_2} \end{bmatrix} \quad \boldsymbol{H} = \begin{bmatrix} e^{x_1} & 0 \\ 0 & e^{x_2} \end{bmatrix}$$

$\boldsymbol{H}$ is positive definite, because $e^x > 0$ everywhere on the finite real axis. Thus, f is strictly convex over finite values of x_1 and x_2, and thus convex.

Problem 4.18

We will show that

$$|(1-\theta)x_1+\theta x_2| \le (1-\theta)|x_1|+\theta|x_2|$$
for all $x_1, x_2,$ and $0 \le \theta \le 1$

Let $f_L = |(1-\theta)x_1+\theta x_2|$ and $f_R = (1-\theta)|x_1|+\theta|x_2|$

(a) $x_1 \ge 0,\ x_2 \ge 0.$ This means that
$(1-\theta)x_1+\theta x_2 = f_L = f_R \Rightarrow$ function is convex.

(b) $x_1 = 0,\ x_2 \ge 0.$ We have $f_L = \theta x_2 = f_R \Rightarrow f$ is convex

(c) $x_1 \le 0,\ x_2 \ge 0.$ We have $(1-\theta)x_1 \le 0$ and $\theta x_2 \ge 0$.

$f_R = (1-\theta)|x_1|+\theta|x_2| = (1-\theta)(-x_1)+\theta x_2$. f_L must be less than f_R because the term $(1-\theta)x_1+\theta x_2$ involves subtraction of $(1-\theta)\,|x_1|$ from θx_2. Thus $f_L \le f_R$, and f is convex for $0 \le \theta \le 1$.

For $\theta = 0,\ f_L = |(1-\theta)x_1| = (1-\theta)|x_1| = f_R$

For $\theta = 1,\ f_L = |(\theta x_2)| = \theta)|x_2| = f_R$

f is convex for $0 \le \theta \le 1$.

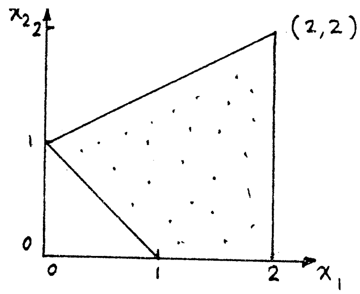
(d) $x_1 \le 0,\ x_2 \le 0.$ $f_L = |(1-\theta)x_1+\theta x_2| = |-[(1-\theta)(-x_1)+\theta(-x_2)]|$

$f_L - (1-\theta)(-x_1)+\theta(-x_2).$

$f_R = (1-\theta)|x_1|+\theta|x_2| = (1-\theta)(-x_1)+\theta(-x_2) = f_L.$

f is convex.

Problem 4.19



All the constraints are linear, and thus concave functions. The region is thus convex. It is also a closed region as seen from the figure.

Problem 4.20

$$g_1 = -(x_1^2 + x_2^2) + 9 \ge 0, \quad g_2 = -x_1 - x_2 + 1 \ge 0$$

$\boldsymbol{\nabla} g_1 = \begin{bmatrix} -2x_1 \\ -2x_2 \end{bmatrix}$ $\boldsymbol{\nabla}^2 g_1 = \begin{bmatrix} -2 & 0 \\ 0 & -2 \end{bmatrix}$ eigenvalues are –2, -2 $\Rightarrow g_1$, is strictly concave; g_2 is concave because it is linear. Thus, the two constraints form a convex region.

Problem 4.21

$$g_1 = x_1^2 - x_2^2 + 9 \ge 0$$

$\nabla g_1 = \begin{bmatrix} -2x_1 \\ -2x_2 \end{bmatrix}$ $\boldsymbol{H}_1 = \begin{bmatrix} -2 & 0 \\ 0 & -2 \end{bmatrix}$ eigenvalues are –2, -2 $\Rightarrow g_1$ is strictly concave.

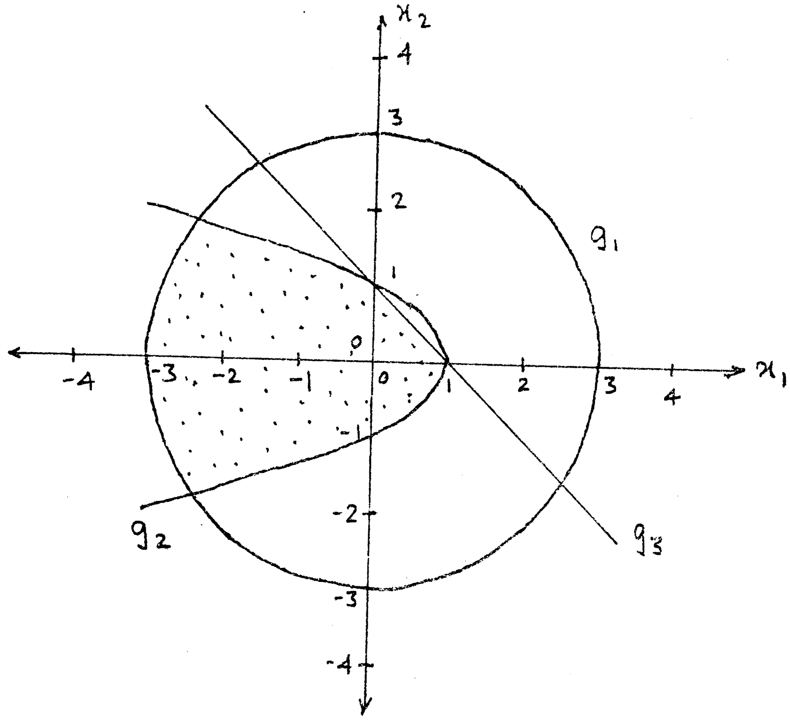
$$g_2 = x_1 - x_2^2 + 1 \ge 0$$

$\nabla g_2 = \begin{bmatrix} -1 \\ -2x_2 \end{bmatrix}$ $\boldsymbol{H}_2 = \begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix}$ eigenvalues are 0, -2 $\Rightarrow g_2$ is concave.

$$g_3 = -x_1 - x_2 + 1 \ge 0$$

$\nabla g_3 = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$ $\boldsymbol{H}_3 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$ eigenvalues are 0, 0. $\Rightarrow g_3$ is concave and convex.

Thus, the region is convex. That it is closed can be seen from the figure.



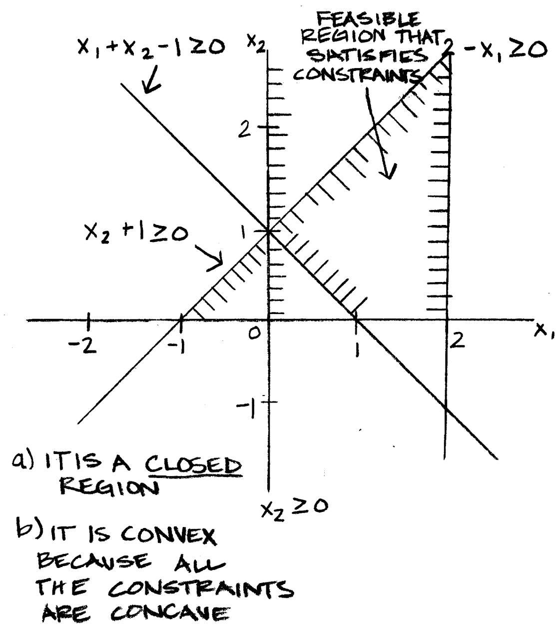
Problem 4.22

$f(x) = \ln x_1 + \ln x_2 \qquad \ln x_i$ is not defined for $x_i \le 0$

$$\nabla f(x) = \begin{bmatrix} \dfrac{1}{x_1} \\ \dfrac{1}{x_2} \end{bmatrix} \qquad \boldsymbol{H}(x) = \begin{bmatrix} -\dfrac{1}{x_1^2} & 0 \\ 0 & -\dfrac{1}{x_2^2} \end{bmatrix}$$

For any $x_i \ne 0, \boldsymbol{H}(\boldsymbol{x})$ is neg. def. At $x_i = 0, \boldsymbol{H}(\boldsymbol{x})$ is undefined, but the conclusion is that $f(\boldsymbol{x})$ is *concave*.

Problem 4.23



Problem 4.24

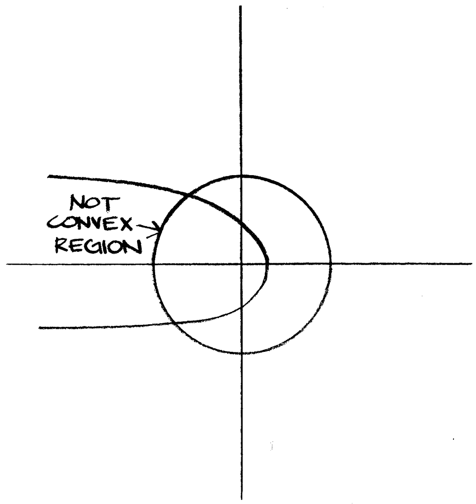
If the region is convex, all the constraints must be concave, i.e., the Hessian matrix must be neg. def.

(a) $h(x) = x_1^{\ 2} + x_2^{\ 2} - 9$

$$\frac{\partial h}{\partial x_1} = 2x_1 \ \frac{\partial h}{\partial x_2} = 2x_2 \ \ \frac{\partial^2 h}{\partial x_1^{\ 2}} = 2 \ \ \frac{\partial^2 h}{\partial x_2^{\ 2}} = 2$$

$H = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$ is pos def. And hence $h(x)$ is not concave (it is convex).

Answer:
No.



Problem 4.25

The Hessian of the each term of $\psi(\boldsymbol{x})$ is pos def. or pos. semi-def. If the term is convex. The Hessian of a sum of convex terms is the sum of the individual Hessians, hence the matrix of $\psi(\boldsymbol{x})$ is convex. For example:

$$f(\boldsymbol{x}) = x_1^2 + x_2^2$$

H of the first term alone is $\begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}$

H of the second term alone is $\begin{bmatrix} 0 & 0 \\ 0 & 2 \end{bmatrix}$

and the sum of the two *H*'s is $\begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$.

Problem 4.26

Note the solution is wrong if $x = 0$.

Determine if $f(x)$ is convex and $g_1(x) \le 0$ is convex.

The Hessian matrix of $f(x)$ is

$$H(x) = \begin{bmatrix} \dfrac{400}{x_1^3 x_2} & \dfrac{200}{x_1^2 x_2^2} \\ \dfrac{200}{x_1^2 x_2^2} & \dfrac{400}{x_1 x_2^3} \end{bmatrix} \text{ is } f(x) \text{ convex?}$$

The principal minors are

$$\det H = \left[\left(\frac{400}{x_1^3 x_2} \right) \left(\frac{400}{x_1 x_2^3} \right) - \left(\frac{200}{x_1^2 x_2^2} \right) \left(\frac{200}{x_1^2 x_2^2} \right) \right] \geq 0$$

$$\frac{400}{x_1 x_2^3 \geq 0} \quad \text{and} \quad \frac{400}{x_1^3 x_2} \geq 0 \quad \text{for } x_i \geq 0 \quad \text{so } f(x) \text{ is convex}$$

Is the constraint $g \leq 0$ convex?

The Hessian matrix of $g(x)$ is

$$H_g(x) = \begin{bmatrix} \dfrac{600}{x_1^3 x_2} & \dfrac{300}{x_1^2 x_2^2} \\ \dfrac{300}{x_1^2 x_2^2} & \dfrac{600}{x_1 x_2^3} \end{bmatrix}$$

$$\det\ H_g = \left[\frac{3.6\text{x}10^5 - 9\text{x}10^4}{x_1^4 x_2^4} \right] \geq 0$$

$$\frac{600}{x_1^3 x_2} \geq 0 \text{ for } x_i \geq 0 \qquad \frac{600}{x_1 x_2^3} \geq 0 \text{ for } x_i \geq 0$$

so that $g(x)$ is convex

The $x_i \geq 0$ are convex functions. Consequently, the problem is a convex programming problem for $x_i > 0$. as $x_i \to 0$, $g \to \infty$, but the function asymptodically is convex.

Problem 4.27

(a) $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ positive definite

(b) $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ neither

(c) $\begin{bmatrix} \text{oil} & 0 \\ 3 & 1 \end{bmatrix}$ not symmetric hence change to $\begin{bmatrix} \text{oil} & 3/2 \\ 3/2 & 1 \end{bmatrix}$ which is not positive definite, so that neither is the answer

(d) $\begin{bmatrix} 1 & -2 \\ -2 & 1 \end{bmatrix}$ $\left.\begin{cases} 1 > \\ (1-4) = -3 < 0 \end{cases}\right\}$ neither

---

Problem 4.28

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

Use principal minors:
det A = 0

delete 1st col. and row $A_1 = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$

The elements on the main diagonal are positive: 1, 1, 0

Thus, *none* is the answer

Or *Use eigenvalues*

$$\det \begin{bmatrix} 1-\partial & 1 & 1 \\ 1 & (1-\partial) & 1 \\ 1 & 1 & (0-\partial) \end{bmatrix} = 0$$

$$(1-\lambda)[(1-\lambda)(0-\lambda)-1]-1[1(0-\lambda)-1+1[1-(1-\lambda)]=0$$

$$\left.\begin{matrix} \lambda_1 = 0 \\ \lambda_2 = 2.73 \\ \lambda_3 = -0.73 \end{matrix}\right\} \text{same conclusion}$$

Problem 4.29

$$f(D,h) = \pi Dh + \frac{\pi}{2}D^2$$

$$\nabla f(D,h) = \pi \begin{bmatrix} (h+D) \\ D \end{bmatrix}$$

$$\boldsymbol{H}(D,h) = \pi \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$$

H is not pos. def. so no minium exists (except at ∞ limits).

The eigenvalues of ***H*** are $\frac{1+\sqrt{5}}{2}$, $\frac{1-\sqrt{5}}{2}$, hence one is + and the other is -.

Based on the above

a. neither
b. is continuous
c. neither
d. does not
e. The trivial constraints (bounds) are linear and concave

$$g = \frac{\pi}{4}D^2h - 400 \geq 0$$

$$\nabla g = \frac{\pi}{4}\begin{bmatrix} 2Dh \\ D^2 \end{bmatrix}$$

$$\boldsymbol{H} = \frac{\pi}{4}\begin{bmatrix} 2h & 2D \\ 2D & 0 \end{bmatrix} \quad \begin{matrix} h > 0 \\ \text{but } 0 = 0 \end{matrix}$$

det ***H*** = -4D^2 and is negative always
so that ***H*** is concave

Thus, the constraints do form a convex region (they all must be concave).

Problem 4.30

Basis: 1 lb mol feed

Income: 50 (0.1 + 0.3x_A + 0.001S + 0.0001 x_AS)(1) [$]

Expenses: Assume the cost of the additive is $/1b mol feed, not additive

Additive: (2.0 + 10x_A + 20x_A^2) (1) [$]

Steam: $(1.0 + 0.003S + 2.0 \text{ x } 10^{-6}S^2)$ (1) [$]

$f = (5 + 15x_A + 0.05S + 0.005x_AS) – (2.0 + 0.003S + 2.0\text{x}10^{-6}S^2)$
$-(2.0 + 10x_A + 20x_A^2)$

(a) $f = 1 + 5x_A – 20x_A^2 + 0.047S – 2.0 \text{ x}10^{-6}S^2 + 0.005x_AS$

$$\nabla f = \begin{bmatrix} (5-40x_A+0.005S) \\ (.047-4.0\text{x}10^{-6}S+0.005x_A) \end{bmatrix}$$

$$\nabla^2 f = \boldsymbol{H} = \begin{bmatrix} -40 & 0.005 \\ .005 & -4.0\text{x}10^{-6} \end{bmatrix}$$

(b) ***H*** is negative definite, hence concave.

The eigenvalues are –40 and $–3.375\text{x}10^{-6}$ (almost zero but not zero).

(c) The search region is linear because the constraints

$0 \leq x_A \leq 1$

$S \geq 0$

are linear, hence concave, and form a convex region.

Problem 4.31

$$f = (P_2/P_1)^{0.286} + (P_3/P_2)^{0.286} + (P_4/P_3)^{0.286}$$

with $P_1 = 1$ atm and $P_4 = 10$ atm, this becomes

$$f = P_2^{0.286} + P_3^{0.286}P_2^{-0.286} + 1.932P_3^{-0.286}$$
$$\partial f/\partial P_2 = 0.286P_2^{-0.714} - 0.286P_3^{0.286}P_2^{-1.286}$$
$$\partial^2 f/\partial P_2^2 = -0.2042P_2^{-1.714} + 0.3678P_3^{0.286}P_2^{-2.286}$$
$$\partial f/\partial P_3 = 0.286P_3^{-0.714}P_2^{-0.286} - 0.5526P_3^{-1.286}$$
$$\partial^2 f/\partial P_3^2 = -0.2042P_3^{-1.714}P_2^{-0.286} + 0.7106P_3^{-2.286}$$
$$\partial^2 f/\partial P_2\partial P_3 = -0.0818P_3^{-0.714}P_2^{-1.286}$$

$$\boldsymbol{H} = \begin{bmatrix} \partial^2 f / \partial P_2^{\ 2} & \partial^2 f / \partial P_2 \partial P_3 \\ \partial^2 f / \partial P_2 \partial P_3 & \partial^2 f / \partial P_3^{\ 2} \end{bmatrix}$$

For convexity, must have $\partial^2 f / \partial P_2^{\ 2} \geq 0$ (as well as some other conditions also).
$\partial^2 f / \partial P_2^{\ 2} = -0.2042 P_2^{-1.714} + 0.3678 P_3^{0.286} P_2^{-2.286}$
$P_2^{1.714}(\partial^2 f / \partial P_2^{\ 2}) = -0.2042 + 0.3678 P_3^{0.286} P_2^{-0.572}$
This has its lowest value at $P_2 = 10$ atm, $P_3 = 1$ atm.
$P_2^{1.714}(\partial^2 f / \partial P_2^{\ 2}) = -0.1057 \ < 0.$
Therefore, $\boldsymbol{H}$ is not positive semi-definite over the range $1 \leq P_2 \leq 10,\ 1 \leq P_3 \leq 10,$ and *f* is not convex over this entire range.

Problem 4.32

(a) $$f(x) = 100 x_1 + \frac{200}{x_1 x_2}$$

$$\boldsymbol{H}(x) = \begin{bmatrix} \dfrac{400}{x_1^{\ 3} x_2} & \dfrac{200}{x_1^{\ 2} x_2^{\ 2}} \\ \dfrac{200}{x_1^{\ 2} x_2^{\ 2}} & \dfrac{400}{x_1 x_2 3} \end{bmatrix}$$

$$\det(\boldsymbol{H}) = \left[\left(\frac{400}{x_1^{\ 3} x_2}\right)\left(\frac{400}{x_1 x_2^{\ 3}}\right) - \left(\frac{200}{x_1^{\ 2} x_2^{\ 2}}\right)\left(\frac{200}{x_1^{\ 2} x_2^{\ 2}}\right)\right]$$

$\dfrac{400}{x_1 x_2^{\ 3}} \geq 0$ and $\dfrac{400}{x_1^{\ 3} x_2} \geq$ for $x_i > 0$ and asymptodically as $x_i \to 0.$ $f(\boldsymbol{x})$ is convex (a)

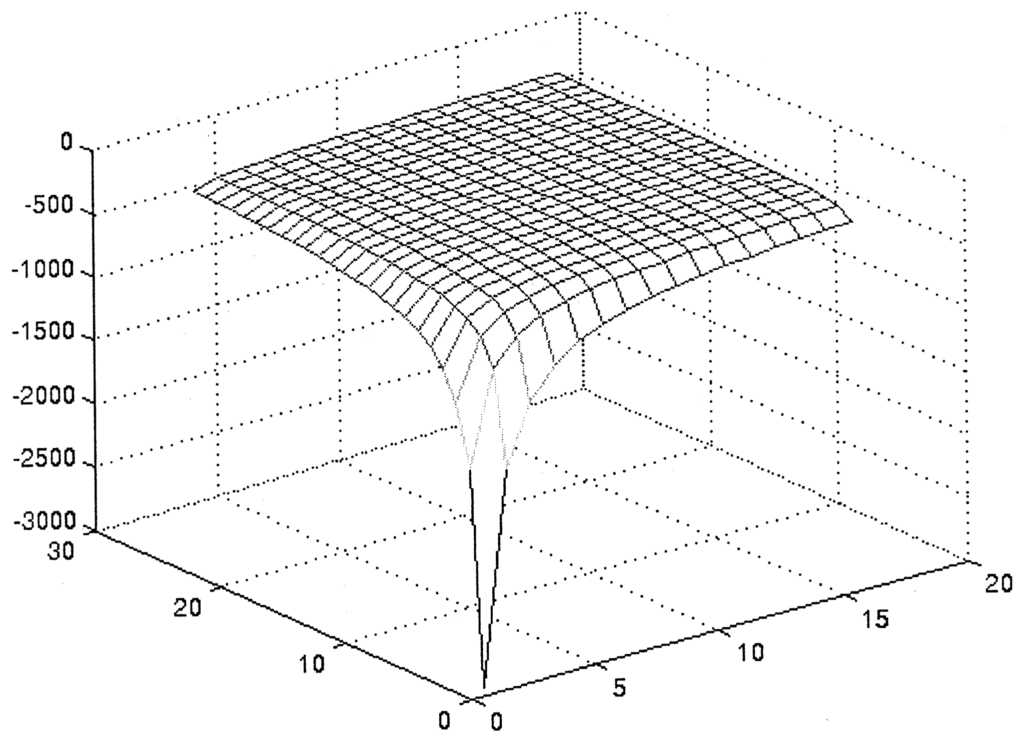
(b) $$g(\boldsymbol{x}) = 2x_2 + \frac{300}{x_1 x_2} - 1 \geq 0$$

$$\boldsymbol{\nabla}^2 g(\boldsymbol{x}) = \begin{bmatrix} +\dfrac{600}{x_1^{\ 3} x_2} & +\dfrac{300}{x_1^{\ 2} x_2^{\ 2}} \\ +\dfrac{300}{x_1^{\ 2} x_2^{\ 2}} & +\dfrac{600}{x_1 x_2^{\ 3}} \end{bmatrix}$$

$+\dfrac{600}{x_1^{\ 3} x_2} \geq 0$ and $+\dfrac{600}{x_1 x_2^{\ 3}} \geq 0$ for $x_i > 0$ and asymptodically as $x_i \to 0.$
so that $g(\boldsymbol{x})$ is convex

Also $x_i \geq 0$ are $\begin{Bmatrix} \text{concave} \\ \text{convex} \end{Bmatrix}$

but the constraint region is not a convex region because $g(\boldsymbol{x}) \geq 0$ has to be a concave function for the region to be convex. The following figure (with $300/x_1x_2$ changed to $30/x_1x_2$ to reduce the scale) illustrate the surface for $g(\boldsymbol{x}) = 1$. Note that the region above $g(\boldsymbol{x}) = 1$ is not convex. In P. 4.26 $g(\boldsymbol{x}) \leq 1$.



Problem 4.33

(a) $\dfrac{\partial f(\boldsymbol{x})}{\partial x_1} = x_1^{\,3} - x_1 \qquad \dfrac{\partial f(\boldsymbol{x})}{\partial x_2} = -2x_2 \qquad \dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_1^{\,2}} = 3x_1^{\,2} - 1$

$$\frac{\partial^2 f(\boldsymbol{x})}{\partial x_2^{\,2}} = -2 \qquad\qquad \frac{\partial^2 f(\boldsymbol{x})}{\partial x_1 \partial x_2} = 0$$

$$\boldsymbol{H}(\boldsymbol{x}) = \begin{pmatrix} 3x_1^{\,2} - 1 & 0 \\ 0 & -2 \end{pmatrix}$$

$f(\boldsymbol{x})$ is not a convex function for all *x*, hence the answer is no.

(b) no: $h_1(\boldsymbol{x})$ is not satisfied $1 + 1 \neq 4$

(c) yes: $\boldsymbol{x}^{\mathrm{T}} = [2 \;\; 2]$ lies in the interior of the inequality $g_2(\boldsymbol{x}^*) = x_1 - x_2 - 2 \leq 2$

Problem 4.34

$f = 14720(100 - P) + 6560R - 30.2PR + 6560 - 30.2P + 19.5ny^{.5} + 23.2y^{.62}$ where $y = 5000R - 23PR + 5000 - 23P$

Differentiation gives

$$\partial^2 f / \partial P^2 = 529(-4.875ny^{-1.5} - 5.46592y^{-1.38})(R+1)^2$$
$$\partial^2 f / \partial P \partial R = -30.2 + (112.125ny^{-1.5} + 125.71616y^{-1.38})(R+1) \text{ x}$$
$$(5000 - 23P) - 224.25ny^{-0.5} - 330.832y^{-0.38}$$
$$\partial^2 f / \partial P \partial n = -224.25y^{-0.5}(R+1)$$
$$\partial^2 f / \partial R^2 = (-4.875ny^{-1.5} - 5.46592y^{-1.38})(5000 - 23P)^2$$
$$\partial^2 f / \partial R \partial n = 9.75y^{-0.5}(5000 - 23P)$$
$$\partial^2 f / \partial n^2 = 0$$

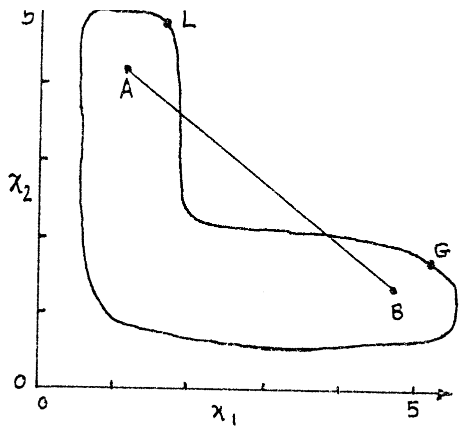
For $P = 99$, $R = 8$ and $n = 55$, we have

$$\boldsymbol{H} = \begin{bmatrix} \partial^2 f / \partial P^2 & \partial^2 f / \partial P \partial R & \partial^2 f / \partial P \partial n \\ \partial^2 f / \partial P \partial R & \partial^2 f / \partial R^2 & \partial^2 f / \partial R \partial n \\ \partial^2 f / \partial P \partial n & \partial^2 f / \partial R \partial n & \partial^2 f / \partial n^2 \end{bmatrix}$$

$$= \begin{bmatrix} -3.2 & -74 & -12.9 \\ -74 & -553.7 & 169.6 \\ -12.9 & 169.6 & 0 \end{bmatrix}$$

For $\boldsymbol{H}$ to be positive definite, all diagonal elements must be positive, which is not the case here. Thus *f* is not convex at *P* = 99, *R* = 8 and *n* = 55. It is therefore, not convex in some small neighborhood of the optimum.

Problem 4.35



If the search is started in the vicinity of point *A*, it is likely to terminate at point *L* which is a local maximum. The global maximum is at point *G*. The region is not convex because the line segment *AB* does not entirely lie within the region, even though the endpoints *A* and *B* lie inside the region.

Problem 4.36

$f(\alpha)$ is a continuous function because it is the sum of continuous functions.

If $f(x)$ is continuos for $a \le x \le b$ and $f\,'(x)$ is positive for $a < x < b,$ then $f(b) > f(a).$ The corresponding fact occurs for $f\,'(\boldsymbol{x})$ being negative. On the interval $x^{(k)} < \alpha < x^{(k+1)}$. We have

$$f(\alpha) = \sum_{i=1}^{n} \left| x^{(i)} - \alpha \right|$$

$$\begin{aligned} &= (\alpha - x^{(1)}) + (\alpha - x^{(2)}) + \cdots + (\alpha - x^{(k)}) \\ &\quad + (x^{(k+1)} - \alpha) + (x^{(k+2)} - \alpha) + \cdots + (x^{(n)} - \alpha) \\ &= k\alpha - \sum_{i=1}^{k} x^{(i)} + \sum_{i=k+1}^{n} x^{(i)} - (n-k)\alpha \end{aligned}$$

Differentiation gives

$$f\,'(\alpha) = k - (n-k) = 2(k - n/2)$$

which is negative for $k < n/2$ and positive for $k > n/2$. $f\,''(\alpha) = 0,$ hence f is convex.

Repeat the above analysis with c_i in the sum. (Assume $c_i > 0$)

Problem 4.37

(a) $f = -x^4 + x^3 + 20$

$f' = -4x^3 + 3x^2 = x^2(-4x+3) = 0$

$x^* = 0, \quad 3/4$

$f'' = -12x^2 + 6x$

$f''(0) = 0 \qquad x = 0$ is a saddle point (inflection)

$f''(3/4) = -2.25 < 0 \qquad x = 3/4$ is a maximum

(b) $f = -x^3 + 3x^2 + x + 5$

$f' = -3x^2 + 6x + 1 = 0 \;\Rightarrow\; x^* = -1 \pm \sqrt{2/3}$

$f'' = 6x + 6$

$f''(-1+\sqrt{2/3}) = 4.9 > 0. \qquad x = -1 + \sqrt{2/3}$ is a minimum

$f''(-1-\sqrt{2/3} = -4.9 < 0. \qquad x = -1 - \sqrt{2/3}$ is a maximum.

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

$f' = 4x^3 - 4x = 4x(x^2 - 1) = 0 \quad \Rightarrow x^* = -1, \quad 0, \quad 1$

$f'' = 12x^2 - 4$

$f''(-1) = 8 > 0 \qquad x = -1$ is a minimum

$f''(0) = -4 < 0 \qquad x = 0$ is a maximum

$f''(1) = 8 > 0 \qquad x = 1$ is a minimum

(d) $f = x_1{}^2 - 8x_1x_2 + x_2{}^2$

$$\nabla f = \begin{bmatrix} 2x_1 - 8x_2 \\ 2x_2 - 8x_1 \end{bmatrix} = \mathbf{0} \Rightarrow \quad \boldsymbol{x}^* = [0 \;\; 0]^{\mathrm{T}}$$

$\boldsymbol{H} = \begin{bmatrix} 2 & -8 \\ -8 & 2 \end{bmatrix}$ Eigenvalues are $(\lambda - 2)^2 - 8^2 = 0$

or $\lambda = -6, \quad 10$

$\boldsymbol{H}$ is indefinite, and $\boldsymbol{x} = [0 \; 0]^{\mathrm{T}}$ is a saddle point.

Problem 4.38

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

$$\nabla f = \begin{bmatrix} 2x_1 + 2 \\ 6x_2 + 6 \end{bmatrix} = 0 \quad \Rightarrow \; \boldsymbol{x}^* = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

$\boldsymbol{H} = \begin{bmatrix} 2 & 0 \\ 0 & 6 \end{bmatrix}$. Eigenvalues are λ=2, 6.

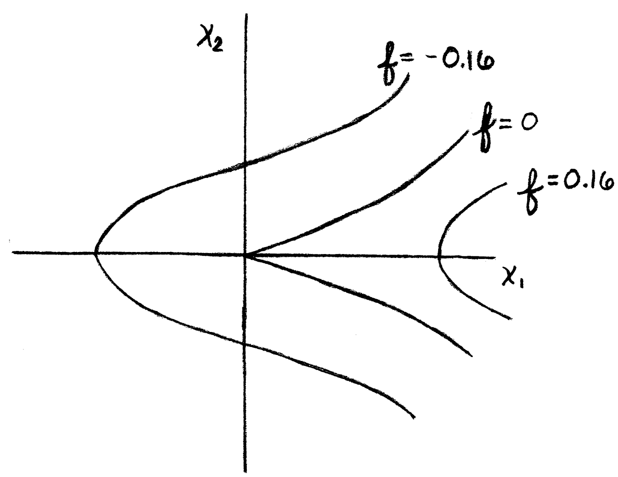
$\boldsymbol{H}$ is positive definite, and $\boldsymbol{x} = [\text{-1 -1}]^T$ is a minimum.

Problem 4.39

$$f(\boldsymbol{x}) = 2x_1^2 x_2 - 2x_2^2 + x_1^3$$

$$\frac{\partial f(\boldsymbol{x})}{\partial x_1} = 4x_1x_2 + 3x_1^2 \qquad \frac{\partial^2 f}{\partial x_1^2} = 4x_2 + 6x_1 \qquad \frac{\partial^2 f}{\partial x_2 \partial x_1} = 4x_1$$

$$\frac{\partial f(\boldsymbol{x})}{\partial x_2} = 2x_1^2 - 4x_2 \qquad \frac{\partial^2 f}{\partial x_1 \partial x_2} = 4x_1 \qquad \frac{\partial^2 f}{\partial x_2^2} = -4$$



at (0, 0)

$$\boldsymbol{H} = \begin{bmatrix} (4x_2 + 6x_1) & 4x_1 \\ 4x_1 & -4 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & -4 \end{bmatrix}$$

$$\lambda_1 = 0 \qquad \lambda_2 = -4$$

So that probably case 10 or 11 is the outcome. Evaluate $f(\boldsymbol{x})$ on both sides of zero to see how the value of $f(\boldsymbol{x})$ changes.

$$\left.\begin{array}{ll} \boldsymbol{x} = [1 \quad 0]^{\mathrm{T}} & f(\boldsymbol{x}) = 1 \\ \boldsymbol{x} = [-1 \quad 0]^{\mathrm{T}} & f(\boldsymbol{x}) = -1 \end{array}\right\} \begin{array}{l} \text{declining ridge toward } x_1 \to -\infty, \\ \text{rising ridge toward } x_1 \to +\infty \end{array}$$

$$\boldsymbol{x} = [0 \quad 1]^{\mathrm{T}} \qquad f(\boldsymbol{x}) = -2$$

$$\boldsymbol{x} = [0 \quad -1]^{\mathrm{T}} \qquad f(\boldsymbol{x}) = -2$$

Problem 4.40

$$f(\boldsymbol{x}) = 3x_1^3 x_2$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 9x_1^2 x_2 \\ 3x_1^3 \end{bmatrix}$$

$$\boldsymbol{H}(\boldsymbol{x}) = \begin{bmatrix} 18x_1x_2 & 9x_1^2 \\ 9x_1^2 & 0 \end{bmatrix}$$

principal minors: 18 x_1 x_2 is not always definite unless $x_i > 0$

$$\det \ \boldsymbol{H} = (18x_1x_2)(0) - 81x_1^4 \ \text{(concave function)}$$

Get eigenvalues

$$(18x_1x_2 - \lambda)(0 - \lambda) - 81x_1^4 = 0$$

$$\lambda = \frac{-(-18x_1x_2) \pm \sqrt{(-18x_1x_2)^2 - 4(1)(-81x_1^4)}}{2}$$

λ depends on the values of x_1 and x_2, but at the stationary point (0, 0)

$$\left(\nabla f(\boldsymbol{x}) = [\mathbf{0}] = \begin{bmatrix} 9x_1^2 x_2 \\ 3x_1^3 \end{bmatrix} \text{ yields } x_1 = x_2 = 0, \text{ or } x_1 = 0, \ x_2 = \text{anything}\right)$$

$\lambda_i = 0$, hence some degenerate surface occurs

Problem 4.41

$$f(\boldsymbol{x}) = 10x_1 - x_1^{\,2} - 10x_2 - x_2^{\,2} - x_1x_2 - x_1^{\,3} - 34$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 10 - 2x_1 - x_2 + 3x_1^{\,2} \\ 10 - 2x_2 - x_1 \end{bmatrix} \qquad \boldsymbol{H}(\boldsymbol{x}) = \begin{bmatrix} (-2 + 6x_1 & -1 \\ -1 & -2 \end{bmatrix}$$

Find two eigenvalues (in terms of x_1)

$$(-2 + 6x_1 - \lambda)(-2 - \lambda) - 1 = 0 \qquad \lambda^2 + (4 - 6x_1)\lambda + (4 - 12x_1) = 0$$

$$\lambda = \frac{-(4 - 6x_1) \pm \sqrt{4 - 6x_1)^2 - 4(1)(4 - 12x_1)}}{2}$$

Solve for λ in terms of x_1; the value of λ depends on the value of x_1

Problem 4.42

(a) $$u(r) = 4 \in \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$$

at the stationary point

$$\left. \frac{du}{dr} \right|_{r^*} = 0 \quad \Rightarrow \quad \left. \frac{du}{dr} \right|_{r^*} = 4 \in \left[-12 \left(\frac{\sigma}{r^*} \right)^{12} \frac{1}{r^*} + 6 \left(\frac{\sigma}{r^*} \right)^{6} \frac{1}{r^*} \right] = 0$$

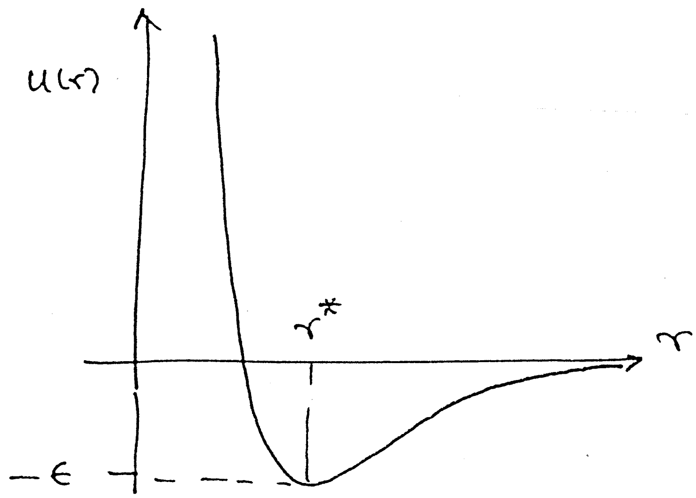
$$\frac{\sigma}{r^*} = \left(\frac{1}{2} \right)^{1/6} \quad \Rightarrow \quad \boxed{r^* = 2^{1/6} \sigma}$$

(b) $$\left. \frac{d^2u}{dr^2} \right|_{r^*} = 4 \in \left[156 \left(\frac{\sigma}{r^*} \right)^{12} \frac{1}{r^{*2}} - 42 \left(\frac{\sigma}{r^*} \right)^{6} \frac{1}{r^{*2}} \right]$$

$$= \frac{72}{\sqrt[3]{2}} \left(\frac{\in}{\sigma^2} \right) > 0 \text{ as long as } \in > 0$$

The Lennard-Jones potential has a minimum at r^*

(c) $u(r^*) = 4\in\left[\left(\frac{1}{2}\right)^2 - \frac{1}{2}\right] \quad = -\in$



Lennard-Jones potential

Problem 4.43

The solution of $y = (x-a)^2 = 0,$ or $x = a$ is misleading. The necessary condition is
$dy/dx = 2(x-a) = 0$
that coincidentally corresponds to the solution of the equation. For
$z = x^2 - 4x + 16,\ \ dz/dx = 2x - 4 = 0$
that differs from
$x^2 - 4x + 16 = 0.$
$x = 2 \pm j\sqrt{3}$ does not satisfy $2x - 4 = 0,$ and is thus not the minimum. $x = 2$ is the minimum.

Problem 4.44

No. $f(x)$ is not differentiable at $x^* = 0$ where the minimum of $f(x)$ is located.

Problem 4.45

(a) $f = 6x_1^2 + x_2^3 + 6x_1x_2 + 3x_2^2$

$$\nabla f = \begin{bmatrix} 12x_1 + 6x_2 \\ 3x_2^2 + 6x_1 + 6x_2 \end{bmatrix} = \mathbf{0} \quad \Rightarrow \boldsymbol{x}^* = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \text{or} \begin{bmatrix} 1/2 \\ -1 \end{bmatrix}$$

$$\boldsymbol{H} = \begin{bmatrix} 12 & 6 \\ 6 & 6x_2 + 6 \end{bmatrix}$$

at $\boldsymbol{x}^* = \begin{bmatrix} 0 & 0 \end{bmatrix}^{\mathrm{T}}, \boldsymbol{H} = \begin{bmatrix} 12 & 6 \\ 6 & 6 \end{bmatrix}$

$\Delta_i = 12$ and 6 are greater than 0 $;\Delta_2 = \begin{bmatrix} 12 & 6 \\ 6 & 0 \end{bmatrix} = 36 > 0.$

$\boldsymbol{H}$ is positive definite, and $[0\ 0]^{\mathrm{T}}$ is a minimum

At $\boldsymbol{x}^* = \begin{bmatrix} 1/2x & -1 \end{bmatrix}^{\mathrm{T}}$, $\boldsymbol{H} = \begin{bmatrix} 12 & 6 \\ 6 & 0 \end{bmatrix}$

$\Delta_i = 12$ and 0 ; $\Delta_2 = \begin{vmatrix} 12 & 6 \\ 6 & 0 \end{vmatrix} = -36 \le 0.$

$\boldsymbol{H}$ is indefinite, and $\begin{bmatrix} 1/2 & -1 \end{bmatrix}^{\mathrm{T}}$ is a saddle point.

(b) $f = 3x_1^2 + 6x_1 + x_2^2 + 6x_1x_2 + x_3 + 2x_3^2 + x_2x_3 + x_2$

$$\nabla f = \begin{bmatrix} 6x_1 + 6 + 6x_2 \\ 2x_2 + 6x_1 + x_3 + 1 \\ 4x_3 + x_2 + 1 \end{bmatrix} = \mathbf{0} \quad \Rightarrow \boldsymbol{x}^* = \begin{bmatrix} 4/17 \\ -21/17 \\ 1/17 \end{bmatrix}$$

$$\boldsymbol{H} = \begin{bmatrix} 6 & 6 & 0 \\ 6 & 2 & 1 \\ 0 & 1 & 4 \end{bmatrix}$$

$\Delta_i = 6, 2,$ and 4 $;\Delta_2 = \begin{vmatrix} 6 & 6 \\ 6 & 2 \end{vmatrix} = -24 \quad \begin{vmatrix} 6 & 0 \\ 0 & 4 \end{vmatrix} = 24, \quad \begin{vmatrix} 2 & 1 \\ 1 & 4 \end{vmatrix} = 7;$

$$\Delta_3 = \begin{vmatrix} 6 & 6 & 0 \\ 6 & 2 & 1 \\ 0 & 1 & 4 \end{vmatrix} = -102$$ $\boldsymbol{H}$ is indefinite, and $\boldsymbol{x}^*$ is a sadlepoint

(c) $f = a_0 x_1 + a_1 x_2 + a_2 x_1^2 + a_3 x_2^2 + a_4 x_1 x_2$

$$\nabla f = \begin{bmatrix} a_0 + 2a_2 x_1 + a_4 x_2 \\ a_1 + 2a_3 x_2 + a_4 x_1 \end{bmatrix} = 0 \quad \Rightarrow \boldsymbol{x}^* = \begin{bmatrix} \dfrac{-2a_0 a_3 + a_0 a_4}{4a_2 a_3 - a_4^2} \\ \dfrac{-2a_0 a_2 + a_0 a_4}{4a_2 a_3 - a_4^2} \end{bmatrix}$$

$$\boldsymbol{H} = \begin{bmatrix} 2a_2 & a_4 \\ a_4 & 2a_3 \end{bmatrix}$$

$\boldsymbol{H}$ must be pos. def. to get a minimum and neg. def. to get a maximum. Otherwise, $\boldsymbol{x}^*$ is a saddle point.

For $\boldsymbol{x}^*$ to be a minimum, must have $a_2 \geq 0,\ a_3 \geq 0,\ 4a_2 a_3 - a_4^2 \geq 0$.

For $\boldsymbol{x}^*$ to be a maximum, must have $a_2 \leq 0,\ a_3 \leq 0,\ 4a_2 a_3 - a_4^2 \geq 0$.

Problem 4.46

The necessary and sufficient conditions are

1) $f(\boldsymbol{x})$ is twice differentiable

$$\left.\begin{array}{l} \dfrac{\partial f}{\partial x_1} = 2(x_1 - 8) \\ \dfrac{\partial f}{\partial x_2} = 2(x_2 - 5) \\ \dfrac{\partial^2 f}{\partial x_1^2} = 2 \qquad \dfrac{\partial^2 f}{\partial x_2^2} = 2 \end{array}\right\} \text{ok}$$

2) $\nabla f(\boldsymbol{x}^*) = \boldsymbol{0}$

$$\left.\begin{array}{l} 2(x_1 - 8) = 0 \\ 2(x_2 - 5) = 0 \end{array}\right\} \left.\begin{array}{l} x_1^* = 8 \\ x_2^* = 5 \end{array}\right\} \text{ok}$$

3) $\boldsymbol{H}(\boldsymbol{x}^*)$ is pos def.

$$\boldsymbol{H} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \quad \text{which is pos. def. ok}$$

Problem 4.47

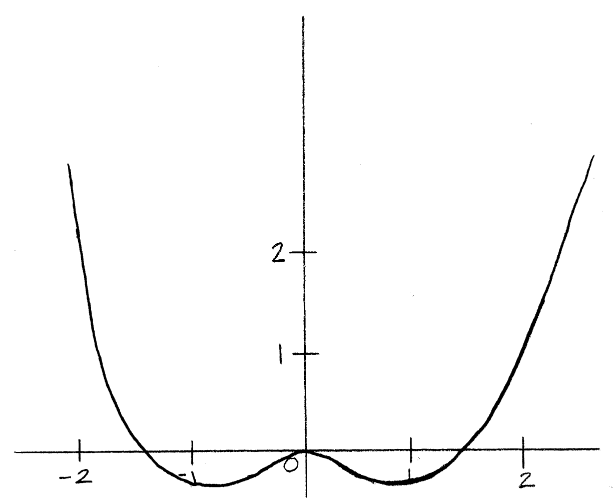
The stationary points of $f(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2$ are obtained from $f^{'}(x) = 0 = x^3 - 1 = 0$

Factor to get: $x(x+1)(x-1) = 0$

Solutions: $x = 0,\ \ x = 1,\ x = -1$

To identify status of these points determine $f\,''(x)$ at each point

$$f\,''(x) = 3x^* - 1 \qquad \begin{aligned} &x = 0: \quad 0 - 1 = -1 \ \ a\max \\ &x = 1: \quad 3 - 1 = 2 \quad a\min \\ &x = -1: \ 3 - 1 = 2 \quad a\min \end{aligned}$$



Problem 4.48

$f(\boldsymbol{x}) = 2x_1^{\,3} + x_2^{\,2} + x_1^{\,2}x_2^{\,2} + 4x_1x_2 + 3$

$$\frac{df}{dx_1} = 6x_1^{\ 2} + 2x_1x_2^{\ 2} + 4x_2$$

$$\frac{df}{dx_2} = 2x_2 + 2x_2x_1^{\ 2} + 4x_1$$

For an optimal solution

$$\frac{df}{dx_1} = 0 \ = 6x_1^{\ 2} + 2x_1x_2^{\ 2} + 4x_2$$

$$\frac{df}{dx_2} = 0 \ = 2x_2 + 2x_2x_1^{\ 2} + 4x_1$$

An obvious solution: $(x_1, x_2) = (0,0)$

Another solution: $(x_1, x_2) = (0.654, -0.916)$

$$\boldsymbol{H}(x) = \begin{bmatrix} 12x_1 + 2x_2^{\ 2} & 4x_1x_2 + 4 \\ 4x_1x_2 + 4 & 2 + 2x_1^{\ 2} \end{bmatrix}$$

$$\boldsymbol{H}(0,0) = \begin{bmatrix} 0 & 4 \\ 4 & 2 \end{bmatrix}$$

$$(-\alpha)(2-\alpha) \ -16 = 0 \qquad \text{or} \qquad \alpha^2 - 2\alpha \ -16 = 0$$

The eigenvalues are

$$\alpha = +2 \pm \sqrt{4+64} = \frac{+2 \pm \sqrt{+68}}{2}$$

$\alpha_1 = 5.123$ $\qquad\qquad$ $\alpha_2 = -3.123$

This is a saddle point

For the other point

$$\boldsymbol{H}(0.654, -0.916) = \begin{bmatrix} 9.53 & 1.60 \\ 1.60 & 2.86 \end{bmatrix}$$

$$\det(\boldsymbol{H}) = 24.7$$

The eigenvalues are

$$(9.53-\alpha)(2.86-\alpha)-2.56=0 \quad \text{or} \quad +\alpha^2-12.39\alpha+24.70=0$$

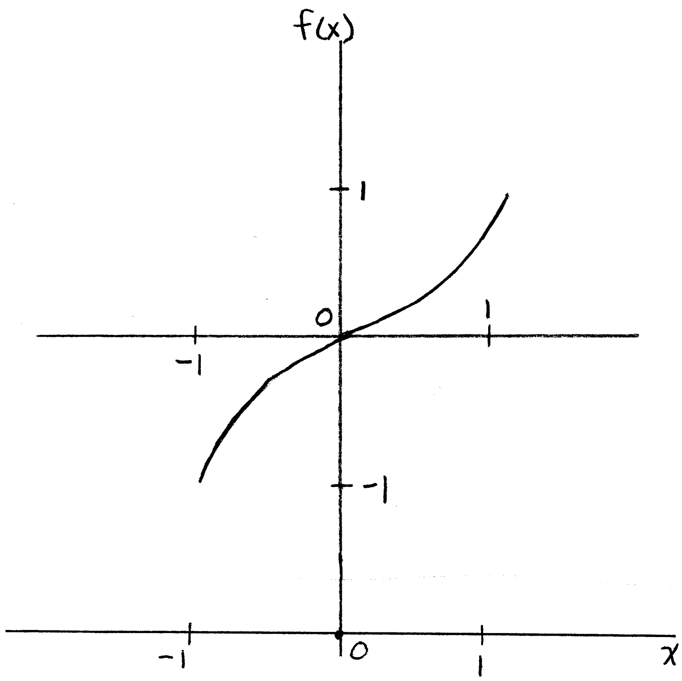
$$\alpha_1=\frac{12.39+7.40}{2}=9.89$$

$\alpha_2,\ \alpha_2>0$ the function is strictly convex at (0.654, -0.916)

Problem 4.49

$$f(x)=\begin{cases}-x^2 & -\infty\le x\le 0\\ x^2 & 0\le x\le 1\\ e^{x-1} & 1\le x\le\infty\end{cases} \qquad f'(x)=\begin{cases}-2x & \text{always+}\\ 2x & \text{always}+\\ e^{x-1} & \text{always}+\end{cases}$$

Look at $f'(x)$ and note that there is one minimum. Or, plot the function



In either case you can determine that the function is not unimodel.

Problem 4.50

Is $\boldsymbol{x}^* = [-0.87 \; -0.8]^{\mathrm{T}}$ a maximum of $f(\boldsymbol{x}) = x_1^4 - 12x_2^3 - 15x_1^2 - 56x_2 + 60$

See if $-f(\boldsymbol{x})$ is convex

$$-\nabla f(\boldsymbol{x}) = -\begin{bmatrix} (4x_1^3 \quad -30x_1) \\ (36x_2^2 - 56) \end{bmatrix}$$

$$-\boldsymbol{H}(\boldsymbol{x}) = -\begin{bmatrix} 12x_1^2 - 30 & 0 \\ 0 & 72x_2 \end{bmatrix}$$

Apparently $\nabla f \neq \mathbf{0}$ at the proposed solution! Hence $\boldsymbol{x}^*$ is not a maximum.

Introduce $\boldsymbol{x}^*$ into $\boldsymbol{H}(\boldsymbol{x})$

$$-\boldsymbol{H}(\boldsymbol{x}^*) = -\begin{bmatrix} -20.917 & 0 \\ 0 & -57.6 \end{bmatrix}$$

$\boldsymbol{H}(\boldsymbol{x}^*)$ is neg. def., but $\boldsymbol{x}^*$ is not a maximum even if $\boldsymbol{H}$ is neg. def. at the point.

Problem 4.51

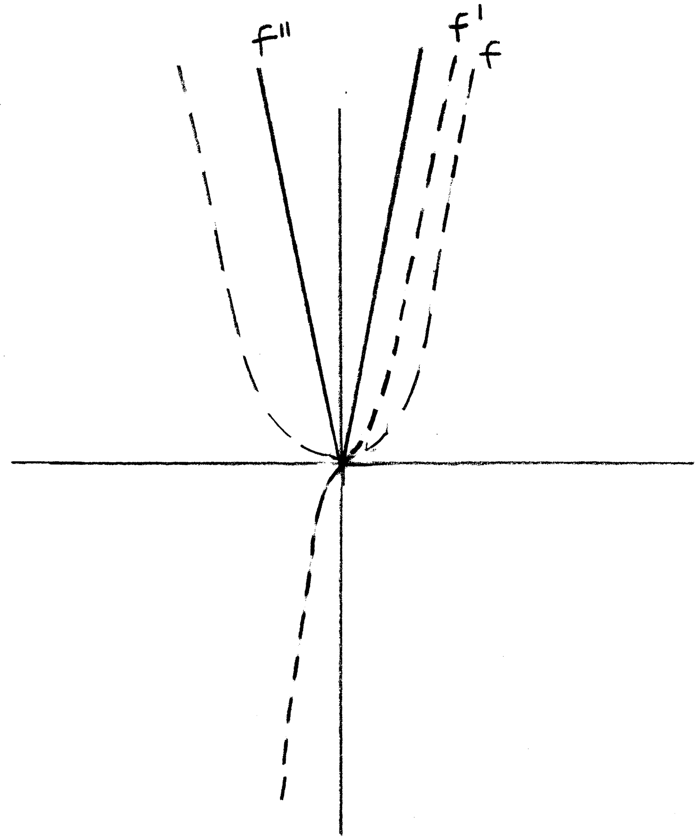
$$f(x) = \left|x^3\right|$$

Differentiate $f(x)$

$$f' = 3x^2 \quad x \geq 0$$
$$f' = -3x^2 \quad x \leq 0$$

$$f'' = 6x \quad x \geq 0 \qquad f''' = 6 \quad x > 0$$
$$f'' = -6x \quad x \leq 0 \qquad f'' = -6 \quad x < 0$$

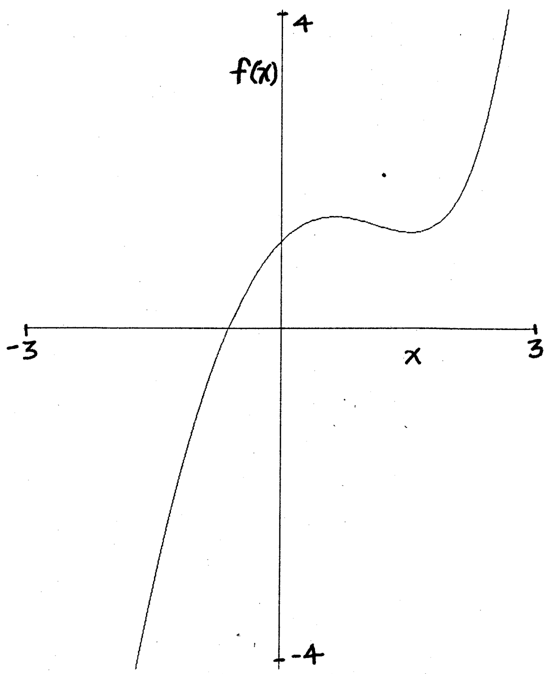
But because the derivatives are decontinuous at $x^* = 0$, even though the function is twice differentiable, you cannot demonstrate that the necessary and sufficient conditions are met because the derivative is not defined at $x^* = 0$.


f''
f'
f

CHAPTER 5

Problem 5.1

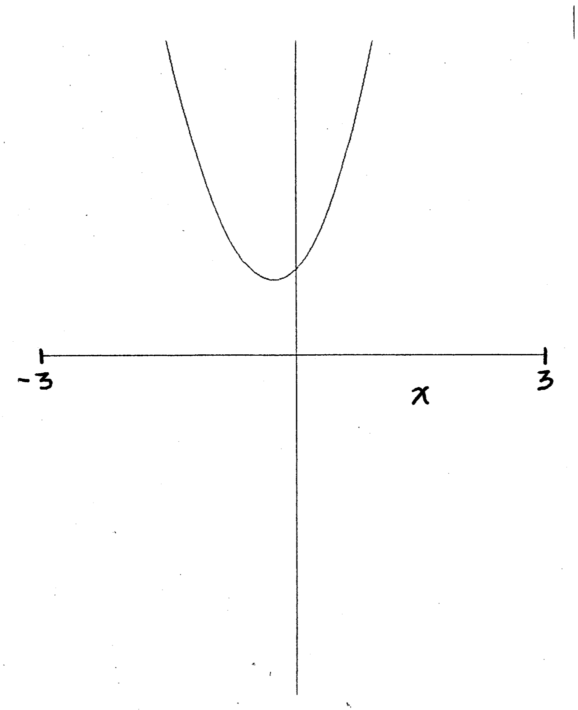
$f(x) = e^* - 1.5x^2$



A local maximum occurs between $x = 0$ and $x = 1$. Consequently if you start to bracket the local minimum at values of $x > 1$ and use reasonable step sizes, you can bracket the local minimum, but if you start with values of *x* before the local maximum occurs, you will most likely proceed to $x \to -\infty$ (the global minimum).

Problem 5.2a

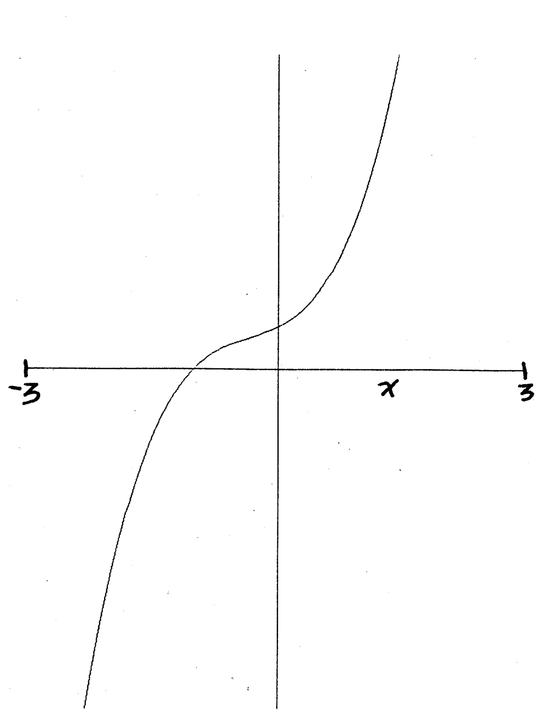
(a) $f(x) = e^{*} + 1.5x^2$



The minimum will be reached from any starting point.

Problem 5.2b

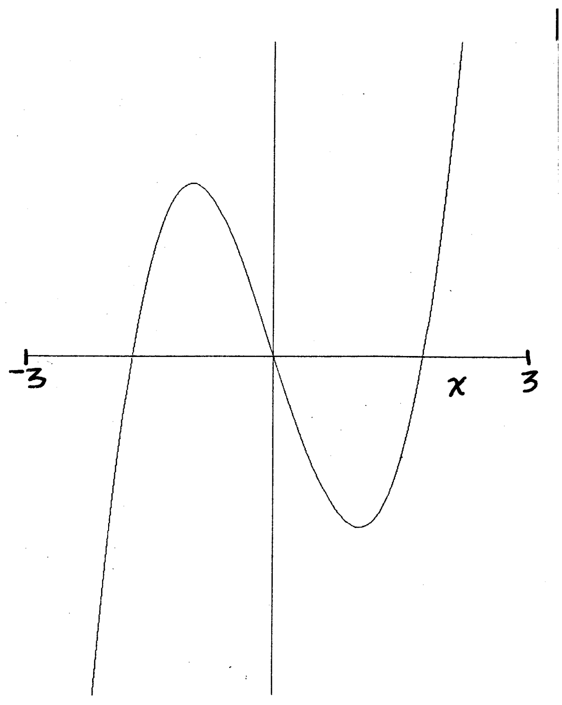
(b) $f(x) = 0.5(x^2 + 1)(x + 1)$



No matter where you start, the minimum (at $-\infty$) cannot be bracketed.

Problem 5.2c

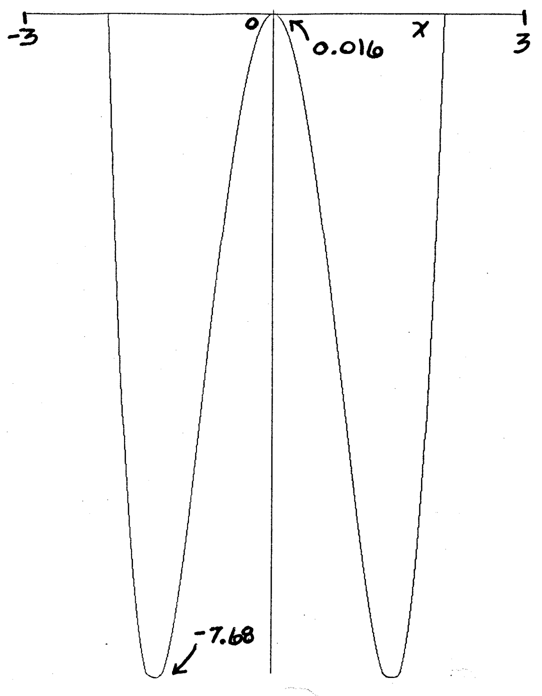
(c) $f(x) = x^3 - 3x$



Because both a local minimum and a global minimum (at $-\infty$) exist, the remarks in P5.1 apply here.

Problem 5.2d

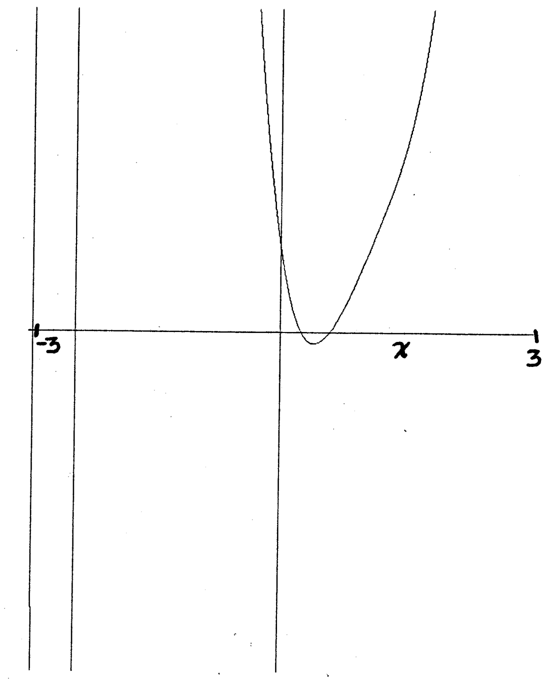
(d) $f(x) = 2x^2(x-2)(x+2)$

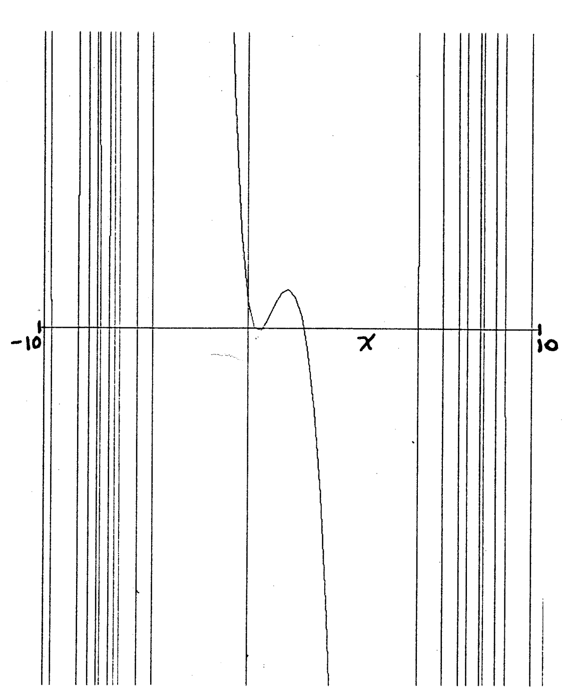


Because this function has two minima, and one maximum, various starting points and step sizes will yield different results.

Problem 5.2e

(e) $f(x) = 0.1x^6 - 0.29x^5 + 2.31x^4 - 8.33x^3 + 12.89x^2 - 6.8x + 1$





A large scale figure shows one minimum, but a small scale figure shows many minima and maxima exist. Starting near $x = 0$ you would reach the local minimum shown in both figures.

Problem 5.3

Use the analytical derivative to get the solution by which the numerical methods can be checked.

$$\text{Minimize}: f = (x-1)^4$$

$$f' = 4(x-1)^3 \qquad x = 1 \text{ is a solution of } f' = 0$$

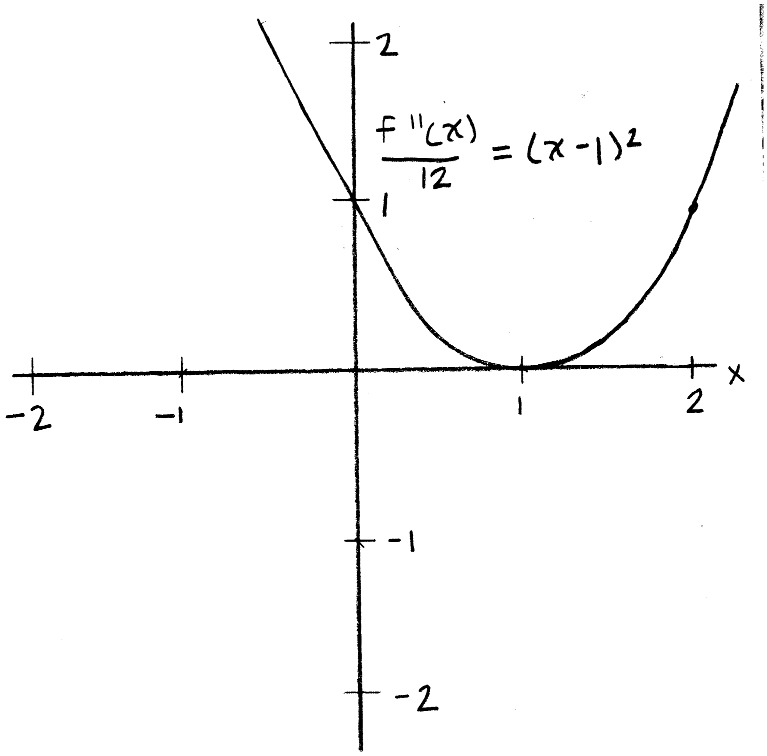
$$f'' = 12(x-1)^2$$

$$f''' = 24(x-1)$$

The fourth derivative is an even number, so you have a minimum as f'''' is positive. You can never have a maximum as f'' is pos. def. at all x except x = 1.

$$f'''' = 24$$

The figure for the second derivative looks as follows



Bracket the minimum

$$f = (x-1)^4$$

x	0	0.5	1	1.5	0.95	1.05
f	1	0.0625	0	0.0625	6.25x10^{-6}	6.25x10^{-6}

A bracket is: 0.95 $< x <$ 1.05

(a) Newton's method (using finite differences instead of analytical derivatives)

If you use $h = 0.5$ and $x^0 = 0$ at the start, the relation is:

$$x^1 = x^0 - \frac{\left[f(x+h) - f(x-h)\right]/2h}{\left[f(x+h) - 2f(x) + f(x-h)\right]/h^2} \quad = 0 - \frac{\left[(0+0.5-1)^4 - (0-0.5-1)^4\right]/(2)(0.5)}{\left[(0+0.5-1)^4 - 2(0+1)^4 + (0-0.5-1)^4\right]/0.5^2}$$

It is better to use a bracket value instead of x^0 = 0, say use $x^0 = 0.95$

$x^1 = 0.9738$

$x^2 = 0.9867$

$x^3 = 0.99336$

$x^4 = 0.9967$

$x^5 = 0.99835$

$x^6 = 0.99917$

$x^7 = 0.99959$

$x^8 = 0.9998$

$x^9 = 0.9999$

$x^{10} = 0.99995$

etc.

$x_{\min} = 1$

(b) Secant (Quasi-Newton) method

$$f = (x-1)^4$$
$$f' = 4(x-1)^3$$

$$\tilde{x}^* = x^q - \frac{f'(x^q)}{\left[f'(x^q) - f'(x^p)\right]/(x^q - x^p)}$$

$x^q = 1.05 \quad x^p = 0.95$

$$x^1 = 1.05 - \frac{4(1.05-1)^3}{\left[4(1.05-1)^3 - 4(0.95-1)^3\right]/(1.05-0.95)} = 1$$

$x^2 = 1$

The minimum $x_{min} = 1$

Problem 5.4

$f = 6.64 + 1.2x - x^2$

The precise values at the solution will depend on the method used.

The final interval is [0.5917, 0.6049], and f = 6.9999 with $\mathbf{x}^* = [0.598 \;\; 0.600]^T$.

Problem 5.5

1. The problem has no minimum

2. It has a minimum but
   a. A bracket on the derivative of f (+ and -) is not maintained.
   b. Numerical and round off errors gives nonsense numbers.
   c. The function was not unimodel.

3. The bracketing procedure at the start is not successful in bracketing a minimum.

Problem 5.6

$f = (x-1)^4$

$$x^{opt} = \frac{1}{2}\left[\frac{(x_2^2 - x_3^2) f_1 + (x_3^2 - x_1^2) f_2 + (x_1^2 - x_2^2) f_3}{(x_2 - x_3) f_1 + (x_3 - x_1) f_2 + (x_1 - x_2) f_3}\right]$$

$x_1 = 0.0 \quad f_1 = 1.0$

$x_2 = 0.5 \quad f_2 = 0.0625$

$x_3 = 2.0 \quad f_3 = 1.0$

Iter.	Points used	x^{opt}	f^{opt}	Point to be discarded
1	x_1, x_2, x_3	$x_4 = 1.0$	$f_4 = 0.0$	x_1
2	x_2, x_3, x_4	$x_5 = 0.833$	$f_5 = 7.7\text{x}10^{-4}$	x_2

3	x_3, x_4, x_5	$x_6 = 0.9194$	$f_6 = 4.2\text{x}10^{-5}$	x_5
4	x_3, x_4, x_6	$x_7 = 0.9600$	$f_7 = 2.6\text{x}10^{-6}$	x_6
5	x_3, x_4, x_7	$x_8 = 0.9800$	$f_8 = 1.6\text{x}10^{-7}$	x_7
6	x_3, x_4, x_8	$x_9 = 0.9900$	$f_9 = 1.0\text{x}10^{-8}$	x_8
7	x_3, x_4, x_9	$x_{10} = 0.9950$	$f_{10} = 6.2\text{x}10^{-10}$	x_9
8	x_3, x_4, x_{10}	$x_{11} = 0.9975$		

$$x^* = 0.9975$$

Problem 5.7

$$f = (x-1)^4$$
$$g = 4(x-1)^3$$

$$x^{opt} = x_2 - \left[\frac{g_2 + w - z}{g_2 - g_1 + 2w} \right](x_2 - x_1)$$

$$z = 3(f_1 - f_2)/(x_2 - x_1) + g_1 + g_2$$
$$w = (z^2 - g_1 g_2)^{1/2}$$
$$x_1 = 0.5$$
$$x_2 = 2.0$$

Iter.	Points used	x^{opt}	Point discarded
1	x_1, x_2	$x_3 = 1.2287$	x_2
2	x_1, x_3	$x_4 = 0.8780$	x_1
3	x_3, x_4	$x_5 = 1.0494$	x_3
4	x_4, x_5	$x_6 = 0.982$	x_4
5	x_5, x_6	$x_7 = 1.0084$	x_5
6	x_6, x_7	$x_8 = 0.9905$	x_6
7	x_7, x_8	$x_9 = 0.9994$	x_7
8	x_7, x_9	$x_{10} = 1.0028$	x_9
9	x_9, x_{10}	$x_{11} = 1.0009$	x_{10}
10	x_9, x_{11}	$x_{12} = 1.0002$	x_{11}

$x^* = 1.0002$

Problem 5.8

$$f(x-1)^4$$
$$x_1 = 1.5 \qquad f_1 = 0.0625$$
$$x_2 = 3.0 \qquad f_2 = 16.0$$
$$x_3 = 4.0 \qquad f_3 = 81.0$$
$$x_4 = 4.5 \qquad f_4 = 150.0625$$

Fitting a cubic equation through these four points gives

$$f = 9x^3 - 54.75x^2 + 115.25x - 80$$
$$df/dx = 27x^2 - 109.5x + 115.25 = 0$$

This quadratic equation does not have real roots, and the problem cannot be solved. The difficulty arises because x_1, x_2, x_3 and x_4 do not bracket the minimum.

Problem 5.9

Minimize: $f(x) = 2\text{x}^3 - 5\text{x}^2 - 8$ $\qquad x \geq 1$

Information about the problem (not required)

$$f'(x) = 6x^2 - 10x$$

$$f''(x) = 12x - 10 \quad \text{is pos def. if } x > \frac{10}{12}$$

$f'(x) = 0 = (6x - 10)x$ yields as solutions $x = 0$ and $x = \frac{10}{6} = 1.67$;
the latter is a minimum for $x \geq 1$

(a) Newton's method

$$x^1 = x^0 - \frac{f'(x^0)}{f''(x^0)} = 1 - \frac{6-10}{12-10} = 1 - (-2) = 3$$

$$x^2 = x^1 - \frac{f'(x^1)}{f''(x^1)} = 3 - \frac{24}{26} = 2.08$$

(b) Secant (Quasi-Newton) method

At $x_A = 2, \quad f'(2) = 4$ positive; $x_B = 1\frac{1}{2}, \quad f'(1.5) = -1.50$ negative — use them as they bracket the derivative value of 0

$$x^1 = x^0 - \frac{f'(x^0{}_A)}{\dfrac{f'(x^0{}_A) - f'(x^0{}_B)}{x_A - x_B}} = 2 - \frac{4}{\dfrac{4-(1-1.5)}{2-1,5}} = 1.636$$

$f'(1.636) = -0.301$ negative; keep $x_A = 2,$ and let $x_B = -0.301$

$$x^2 = 1.636 - \frac{4}{\dfrac{4-(-0.304)}{2-1.636}} = 1.30$$ Error caused by round off

(c) $f(x) = 2x^3 - 5x^2 - 8 \quad x \geq 1$

For polynomial approximation (use a quadratic function) start with 3 points possibly evenly spaced that bracket the minimum

	$f(x)$
Start at $x = 1$	-11
$x = 2$	-12
$x = 1.5$	-12.5

Thus $1 \leq x \leq 2$ brackets the min of $f(x)$.

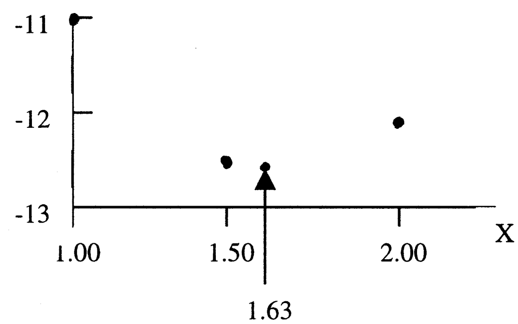
Step 1

Solve the quadratic $f(x) = a + bx + cx^2$ using the 3 above points

-11 = a + b + c
-12.5 = a + 1.5b + 2.25c
-12 = a + 2b + 4c

$$\min x = -\frac{b}{2c} = -\frac{-13}{2\frac{1}{4}} = \frac{13}{8} = 1.63$$

$$f(x) = -12.62$$



Save $x_1 = 1.50,\ x_2 = 1.63,\ x_3 = 2.0$ and repeat

	$f(x)$
$x = 1.5$	-12.5
$x = 1.63$	-12.63
$x = 2$	-12.00

Solve

$$\left.\begin{aligned} -12.5 &= a + 1.5b + 2.25c \\ -12.63 &= a + 1.63b + 2.66c \\ -12.00 &= a + 2.00b + 4c \end{aligned}\right\} \text{ solve for } b \text{ and } c\text{, and get}$$

$$x^* = -\frac{b}{2c}$$

and continue to improve the values of x^*.

Problem 5.10

$$f(x) = 1 - 8x + 2x^2 - \frac{10}{3}x^3 - \frac{1}{4}x^4 + \frac{4}{6}x^5 - \frac{1}{6}x^2$$

$$f' = 8 + 4x - 10x^2 - x^3 + 4x^4 - x^5 = (1+x)^2(2-x)^3$$

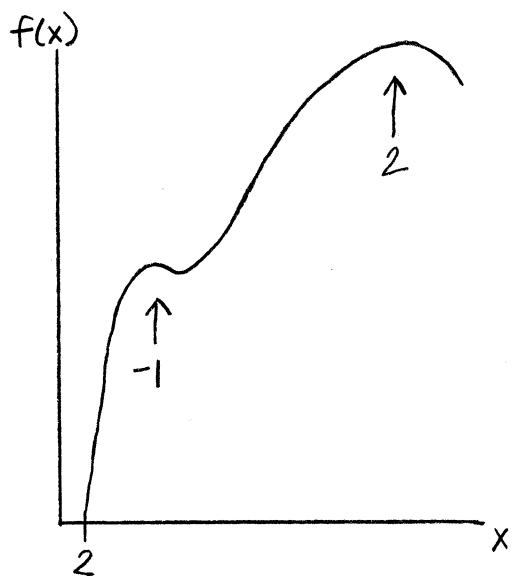
$$= 0 \text{ at } x = -1 \text{ and } x = 2$$

a. $f'' = (1-5x)(1+x)(2-x)^2 \quad = 0$ for $x = -1$ and $x = 2$

$f''' = -2(2-x)(5+4x-10x^2)$ $\neq 0$ for $x = -1$, so $x = -1$ is a saddle point, but f' = 0 for x = 2

$f'''' = -6(1-16x+10x^2)$ is negative at x = 2, so x = 2 is a maximum.

b. Newton method



$$x^{k+1} = x^k - \frac{f'(x^k)}{f''(x^k)}$$

$$x^1 = -2 - \frac{16}{-176} = -1.910$$

$$x^2 = -1.190 + \frac{12.66}{146.7} = -1.104$$

c. Quadratic interpolation

$$x^* = \frac{1}{2}\left[\frac{(x_2^{\,2} - x_3^{\,2})\, f_1 + (x_3^{\,2} - x_1^{\,2})\, f_2 + (x_1^{\,2} - x_2^{\,2})\, f_3}{(x_2 - x_3)\, f_1 + (x_3 - x_1)\, f_2 + (x_1 - x_2)\, f_3}\right]$$

Starting with $x_1 = -2$, pick $x_2 = 0$ and $x_3 = 2$ arbitrarily.

$$f_1 = 1 - 8(-2) + 2(-2)^2 - \frac{10}{3}(-2)^3 + \frac{1}{4}(-2)^4 + \frac{4}{5}(-2)^5 - \frac{1}{6}(-2)^6 = 95.9$$

$$f_2 = 1$$

$$f_3 = 1 - 8(2) + 2(2)^2 - \frac{10}{3}(2)^3 + \frac{1}{4}(2)^4 + \frac{4}{5}(2)^5 - \frac{1}{6}(2)^6 = -14.73$$

$$x^1 = \frac{1}{2}\left[\frac{(0^2 - 2^2)(95.9) + [2^2 - (-2)^2](1) + [(-2)^2 - 0^2](-14.73)}{(0 - 2)(95.9) + [2 - (-2)](1) + [(-2) - 0](-14.73)}\right]$$

and repeat

Problem 5.11

(a) $f = x^2 - 6x + 3$

(i) Newton's method: $x^0 = 1;$ converges in one iteration to $x^* = 3$

(ii) Finite differences Newton method: $x^0 = 1,\ h = 0.001$
Converged in one iteration to $x^* = 3$

(iii) Quasi-Newton (Secant) method: $x^0 = 1,\ x^1 = 5.$ Converged in one iteration to $x^* = 3.$

(iv) Quadratic interpolation: Started with $x^1 = 1,\ x^2 = 2,\ x^3 = 5.$ Converged in one iteration to $x^* = 3.$

(v) Cubic interpolation: Initial prints: 1, 2, 5, 6

$\underline{x}$	$\lVert\cdot\rVert_1$	$\lVert\cdot\rVert_2$
3.047619		
3.028532	0.599	12.583
3.00000	0	0

convergence is linear

Here

$$\|\cdot\|_1 = \frac{\|x^{k+1} - x^*\|}{\|x^k - x^*\|} \qquad \text{and} \qquad \|\cdot\|_2 = \frac{\|x^{k+1} - x^*\|}{\|x^k - x^*\|^2}$$

(b) $f = \sin x$

(i) Newton's method.

x	$\|\cdot\|_1$	$\|\cdot\|_2$
5.0		
4.86369	0.526	1.83
4.71122	0.008	0.051
4.71239	0	0

The rate of convergence is superlinear.

(ii) Finite difference Newton method.

x	$\|\cdot\|_1$	$\|\cdot\|_2$
5.0		
4.70419	0.029	0.100
4.71239	0	0

The rate of convergence seems to be quadratic, but there are two few points to be certain.

(iii) Quasi-Newton (Secant) method. Initial points were $x^1 = 3,\ x^2 = 5$

x	$\|\cdot\|_1$	$\|\cdot\|_2$
4.55457		
4.71338	0.006	0.04
4.71238	0.010	3.06
4.71239	0	0

Rate of convergence is linear.

(iv) Quadratic interpolation. Initial points were $x^1 = 3,\ x^2 = 5,\ x^3 = 5.5$

x	$\|\cdot\|_1$	$\|\cdot\|_2$
4.65058		
4.68558	0.433	7.02
4.71261	0.206	0.306
4.71247	0.364	0.165
4.71239	0	0

Rate of convergence is linear.

(v) Cubic interpolation. Initial points were $x^1 = 3, x^2 = 4, x^3 = 5, x^4 = 5.5$.

x	$\|\cdot\|_1$	$\|\cdot\|_2$
4.74334		
4.70481	0.245	7.91
4.71219	0.026	3.48
4.71239	0	0

Rate of convergence is superlinear.

(c) $f = x^4 - 20x^3 + 0.1x$

(i) Newton's method.

x	$\|\cdot\|_1$	$\|\cdot\|_2$
20.0		
18.312	0.662	0.132
17.191	0.661	0.200
16.448	0.661	0.302
15.956	0.660	0.456
15.631	0.660	0.691
15.416	0.659	1.05
15.275	0.660	1.59
15.181	0.657	2.40
15.119	0.656	3.64
15.079	0.661	5.60
15.052	0.654	8.38
15.034	0.647	12.7
15.022	0.636	19.3
15.015	0.667	31.7
15.010	0.643	45.9
15.006	0.556	61.7
15.004	0.600	120
15.003	0.667	222
15.002	0.500	250
15.001	0	0
15.001		

The rate of convergence is linear.

(ii) Finite difference Newton method. $h = 0.001$

x	$\|\cdot\|_1$	$\|\cdot\|_2$
20.0		
16.667	0.333	0.067
15.278	0.167	0.100
15.010	0.036	0.129
15.000	0	0

The rate of convergence is quadratic.

(iii) Quasi-Newton (Secant) method. Initial points are $x^1 = 10, x^2 = 20.$

$\underline{x}$	$\underline{\lVert\cdot\rVert_1}$	$\underline{\lVert\cdot\rVert_2}$
12.000		
13.421	0.526	0.175
14.240	0.481	0.305
14.652	0.457	0.602
14.845	0.444	1.28
14.931	0.442	2.87
14.970	0.426	6.27
14.987	0.414	14.3
14.994	0.417	34.7
14.997	0.400	80.0
14.999	0	0

The rate of convergence is linear.

(iv) Quadratic interpolation. Initial points are $x^1 = 10,\ x^2 = 16,\ x^3 = 20.$

$\underline{x}$	$\underline{\lVert\cdot\rVert_1}$	$\underline{\lVert\cdot\rVert_2}$
14.031		
14.920	0.08	0.085
14.957	0.53	6.72
14.995	0.10	2.27
14.998	0.25	62.5
14.999	0	0

The rate of convergence is linear

(v) Cubic interpolation. Initial points are $x^1 = 10,\ x^2 = 13,\ x^3 = 16,\ x^4 = 20$

$\underline{x}$	$\underline{\lVert\cdot\rVert_1}$	$\underline{\lVert\cdot\rVert_2}$
14.974		
14.989	0.423	16.27
15.000	0	0

The rate of convergence is linear. There are not enough points to tell whether it is superlinear.

Problem 5.12

$$C = \$500 + \$0.9x + \frac{\$0.03}{x}(150000)$$
$$= 500 + 0.9x + \frac{4500}{x}$$
$$dC/dx = 0 = 0.9 - \frac{4500}{x^2}$$
$$x = 70.71 \text{ hp.}$$

Problem 5.13

At least squares fit gives

$$E = 74.764 - 0.0853R + 1.551\text{x}10^{-3}R^2 - 7.613\text{x}10^{-6}R^3 + 9.605\text{x}10^{-9}R^4$$

$$\text{Coal cost} = 7\left(\frac{\$}{\text{ton}}\right)\text{x}\frac{1}{2240}\left(\frac{\text{ton}}{\text{lb}}\right)\text{x}\frac{1}{14000}\left(\frac{\text{lb}}{\text{Btu}}\right)\text{x5}$$

$$\text{x}\frac{300R}{E}\text{ x } 2544.43\left(\frac{\text{Btu}}{\text{hr.hp}}\right)\text{ x8550}\left(\frac{\text{hr}}{\text{yr}}\right) = 7284\frac{R}{E}\ \$/\text{yr.}$$

Fixed cost = 14000 + 0.04R^2 \$/yr.

$$\text{Total cost}\left(\frac{\$}{\text{yr}\cdot\text{hp}}\right) = \frac{7284(R/E) + 14000 + 0.04R^2}{(5)(300)(0.01R)}$$

$$C = \frac{485.6}{E} + \frac{933.33}{R} + 2.67\text{x}10^{-3}R$$

Introducing the least squares expression for *E* into the expression for *C* and minimizing gives

$$C^* = 11.44$$
$$R^* = 244.09$$
$$E^* = 69.7$$

Problem 5.14

$$t_f = [\Delta P_c A^2 / \mu M^2 c] x_c \exp(-a x_c + b)$$
$$\text{Let } c_1 = \Delta P_c A^2 / \mu M^2 c$$

Then:

$$t_f' = c_1 \exp(-a x_c + b)(1 - a x_c)$$
$$t_f'' = -a c_1 (2 - a x_c) \exp(-a x_c + b)$$

Newton's method gives

$$x_c^{k+1} = x_c^k - (t_f' / t_f'')$$
$$= x_c^k + \frac{1 - a x_c}{a(2 - a x_c)}$$

Substituting numerical values,

$$x_c^{k+1} = x_c^k + \frac{1 - 3.643 x_c}{7.286 - 13.2714 x_c}$$

k	x_c
0	0
1	0.1372
2	0.2332
3	0.2791
4	0.2884
5	0.2888
6	0.2888

$$x_c^* = 0.2888, \text{ and}$$
$$t_f^* = 1634 \text{ minimum}$$

Problem 5.15

The authors of the paper cited report $T^* = 453K$, but several procedures in this book indicate that the problem does not have a realistic solution to get the minimum cost as a function of T, probably because the function for β is incorrect.

Problem 5.16

The comment is true

CHAPTER 6

Problem 6.1

If each step is 1/20 of the interval, then there are 21 values for each variable. The number of function evaluations is

$$(21)^5 = 4084101$$

Problem 6.2

(a)

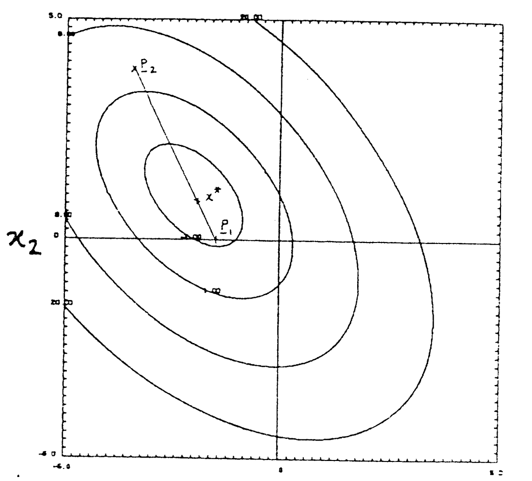
$$f(\boldsymbol{x}) = x_1^{\,2} + x_1 x_2 + x_2^{\,2} + 3x_1$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 2x_1 + x_2 + 3 \\ x_1 + 2x_2 \end{bmatrix} = 0 \quad \Rightarrow x^* = \begin{bmatrix} -2 \\ 1 \end{bmatrix}$$

$\boldsymbol{H} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$ $\boldsymbol{H}$ is positive definite, so x^* is a minimum.

(b) Since $f(x)$ has only one stationary point, it is a global minimum.

(c)



(d) A univariate search will be a good method because the function is quadratic and well scaled. The search directions must be chosen appropriately.

(e) Let λ be the step-size. Then, starting from $[0 \; 0]^T$, the next point is $[\lambda \; 0]^T$.

$$f = \lambda^2 + 3\lambda$$

$$df/d\lambda = 2\lambda + 3 = 0 \quad \Rightarrow \lambda = -3/2$$

$$P_1 = [3/2 \;\; 0]^T$$

If we start from $[0 \;\; 4]^T$, and α is the step size, then $P_2 = [\alpha \;\; 4]^T$

$$f = \alpha^2 + 4\alpha + 4^2 + 3\alpha = \alpha^2 + 7\alpha + 16$$
$$df/d\alpha = 2\alpha + 7 = 0 \quad \Rightarrow \quad \alpha = -7/2$$
$$P_2 = [-7/2 \;\; 4]^T$$

(f) See the figure. A line joining P_1 and P_2 passes through the optimum. This is analogous to the method of conjugate directions.

Problem 6.3

We need a regular tetrahedron with each side 0.2 units long, and one vertex at (-1, 2, -2). Let one face of the regular tetrahedron (an equilateral triangle) be parallel to the *x*-*y* plane with one vertex at (-1, 2, -2). We may place the second vertex at (-1.2, 2, -2). By symmetry, the *x*-coordinate of the third vertex, x_3 is -1.1. The *y* coordinate is given by

$$[(-1.1)-(-1)]^2 + [y_3 - 2]^2 = (0.2)^2$$

$$y_3 = 1.8628 \text{ or } 2.1732$$

Select y_3 = 2.1732. Thus, the equilateral triangle has vertices (-1, 2, -2), (-1.2, 2, -2) and (-1.1, 2.1732, -2). The *x* and *y* coordinates of the centroid of this triangle are the *x* and *y* coordinates.

$$x_4 = \frac{x_1 + x_2 + x_3}{3} = -1.1$$

$$y_4 = \frac{y_1 + y_2 + y_3}{3} = 2.0577$$

Then, the *z*-coordinate, z_4 is given by

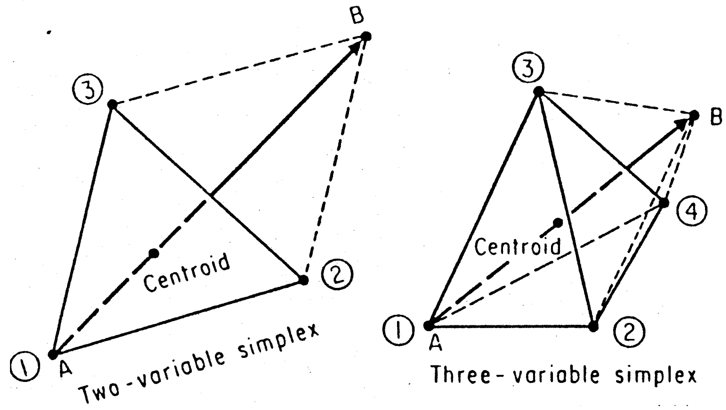
$$[(-1.1)-(-1)]^2 + [2.0577 - 2.1732]^2 + [z_4 - (-2)]^2 = (0.2)^2$$

$$z_4 = -2.1633 \text{ or } -1.8367.$$

Say z_4 = -2.1633. Then the required simplex has its four vertices at

(-1, 2, -2), (-1.2, 2, -2), (-1.1, 2.1732, -2) and (-1.1, 2.0577, -2.1633)

Recall that regular polyhedrons in E^n are simplexes. For example, as indicated in Fig 1, for two variables a regular simplex is an equilateral triangle (three points); for three variables, the regular simplex is a regular tetrahedron (four points), and so forth.



Regular simplexes for two and three independent variables. (1) indicates the highest value of $f(\boldsymbol{x})$. The arrow points in the direction of greatest improvement.

Coordinates for a Set of Simplex Vertices

	n coordinates of each point						
Point j	$\zeta_{1,j}$	$\zeta_{2,j}$	$\zeta_{3,j}$	$\zeta_{4,j}$	$\cdots$	$\zeta_{n=1,j}$	$\zeta_{n,j}$
1	0	0	0	0	$\cdots$	0	0
2	p	q	q	q	$\cdots$	q	q
3	q	p	q	q	$\cdots$	q	q
. . . .							
n	q	q	q	q	$\cdots$	p	q
n+1	q	q	q	q	$\cdots$	q	p

$$p = \frac{a}{n\sqrt{2}}\left(\sqrt{n+1}+n-1\right)$$

$$q = \frac{a}{n\sqrt{2}}\left(\sqrt{n+1}-1\right)$$

a = distance between two vertices

Note: The table starts at (0, 0, 0); for another starting vertex such as (-1, 2, -1), you have to translate these values.

For example, for n = 2 and a = 1, the triangle given in Figure 1 has the following coordinates:

Vertex	$x_{1,i}$	$x_{2,i}$
1	0	0
2	0.965	0.259
3	0.259	0.965

The objective function can be evaluated at each of the vertices of the simplex, and a projection made from the point yielding the highest value of the objective function, point *A* in Figure 1, through the centroid of the simplex. Point *A* is deleted, and a new simplex, termed a *reflection*, is formed, composed of the remaining old points and the one new point, *B*, located along the projected line at the proper distance from the centroid. Continuation of this procedure, always deleting the vertex that yields the highest value of the objective function, plus rules for reducing the size of the simplex and for preventing cycling in the vicinity of the extremum, permit a derivative-free search in which the step size on any stage *k* is fixed but the direction of search is permitted to change.

Problem 6.4

$\boldsymbol{x}_1 = [1\ \ 1]^{\mathrm{T}}$

$\boldsymbol{x}_2 = [1\ \ 2]^{\mathrm{T}}$

Select $\boldsymbol{x}_3$ so that $\boldsymbol{x}_1, \boldsymbol{x}_2$ and $\boldsymbol{x}_3$ form an equilateral triangle. Say

$\boldsymbol{x}_3 = [1.8660\ 1.5]^{\mathrm{T}}$

Stage 1:

$f(\boldsymbol{x}_1) = 4.00$
$f(\boldsymbol{x}_2) = 13.00$
$f(\boldsymbol{x}_3) = 10.23$
discard $\boldsymbol{x}_2$.

Stage 2: $\boldsymbol{x}_4$ is the reflection of $\boldsymbol{x}_2$ in the line joining $\boldsymbol{x}_1$ and $\boldsymbol{x}_3$.

$\boldsymbol{x}_4 = [1.8660\ \ 0.5]^{\mathrm{T}}$
$f(\boldsymbol{x}_4) = 4.23$
discard $\boldsymbol{x}_3$.

Stage 3: $\boldsymbol{x}_5$ is the reflection of $\boldsymbol{x}_3$ in the line joining $\boldsymbol{x}_1$ and $\boldsymbol{x}_4$.

$\boldsymbol{x}_5 = [1\ \ \ 0]^{\mathrm{T}}$

$f(\boldsymbol{x}_5) = 1$

discard $\boldsymbol{x}_2$.

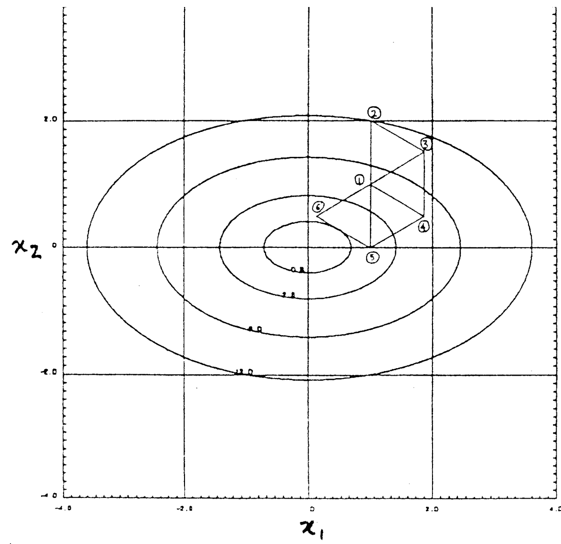
Stage 4: $\boldsymbol{x}_6$ is the reflection of $\boldsymbol{x}_2$ in the line joining $\boldsymbol{x}_1$ and $\boldsymbol{x}_5$.

$\boldsymbol{x}_6 = [0.134 \quad 0.5]^{\mathrm{T}}$

$f(\boldsymbol{x}_6) = 0.768$

discard $\boldsymbol{x}_1$.

And so on.



Problem 6.5

$\boldsymbol{x}_1 = [0 \quad 0 \quad 0]^{\mathrm{T}}$ $\quad f(\boldsymbol{x}_1) = 4$

$\boldsymbol{x}_2 = [-4/3 \;\; -1/3 \;\; -1/3]^{\mathrm{T}}$ $\quad f(\boldsymbol{x}_2) = 7$

$\boldsymbol{x}_{3=}[-1/3 \quad -4/3 \;\; -1/3]^{\mathrm{T}}$ $\quad f(\boldsymbol{x}_3) = 10$

$\boldsymbol{x}_{4=}[-1/3 \quad -1/3 \quad 4/3]^{\mathrm{T}}$ $\quad f(\boldsymbol{x}_4) = 5$

$\boldsymbol{x}_3$ is dropped. The next point, $\boldsymbol{x}_5$, is the reflection of $\boldsymbol{x}_3$ in the plane containing $\boldsymbol{x}_{1,}$ $\boldsymbol{x}_2$ and $\boldsymbol{x}_4$. The centroid of the equilateral triangle formed by $\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_4$ is

$$\boldsymbol{x}_C = \frac{1}{3}(\boldsymbol{x}_1 + \boldsymbol{x}_2 + \boldsymbol{x}_4) = [-0.556 \;\; -0.222 \;\; -0.556]^{\mathrm{T}}$$

$$\boldsymbol{x}_3 + \boldsymbol{x}_5 = 2\boldsymbol{x}_C$$

$$\boldsymbol{x}_5 = 2\boldsymbol{x}_C - \boldsymbol{x}_s$$

$$\boldsymbol{x}_5 = [-7/9 \quad 8/9 \quad -7/9]^{\mathrm{T}}$$

Problem 6.6

(a) $\boldsymbol{s}_1 = \left[1/\sqrt{3} \;\; -1/\sqrt{3} \;\; -1/\sqrt{3}\right]$

Let $\boldsymbol{s}_2 = [a\ b\ c]^{\mathrm{T}}$

Then, for $\boldsymbol{s}_2$ to be orthogonal to $\boldsymbol{s}_1$.

$$\boldsymbol{s}_2^T \boldsymbol{s}_1 = \frac{1}{\sqrt{3}}(a - b - c) = 0$$

Any values of *a*, *b* and *c* which satisfy this equation gives $\boldsymbol{s}_2$ orthogonal to $\boldsymbol{s}_1$.
Say, $s_2 = [1 \;\; 1 \;\; 0]^{\mathrm{T}}$ (No unique solution)

(b) $f(\boldsymbol{x}) = x_1 + 2x_2^{\,2} - x_1 x_2$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 1 - x_2 \\ 4x_2 - x_1 \\ 0 \end{bmatrix} \qquad \boldsymbol{H} = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 4 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

H is not positive definite, so s_1 cannot have a conjugate direction with respect to ***H*.**

Problem 6.7

$f(\boldsymbol{x}) = x_1^{\,2} + x_2^{\,2} + 2x_3^{\,2} - x_1 x_2$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 2x_1 - x_2 \\ 2x_2 - x_1 \\ 4x_3 \end{bmatrix} \qquad \boldsymbol{H} = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 4 \end{bmatrix}$$

H is positive definite, and the stationary point $[0 \;\; 0 \;\; 0]^{\mathrm{T}}$ is a minimum.

Let $\boldsymbol{x}^0 = [1 \;\; 1 \;\; 1]^{\mathrm{T}}$ and $\boldsymbol{s}^0 = [1 \;\; 0 \;\; 0]^{\mathrm{T}}$. If $\boldsymbol{s}^1$ is conjugate to $\boldsymbol{s}^0$ with respect to ***H***, then

$$(\boldsymbol{s}^1)^{\mathrm{T}}\ \mathrm{H}\, s^0 = 0$$
$$\boldsymbol{s}^1 = [1 \;\; 2 \;\; 0]^{\mathrm{T}} \quad \text{(say)}$$

Step 1: start at $\boldsymbol{x}^0$ and minimize *f* along the $\boldsymbol{s}^0$ direction. The optimum step size is

$$\lambda^0 = -\frac{[\nabla f(\boldsymbol{x}^0)]^{\mathrm{T}} \boldsymbol{s}^0}{(\boldsymbol{s}^0)^{\mathrm{T}} \; \boldsymbol{H} \; \boldsymbol{s}} = -\frac{1}{2}$$

$$\boldsymbol{x}^1 = \boldsymbol{x}^0 + \lambda^0 \boldsymbol{s}^0 = [1/2 \quad 1 \quad 1]^{\mathrm{T}}$$

Step 2: start at $\boldsymbol{x}^1$ and minimize f along the $\boldsymbol{s}^1$ direction. The optimum step size is

$$\lambda^1 = -\frac{[\nabla f(\boldsymbol{x}^1)]^{\mathrm{T}} \boldsymbol{s}^1}{(\boldsymbol{s}^1)^{\mathrm{T}} \; \boldsymbol{H} \; \boldsymbol{s}^1} = -\frac{1}{2}$$

$$x^2 = x^1 + \lambda^1 s^1 = [0 \quad 0 \quad 1]^{\mathrm{T}}$$

The minimum is not reached in two steps. For a quadratic function of three independent variables, three steps will be required to reach the minimum.

Problem 6.8

$$f(\boldsymbol{x}) = x_1^{\;2} + x_1 x_2 + 16 x_2^{\;2} + x_3^{\;2} - x_1 x_2 x_3$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 2x_1 + x_2 - x_2 x_3 \\ 32 x_2 + x_1 - x_1 x_3 \\ 2x_3 - x_1 x_2 \end{bmatrix}$$

$$\boldsymbol{H}(\boldsymbol{x}) = \begin{bmatrix} 2 & 1 - x_3 & -x_2 \\ 1 - x_3 & 32 & -x_1 \\ -x_2 & -x_1 & 2 \end{bmatrix}$$

$\boldsymbol{s}^1$ and $\boldsymbol{s}^2$ are conjugate with respect to $\boldsymbol{H}(\boldsymbol{x})$ when

$$(\boldsymbol{s}^1)^{\mathrm{T}} \; \boldsymbol{H}(\boldsymbol{x}) \boldsymbol{s}^2 = 0$$

The det $\boldsymbol{H} > 0$, and all the principal minors must be >0, or all the eigenvalues must be positive.

Insert the two given vectors to get an equation in x_i that must be satisfied.

i.e. $2x_1 - x_2 + 3x_3 + 63 = 0$

and $\boldsymbol{H}(x)$ has to be positive definite. Thus, $\boldsymbol{x}$ must lie on the above plane, and satisfy

$$(1-x_3)^2 \le 64 \quad \text{or} \quad -7 \le x_3 \le 9$$
$$x_2^{\ 2} \le 4 \qquad -2 \le x_2 \le 2$$
$$x_1^{\ 2} \le 64 \qquad -8 \le x_1 \le 8$$

and $128 - 2x_1^{\ 2} - 32x_2^{\ 2} + 2x_1x_2(1-x_3) - 2(1-x_3)^2 > 0$

Problem 6.9

$$f(\boldsymbol{x}) = 5x_1^{\ 2} + x_2^{\ 2} + 2x_1x_2 - 12x_1 - 4x_2 + 8$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 10x_1 + 2x_2 - 12 \\ 2x_1 + 2x_2 - 4 \end{bmatrix}$$

$\boldsymbol{H} = \begin{bmatrix} 10 & 2 \\ 2 & 2 \end{bmatrix}$ is positive definite

If $\boldsymbol{s}^1$ is conjugate to $\boldsymbol{s}^0 = [1 \quad 0]^{\mathrm{T}}$ (the x_i axle); then

First direction: $\quad (s^1)^{\mathrm{T}} \begin{bmatrix} 10 & 2 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 10s_1^1 + 2s_2^1 = 0$

Say $\boldsymbol{s}^1 = [1 \ -5]^{\mathrm{T}}$

For $\boldsymbol{s}^2$ to be conjugate to $\boldsymbol{s}^1$

$$\boldsymbol{s}^2 \begin{bmatrix} 10 & 2 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ -5 \end{bmatrix} = -8s_2^2 = 0, \text{ or } s_2^2 = 0$$

Second direction: $\quad \boldsymbol{s}^2 = [1 \quad 0]^{\mathrm{T}}$ (say).

(Note that you get back the original direction for a quadratic function)

Problem 6.10

a. The conditions for orthogonality are

$$\left.\begin{aligned}\boldsymbol{x}^{\mathrm{T}}\boldsymbol{y}=0\\ \boldsymbol{y}^{\mathrm{T}}\boldsymbol{z}=0\\ \boldsymbol{z}^{\mathrm{T}}\boldsymbol{x}=0\end{aligned}\right\}$$ solve simultaneously. An example is

$$[2/3\ \ -1/3\ \ -2/3]\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = 2/3y_1\ \ -1/3y_2\ \ -2/3y_3 = 0$$

$$[y_1 y_2 y_3]\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = y_1 z_1 + y_2 z_2 + y_3 z_3 = 0$$

$$[z_1 z_2 z_3]\begin{bmatrix} 2/3 \\ -1/3 \\ -2/3 \end{bmatrix} = 2/3z_1 - 1/3z_2 - 2/3z_3 = 0$$

Let $y_1 = 1, y_2 = 1,$ then $y_3 = 1/2$

$$\left.\begin{aligned} z_1 + z_2 + 1/2z_3 = 0 \\ 2/3z_1 - 1/3z_2 - 2/3z_3 = 0 \end{aligned}\right\}$$ Let $z_1 = 1$

Then $z_2 = -2$ and $z_3 = 2$

The vectors are $\boldsymbol{y} = \begin{bmatrix} 1 \\ 1 \\ 1/2 \end{bmatrix}$ $\boldsymbol{z} = \begin{bmatrix} 1 \\ -2 \\ 2 \end{bmatrix}$ (not unique)

$$\boldsymbol{H} = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 3 \end{bmatrix}$$

$$\boldsymbol{H} = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 3 \end{bmatrix}$$

b. The two directions for conjugacy are

$$\left.\begin{aligned} \boldsymbol{x}^{\mathrm{T}}\boldsymbol{H}\boldsymbol{y} &= 0 \\ \boldsymbol{y}^{\mathrm{T}}\boldsymbol{H}\boldsymbol{z} &= 0 \\ \boldsymbol{z}^{\mathrm{T}}\boldsymbol{H}\boldsymbol{x} &= 0 \end{aligned}\right\}$$ solve simultaneously to get a non unique solution. An example is:

$$[2/3\ \ -1/3\ \ -2/3]\begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 3 \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = 0 = [1\ \ -2/3\ \ -7/3]\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

$$[y_1 y_2 y_3]\begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 3 \end{bmatrix}\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = 0 = \left[(2y_1 + y_2)\ \ (y_1 + 2y_2 + y_3)\ \ (y_2 + 3y_3)\right]\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix}$$

$$[z_1 z_2 z_3]\begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 3 \end{bmatrix}\begin{bmatrix} 2/3 \\ -1/3 \\ -2/3 \end{bmatrix} = 0 = \left[(2z_1 + z_2)\ \ (z_1 + 2z_2 + z_3)\ \ (z_2 + 3z_3)\right]\begin{bmatrix} 2/3 \\ -1/3 \\ -2/3 \end{bmatrix}$$

Let $y_1 = 1, y_2 = 1, y_3 = 7$. Then

$$\left.\begin{aligned} 3z_1 + \frac{16}{3}z_2 + 8z_3 &= 0 \\ 2z_1 - 4/3z_2 + 4/3z_3 &= 0 \end{aligned}\right\}$$ Let $z_1 = 1$ and solve for z_2 and z_3.

$$z_3 = -.826$$
$$z_2 = .677$$

Problem 6.11

$$f(\boldsymbol{x}) = x_1^2 + x_1 x_2 + x_2^2 - 3x_1 - 3x_2$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 2x_1 + x_2 - 3 \\ x_2 + 2x_2 - 3 \end{bmatrix} \quad \text{at } (2,2)\ \ \nabla f(x) = \begin{bmatrix} 3 \\ 3 \end{bmatrix}$$

$$\boldsymbol{H}(\boldsymbol{x}) = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \quad \text{(pos. def.)}$$

$$[-3\ -3]\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} s_1^{\,1} \\ s_2^{\,1} \end{bmatrix} = 0$$ gives a conjugate direction

$$[-9\ -9]\begin{bmatrix} s^1{}_1 \\ s^1{}_2 \end{bmatrix} = 0 \qquad\qquad -9s_1^{\,1} - 9s_2 = 0$$

$$\left.\begin{array}{l} \text{Let } s_1^{\,1} = 1 \\ \text{then } s_2 = -1 \end{array}\right\}$$ Direction is unique because for a quadratic function you can only have two conjugate directions, and one was fixed by s_o. The values of elements in $\boldsymbol{s}$ are usually not unique.

Problem 6.12

$$f(\boldsymbol{x}) = (x_1 + x_2)^3 x_3 + x_3^{\,2} x_2^{\,2} x_1^{\,2}$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 3(x_1 + x_2)^2 x_3 + 2x_1 x_2^{\,2} x_3^{\,2} \\ 3(x_1 + x_2)^2 x_3 + 2x_1^{\,2} x_2 x_3^{\,2} \\ (x_1 + x_2)^3 + 2x_1^{\,2} x_2^{\,2} x_3 \end{bmatrix}$$

at $\boldsymbol{x} = [1\ \ 1\ \ 1]^T$, $\nabla f(\boldsymbol{x}) = [14\ \ \ 14\ \ \ 10]^T$

Problem 6.13

Max $\quad f(\boldsymbol{x}) = x_1 + x_2 - \dfrac{1}{2}(x_1^{\,2} + 2x_1 x_2 + 2x_2^{\,2})$

Start at $\boldsymbol{x} = [1\ \ \ 1]$

$$\nabla f(1,1) = \begin{bmatrix} 1 - x_1 - x_2 \\ 1 - x_1 - 2x_2 \end{bmatrix} = \begin{bmatrix} -1 \\ -2 \end{bmatrix}$$

A second search direction is $[-1\ \ -2]\left[\boldsymbol{H}\right]\begin{bmatrix} s_1^{\,2} \\ s_2^{\,2} \end{bmatrix} = 0$

$$\boldsymbol{H} = \begin{bmatrix} -1 & -1 \\ -1 & -2 \end{bmatrix}$$ is neg. def.

$$\begin{bmatrix} 3 & 5 \end{bmatrix} \begin{bmatrix} s_1{}^2 \\ s_1{}^2 \end{bmatrix} = 0 \qquad \text{or} \quad 3s_1{}^2 - 5s_2{}^2 = 0$$

Pick any $s_1{}^2$; determine $s_2{}^2$

Problem 6.14

$$f(\boldsymbol{x}) = 10x_1{}^2 + x_2{}^2$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 20x_1 \\ 2x_2 \end{bmatrix}$$

$$\boldsymbol{x}^0 = [1 \quad 1]^{\mathrm{T}}$$

$$\boldsymbol{s}^0 = -\nabla f(\boldsymbol{x}^0) = [\text{-}20 \quad \text{-}2]^{\mathrm{T}}$$

$$\boldsymbol{x}^1 = \boldsymbol{x}^0 + \lambda_0 \boldsymbol{s}^0 = \left[1 - 20\lambda_0 \quad 1 - 2\lambda_0\right]^{\mathrm{T}}$$

$$f(\boldsymbol{x}^1) = 10(1 - 20\lambda_0)^2 + (1 - 2\lambda_0)^2$$

$$df/d\lambda_0 = 8008\lambda_0 - 404 = 0 \qquad \lambda_0 = 0.05045$$

$$\boldsymbol{x}^1 = \left[-8.991\text{x}10^{-3} \quad 0.8991\right]^{\mathrm{T}}$$

$$\boldsymbol{s}^1 = -\nabla f(\boldsymbol{x}^1) = \left[0.1798 \quad -1.798\right]$$

$$\boldsymbol{x}^2 = \boldsymbol{x}^1 + \lambda_1 \boldsymbol{s}^1 = \left[-8.991\text{x}10^{-3} \ + 0.1798\lambda_1 \ +0.8991 \ - 1.798\lambda_1\right]^{\mathrm{T}}$$

$$f(\boldsymbol{x}^2) = 10(-8.991\text{x}10^{-3} + 0.1798\lambda_1)^2 + (0.8991 - 1.798\lambda_1)^2$$

$$df/d\lambda_1 = 7.112168\ \lambda_1 - 3.26549 = 0 \qquad \lambda_1 = 0.459$$

$$\boldsymbol{x}^2 = \left[0.07354 \quad 0.07382\right]^{\mathrm{T}}$$

This is not the optimum $(\boldsymbol{x}^* = [0 \quad 0]^{\mathrm{T}})$. Thus more than two iterations are needed.

Note: The answer to the problem is easily obtained by first calculating the eigenvalues of ***H***, noting that they are positive, and stating that their ratio is 10, hence steepest decent will take more than two iterations.

Problem 6.15

$$f(\boldsymbol{x}) = e^{x_1 x_2} - 2e^{x_1} + 2e^{x_2} + (x_1 x_2)^2$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} x_2 e^{x_1 x_2} - 2e^{x_1} + 2x_1 x_2^{\,2} \\ x_1 e^{x_1 x_2} + 2e^{x_2} + 2x_1^{\,2} x_2 \end{bmatrix}$$

at $\boldsymbol{x} = [0 \ 0]^{\mathrm{T}}$, $\nabla f(\boldsymbol{x}) = [-2 \quad 2]^{\mathrm{T}}$

Problem 6.16

$$f(\boldsymbol{x}) = x_1^{\,2} + x_2^{\,2}$$

$$\nabla f(\boldsymbol{x}) = [2x_1 \ \ 2x_2]^{\mathrm{T}}$$

$$\boldsymbol{x}_{\text{old}} = [3 \quad 5]^{\mathrm{T}}$$

$$\nabla f(\boldsymbol{x}_{\text{old}}) = [6 \quad 10]^{\mathrm{T}}$$

$$\boldsymbol{x}_{\text{new}} = [3 \quad 5]^{\mathrm{T}} - \alpha[6 \quad 10]^{\mathrm{T}} = [3 - 6\alpha \quad 5 - 10\alpha]^{\mathrm{T}}$$

$$f(\boldsymbol{x}_{\text{new}}) = (3-6\alpha)^2 + (5-10\alpha)^2 \qquad = 136\alpha^2 - 136\alpha + 34$$

$$df/d\alpha = 272\alpha - 136 = 0 \quad \Rightarrow \alpha = 1/2$$

$\boldsymbol{x}_{\text{new}} = [0 \quad 0]^{\mathrm{T}}$ which is the optimum

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Problem 6.17

The direction of search calculated by the negative gradient does not point toward the extremum in poorly scaled functions, hence steepest decent search directions will require more iterations to reach the extremum than many other methods.

Problem 6.18

(a) $f(\boldsymbol{x}) = 3x_1^{\,2} + x_2^{\,2}$

$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 6x_1 & 2x_2 \end{bmatrix}^{\mathrm{T}}$ $\qquad \boldsymbol{H} = \begin{bmatrix} 6 & 0 \\ 0 & 2 \end{bmatrix}$

$\boldsymbol{x}^0 = \begin{bmatrix} 1 & 1 \end{bmatrix}^{\mathrm{T}}$

$\boldsymbol{s}^0 = -\nabla f(\boldsymbol{x}^0) = \begin{bmatrix} -6 & -2 \end{bmatrix}^{\mathrm{T}}$

$$\lambda_0 = -\frac{\nabla^T f(\boldsymbol{x}^0)\boldsymbol{s}^0}{(\boldsymbol{s}^0)^{\mathrm{T}}\boldsymbol{H}\boldsymbol{s}^0} = 0.1785$$

$\boldsymbol{x}_1 = \begin{bmatrix} -0.07142 & 0.6428 \end{bmatrix}^{\mathrm{T}}$

$\nabla f(\boldsymbol{x}^1) = \begin{bmatrix} -0.4285 & 1.2857 \end{bmatrix}^{\mathrm{T}}$

$$\omega_0 = \frac{\nabla^{\mathrm{T}} f(\boldsymbol{x}^1)\nabla f(\boldsymbol{x}^1)}{\nabla^{\mathrm{T}} f(\boldsymbol{x}^0)\nabla f(\boldsymbol{x}^0)} = 0.04591$$

$\boldsymbol{s}^1 = -\nabla f(\boldsymbol{x}^1) + \omega_0 \boldsymbol{s}^0 = \begin{bmatrix} 0.1530 & -1.3775 \end{bmatrix}^{\mathrm{T}}$

$$\lambda_1 = -\frac{\nabla^{\mathrm{T}} f(\boldsymbol{x}^1)\boldsymbol{s}^1}{(\boldsymbol{s}^1)^{\mathrm{T}}\boldsymbol{H}\boldsymbol{s}^1} = 0.4666$$

$\boldsymbol{x}^2 = \boldsymbol{x}^1 + \lambda_1 \boldsymbol{s}^1 = \begin{bmatrix} -1.203\text{x}10^{-7} & -4.01\text{x}10^{-8} \end{bmatrix}^{\mathrm{T}}$

This is very close to the true minimum, $\boldsymbol{x}^* = \begin{bmatrix} 0 & 0 \end{bmatrix}^{\mathrm{T}}$

(b) $f(\boldsymbol{x}) = 4(\boldsymbol{x}_1 - 5)^2 + (\boldsymbol{x}_2 - 6)^2$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 8(\boldsymbol{x}_1 - 5) \\ 2(\boldsymbol{x}_2 - 6) \end{bmatrix} \quad \boldsymbol{H} = \begin{bmatrix} 8 & 0 \\ 0 & 2 \end{bmatrix}$$

$$\boldsymbol{x}^0 = [1 \quad 1]^{\mathrm{T}}$$

$$\nabla f(\boldsymbol{x}^0) = [-32 \;\; -10]^{\mathrm{T}}$$

$$\boldsymbol{s}^0 = -\nabla f(\boldsymbol{x}^0) = [32 \;\; 10]^{\mathrm{T}}$$

$$\lambda_0 = -\frac{\nabla^{\mathrm{T}} f(\boldsymbol{x}^0)\boldsymbol{s}^0}{(\boldsymbol{s}^0)^{\mathrm{T}} \boldsymbol{H}\boldsymbol{s}^0} = 0.1339$$

$$\boldsymbol{x}^1 = \boldsymbol{x}^0 + \lambda_0 \boldsymbol{s}^0 = [5.2859 \;\; 2.3393]^{\mathrm{T}}$$

$$\omega_0 = \frac{\nabla^{\mathrm{T}} f(\boldsymbol{x}^1)\nabla f(\boldsymbol{x}^1)}{\nabla^{\mathrm{T}} f(\boldsymbol{x}^0)\nabla f(\boldsymbol{x}^0)} = 0.05234$$

$$\boldsymbol{s}^1 = -\nabla f(\boldsymbol{x}^1) + \omega_0 \boldsymbol{s}^0 = [-0.6125 \;\; 7.8446]^{\mathrm{T}}$$

$$\lambda_1 = -\frac{\nabla^{\mathrm{T}} f(\boldsymbol{x}^1)\boldsymbol{s}^1}{(\boldsymbol{s}^1)^{\mathrm{T}} \boldsymbol{H}\boldsymbol{s}^1} = 0.4666$$

$$\boldsymbol{x}^2 = \boldsymbol{x}^1 + \lambda_1 \boldsymbol{s}^1 = [5.0001204 \;\; 6.0000262]^{\mathrm{T}}$$

This is very close to the true minimum at $\boldsymbol{x}^* = [5 \quad 6]^{\mathrm{T}}$.

Problem 6.19

(a) Fixed step gradient: The move from a point $\boldsymbol{x}^k$ to the next point $\boldsymbol{x}^{k+1}$ is given by $\boldsymbol{x}^{k+1} = \boldsymbol{x}^k + \alpha\nabla f(\boldsymbol{x}^k)$. The gradient at $\boldsymbol{x}^k$ gives the search direction. The step-size, α is prespecified, and remains fixed from iteration to iteration.

(b) Steepest descent: This is similar to (a) in that the search direction is given by $\nabla f(\boldsymbol{x}^k)$, but α is determined at each iteration a unidimensional search to minimize *f*.

(c) Conjugate gradient: The new search direction is a linear combination of the gradient at the current point and the previous search direction. The weighting factor depends upon the magnitude of the previous gradient. The step-size is determined by a one dimensional search.

Problem 6.20

The solution is: $f = 0$ at (1, 1, 1, 1)

Problem 6.21

$$f(h,r) = \frac{1}{\pi r^2 h} + 2\pi rh + 10\pi r^2$$

Check to see if ***H*** is pos. def. for $r \geq 0$, $h \geq 0$

$$\frac{\partial f}{\partial r} = \frac{-2}{\pi h r^3} + 2\pi h + 20\pi r$$

$$\frac{\partial f}{\partial h} = \frac{-1}{\pi r^2 h^2} + 2\pi r$$

$$\frac{\partial^2 f}{\partial r^2} = \frac{6}{\pi r^4} + 20\pi \qquad \frac{\partial^2 f}{\partial r \partial h} = \frac{2}{\pi r^3 h^2} + 2\pi$$

$$\frac{\partial^2 f}{\partial h \partial r} = \frac{2}{\pi h^2 r^3} + 2\pi \qquad \frac{\partial^2 f}{\partial h^2} = \frac{2}{\pi r^2 h^3}$$

The elements on the diagonal of ***H*** are positive, and the determinant

$$\left[\left(\frac{6}{\pi r^4} + 20\pi\right)\left(\frac{2}{\pi r^2 h^3}\right)\right] - \left(\frac{2}{\pi r^3 h^2} + 2\pi\right)^2 > 0 \ \ ?$$

has to be positive for ***H*** to be positive definite. At (0.22, 2.16). The value is 112770, hence Newton's method will converge in the vicinity of (0.22, 2.16). If det ***H*** is not pos. def. at some (*r*, *h*) during the search, Newton's method may not converge.

Problem 6.22

No, but it must be positive definite at the minimum for the extremum to be a minimum.

Problem 6.23

Possible answers are:

(1) If more than one extremum exists, the Simplex method may converge to a better local minimum than the Quasi-Newton (secant) method.

(2) If the variables in the objective function are random variables as in experimentation.

(3) Simple method to understand (no complicated mathematics involved) and program.

(4) Requires only one function evaluation per search step.

Problem 6.24

They would both be equally fast, as far as the number of iterations is concerned, because the search direction is the same for both, and both yield the optimum in one step.

Problem 6.25

You must consider both minima and maxima

(a) $f = 1 + x_1 + x_2 + (4/x_1) + (9/x_2)$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 1-(4/x_1^{\ 2}) \\ 1-(9/x_2^{\ 2}) \end{bmatrix}$$

$$\boldsymbol{H} = \begin{bmatrix} 8/x_1^3 & 0 \\ 0 & 18/x_2^{\ 3} \end{bmatrix}$$

H is not positive definite or negative definite for all ***x***, so Newton's method is not guaranteed to converge to minimum nor a maximum. From a positive starting point. The search for a minimum can go to $-\infty$ as $x_i \to \infty$.

(b) $f(\boldsymbol{x}) = (x_1+5)^2 + (x_2+8)^2 + (x_3+7)^2 + 2x_1^{\ 2}x_2^{\ 2} + 4x_1^{\ 2}x_3^{\ 2}$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 2(x_1+5)+4x_1x_2^{\ 2}+8x_1x_3^{\ 2} \\ 2(x_2+8)+4x_1^{\ 2}x_2 \\ 2(x_3+7)+8x_1^{\ 2}x_3 \end{bmatrix}$$

$$\boldsymbol{H}(\boldsymbol{x}) = \begin{bmatrix} 2+4x_2^{\ 2}+8x_3^{\ 2} & 8x_1x_2 & 16x_1x_3 \\ 8x_1x_2 & 2+4x_1^{\ 2} & 0 \\ 16x_1x_3 & 0 & 2+16x_3^{\ 2} \end{bmatrix}$$

It is hard to tell by inspection if $\boldsymbol{H}$ is positive definite for all $\boldsymbol{x}$, so that Newton's method can be guaranteed to converge to the minimum. However, by inspection of $f(\boldsymbol{x})$ you can see that each term in the function is positive so that Newton's method should reach a local minimum. One exists at (-0.0154, 7.996, -6.993) with f = 24.92.

Problem 6.26

$$f(\boldsymbol{x}) = x_1^{\ 3}+x_1x_2-x_2^{\ 2}x_1^{\ 2}$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 3x_1^{\ 2}+x_2-2x_1x_2^{\ 2} \\ x_1-2x_1^{\ 2}x^2 \end{bmatrix}$$

$$\boldsymbol{H}(\boldsymbol{x}) = \begin{bmatrix} 6x_1-2x_2^{\ 2} & 1-4x_1x_2 \\ 1-4x_1x_2 & -2x_1^{\ 2} \end{bmatrix}$$

at $\boldsymbol{x}^* = [1 \;\; 1]$,

$$\boldsymbol{H}(\boldsymbol{x}^*) = \begin{bmatrix} 4 & -3 \\ -3 & 2 \end{bmatrix}$$

$\boldsymbol{H}$ is not positive definite at $\boldsymbol{x}^0$, which is the probable reason why the code fails.

Problem 6.27

$$f(\boldsymbol{x}) = 2x_1^{\ 2}+2x_2^{\ 2}$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 4x_1 & 4x_2 \end{bmatrix}^{\mathrm{T}}$$

$$\boldsymbol{H} = \begin{bmatrix} 4 & 0 \\ 0 & 4 \end{bmatrix}$$

The initial search direction is

$$\boldsymbol{s}^0 = -\boldsymbol{H}^{-1}\nabla f(\boldsymbol{x}^0) = -\begin{bmatrix} 1/4 & 0 \\ 0 & 1/4 \end{bmatrix}\begin{bmatrix} 4x_1^{\,0} \\ 4x_2^{\,0} \end{bmatrix} = \begin{bmatrix} -x_1^{\,0} \\ -x_2^{\,0} \end{bmatrix}$$

The step size is always $\lambda = 1$ for Newton's method. Only one step is needed to reach the minimum, because *f* is quadratic.

$\boldsymbol{x}^1 = \boldsymbol{x}^0 + \lambda \boldsymbol{s}^0 = \begin{bmatrix} 0 & 0 \end{bmatrix}^{\mathrm{T}}$ which is the optimum.

Problem 6.28

The Hessian matrix of *f(**x**)* is positive definite at the starting point, but does not remain positive definite as the search progresses. Therefore Newton's method does not converge at all with $\lambda = 1$. Adjusting λ in the search direction will not help much.

Problem 6.29

(a) *Newton's Method*

$$f(\boldsymbol{x}) = 8x_1^{\,2} + 4x_1x_2 + 5x_2^{\,2}$$

$$\nabla^{\mathrm{T}} f(\boldsymbol{x}) = \begin{bmatrix} (16x_1 + 4x_2)(10x_2 + 4x_1) \end{bmatrix}^{\mathrm{T}}$$

at (10, 10) $\qquad \nabla f = \begin{bmatrix} 200 \\ 140 \end{bmatrix}$

$$\nabla^2 f(\boldsymbol{x}) = \begin{bmatrix} 16 & 4 \\ 4 & 10 \end{bmatrix}$$

$$\boldsymbol{x}^{(1)} = \begin{bmatrix} 10 \\ 10 \end{bmatrix} - \begin{bmatrix} 16 & 4 \\ 4 & 10 \end{bmatrix}^{-1} \begin{bmatrix} 200 \\ 140 \end{bmatrix} \qquad \begin{bmatrix} 16 & 4 \\ 4 & 10 \end{bmatrix}^{-1} = \frac{1}{144}\begin{bmatrix} 16 & -4 \\ -4 & 10 \end{bmatrix}$$

or solve

$$\begin{bmatrix}200\\140\end{bmatrix}+\begin{bmatrix}16 & 4\\4 & 10\end{bmatrix}\begin{pmatrix}10-x_1^1\\10-x_1^2\end{pmatrix}=0$$

solution: $\boldsymbol{x}=\begin{bmatrix}0 & 0\end{bmatrix}^{\mathrm{T}}$

(b) *Fletcher-Reeves Method*

Use an algorithm code such as shown in the text. Start with

$$s^0=-\nabla f(\boldsymbol{x}^0)=-\begin{bmatrix}200\\140\end{bmatrix}$$

$$\boldsymbol{x}^1=\begin{bmatrix}10\\10\end{bmatrix}-\lambda^0\begin{bmatrix}200\\140\end{bmatrix}$$

Minimize exactly in the $\boldsymbol{s}^0$ direction to get λ^0

$$\lambda^0=-\frac{\nabla^{\mathrm{T}} f(\boldsymbol{x})\boldsymbol{s}}{\boldsymbol{s}^{\mathrm{T}}\boldsymbol{Hs}}=+\frac{\begin{bmatrix}200 & 140\end{bmatrix}\begin{bmatrix}200\\140\end{bmatrix}}{\begin{bmatrix}200 & 140\end{bmatrix}\begin{bmatrix}164\\410\end{bmatrix}\begin{bmatrix}200\\140\end{bmatrix}}=\frac{59{,}600}{1.06\text{x}10^6}=0.05623$$

Then

$$\boldsymbol{x}^1=\begin{bmatrix}10\\10\end{bmatrix}-0.05623\begin{bmatrix}200\\140\end{bmatrix}=\begin{bmatrix}10\\10\end{bmatrix}-\begin{bmatrix}11.2460\\7.8722\end{bmatrix}=\begin{bmatrix}-1.2460\\+2.1278\end{bmatrix}$$

Next calculate $f(\boldsymbol{x}^1)$, $\nabla f(\boldsymbol{x}^1)$ and calculate the next search direction

$$\boldsymbol{s}^1=-\nabla f(\boldsymbol{x}^1)+\boldsymbol{s}^0\frac{\nabla^{\mathrm{T}} f(\boldsymbol{x}^1)\nabla f(\boldsymbol{x}^1)}{\nabla^{\mathrm{T}} f(\boldsymbol{x}^0)\nabla f(\boldsymbol{x}^0)}$$

and continue. A computer program is needed to save user time.

Problem 6.30

(a) From both starting points, Newton's method converges to

$$\boldsymbol{x}^* = \begin{bmatrix} -0.2 & -0.2 & -0.2 & -0.2 \end{bmatrix}^{\mathrm{T}}, \quad f^* = 0.6$$

(b) $\boldsymbol{x}^* = \begin{bmatrix} 17.27 & 7.350 & 0.3483 & 0.7196 \end{bmatrix}^{\mathrm{T}}, \quad f^* = 0.74\text{x}10^{-10} \approx 0$

Problem 6.31

(a) Sequential Simplex

Advantages:

(1) If more than one extremum exists, the Simplex method may converge to a better local minimum than the Quasi-Newton (secant) method.

(2) If the variables in the objective function are random variables as in experimentation.

(3) Simple method to understand (no complicated mathematics involved) and program.

(4) Requires only one function evaluation per search step.

Disadvantages:

(1) Slow to converge

(2) Not efficient for problems with many variables

(3) Will not work for problems with constraints without modification

(b) Conjugate gradient

Advantages:

(1) Uses only first derivatives

(2) Low storage required

Disadvantages:

(1) Have to reset directions after one cycle

(2) Hessian may become ill-conditioned

(c) Newton's Method

Advantages:

(1) Fast for reasonably scaled problems with one extremum

(2) Simple algorithm

Disadvantages:

(1) Can perform poorly on problems with multiple extrema

(2) Converges to a local extremum (as opposed to a global algorithm)

(3) Requires second partial derivatives for a strict Newton method.

Twenty independent variables makes a Simplex search not practical. The other two methods would converge more slowly, but are not affected otherwise.

Problem 6.32

Let $-\left[f(\boldsymbol{x}) = 100 - (10 - x_1)^2 - (5 - x_2)^2 \right]$ be maximized

$$\hat{f}(\boldsymbol{x}) = -100 + (10 - x_1)^2 + (5 - x_2)^2$$

$$\nabla \hat{f}(\boldsymbol{x}) = \begin{bmatrix} -2(10 - x_1) \\ -2(5 - x_2) \end{bmatrix} \qquad \hat{\boldsymbol{H}}(\boldsymbol{x}) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \text{ pos. def.}$$

$$\boldsymbol{x}^0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

The maximum is at $\boldsymbol{x} = [10 \quad 5]^{\mathrm{T}}$.

The minimum is at $\hat{f}(0, \ 0) = \ 25$

a. *Simplex Method* Pick a suitable sized triangle.

Point	$x_1^{(k)}$	$x_2^{(k)}$	$\hat{f}(\boldsymbol{x}^{(k)})$		$f(\boldsymbol{x})$
1	0	0	25	starting Simplex	–25
2	1.9314	0.5174	–14.9		14.9
3	0.5174	1.9314	–0.6		0.6
	Drop Point No. 1				
4	2.4488	2.4488	-26.5		26.5
	Drop Point No. 3				
5	3.8628	1.0348	-46.6		46.6

Or use a graphical procedure.

b. *Newton's method* Start at (0, 0) $\lambda = 1$

$$\Delta \boldsymbol{x}^{(0)} = -\lambda \hat{\boldsymbol{H}}^{-1} \nabla \hat{f}(\boldsymbol{x}) = -(1) \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix} \begin{bmatrix} -20 \\ -10 \end{bmatrix} = \begin{bmatrix} 10 \\ 5 \end{bmatrix}$$

$$\boldsymbol{x}^{(1)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 10 \\ 5 \end{bmatrix} = \begin{bmatrix} 10 \\ 5 \end{bmatrix}$$

c. *BFGS method*

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} - \lambda^{(k)} \hat{\boldsymbol{H}}^{-1}(\boldsymbol{x}^{(k)}) \nabla \hat{f}(\boldsymbol{x}^{(k)}) \qquad \text{Let } \hat{\boldsymbol{H}}^{(0)} = \boldsymbol{I}$$

At (0, 0), f = -25.

$$\mathbf{x}^{(1)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \lambda^{(0)} \overbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -20 \\ -10 \end{bmatrix}}^{\mathbf{s}^{(0)}}$$ ($\mathbf{s}^{(0)}$ is the negative gradient direction)

Pick a $\lambda = 1$ or maximize in $s = \mathbf{H}^{-1}(\mathbf{x})\nabla f(\mathbf{x})$ direction to get λ.

For $\lambda = 1$: $\mathbf{x}^{(1)} = -\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -20 \\ -10 \end{bmatrix} = \begin{bmatrix} 20 \\ 10 \end{bmatrix}$

$\hat{f}(20,\ 10) = 25$

Alternately, pick λ to maximize $\hat{f}(\mathbf{x})$ in the search direction

$$\lambda^{opt} = -\frac{\nabla^{\mathrm{T}} f(\mathbf{x}^{(k)})\mathbf{s}^{(k)}}{(\mathbf{s}^{(k)\mathrm{T}}\hat{\mathbf{H}}^{(k)}\mathbf{s}^{(k)})} = -\frac{\begin{bmatrix} -20 & -10 \end{bmatrix} \begin{bmatrix} -20 \\ -10 \end{bmatrix}}{\begin{bmatrix} -20 & -10 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} -20 \\ -10 \end{bmatrix}} = -\frac{1}{2}$$

$$\mathbf{x}^{(1)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \left(\frac{1}{2}\right) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -20 \\ -10 \end{bmatrix} = \begin{bmatrix} 10 \\ 5 \end{bmatrix}$$ (This is the optimum)

If $\mathbf{x}^{(1)}$ were not the optimum, the next stage via BFGS gives the approximate $\hat{\mathbf{H}}^{-1}$

$$\left(\Delta\hat{\mathbf{H}}^{k}\right)^{-1} = \frac{(\Delta\mathbf{x}^{(k)})\Delta\mathbf{x}^{(k)}}{(\Delta\mathbf{x}^{k})^{\mathrm{T}}\Delta\mathbf{g}^{(k)}} - \frac{(\hat{\mathbf{H}}^{(k)})^{-1}\Delta\mathbf{g}^{(k)}(\Delta\mathbf{g}^{(k)})^{\mathrm{T}}\left[(\Delta\hat{\mathbf{H}}^{(k)})^{-1}\right]^{\mathrm{T}}}{(\Delta\mathbf{g}^{(k)})^{\mathrm{T}}(\hat{\mathbf{H}}^{(k)})^{-1}\Delta\mathbf{g}^{(k)}}$$

but $\nabla^{\mathrm{T}} f(10,\ 5) = \begin{bmatrix} 0 & 0 \end{bmatrix}^{\mathrm{T}}$ so $\Delta x^{(1)}$ will be **0** whatever $(\hat{\mathbf{H}}^{(1)})^{-1}$ is.

Problem 6.33

$f(x) = x^2 - 200x + 10^4$

$f'(x) = 2x - 200$ hence a minimum exists at $x = 100$

$f''(x) = 2$ (pos. def.)

Bracket the minimum start at $x = 0$, and bracket the minimum for all methods.

Let $\Delta^0 = 10$

	$x + \Delta$	$f(x)$
$x =$	0	10,000
	0 + 10	8,000
	10 + 20	4, 900
	30 + 40	900
	70 + 80	2500

Newton's Method

$$x^{(1)} = 0 - \frac{f'(0)}{f''(0)} = -\frac{-200}{2} = 100$$

$$x^{(2)} = 100 - \frac{f'(100)}{f''(100)} = 100 - \frac{(200-200)}{2} = 100$$

(one step for a quadratic function)

Quasi-Newton (Secant) Method

$$x^{(1)} = 0 - \frac{f'(0)}{\frac{f'(q) - f'(p)}{q-p}}$$

Let $p = 0$ and $q = 150$

$$x^{(1)} = 0 - \frac{-200}{\frac{100-(-200)}{150-0}} = \frac{200}{2} = 100$$

At 100, $f' = 0$, hence can stop.

Quadratic interpolation

Pick 3 points, bracketing minimum

x	$f(x)$
0	10,000

100	0
150	2500

Fit $f(x) = a + bx + cx^2$ with min at $x^* = -\dfrac{b}{2c}$

$$10^4 = a$$

$$\left.\begin{aligned} 0 &= a + b(100) + c(100)^2 \\ 2500 &= a + b(150) + c(150)^2 \end{aligned}\right\} \quad \begin{aligned} b &= -200 \\ c &= 1 \end{aligned}$$

$$x^* = -\frac{-200}{2(1)} = 100$$

Problem 6.34

$$f(x) = (x-100)^3$$

$f'(x) = 3(x-100)^2$ so an extremum is at $x = 100$

$f''(x) = 6(x-100)$ at $x = 100$, $f'' = 0$ (not pos. def.)
$f''' = 6$ hence $x = 100$ is an inflection.
The problem has a minimum at $x = -\infty$.

Start at $x = 0$

a. *Steepest descent*

At $x = 0$, $f'(0) = \quad -3\text{x}10^6$

$$x^{(1)} = 0 + \lambda(-3\text{x}10^6)$$

$$\left.\begin{aligned} &\text{Select } \lambda = 1 \\ &\text{or} \quad \lambda = \min f(x) \end{aligned}\right\} \text{or any other suitable choice}$$

Select $\lambda^{opt} = -\dfrac{(-3\text{x}10^6)(-3\text{x}10^{-6})}{(-3\text{x}10^6)(-600)(-3\text{x}10^6)} = \dfrac{1}{600}$

$$x^{(1)} = 0 + \frac{1}{600}\left(-3\text{x}10^{6}\right) = -0.5\text{x}10^{-4}$$

Select $\lambda = 1$

$$x^{(1)} = 0 + (-3\text{x}10^{6}) = -3\text{x}10^{6}$$

Clearly x^{*} goes to $-\infty$

b. *Newton's method*

$$x^{(1)} = 0 - \frac{f\,'(0)}{f\,''(0)} = -\frac{-3\text{x}10^{6}}{-600} = -.5\text{x}10^{4}$$

Same result as for steepest descent

c. *Quasi-Newton (Secant) method* Let $x^{p} = 0,\ \ x^{q} = 200$

$$x^{(1)} = 0 - \frac{f\,'(0)}{\left(\dfrac{f\,'(q) - f\,'(p)}{q - p}\right)} \qquad x^{(1)} = -\frac{-3\text{x}10^{6}}{\dfrac{3\text{x}10^{6} - (-3\text{x}10^{6})}{200 - 0}} = 100$$

At x = 100, $f\,'(100) = 0$. To maintain + and – bracket on $f\,'$, you would have to pick another x^{p} and x^{q}. The method will then proceed to $-\infty$ for x.

d. *Quadratic interpolation*

Pick 3 points, bracketing minimum

x	$f(x)$
0	$-3\text{x}10^{6}$
100	0
200	$-3\text{x}10^{6}$

Fit $f(x) = a + bx + cx^{2}$ with minimum at $\dfrac{df(x)}{dx} = 0$ or $x^{*} = -\dfrac{b}{2c}$

$$-3\text{x}10^{6} = a$$

$$\left.\begin{aligned} 0 &= a + b(100) + c(100)^2 \\ 3\text{x}10^6 &= a + b(200) + c(200)^2 \end{aligned}\right\} \begin{aligned} c &= 3.123\text{x}10^{-15} \\ b &= 3\text{x}10^4 \end{aligned}$$

$$x^* = -\frac{3\text{x}10^4}{3.123\text{x}10^{-15}} \cong -1\text{x}10^{19} \rightarrow -\infty$$

Problem 6.35

$$f(\boldsymbol{x}) = 2x_1^{\,2} - 2x_2^{\,2} - x_1 x_2$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 4x_1 - x_2 \\ -4x_2 - x_1 \end{bmatrix} \quad \boldsymbol{H} = \begin{bmatrix} 4 & -1 \\ -1 & 4 \end{bmatrix}$$

$\boldsymbol{H}$ is not positive definite.

Let $\hat{\boldsymbol{H}} = \boldsymbol{H} + \beta \boldsymbol{I}$. Then, the eigenvalues of $\hat{\boldsymbol{H}}$ are the roots of

$$\det \begin{pmatrix} \boldsymbol{H} + \beta \boldsymbol{I} \\ -\lambda \boldsymbol{I} \end{pmatrix} = \begin{vmatrix} 4 + \beta - \lambda & -1 \\ -1 & -4 + \beta - \lambda \end{vmatrix} = 0$$

$$(\beta - \lambda)^2 - 17 = 0$$

$$\lambda_1 = \beta + \sqrt{17}, \quad \lambda_2 = \beta - \sqrt{17}$$

If $\beta > \sqrt{17}$, then λ_1 and λ_2 are positive, and $\hat{\boldsymbol{H}}$ is positive definite and its inverse is positive definite.

Alternate solution: Start with $\hat{\boldsymbol{H}}^{-1} = \left[\boldsymbol{H} + \beta \boldsymbol{I}\right]^{-1}$ and proceed as above, but you need to calculate $\boldsymbol{H}^{-1}$.

Problem 6.36

$$f(\boldsymbol{x}) = 2x_1^{\,2} - 4x_1 x_2 + x_2^{\,2}$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 4x_1 - 4x_2 \\ -4x_1 + 2x_2 \end{bmatrix} \quad \boldsymbol{H} = \begin{bmatrix} 4 & -4 \\ -4 & 2 \end{bmatrix}$$

$\boldsymbol{H}$ is not positive definite, so f does not have a stationary point which is a minimum. Thus, it is meaningless to use Marquardt's method to find one. But a positive definite approximation of $\boldsymbol{H}$ is $\hat{\boldsymbol{H}} = \begin{bmatrix} 4-\beta & -4 \\ -4 & 4-\beta \end{bmatrix}$ and choose β to make $\hat{\boldsymbol{H}}$ pos. def. As for example $\beta = -1$. Or, get the eigenvalues of $\boldsymbol{H}$ and add to them to get a pos. def. approximation.

Problem 6.37

$$f(\boldsymbol{x}) = 2x_1^3 - 6x_1x_2 + x_2^2$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 6x_1^2 - 6x_2 \\ -6x_1 + 2x_2 \end{bmatrix}$$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 12x_1 & -6 \\ -6 & 2 \end{bmatrix} \qquad \text{at } \boldsymbol{x} = [1 \;\; 1]^T$$

$$\boldsymbol{H}(1,\ 1) = \begin{bmatrix} 12 & -6 \\ -6 & 2 \end{bmatrix}$$

and det $\boldsymbol{H}$ = -12 so $\boldsymbol{H}$ is not pos. definite

Add $\begin{bmatrix} \beta & 0 \\ 0 & \beta \end{bmatrix}$ to $\boldsymbol{H}(1,\ 1)$ with β given by

$$(12+\beta)(2+\beta) - 36 > 0$$

or at = 0, $\quad \beta^2 + 14\beta - 12 = 0 \qquad \beta = \dfrac{-14 \pm \sqrt{14^2 - 4(1)(-12)}}{2}$

Another way: get the eigenvalues of $\boldsymbol{H}$ and calculate $\beta; \alpha_1 = 14.81, \quad \alpha_2 = -.81$

Problem 6.38

$f(\boldsymbol{x}) = u_1^2 + u_2^2 + u_3^2$

$$u_1 = 1.5 - x_1(1 - x_2)$$
$$u_2 = 2.25 - x_1(1 - x_2^2)$$
$$u_3 = 2.625 - x_1(1 - x_2^3)$$

$$\nabla f(\boldsymbol{x}) = 2\begin{bmatrix} [1.5 - x_1(1-x_2)][-(1-x_2)] + \left[2.25 - x_1(1-x_2^{\,2})\right]\left[-(1-x_2^{\,2})\right] + \left[2.625 - x_1(1-x_2^{\,3})\right]\left[-(1-x_2^{\,3})\right] \\ [1.5 - x_1(1-x_2)][x_1] + \left[2.25 - x_1(1-x_2^{\,2})\right](2x_1x_2) + \left[2.625 - x_1(1-x_2^{\,3})\right](3x_1x_2^{\,2}) \end{bmatrix}$$

Calculate ***H***(***x***). Because ***H***(***x***) is not positive definite:

(1) At $\begin{bmatrix} 0 & 1 \end{bmatrix}^{\mathrm{T}} = \boldsymbol{x},$ add constants to the elements on the main diagonal of ***H***(***x***) so that ***H***(***x***) becomes positive definite, or so that the eigenvalues of ***H***(***x***) become positive.

(2) Or, at $\begin{bmatrix} 0 & 1 \end{bmatrix}^{\mathrm{T}} = \boldsymbol{x},$ decompose $\boldsymbol{H}$ into $\boldsymbol{LDL}^{\mathrm{T}} = \boldsymbol{H} = \alpha_1\boldsymbol{e}_1\boldsymbol{e}_1^{\ \mathrm{T}} + \alpha_2\boldsymbol{e}_2\boldsymbol{e}_2^{\ \mathrm{T}}$ and change all negative (α_1, α_2) to be positive.

Problem 6.39

(a) False. The algorithm may initially use arbitrary search directions.
(b) True
(c) True

Problem 6.40

(a) Maximize $f(\boldsymbol{x}) = -x_1^{\ 2} + x_1 - x_2^{\ 2} + x_2 + 4$

Instead of maximization of $f(\boldsymbol{x}),$ we minimize –*f*(***x***):

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

by the BFGS method.

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 2x_1 - 1 \\ 2x^2 - 1 \end{bmatrix}$$

If you set $\nabla f(\boldsymbol{x}) = \boldsymbol{0},$ you find $\boldsymbol{x}^* = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix}^{\mathrm{T}}$

Steps Pick $\boldsymbol{x}^0 = [1 \ \ 1]^{\mathrm{T}}$. Pick $\boldsymbol{s}^0 = -\nabla f(\boldsymbol{x}^0)$. $\boldsymbol{s}^0(1,1) = [-1 \ \ -1]^{\mathrm{T}}$.

Pick $\hat{\boldsymbol{H}}^0 = \boldsymbol{H}(1,1) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$ (pos. def.)

1. $\boldsymbol{x}^1 = \boldsymbol{x}^0 + \lambda \boldsymbol{s}^0$

$$\lambda^{opt} = -\frac{\nabla^{\mathrm{T}} f(\boldsymbol{x}^k)\boldsymbol{s}^k}{(\boldsymbol{s}^k)^{\mathrm{T}} \hat{\boldsymbol{H}}(\boldsymbol{x}^k)\boldsymbol{s}^k} = -\frac{\begin{bmatrix} 1, & 1 \end{bmatrix} \begin{bmatrix} -1 \\ -1 \end{bmatrix}}{\begin{bmatrix} -1 & -1 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} -1 \\ -1 \end{bmatrix}} = \frac{1}{2}$$

$$\boldsymbol{x}^1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} -1 \\ -1 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix}^{\mathrm{T}}$$

$$\Delta \boldsymbol{x}^0 = \boldsymbol{x}^1 - \boldsymbol{x}^0 = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2} \end{bmatrix}^{\mathrm{T}} \qquad \text{(the solution)}$$

$$\Delta \boldsymbol{g}^0 = \nabla f(\boldsymbol{x}^1) - \nabla f(\boldsymbol{x}^0) = \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

$$\hat{\boldsymbol{H}}^1 = \frac{\Delta \boldsymbol{g}^0 (\Delta \boldsymbol{g}^0)^{\mathrm{T}}}{(\Delta \boldsymbol{g}^0)^{\mathrm{T}} (\Delta \boldsymbol{x}^0)} - \frac{\hat{\boldsymbol{H}}^0 \Delta \boldsymbol{x}^0 (\Delta \boldsymbol{x}^0)^{\mathrm{T}} \hat{\boldsymbol{H}}^0}{(\Delta \boldsymbol{x}^0)^{\mathrm{T}} \hat{\mathbf{H}}^0 \Delta x^0}$$

$$\hat{\boldsymbol{H}}^1 = \frac{\begin{bmatrix} -1 \\ -1 \end{bmatrix} \begin{bmatrix} -1 & -1 \end{bmatrix}}{\begin{bmatrix} -1 & -1 \end{bmatrix} \begin{bmatrix} -1/2 \\ -1/2 \end{bmatrix}} - \frac{\begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} -1/2 \\ -1/2 \end{bmatrix} \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2} \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}}{\begin{bmatrix} -\frac{1}{2} & -\frac{1}{2} \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} -1/2 \\ -1/2 \end{bmatrix}}$$

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

$$\Delta \boldsymbol{x}^1 = -\lambda^1 \hat{\boldsymbol{H}}^{-1}(\boldsymbol{x}^1) \nabla f(\boldsymbol{x}^1) = \mathbf{0}$$

The solution is at $\boldsymbol{x}^* = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix}^{\mathrm{T}}$ (as shown analytically)

(b) (*i*) $f(\boldsymbol{x}) = x_1^{\,3} \exp(x_2 - x_1^{\,2} - 10(x_1 - x_2)^2)$

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} \left\{3x_1^{\,2} + x_1^{\,3}(-2x_1 - 20(x_1 - x_2))\right\}\exp\left[x_2 - x_1^{\,2} - 10(x_1 - x_2)^2\right] \\ x_1^{\,3}\left[1 + 20(x_1 - x_2\ )\right]\exp\left[x_2 - x_1^{\,2} - 10(x_1 - x_2)^2\right] \end{bmatrix}$$

$$\boldsymbol{x}^0 = \begin{bmatrix} 1 & 1 \end{bmatrix}^{\mathrm{T}}$$

Let $\hat{\boldsymbol{H}}^0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

$$\nabla f(\boldsymbol{x}^0) = \begin{bmatrix} -1 & -1 \end{bmatrix}^{\mathrm{T}}$$

$$\boldsymbol{s}^0 = -(\hat{\boldsymbol{H}}^0)^{-1}\nabla f(\boldsymbol{x}^0) = \begin{bmatrix} 1 & 1 \end{bmatrix}^{\mathrm{T}}$$

$$\boldsymbol{x}^1 = \begin{bmatrix} (1+\lambda) & (1+\lambda) \end{bmatrix}^{\mathrm{T}}$$

A search for λ which minimizes $f(\boldsymbol{x}^1)$ gives $\lambda = 0.5$.

$$\boldsymbol{x}^1 = \begin{bmatrix} 1.5 & 1.5 \end{bmatrix}$$

$$\nabla f(\boldsymbol{x}^1) = \begin{bmatrix} 1.5942 & -1.5942 \end{bmatrix}^{\mathrm{T}}$$

$$\Delta\boldsymbol{x}^0 = \boldsymbol{x}^1 - \boldsymbol{x}^0 = \begin{bmatrix} 0.5 & 0.5 \end{bmatrix}^{\mathrm{T}}$$

$$\Delta\boldsymbol{g}^0 = \nabla f(\boldsymbol{x}^1) - \nabla f(\boldsymbol{x}^0) = \begin{bmatrix} 2.5942 \\ -0.5942 \end{bmatrix}$$

$$\boldsymbol{h}^0 = \Delta\boldsymbol{x}^0 - (\hat{\boldsymbol{H}}^0)^{-1}\Delta\boldsymbol{g}^0 = \begin{bmatrix} -2.0942 & 1.0942 \end{bmatrix}^{\mathrm{T}}$$

$$\Delta(\hat{\boldsymbol{H}}^0)^{-1} = \frac{h^0(\Delta x^0)^{\mathrm{T}} + (\Delta x^0)(h^0)^{\mathrm{T}}}{(\Delta g^0)^{\mathrm{T}}\Delta x^0} - \frac{(h^0)^{\mathrm{T}}\Delta g^0 \Delta x^0 (\Delta x^0)^{\mathrm{T}}}{\left[(\Delta g^0)^{\mathrm{T}}\Delta x^0\right]^{\mathrm{T}}\left[\Delta g^0)^{\mathrm{T}}\Delta x^0\right]}$$

$$= \begin{bmatrix} 3.9889 & 5.5831 \\ 5.5831 & 7.177 \end{bmatrix}$$

$$(\hat{\boldsymbol{H}}^1)^{-1} = \begin{bmatrix} 4.9889 & 5.5831 \\ 5.5831 & 8.177 \end{bmatrix}$$

(ii) $f(\boldsymbol{x}) = x_1^{\ 2} + x_2^{\ 2} + x_3^{\ 2} + x_4^{\ 2}$

The procedure is the same as for (i). $\hat{\boldsymbol{H}}$ is invariant and positive definite

$$\hat{\boldsymbol{H}} = \boldsymbol{H} = \begin{bmatrix} -2 & & & 0 \\ & 2 & & \\ & & 2 & \\ 0 & & & 2 \end{bmatrix}$$

The gradient of $f(\boldsymbol{x})$ is

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} 2x_1 \\ 2x_2 \\ 2x_3 \\ 2x_4 \end{bmatrix}$$

and at (1, 1, 1, 1), $\nabla f = \begin{bmatrix} 2 & 2 & 2 & 2 \end{bmatrix}^{\mathrm{T}}$. Then $\boldsymbol{s}^0$ is

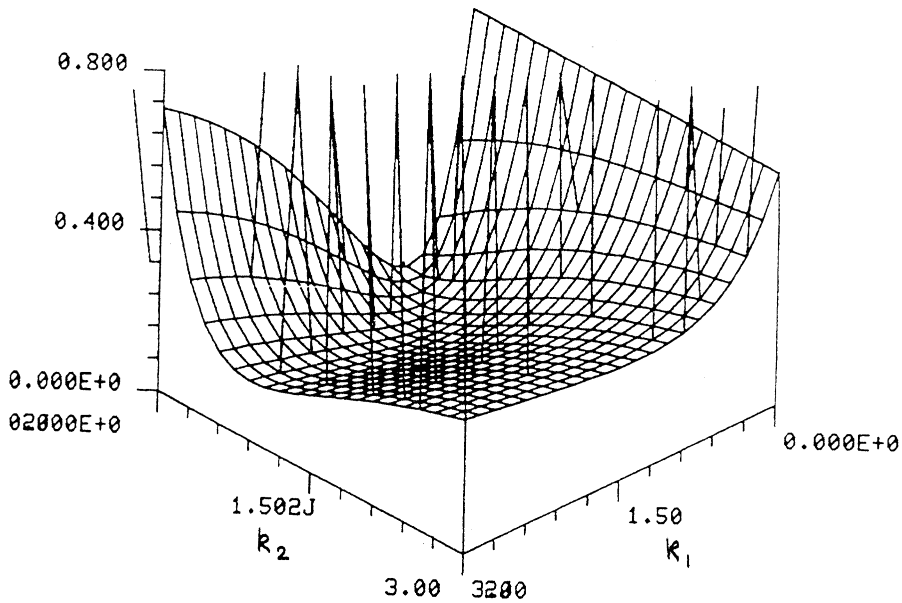
$$\boldsymbol{s}^0 = -\nabla f(\boldsymbol{x}^0) = \begin{bmatrix} -2 & -2 & -2 & -2 \end{bmatrix}^{\mathrm{T}}$$

$\boldsymbol{x}^1 = \boldsymbol{x}^0 + \lambda \boldsymbol{s}^0$, or if pick $\lambda = \dfrac{1}{2}$

$$\begin{bmatrix} x_1^{\ 1} \\ x_2^{\ 1} \\ x_3^{\ 1} \\ x_4^{\ 1} \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} -2 \\ -2 \\ -2 \\ -2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$ The solution.

Problem 6.41

$$k_1\text{opt} = 0.6630$$
$$k_2\text{opt} = 0.1546$$
$$\phi\ \text{opt} = 1.717\text{x}10^{-4}$$



Problem 6.42

The optimum is $k_1 = 2.44277$
$k_2 = 3.13149$
$k_3 = 15.1593$
$\phi = 4.355\text{x}10^{-5}$

Problem 6.43

Let $y = a(1\text{-}x^2)$, a better approximation than $y = a\ (1\text{-}x)$. This function satisfies the boundary conditions. We want to find the value of a which minimizes

$$F_1 = \int_0^1 \left[\left(\frac{dy}{dx} \right)^2 - 2yx^2 \right] dx \;=\; \frac{4}{3}a^2 - \frac{1}{2}a$$

From $dF_1 / da = \frac{8}{3}a - \frac{1}{2} = 0,$ we get $a^* = 3/16,$ and $F_1^* = -0.0469.$

If a more complicated function is chosen, say

$y = a_1(1-x^2) + a_2(1-x^2)^2,$ then

$$F_2 = 1.333a_1^2 + 1.219a_2^2 - 2.133a_1a_2 - 0.267a_1 - 0.152a_2$$

The minimum of this function is

$$a_1^* = 0.5,\quad a_2^* = 0.5,\quad F_2^* = -0.1048.$$

Since $F_2^* < F_1^*$, we conclude that a more complicated function improves the estimate of the minimum of the integral.

Problem 6.44

The optimum is
Expected risk = -0.12794 E11
and b^* = -0.2993 E4

Problem 6.45

The solution is:

(a) $\boldsymbol{x}^0 = \begin{bmatrix} 5 & 5 \end{bmatrix}^T \qquad \boldsymbol{x}^* = \begin{bmatrix} 4 & 2 \end{bmatrix}^T \qquad f^* = 3.428$

(b) $\boldsymbol{x}^0 = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^T \qquad \boldsymbol{x}^* = \begin{bmatrix} 1 & 2 & 1 \end{bmatrix}^T \qquad f^* = 0.299$

$\boldsymbol{x}^0 = \begin{bmatrix} 5 & 4 & 6 \end{bmatrix}^T \qquad \boldsymbol{x}^* = \begin{bmatrix} 4 & 2 & 1 \end{bmatrix}^T \qquad f^* = 0.464$

Problem 6.46

The solution is

(a) $\boldsymbol{x}^0 + \begin{bmatrix} 2 & 1 \end{bmatrix}^T$ $\boldsymbol{x}^* = \begin{bmatrix} 4 & 2 \end{bmatrix}^T$ $f^* = 3.428$

$\boldsymbol{x}^0 = \begin{bmatrix} 2 & 2 \end{bmatrix}^T$ $\boldsymbol{x}^* = \begin{bmatrix} 4 & 2 \end{bmatrix}^T$ $f^* = 3.428$

(b) $\boldsymbol{x}^0 + \begin{bmatrix} 2 & 1 & 1 \end{bmatrix}^T$ $\boldsymbol{x}^* = \begin{bmatrix} 2 & 2 & 1 \end{bmatrix}^T$ $f^* = 0.2686$

$\boldsymbol{x}^0 = \begin{bmatrix} 2 & 2 & 1 \end{bmatrix}^T$ $\boldsymbol{x}^* = \begin{bmatrix} 2 & 2 & 1 \end{bmatrix}^T$ $f^* = 0.2686$

Problem 6.47

The optimum is

$a^* = 0.94089$
$b_1^* = 3.04917$
$b_2^* = 0.47456$
$f^* = 896.719$ (sum of squares of the errors)

Problem 6.48

The optimum is T^* = 446,927 kL
Q^* = 179,840 bbl/day
C^* = 17.88 $/kL

The optimum is flat, and slightly different T and Q give the same C.

CHAPTER 7

Problem 7.1

The yields are bbl product per bbl of crude expressed as a fraction. The problem to maximize the profit.

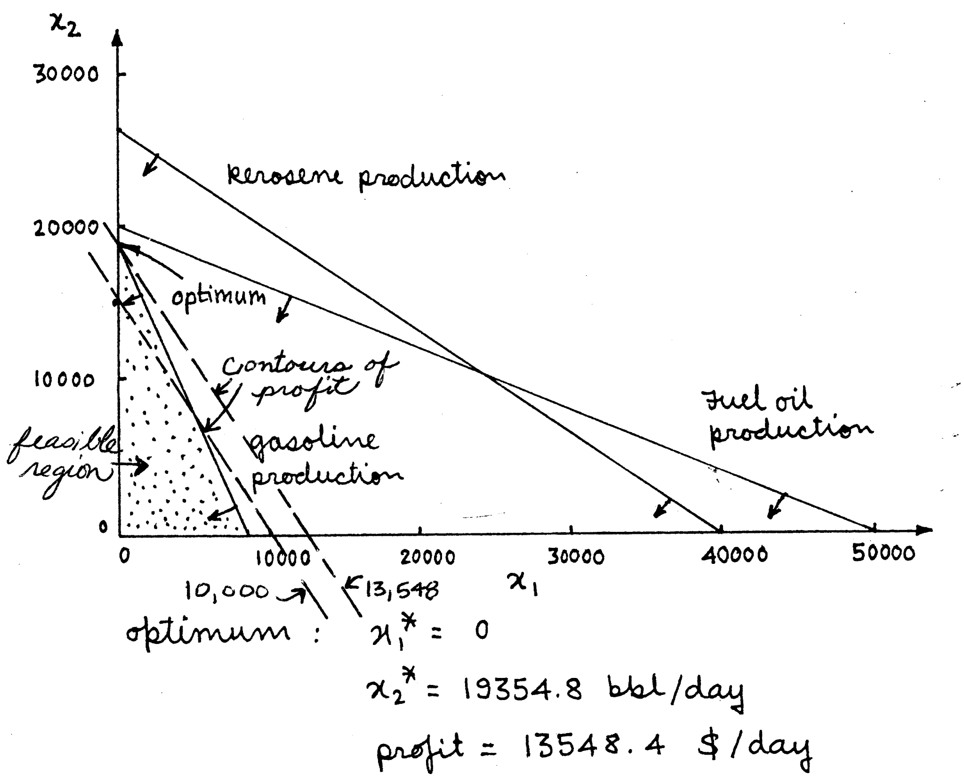
Let x_1 = volume of crude no. 1 used (bbl/day)
x_2 = volume of crude no. 2 used (bbl/day)

Constraints:

Gasoline production	$0.7x_1 + 0.31\,x_2$	≤ 6000	(a)
Kerosene production	$0.06\,x_1 + 0.09\,x_2$	≤ 2400	(b)
Fuel oil production	$0.24\,x_1 + 0.60\,x_2$	≤ 12000	(c)

profit = $1.00\,x_1 + 0.70\,x_2$ ($/day)

Also: $x_1 \ge 0$
$x_2 \ge 0$



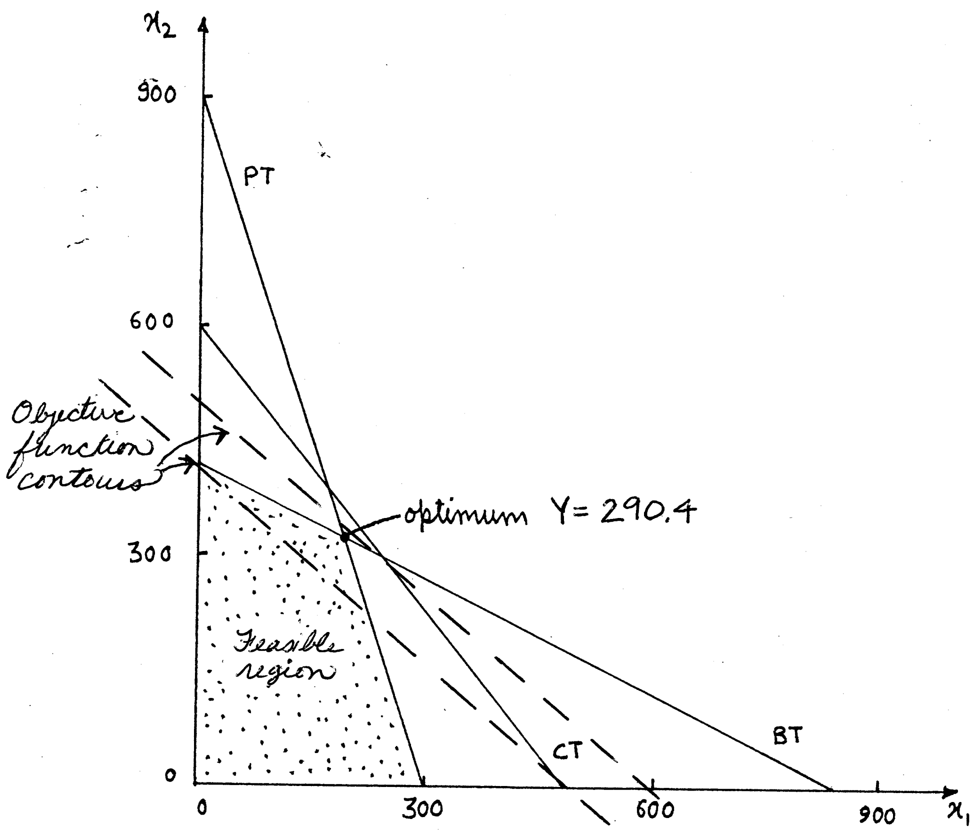
Problem 7.2

Basis: 1 run	hr	x_1 Ergies	1 run
Units:	Ergies produced		

Let x_1 = number of boxes of ERGIES per run
x_2 = number of boxes of NERGIES per run

Maximize: profit $Y = 0.50\, x_1 + 0.60\, x_2$
Constraints:

blending time	$BT = (1/60)\, x_1 + (2/60)\, x_2 \le 14$ hr
cooking time	$CT = (5/60)\, x_1 + (4/60)\, x_2 \le 40$ hr
packing time	$PT = (3/60)\, x_1 + (1/60)\, x_2 \le 15$ hr
	$x_1, x_2 \ge 0$



optimum: $x_1 = 192$ boxes/run
$x_2 = 324$ boxes/run
$Y = 290.4$ \$/run

Problem 7.3

Objective function:

$$y = \$.60P_1 + \$.30P_2 - \$.40F$$

Equality constraints:

$$\text{equality}: \quad F = F_A + F_B + F_C$$

$$P_1 = F_A(.40) + F_B(.30) + F_C(.50)$$
$$P_2 = F_A(.60) + F_B(.70) + F_c(.50)$$

Inequality constraints:

$$F \le 10,000$$
$$F_A \le 5,000$$
$$F_B \le 5,000$$
$$F_C \le 5,000$$
$$P_1 \le 4,000$$
$$P_2 \le 7,000$$

Problem 7.4

The graph is shown below and indicates that the optimal solution is at the extreme point B where $x_1 = 2$, $x_2 = 4$, and $f_{max} = 10$.

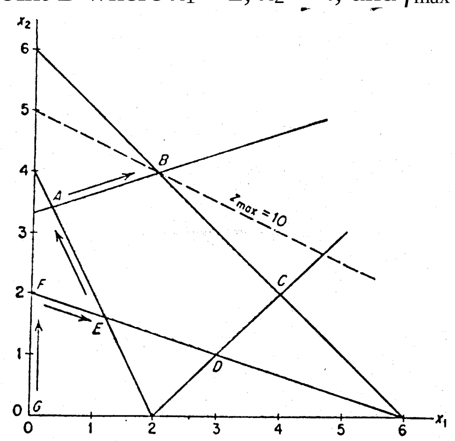


FIG. 3-2

Problem 7.5

Let X_{ij} be the number of batches of product i (i = 1, 2, 3) produced per week on unit j ($j = A, B, C$). We want to maximize the weekly profit.

$$\max: f(\boldsymbol{x}) = 20(X_{1A} + X_{1B} + X_{1C}) + 6(X_{2A} + X_{2B} + X_{2C}) + 8(X_{3A} + X_{3B} + X_{3C})$$

subject to:

sales limits: $X_{3A} + X_{3B} + X_{3C} \le 20$

hours available on each unit:

unit A	$0.8X_{1A} + 0.2X_{2A} + 0.3X_{3A}$	≤ 20
unit B	$0.4X_{1B} + 0.3X_{2B}$	≤ 10
unit C	$0.2X_{1C} + 0.1X_{3C}$	≤ 5

and non-negativity constraints:

$$X_{ij} \ge 0 \quad i = 1,2,3 \quad j = A, B.C$$

Problem 7.6

Let i	designate the constituent index	i = 1 to 4
j	designate the grade index	j = 1 to 3

(A = 1, B = 2, C = 3)

x_i designate a constituent
y_j designate a grade
x_{ij} is bbl/day of constituent i in grade j

Objective function ($/day):

$$f = 16.20y_1 + 15.75y_2 + 15.30y_3 - 13.00\sum_{j=1}^{3} x_{1j}$$

$$-15.30\sum_{j=1}^{3} x_{2j} - 14.60\sum_{j=1}^{3} x_{3j} - 14.90\sum_{j=1}^{3} x_{4j}$$

Constraints:

$$\sum_{j=1}^{3} x_{1j} \le 3{,}000 \qquad \sum_{j=1}^{3} x_{3j} \le 4{,}000$$

$$\sum_{j=1}^{3} x_{2j} \le 2{,}000 \qquad \sum_{j=1}^{3} x_{4j} \le 1{,}000$$

$$\frac{x_{11}}{y_1} \le 0.15 \qquad \frac{x_{12}}{y_2} \le 0.10$$

$$\frac{x_{21}}{y_1} \le 0.40 \qquad \frac{x_{22}}{y_2} \le 0.10$$

$$\frac{x_{31}}{y_1} \le 0.50 \qquad \frac{x_{13}}{y_2} \le 0.20$$

$$y_j \ge 0$$
$$x_{ij} \ge 0$$

$$y_{1=} \sum_{i=1}^{4} x_{i1} \quad y_{2=} \sum_{i=1}^{4} x_{i2} \quad y_{3=} \sum_{i=1}^{4} x_{i3}$$

Problem 7.7

The objective function is: Max: $f(\mathbf{x}) = 5(P + T + F) - 8F$

The constraints are:

Viscosity requirement $5P + 11T + 37F \geq 21(P + T + F)$.

Gravity requirement $8P + 7T + 24F \geq 12(P + T + F)$.

Material balances $P + V = 1000$

$T = 0.8V$

Also:
$P, V, F, T \geq 0$

Note: It would be also ok to let $P + T + F = F^*$ (fuel oil)

profit $f(\mathbf{x}) = 5F^* - 8F = 5(P + T + F) - 8F$

viscosity: $-16P - 10T + 16F \geq 0$

gravity: $-4P - 5T + 12F \geq 0$

$$\left.\begin{array}{ll}\text{material balances on} & P + V = 1000 \\ \text{viscosity breaker:} & T = 0.8V\end{array}\right\} P + \frac{T}{.8} = 1000$$

The number of equality constraints depends on the number of substitutions you make, and the same is true with respect to the number of variables. You can delete F^*, V.

Problem 7.8

After adding slack variable

$$\begin{aligned} x_1 - 2x_2 + x_3 - x_4 &= 11 \\ -4x_1 + x_2 + 2x_3 - x_5 &= 3 \\ 2x_1 - x_3 &= -1 \end{aligned}$$

There is no basic feasible solution because with

$x_1 = x_2 = x_3 = 0$, $x_4 = 11$ but $x_5 = -3$(not feasible).

Problem 7.9

(a) Choose the largest positive coefficient in the bottom row, since this will decrease f the fastest. x_1 should be increased first.

(b) Part (a) designated x_1 as the pivotal column. Check the ratios to find the limiting constraint. Choose the smallest positive ratio from –3/2, 11/5 and 4/1. It is 11/5. Therefore, x_4 is the pivotal row, and "5" is the pivotal element.

(c) The limiting value of x_1 is found from the ratio test; it is 11/5.

Problem 7.10

Start with the following matrix:

	x_1	x_2	x_3	x_4	x_5	f	b
x_3	-2	2	1	0	0	0	3
x_4	5	2	0	1	0	0	11
x_5	1	-1	0	0	1	0	4
f	4	2	0	0	0	1	0

Let x_1 replace x_4 as a basic variable.

step 1: divide row 2 by 5
step 2: multiply row 2 by 2 and add to row 1
step 3: multiply row 2 by –1 and add to row 3
step 4: multiply row 2 by –4 and add to row 4

The next matrix is:

	x_1	x_2	x_3	x_4	x_5	f	b
x_3	0	14/5	1	2/5	0	0	7.4
x_1	1	2/5	0	1/5	0	0	11/5
x_5	0	-7/5	0	-1/5	1	0	1.8
f	0	2/5	0	-4/5	0	1	-8.8

The basic variables are: x_1, x_3, x_5 The non-basic variables are: x_2, x_4

Problem 7.11

The constraints are:

$$x_1 - 2x_2 + x_3 \le 11 \qquad \text{(a)}$$
$$-4x_1 + x_2 + 2x_3 \ge 3 \qquad \text{(b)}$$
$$2x_1 - x_3 = -1 \qquad \text{(c)}$$
$$x_1, x_2, x_3 \ge 0.$$

From (c), get $x_3 = 2x_1 + 1$ (d)

From (a) and (d) get $3x_1 - 2x_2 \le 10$ (e)

From (b) and (d) get $x_2 \ge 1$, say $x_2 = 1$.

Then from *(e)*, $x_1 \le 4$, say $x_1 = 4$

Then from *(d)*, $x_3 = 9$.

Therefore, $x_1 = 4$, $x_2 = 1$, $x_3 = 9$ is a basic feasible solution, and thus, there exists a basic feasible solution.

Problem 7.12

A phase I procedure can be used to obtain a feasible basic solution. Add an artificial variable x_6, to the second equality constraint. Now solve the LP

Minimize: x_6

Subject to:
$$x_1 + 2x_2 + 2x_3 + x_4 = 8$$
$$3x_1 + 4x_2 + x_3 - x_5 + x_6 = 7$$
$$x_1, \ldots, x_6 \geq 0$$

The solution to this LP gives a feasible solution to the original LP provided $x_6^* = 0$. If $x_6^* \neq 0$, then the original LP does not have a feasible solution. In our case, $x_1^* = x_4^* = x_5^* = x_6^* = 0,\ x_2^* = 1,\ x_3^* = 3$. This is a feasible solution.

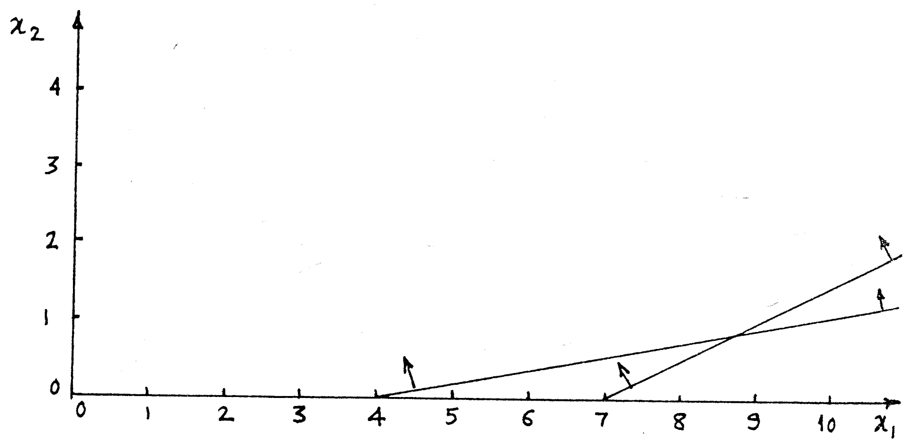
Problem 7.13

(a) The basic variables have negative values: $x_3 = -6$ and $x_4 = -4$. This violates the non-negativity constraints.

(b) The constraints are

$$\begin{aligned} x_1 - 2x_2 + x_3 &= 7 \\ x_1 - 3x_2 + x_4 &= 4 \end{aligned} \quad \text{or} \quad \begin{aligned} x_1 - 2x_2 &\leq 7 \\ x_1 - 3x_2 &\leq 4 \end{aligned}$$

$$x_1 - 3x_2 + f = 0 \qquad\qquad f = x_1 - 3x_2$$



The problem is unsolvable, because the optimum is unbounded.

(c) x_2 is the incoming variable. The ratio test says that either of x_3 and x_4 can leave the basic set. If x_3 leaves the basic set, the final matrix is:

	x_1	x_2	x_3	x_4	f	b
x_2	2	1	0.5	0	0	3
x_4	0	0	-1.5	1	0	0
f	-5	0	-1.5	0	1	-9

The solution is: $x_1^* = x_3^* = x_4^* = 0,\ \ x_2^* = 3,\ f^* = -9$

If x_2 replaces x_4, the final matrix is

	x_1	x_2	x_3	x_4	f	b
x_3	0	0	1	-0.67	0	0
x_2	2	1	0	0.33	0	3
f	-5	0	0	-1	1	-9

The solution is: $x_1^* = x_3^* = x_4^* = 0,\ \ x_2^* = 3,\ \ f^* = -9$

Thus, the solution is unique.

(d) The given problem is already at an optional solution:

$$x_1^* = x_2^* = 0,\ \ x_3^* = 7,\ x_4^* = 5,\ f^* = 0$$

We can also pivot around "3" (x_4 row, x_2 column) to get

	x_1	x_2	x_3	x_4	f	b
x_3	0	0	0	-2/3	0	11/3
x_2	2	1	0	1/3	0	5/3
f	-1	0	1	0	1	0

$x_1^* = x_4^* = 0,\ x_2^* = 5/3, x_3^* = 11/3,\ f^* = 0.$

This means the any point on the line segment joining the points

$\begin{bmatrix} 0 & 0 & 7 & 5 \end{bmatrix}^T$ and $\begin{bmatrix} 0 & 5/3 & 11/3 & 0 \end{bmatrix}^T$ is optimal

---

Problem 7.14

Add slack variables x_3, x_4, x_5 and x_6. Now solve

$$\begin{aligned} \text{Minimize: } & f = x_1 + x_2 \\ \text{Subject to: } & x_1 + 3x_2 + x_3 = 12 \\ & x_1 - x_2 + x_4 = 1 \\ & 2x_1 - x_2 + x_5 = 4 \\ & 2x_1 + x_2 + x_6 = 8 \\ & x_1, ..., x_6 \geq 0 \end{aligned}$$

The beginning matrix is

	x_1	x_2	x_3	x_4	x_5	x_6	f	b
x_3	1	3	1	0	0	0	0	12
x_4	1	-1	0	1	0	0	0	1
x_5	2	-1	0	0	1	0	0	4
x_6	2	1	0	0	0	1	0	8
f	-1	-1	0	0	0	0	1	0

This is already at the optimal point!

$x_1^* = x_2^* = 0,\ f^* = 0$

The Simplex method did not exhibit cycling.

Problem 7.15

Problem 7.1 was

Maximize: $x_1 + 0.7x_2$

Subject to: $0.7x_1 + 0.31x_2 \le 6000$

$0.06x_1 + 0.09x_2 \le 2400$

$0.24x_1 + 0.60x_2 \le 12000$

which is the same as

Minimize $-x_1 - 0.7x_2$

Subject to: $0.7x_1 + 0.31x_2 + x_3 = 6000$

$0.06x_1 + 0.09x_2 + x_4 = 2400$

$0.24x_1 + 0.60x_2 + x_5 = 12000$

where x_3, x_4 and x_5 are slack variables. The initial matrix is (the origin is a feasible solution):

	x_1	x_2	x_3	x_4	x_5	f	b
x_3	0.7	0.31	1	0	0	0	6000
x_4	0.06	0.09	0	1	0	0	2400
x_5	0.24	0.60	0	0	1	0	12000
f	1	0.7	0	0	0	1	0

Now, use the Simplex method:

	x_1	x_2	x_3	x_4	x_5	f	b
x_1	1	0.4428571	1.4285714	0	0	0	8571.43
x_4	0	0.0634285	-0.0857142	1	0	0	1885.71
x_5	0	0.4937143	-0.3428571	0	1	0	9942.86
f	0	0.2571429	-1.428571	0	0	1	-8571.43

	x_1	x_2	x_3	x_4	x_5	f	b
x_2	2.2580647	1	3.2258067	0	0	0	19354.84
x_4	-0.1432256	0	-0.2903222	1	0	0	658.07
x_5	-1.1148388	0	-1.935484	0	1	0	387.10
f	-0.5806453	0	-2.2580647	0	0	1	-13548.39

This last matrix gives the optimal solution. At the optimum, x_2 (crude # 2) is a basic variable, and x_1 (crude # 1) is a non-basic variable. Thus a small change in the profit coefficient of x_1 does not affect the optimum (Note that if the profit coefficient were 1.1, its shadow price would still be negative, which implies that the optimum, $\boldsymbol{x}^*$ and f^* are unchanged). A five percent increase in the profit coefficient of x_2 influences the objective function the most. (Note: if the profit coefficient x_2 were 0.735 instead of 0.7, the current $\boldsymbol{x}^*$ would still be optimal).

Problem 7.16

Start with the matrix that has been converted to standard canonical form by the addition of slack variables, and has a basic feasible solution (with $x_1 = x_2 = 0$):

	x_1	x_2	x_3	x_4	x_5	Constants
obj. function:	4	2	0	0	0	0
constraints:	-2	2	1	0	0	3
	5	2	0	1	0	11
	1	-1	0	0	1	4

Next

(a) Increase x_1 first as it has largest positive coefficient.

(b) Column no. is 1. Row no. comes from the first constraint that is encountered

Look at each one: $b_s - a_s x_s = 0$

2nd row $\quad 3-(-2)x_1 = 0 \quad x_1 < 0$ ok to increase

3rd row $\quad 11–5x_1 = 0 \quad$ so $x_1 = \dfrac{11}{5}$ (is the limit)

4th row $\quad 4-x_1 = 0 \quad$ so $x_1 = 4$

Row no. to choose is 3 (2nd constraint)

(c) Limiting value is $x_1 = \dfrac{11}{5}$.

(d) The next basis will be $x_2 = 0,\ x_4 = 0;\ x_1, x_3, x_4$ will be non-basic.

(e) Use elementary operations to make the x_1 column a unit vector

	x_1	x_2	x_3	x_4	x_5	Constants
1	0	$\left(2-\frac{8}{5}\right)$	0	-4/5	0	-44/5
2	0	$\left(2+\frac{2}{5}\right)$	1	$\frac{2}{5}$	0	$\left(3+\frac{22}{5}\right)$
3	1	$\frac{2}{5}$	0	$\frac{1}{5}$	0	$\frac{11}{5}$
4	0	$-\frac{7}{5}$	0	$-\frac{1}{5}$	1	$\left(4-\frac{11}{5}\right)$

Problem 7.17

An LP code gives

$$f(\boldsymbol{x}) = 6 \quad x_1 = 0 \quad x_2 = 2 \quad x_3 = 0$$

Problem 7.18

To solve this problem, introduce slack variables $x_4 \geq 0$ and $x_5 \geq 0$ so that the constraints become

$$\begin{aligned} 2x_1 + 2x_2 + x_3 + x_4 &= 16, \\ 4x_1 + 8x_2 + x_3 + x_5 &= 40, \\ x_i \geq 0 \quad &\text{for } 1 \leq i \leq 5. \end{aligned}$$

Now consider the following array

E_1	$2x_1 + 2x_2 + x_3 + x_4$	= 16
E_2	$4x_1 + 8x_2 + x_3 \quad + x_5$	= 40
E_3	$7x_1 + 12x_2 + 3x_3$	-Z = 0

Clearly, a basic feasible solution is given by

$$x_1 = x_2 = x_3 = 0, \; x_4 = 16, \text{ and } x_5 = 40.$$

According to the above algorithm we do not have an optimal solution because the coefficient of each x_i in equation E_3 is positive. Since 12 is the largest relative cost factor, we choose column 2. Furthermore, since $16/a_{12}=8$ and $40/a_{22}=5$, we choose row 2 and pivot about $8x_2$. This yields the following array:

$$E_4 = \frac{E_2}{8} \qquad \frac{1}{2}x_1 + x_2 + \frac{1}{8}x_3 \qquad + \frac{1}{8}x_5 \qquad = 5,$$

$$E_5 = E_1 - 2E_4 \qquad x_1 \qquad + \frac{3}{4}x_3 + x_4 - \frac{1}{4}x_5 \qquad = 6,$$

$$E_6 = E_3 - 12E_4 \qquad x_1 \qquad + \frac{3}{2}x_3 \qquad - \frac{3}{2}x_5 - \text{Z} = -60 \;.$$

This yields another basic feasible solution given by

$$x_1 = x_3 = x_5 = 0,\ x_2 = 5,\ \text{and } x_4 = 6$$

Since there are still positive cost factors (in E_6), then we know that this solution is not optimal. Since 3/2 is the largest relative cost factor we choose column 3 and observe that we must pivot about (3/4) x_3. Doing this, we obtain

$$E_7 = \frac{4E_5}{3} \qquad \frac{4}{3}x_1 \quad + x_3 + \frac{4}{3}x_4 - \frac{1}{3}x_5 \qquad = 8,$$

$$E_8 = E_4 - \frac{1}{8}E_7 \quad \frac{1}{3}x_1 + x_2 \quad - \frac{1}{6}x_4 + \frac{1}{6}x_5 \qquad = 4,$$

$$E_9 = E_6 - \frac{3}{2}E_7 \quad -x_1 \qquad - \frac{3}{2}x_4 - \quad x_5 - Z \quad = \quad -72$$

Continuing on until all the variables in the *Z* function have negative coefficients (so the variables cannot be increased), the optimal solution is

$$x_1 = 0 \quad x_2 = 4 \quad x_3 = 8 \quad z = 72$$

In this case we obtain as a basic solution

$$x_1 = x_4 = x_5 = 0,\ x_2 = 4,\ x_3 = 8,\ \text{and } Z = 72.$$

This solution is optimal since all cost factors (in E_9) are negative. Thus, the maximum value of the objective function is 72.

Some comments are necessary with regard to the simplex algorithm as stated. First, the problem must be feasible, and this is why the initial solution has to be feasible. This suggests that it might be desirable to have some test of feasibility before applying the algorithm unless it is known a priori that a physically realizeable solution must exist. Second, the assumption was made that all b_i are nonnegative. If any b_i is negative, we multiply each equation by –1 to obtain a positive constant on the right-hand side of the inequality. In particular, if $b_1 < 0$, then from the constraint $\sum_{j=1}^{n} a_{1j} x_j \le b_1$ we obtain $-\sum_{j=1}^{n} a_{1j} x_j \ge -b_1$. To make this an equality, we must subtract a non-negative variable x_{n+1} from the left-hand side to obtain $-\sum_{j=1}^{n} a_{1j} x_j - x_{n+1} = -b_1$. Inserting this equation into the system of equations defined by the constraint inequalities shows that the basic solution of the resulting canonical system is not feasible since we would have $x_{n+1} = b_1 < 0$ as part of the basic solution. Therefore, in order to apply the simplex algorithm directly, we must perform at least one pivot operation to obtain a basic feasible solution as a starting point. This requires, in general, a trial and error process that may require considerable time before obtaining a suitable basic solution as a starting point.

Problem 7.19

You want to have all of the *b's* (the right hand sides of the inequalities) be positive at the start. If you multiply the last two in equalities by –1, you change the values of the *b's* to positive and reverse the direction of the inequalities, but $f \to \infty$. It is better to translate x_1 and x_2 (by addition) to get new variables for which the origin is a feasible point.

Problem 7.20

(a) True
(b) True
(c) True

Problem 7.21

Let x_{ij} = tons/day of product from refinery *i* transported to customer *j*.

i = 1, 2 and *j* = 1, 2, 3.

Capacity constraints:

$x_{11} + x_{12} + x_{13} \leq 1.6$
$x_{21} + x_{22} + x_{23} \leq 0.8$

Minimum demand constraints:

$x_{11} + x_{21} \geq 0.9$
$x_{12} + x_{22} \geq 0.7$
$x_{13} + x_{23} \geq 0.3$

Production cost = $P_1(x_{11} + x_{12} + x_{13}) + 35(x_{21} + x_{22} + x_{23})$ ($/day)

where $P_1 = \$30/\text{ton if } x_{11} + x_{12} + x_{13} \leq 0.5 \text{ ton/day}$
$= \$40/\text{ton if } x_{11} + x_{12} + x_{13} > 0.5 \text{ ton/day}$

Transportation cost = $25x_{11} + 60x_{12} + 75x_{13} + 20x_{21} + 50x_{22} + 85x_{23}$ ($/day)

Total cost = Production cost + Transportation cost
(to be minimized).

If we assume that $P_1 = \$30/\text{ton}$, then the solution to the LP is $x_{11} = 0.9,\ x_{13} = 0.3,\ x_{22} = 0.7,\ x_{12}, x_{21} x_{23} = 0.$ But, $x_{11} + x_{12} + x_{13} = 1.2$ tons/day $>$ 0.5 tons/day. So, we cannot use P_1 = $30/ton.

If we use $P_1 = \$40/\text{ton}$, then the optimum is $x_{11} = 0.8, x_{13} = 0.3, x_{21} = 0.1, x_{22} = 0.7, x_{12} = x_{23} = 0.$ Total cost = $151.50/day. $x_{11} + x_{12} + x_{13} = 1.1$ ton/day. So, we used the correct value for P_1. The solution is

$x_{11}^* = 0.8$ tons/day
$x_{13}^* = 0.3$ tons/day
$x_{21}^* = 0.1$ tons/day
$x_{22}^* = 0.7$ tons/day
$x_{12}^* x_{23}^* = 0.$

Total cost = $151.50/day.

Problem 7.22

Let x_{ij} = bbl/day of stream *i* used to make product *j*

$i =$ A alkylate
C cat cracked gas
S s.r. gas
$j =$ A aviation gas A
B aviation gas B
L leaded motor gas
U unleaded motor gas

Maximize:

profit (\$/day) = 5.00 $(x_{AA} + x_{CA} + x_{SA})$ $+5.50(x_{AB} + x_{CB} + x_{SB}) + 4.50(x_{AL} + x_{CL} + x_{SL})$
$+4.50(x_{AU} + x_{CU} + x_{SU})$

Subject to:

(i) availability constraints

$x_{AA} + x_{AB} + x_{AL} + x_{AU} \le 4000$ bbl/day (a)

$x_{CA} + x_{CB} + x_{CL} + x_{CU} \le 2500$ bbl/day (b)

$x_{SA} + x_{SB} + x_{SL} + x_{SU} \le 4000$ bbl/day (c)

(ii) RVP constraints

$5x_{AA} + 8x_{CA} + 4x_{SA} \le 7(x_{AA} + x_{CA} + x_{SA})$

$5x_{AB} + 8x_{CB} + 4x_{SB} \le 7(x_{AB} + x_{CB} + x_{SB})$

or

$-2x_{AA} + x_{CA} - 3x_{SA} \le 0$ (d)

$-2x_{AB} + x_{CB} - 3x_{SB} \le 0$ (e)

(iii) ON constraints

$94x_{AA} + 84x_{CA} + 74x_{SA} \ge 80(x_{AA} + x_{CA} + x_{SA})$

$94x_{AU} + 84x_{CU} + 74x_{SU} \ge 91(x_{AU} + x_{CU} + x_{SU})$

$108x_{AB} + 94x_{CB} + 86x_{SB} \ge 91(x_{AB} + x_{CB} + x_{SB})$

$108x_{AL} + 94x_{CL} + 86x_{SL} \ge 87(x_{AL} + x_{CL} + x_{SL})$

or

$14x_{AA} + 4x_{CA} - 6x_{SA} \ge 0$ (f)

$3x_{AU} + 7x_{CU} - 17x_{SU} \ge 0$ (g)

$17x_{AB} + 3x_{CB} - 5x_{SB} \ge 0$ (h)

$21x_{AL} + 7x_{CL} - x_{SL} \ge 0$ (i)

(iv) Non-negativity constraints

all $x_{ij} \ge 0$

Solution: $x^*_{AB} = 4000$ bbl/day
$x^*_{CB} = 2500$ bbl/day
$x^*_{SB} = 4000$ bbl/day
all other $x^*_{ij} = 0$ $x^*_{ij} = 0$
Profit = \$57750/day.

Problem 7.23

Let $x_i = 100\ \text{lb/day of material } i$ produced or consumed i = A, B, C, E, F, G

Total income (\$/day) = $4x_4 + 3.3x_5 + 3.8x_6$
Cost of raw material (\$/day) = $1.5x_1 + 2x_2 + 2.5x_3$
Operating cost (\$/day) = $\frac{2}{3}x_4 + \frac{1}{3}x_5 + x_6$

From the material balances, we have

$$x_1 = \frac{2}{3}x_4 + \frac{2}{3}x_5 + \frac{1}{2}x_6$$

$$x_2 = \frac{1}{3}x_4 + \frac{1}{3}x_5 + \frac{1}{6}x_6 \qquad x_3 = \frac{1}{3}x_6$$

Using these to eliminate x_1, x_2 and x_3 from the cost-of-raw material expression, we get the cost of raw material (\$/day) = $\frac{5}{3}x_4 + \frac{5}{3}x_5 + 1.92x_6$
The objective is to maximize the profit:
Profit = total income – raw material cost - operating cost

The LP is, therefore,
Maximize: $1.67x_4 + 1.3x_5 + 0.88x_6$
Subject to availability of raw materials:

$$\frac{2}{3}x_4 + \frac{2}{3}x_5 + \frac{1}{2}x_6 \le 40$$

$$\frac{1}{3}x_4 + \frac{1}{3}x_5 + \frac{1}{6}x_6 \le 30$$

$$\frac{1}{3}x_6 \le 25$$

$$x_4, x_5, x_6 \ge 0$$

An equivalent objective is

Minimize: $-1.67x_4 - 1.3x_5 - 0.88x_6$

Introducing the slack variables x_7, x_8, x_9. The inequalities are converted to equality constraints:

$$\frac{2}{3}x_4 + \frac{2}{3}x_5 + \frac{1}{2}x_6 + x_7 = 40$$
$$\frac{1}{3}x_4 + \frac{1}{3}x_5 + \frac{1}{6}x_6 + x_8 = 30$$
$$\frac{1}{3}x_6 + x_9 = 25$$

$x_4 = x_5 = x_6$ gives an initial feasible solution. The initial matrix is

	x_4	x_5	x_6	x_7	x_8	x_9	f	b
x_7	2/3	2/3	½	1	0	0	0	40
x_8	1/3	1/3	1/6	0	1	0	0	30
x_9	0	0	1/3	0	0	1	0	25
f	1.67	1.3	0.88	0	0	0	1	0

x_4 is the incoming variable. x_7 leaves the basic set. The next matrix is

	x_4	x_5	x_6	x_7	x_8	x_9	f	b
x_4	1	1	¾	3/2	0	0	0	60
x_8	0	0	-1/12	-1/2	1	0	0	10
x_9	0	0	1/3	0	0	1	0	25
f	0	-0.37	-0.37	-2.51	0	0	1	-100.2

This matrix gives the optimal solution

$x_4 = 60$

$x_8 = 10$

$x_9 = 25$

$x_5, x_6, x_7 = 0$

The optimum distribution is to produce 6000 lb/day of E, and no F and G.

Problem 7.24

(profit or loss of each refinery cpb)

Crude / Refinery	*a*	*b*	*c*	*d*	*e*	*f*	*g*	*h*	*i*	*j*	Required *M* bpd
X_1	-6	3	17	10	63	34	15	22	-2	15	30
X_2	-11	-7	-16	9	49	16	4	10	-8	8	40
Y	-7	3	16	13	60	25	12	19	4	13	50
Z	-1	0	13	3	48	15	7	17	9	3	60
Available *M* bpd	30	30	20	20	10	20	20	10	30	10	200

Refinery X_1

$$P_{X1} = -6X_{1a} + 3X_{1b} + 17X_{1c} + 10X_{1d} + 63X_{1e} + 34X_{1f} + 15X_{1g} + 22X_{1h} - 2X_{1i} + 15X_{ij}$$

where P_{X1} = net profit of Refinery X_1

X_{1a} = crude *a* used in X_1

X_{1j} = crude *j* used in X_1

Refinery X_2

$$P_{X2} = -11X_{2a} - 7X_{2b} - 16X_{2c} + 9X_{2d} + 49X_{2e} + 16X_{2f} + 4X_{2g} + 10X_{2h} - 8X_{2i} + 8X_{2j}$$

Refinery Y

$$P_Y = -7Y_a - 3Y_b - 16Y_c + 13Y_d + 60Y_e + 25Y_f + 12Y_g + 19Y_h + 4Y_i + 13Y_j$$

Refinery Z

$$P_Z = -Z_a + 13Z_c + 3Z_d + 48Z_e + 15Z_f + 7Z_g + 17Z_h + 9Z_i + 3Z_j$$

$$P_{tot} = P_{X1} + P_{X2} + P_Y + P_Z \leftarrow \text{objective function}$$

$$\begin{aligned} P_{tot} = & -6X_{1a} + 3X_{1b} + 17X_{1c} + 10X_{1d} + 63X_{1e} + 34X_{1f} + 15X_{1g} + 22X_{1h} - 2X_{1i} + 15X_{1j} \\ & -11X_{2a} - 7X_{2b} - 16X_{2c} + 9X_{2d} + 49X_{2e} + 16X_{2f} + 4X_{2g} + 10X_{2h} - 8X_{2i} + 8X_{2j} \\ & -7Y_a + 3Y_b + 16Y_c + 13Y_d + 60Y_e + 25Y_f + 12Y_{g+}19Y_h + 4Y_i + 13Y_j \\ & -Z_a + 0 + 13Z_c + 3Z_d + 48Z_e + 15Z_f + 7Z_g + 17Z_h + 9Z_i + 3Z_j \end{aligned}$$

Contraints

1) equality constraints:

$$X_{1a}+X_{1b}+X_{1c}+X_{1d}+X_{1e}+X_{1f}+X_{1g}+X_{1h}+X_{1i}+X_{1j}=30$$
$$X_{2a}+X_{2b}+X_{2c}+X_{2d}+X_{2e}+X_{2f}+X_{2g}+X_{2h}+X_{2i}+X_{2j}=40$$
$$Y_a+Y_b+Y_c+Y_d+Y_e+Y_f+Y_g+Y_h+Y_i+Y_j=50$$
$$Z_a+Z_b+Z_c+Z_d+Z_e+Z_f+Z_g+Z_h+Z_i+Z_j=60$$

2) inequality constraints:

$$X_{1a}+X_{2a}+Y_a+Z_a\le 30$$
$$X_{1b}+X_{2b}+Y_b+Z_b\le 30$$
$$X_{1c}+X_{2c}+Y_c+Z_c\le 20$$
$$X_{1d}+X_{2d}+Y_d+Z_d\le 20$$
$$X_{1e}+X_{2e}+Y_e+Z_e\le 10$$
$$X_{1f}+X_{2f}+Y_f+Z_f\le 20$$
$$X_{1g}+X_{2g}+Y_g+Z_g\le 20$$
$$X_{1h}+X_{2h}+Y_h+Z_h\le 10$$
$$X_{1i}+X_{2i}+Y_i+Z_i\le 30$$
$$X_{1j}+X_{2j}+Y_j+Z_j\le 10$$

Solved by Lindo:

$$P_{\max}=2540\text{x}10^3$$

```
max -6 X1A+3 X1B+17 X1C+10 X1D+63 X1E+34 X1F+15 X1G+22 X1H-2 X1I+15 X1J
:    -11 X2A-7 X2B-16 X2C+9 X2D+49 X2E+16 X2F+4 X2G+10 X2H-8 X2I+8 X2J
:    -7 YA+3 YB+16 YC+13 YD+60 YE+25 YF+12 YG+19 YH+4 YI+13 YJ
:    -ZA+13 ZC+3 ZD+48 ZE+15 ZF+7 ZG+17 ZH+9 ZI+3 ZJ
:SUBJECT TO
:     2) X1A+X1B+X1C+X1D+X1E+X1F+X1G+X1H+X1I+X1J=30
:     3) X2A+X2B+X2C+X2D+X2E+X2F+X2G+X2H+X2I+X2J=40
:     4) YA+YB+YC+YD+YE+YF+YG+YH+YI+YJ=50
:     5) ZA+ZB+ZC+ZD+ZE+ZF+ZG+ZH+ZI+ZJ=60
:     6) X1A+X2A+YA+ZA<=30
:     7) X1B+X2B+YB+ZB<=30
:     8) X1C+X2C+YC+ZC<=20
:     9) X1D+X2D+YD+ZD<=20
:    10) X1E+X2E+YE+ZE<=10
:    11) X1F+X2F+YF+ZF<=20
:    12) X1G+X2G+YG+ZG<=20
:    13) X1H+X2H+YH+ZH<=10
:    14) X1I+X2I+YI+ZI<=30
:    15) X1J+X2J+YJ+ZJ<=10
:END

:BAT
:


LP OPTIMUM FOUND AT STEP      23

       OBJECTIVE FUNCTION VALUE  ( Mbpd )

       1)     2540.000000

 VARIABLE         VALUE           REDUCED COST
      X1A           .000000          11.000000
      X1B           .000000           3.000000
      X1C           .000000           2.000000
      X1D           .000000          10.000000
      X1E           .000000            .000000
      X1F         20.000000            .000000
      X1G         10.000000            .000000
      X1H           .000000           1.000000
      X1I           .000000          17.000000
      X1J           .000000           4.000000
      X2A           .000000           5.000000
      X2B           .000000           2.000000
      X2C           .000000          24.000000
      X2D         20.000000            .000000
      X2E           .000000           3.000000
      X2F           .000000           7.000000
      X2G         10.000000            .000000
--MORE--

      X2H           .000000           2.000000
      X2I           .000000          12.000000
      X2J         10.000000            .000000
```

```
YA              .000000           9.000000
YB            20.000000            .000000
YC            20.000000            .000000
YD              .000000           4.000000
YE            10.000000            .000000
YF              .000000           6.000000
YG              .000000            .000000
YH              .000000           1.000000
YI              .000000           8.000000
YJ              .000000           3.000000
ZA            10.000000            .000000
ZC              .000000            .000000
ZD              .000000          11.000000
ZE              .000000           9.000000
ZF              .000000          13.000000
ZG              .000000           2.000000
ZH            10.000000            .000000
ZI            30.000000            .000000
ZJ              .000000          10.000000
ZB            10.000000            .000000




--MORE--

    ROW   SLACK OR SURPLUS     DUAL PRICES
     2)          .000000          5.000000
     3)          .000000         -6.000000
     4)          .000000          2.000000
     5)          .000000         -1.000000
     6)        20.000000           .000000
     7)          .000000          1.000000
     8)          .000000         14.000000
     9)          .000000         15.000000
    10)          .000000         58.000000
    11)          .000000         29.000000
    12)          .000000         10.000000
    13)          .000000         18.000000
    14)          .000000         10.000000
    15)          .000000         14.000000

NO. ITERATIONS=       23

DO RANGE(SENSITIVITY) ANALYSIS?
?
```

Problem 7.25

Solution (via Berkely LP code on the web):

$f = 19{,}000$ $\quad x_1 = 200\text{hr} \quad x_2 = 300\text{hr} \quad N = 2$

$x_3 = x_4 = x_5 = 0$

Problem 7.26

Solution:

$$x_1 = 0$$
$$x_3 = 0$$
$$x_2 = 1$$

$$f = 8$$

Problem 7.27

Solution:

$$x = [0\ 0\ 7\ 00]^{\mathrm{T}}$$

$$f = 7$$

Problem 7.28

(a) Problem formulation:

Minimize

$$\sum C_{i\,j} + \sum_i C_i I_i$$

Subject to:

for each j, $\quad \sum_i S_{i\,j} \geq R_j$

for each i, $\quad \sum_j S_{i\,j} \leq Q_i$

and $\sum I_i \leq 1 \quad I_1, I_2 .... I_i \text{integer}$.

(b) Numerical solution:

Plant A	Plant B
1	0

Fixed Charge A	Fixed Charge B
700	0

A to C	A to D	B to C	B to D	Production A	Production B
200	250	0	0	450	0

Cost A to C	Cost A to D	Cost B to C	Cost B to D	C	D
200	750	0	0	200	250

Total cost
1650

Build only plant A.

Problem 7.29

The solution is:

VARIABLES

	X111	X112	X113	X121	X122	X123	X131	X132	X133	X211	X212	X213	X221	X222	X223	X231	X232	X233	I12	I13	I22	I23	I32	I33		
Upper Bound	0.5	1.5		0.5	1.5		0.5	1.5		0.5	1.5		0.5	1.5		0.5	1.5		1	1	1	1	1	1		
Lower Bound																			0	0	0	0	0	0		
Objective	80	60	40	80	60	40	80	60	40	80	60	40	80	60	40	80	60	40								
DEM.M1	1	1	1							1	1	1													$\geq$	2.0
DEM.M2				1	1	1							1	1	1										$\geq$	5.0
DEM.M3							1	1	1							1	1	1							$\geq$	4.0
CAP.R1	1	1	1	1	1	1	1	1	1																$\leq$	5.0
CAP.R2										1	1	1	1	1	1	1	1	1							$\leq$	7.5
M1MAXP1	1									1									-.5						$\geq$	0
M1MINP2		-1									-1								1.5						$\geq$	0
M1MAXP2		1									1									-1.5					$\geq$	0
M1MAXP3			-1									-1								0					$\geq$	0
M2MAXP1				1									1								-.5				$\geq$	0
M2MINP2					-1									-1							1.5				$\geq$	0
M2MAXP2					1									1								-1.5			$\geq$	0
M2MAXP3						-1									-1							3.0			$\geq$	0
M3MAXP1							1									1							-.5		$\geq$	0
M3MINP2								-1									-1						1.5		$\geq$	0
M3MAXP2								1									1							-1.5	$\geq$	0
M3MAXP3									-1									-1						2.0	$\geq$	0

CHAPTER 8

Problem 8.1

Starting from the non-feasible point (10, 10), the numerical solution is (0, 0). By substitution of $x_1 = -x_2^{\,4}$, the objective function becomes

$$\tilde{f} = x_2^{\,4}$$

$\tilde{f}\,' = 4x_2^{\,3} = 0$ yields $x_2 = 0$ so that $x_1 = 0$

Problem 8.2

Starting from the non-feasible point (2, 2), the numerical solution is (1, 0). By substitution of $x_1 = 1 - 10^{-5} x_2^{\,2}$, the objective function becomes

$$\tilde{f} = -\left[1 - 10^{-5} x_2^{\,2}\right]^2$$

$\tilde{f}\,' = -2\left[1 - 10^{-5} x_2^{\,2}\right](-10^{-5})(2x_2) = 0$ yields $x_2 = 0$ or $1 - 10^{-5} x_2 = 0$ so that an alternate solution is $x_2 = 10^5$.

If $x_2 = 0, x_1 = 1$. If $x_2 = 10^5, x_1 = 1 - 10^5$.
Check $\tilde{f}\,''$. If $x_2 = 0$, $\tilde{f} = 4\text{x}10^5$ (positive definite, a minimum).
If $x_2 = 10^5$, $\tilde{f} \cong -6\text{x}10^5$ (negative definite, a maximum).

Problem 8.3

Add to the LHS of the equation a variable that is always positive such as

$$x = |x_4|$$
$$x = x_4^{\,2}$$
$$x = e^{x_4}$$

Problem 8.4

The Lagrange function is

$$L(\boldsymbol{x}, \omega) = x_1^{\,2} + x_2^{\,2} + \omega(2x_1 + x_2 - 2)$$

The necessary conditions are:

$$\left.\begin{aligned}\frac{\partial L}{\partial x_1} &= 2x_1 + 2\omega = 0 \\ \frac{\partial L}{\partial x_2} &= 2x_2 + \omega = 0\end{aligned}\right\} \begin{aligned}&\text{eliminate } \omega \\ &2x_1 - 4x_2 = 0\end{aligned} \qquad \text{(a)}$$

$$\frac{\partial L}{\partial \omega} = 2x_1 + x_2 - 2 = 0 \qquad \text{(b)}$$

Solve (a) and (b) to get $x_1 = 0.8$ and $x_2 = 0.4$. Then $\omega = -2x_2 = -0.8$ and $f(\boldsymbol{x}) = 0.80$.

Check to make sure the above solution is a minimum.
$\nabla_x^2 L$ must be pos. def.

$\nabla_x^2 L = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$ which is pos def.

Problem 8.5

$$f(\boldsymbol{x}) = (x_1^{\ 2} + x_2^{\ 2})^{1/2}$$
$$h(\boldsymbol{x}) = 5x_1^{\ 2} + 6x_1x_2 + 5x_2^{\ 2} - 8 = 0$$

$$L = (x_1^{\ 2} + x_2^{\ 2})^{1/2} + \omega(5x_1^{\ 2} + 6x_1x_2 + 5x_2^{\ 2} - 8)$$
$$\partial L/\partial x_1 = \frac{1}{2}(x_1^{\ 2} + x_2^{\ 2})^{-1/2}(2x_1) + 10\omega x_1 + 6\omega x_2 = 0 \qquad \text{(a)}$$
$$\partial L/\partial x_2 = \frac{1}{2}(x_1^{\ 2} + x_2^{\ 2})^{-1/2}(2x_2) + 6\omega x_1 + 10\omega x_2 = 0 \qquad \text{(b)}$$
$$\partial L/\partial \omega = 5x_1^{\ 2} + 6x_1x_2 + 5x_2^{\ 2} - 8 = 0 \qquad \text{(c)}$$

Divide (a) by x_1 and (b) by x_2, and equate the resulting equations.
From (a) and (b):

$$10\omega x_1x_2 + 6\omega x_2^{\ 2} = 10\omega x_1x_2 + 6\omega x_1^{\ 2}$$
$$x_1 = \pm x_2 \qquad \text{(d)}$$

From (c) and (d):

$$5x_1^{\ 2} + 6x_1^{\ 2} + 5x_1^{\ 2} - 8 = 0 \qquad x_1 = x_2 = \pm\sqrt[1]{2}$$

or $\quad 5x_1^{\,2}-6x_1^{\,2}+5x_1^{\,2}-8=0 \qquad x_1=x_2=\pm\sqrt{2}$

The points $\left(\frac{1}{\sqrt{2}},\ \frac{1}{\sqrt{2}}\right)$ and $\left(-\frac{1}{\sqrt{2}},\ -\frac{1}{\sqrt{2}}\right)$ are closest to the origin (distance =1) and the points $(\sqrt{2},\ -\sqrt{2})$ and $(-\sqrt{2}\ \ \sqrt{2})$are the farthest (distance = 2).

Problem 8.6

$$L(x_1,x_2,\omega)=x_1^{\,2}+x_2^{\,2}+\omega\left[(x_1-1)^3-x_2^{\,2}\right]$$

$$\partial L/\partial x_1 = 2x_1+3\omega(x_1-1)^2=0 \qquad \text{(a)}$$
$$\partial L/\partial x_2 = 2x_2-2\omega x_2 = 2x_2(1-\omega)=0 \qquad \text{(b)}$$
$$\partial L/\partial \omega = (x_1-1)^3-x_2^{\,2}=0 \qquad \text{(c)}$$

If $\boldsymbol{x}^{\mathrm{T}}=\left[1\ 0\ \right]$ satisfies eq. (c) but not eq. (a), $\omega=1$ satisfies eq. (b), but eq. (a) gives $2x_1+3(x_1-1)^2=0,$ x_1 is imaginary and eq. (c) will not be satisfied. $x_2=0$ satisfies eq. (b), but eq. (c) is not satisfied except for $x_1=1$. Hence no ω exists.

Problem 8.7

$$f(C,T)=(C-C_r)^2+T^2 \qquad C_0 \text{ is a constant.}$$
$$h(C,T)=C_0+e^{\mathrm{T}}-C=0$$
$$g(C,T)=K-C_0\geq 0$$

Eliminating C using he equality constraint, we may write the Lagrangian as

$$L(C_0,T,\omega,\sigma)=(C_0+e^{\mathrm{T}}-C_r)^2+T^2+u(\sigma^2+C_0-K)$$
$$\partial L/\partial C_0 = 2(C_0+e^{\mathrm{T}}-C_r)+u=0$$
$$\partial L/\partial T = 2(C_0+e^{\mathrm{T}}-C_r)e^{\mathrm{T}}+2T=0$$
$$\partial L/\partial u = \sigma^2+C_0-K=0$$
$$\partial L/\partial \sigma = 2\sigma u=0$$

If u = 0, we have a saddle point; we are not interested in this case. Thus $\sigma=0$.

$$K = C_0 = C_r - 2$$
$$e^{T}(e^{T} - 2) + T = 0$$
$$T = 0.524$$
$$C = C_0 + e^{T} = C_r - 2 + e^{T}$$
$$C - C_r = e^{T} - 2 = -0.311$$
$$f = (-0.311)^2 + (0.524)^2 = 0.371$$

Alternate solution: Use 2 Lagrange multipliers, one for *h* and one for *g*, and the original function for *f*.

Problem 8.8

a.

1. The objective function and constraints are twice differentiable at $\boldsymbol{x}^*$

2. The gradients of the constraints are linearly independent, so that the Lagrange multipliers exist.

3. The constraints are satisfied (the second constraint is $3.98 \neq 4.1$ but close enough).

4. The Lagrange multipliers for any inequality constraints are not involved in the problem. They exist for the equality constraints.

5. To show that x^* is at a stationary point where $\nabla_{\boldsymbol{x}} L = \mathbf{0}$, a set of 4 nonlinear equations obtained by setting the partial derivatives of $L = 0$ must be solved for $\boldsymbol{x}^*$ and $\boldsymbol{\omega}^*$. This problem is as difficult to solve as the original NLP problem, and require the use of a nonlinear equation solver.

6. Additionally, you have to show that the Hessian matrix L is negative semi-definite at $\boldsymbol{x}^*$, i.e., that the eigenvalues of the $\boldsymbol{H}$ of L are negative or zero.

b. The steps for part b are the same as Part a, except that the Hessian matrix of L must be positive semi-definite. You can substitute for V into the objective function, and get P in terms of x_i. Then the necessary conditions for an unconstrained function can be tested. A set of nonlinear equations obtained as in Step 5 of Part a still has to be solved for $\boldsymbol{x}^*$.

Problem 8.9

(a) The Lagrangian is

$$L(x_1, x_2, \omega) = x_1^{\,2} + x_2^{\,2} + 4x_1x_2 + \omega(x_1 + x_2 - 8)$$

$$\partial L / \partial x_1 = 2x_1 + 4x_2 + \omega = 0 \qquad \text{(a)}$$

$$\partial L / \partial x_2 = 2x_2 + 4x_1 + \omega = 0 \qquad \text{(b)}$$

$$\partial L / \partial \omega = x_1 + x_2 - 8 = 0 \qquad \text{(c)}$$

The solution to this set of equations is

$$x_1^{\,*} = 4, \quad x_2^{\,*} = 4, \quad \omega^* = -24.$$

$$f^* = 96$$

(b) $$\frac{\Delta L}{\Delta e} = \frac{\Delta f}{\Delta e} = -\omega$$

$$\Delta L = \Delta f = -(-24)(0.01) = 0.24$$

$$L = f = 96.24$$

Problem 8.10

(a) $$L(x_1, x_2, \omega) = x_1^{\,2} + x_2^{\,2} + 10x_1 + 20x_2 + 25 + \omega(x_1 + x_2)$$

$$\partial L / \partial x_1 = 2x_1 + 10 + \omega = 0 \qquad \text{(a)}$$

$$\partial L / \partial x_2 = 2x_2 + 20 + \omega = 0 \qquad \text{(b)}$$

$$\partial L / \partial \omega = x_1 + x_2 = 0 \qquad \text{(c)}$$

The solution to this set of equations is

$$x_1^{\,*} = +2.5, \quad x_2^{\,*} = -2.5, \quad \omega^* = -15.$$

$$f^* = 12.5$$

(b) $$\Delta f^* = -\omega^* \Delta e = -(15)(0.01) = 0.15$$

f^* increases by 0.15

(c) $$P(x_1, x_2) = x_1^{\,2} + x_2^{\,2} + 10x_1 + 20x_2 + 25 + r(x_1 + x_2)^2$$

$$\partial P / \partial x_1 = 2x_1 + 10 + 2r(x_1 + x_2) = 0$$

$$\partial P / \partial x_2 = 2x_2 + 20 + 2r(x_1 + x_2) = 0$$

Simultaneous solution of these two equations gives

$$x_1 = \frac{5r-5}{2r+1} \quad \text{and} \quad x_2 = \frac{5r-10}{2r+1}$$

As $r \to \infty$, we have $x_1^* = 2.5$ and $x_2^* = -2.5$

(d) From parts (a) and (c), we have

$$\omega = 2r(x_1 - x_2)$$

$$\omega^* = \lim_{r \to \infty} \left[2r \ (x_1 + x_2) \right]$$

(e) $$\nabla^2 P = \begin{bmatrix} 2r+2 & 2r \\ 2r & 2r+2 \end{bmatrix}$$

Now, $r > 0$ always and $2r + 2 > 0$. Also,
det $(\nabla^2 P) = 4(2r+1) > 0$. P is convex, because $\nabla^2 P$ is positive definite

---

Problem 8.11

The Hessian of $f(\boldsymbol{x})$ is $\begin{bmatrix} 6x_1 & 0 \\ 0 & 8 \end{bmatrix}$

This is positive definite or indefinite depending upon the value of x_1. Thus, this problem is not a convex programming problem which requires that $f(\boldsymbol{x})$ be convex and the equality constraint be concave. For convexity, you need the further specification that $x_i \geq 0$.

Problem 8.12

(a) $f(\boldsymbol{x})$, $h(\boldsymbol{x})$, and $g(\boldsymbol{x})$ are twice differentiable

(b) Are the gradients of the binding constraints independent?

$$\nabla h(\boldsymbol{x}) = \begin{bmatrix} 2x_1 + 1 \\ 2x_2 + 1 \end{bmatrix}$$

$$\nabla g(\boldsymbol{x}) = \begin{bmatrix} -1 \\ 2x_2 \end{bmatrix}$$

Is the only solution at $x^{\mathrm{T}} = \begin{bmatrix} 0 & 0 \end{bmatrix}$ of

$$c_1 \begin{bmatrix} 2x_1 + 1 \\ 2x_2 + 1 \end{bmatrix} + C_2 \begin{bmatrix} -1 \\ 2x_2 \end{bmatrix} = 0$$

$C_1 = 0$ and $C_2 = 0$?

$$C_1 \begin{bmatrix} 1 \\ 1 \end{bmatrix} + C_2 \begin{bmatrix} -1 \\ 0 \end{bmatrix} = 0$$

$C_1 + (-1)C_2 = 0$ so $C_1 = C_2$
$C_1 + 0(C_2) = 0$ hence $C_1 = 0$
so $C_2 = 0$

Answer is yes.

(c) The Lagrange multipliers exist because (b) is satisfied.

(d) The constraints are satisfied

(e) The Lagrange multipliers of the inequality constraint is non negative

(f) $u^* g\ (0, 0) = 0$ ok

(g) Is $\nabla Lx(0, 0, w^*, u^*) = 0$?

$$L = (x_1 - 1)^2 + x_2{}^2 + \omega(x_1{}^2 + x_2{}^2 + x_1 + x_2) - u(-x_1 + x_2{}^2)$$

$$\frac{\partial L}{\partial x_1} = 2(x_1 - 1) + \omega(2x_1 + 1) + u = 0$$

$$\frac{\partial L}{\partial x_2} = 2x_2 + \omega(2x_2 + 1) - u(2x_2) = 0$$

at (0, 0)

$$\left.\begin{array}{r} -2 + \omega + u = 0 \\ \omega - u(0) = 0 \end{array}\right\} \omega = 0 \text{ and } u = 2$$

so both (e) and (g) are satisfied

(h) Is the Hessian of L positive definite?

$$\nabla_x^2 L = \begin{bmatrix} (-2+2\omega) & 0 \\ 0 & -2u \end{bmatrix} \qquad \text{for } \omega = 0 \text{ and } u = 2$$

$$\nabla_x^2 L = \begin{bmatrix} -2 & 0 \\ 0 & -4 \end{bmatrix} \qquad \text{not pos def.} \qquad \text{(nor neg. def.)}$$

$$\text{Is } v^T \begin{bmatrix} -2 & 0 \\ 0 & -4 \end{bmatrix} v \geq 0 \qquad \text{No, because}$$

$$v^T \begin{bmatrix} -1 \\ 0 \end{bmatrix} = 0 \quad \text{so } v_1(-1) + v_2(0) = 0 \quad \text{so } v_1 = 0$$

$$v^T \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 0 \quad \text{so } v_1 + v_2 = 0 \quad \text{hence } v_2 = 0$$

The answer to the problem is: No.

Problem 8.13

(h) f is not twice differentiable at x^*. Also g_1, g_2 and g_3 are twice differentiable at x^*.

(ii) All the four constraints are active

$$\nabla h = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad \nabla g_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad \nabla g_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad \nabla g_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \text{ at } \boldsymbol{x}^*$$

but they are not linearly independent.

Thus, the point $\begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T$ does not satisfy the necessary conditions for a minimum. However, this is a problem with three variables and four active constraints. Hence, their intersection, if unique, is the only feasible point, and it is the minimum.

Problem 8.14

(i) The functions are twice differentiable at $\boldsymbol{x}^*$

(ii) The constraints are satisfied at $\boldsymbol{x}^*$

(iii) h_1 is the only active constraint, and

$$\nabla h_1(x^*) = \begin{bmatrix} 4 \\ 2 \end{bmatrix} \text{ is linearly independent}$$

(iv) $$L = -x_1^2 x_2 + \omega(x_1 x_2 + \frac{x_1^2}{2} - 6) - u(x_1 + x_2)$$

$$\partial L / \partial x_1 = -2x_1 x_2 + \omega x_2 + \omega x_1 - u = 0 \quad \Rightarrow 4\omega - u = 8$$

$$\partial L / \partial x_2 = -x_1^2 + \omega x_1 - u = 0 \quad \Rightarrow 2\omega - u = 4$$

$$\omega = 2, \quad u = 0.$$

$$\nabla_{\boldsymbol{x}}^2 L = \begin{bmatrix} -2x_2 + \omega & -2x_1 + \omega \\ -2x_1 + \omega & 0 \end{bmatrix} = \begin{bmatrix} -2 & -2 \\ -2 & 0 \end{bmatrix}$$

$\nabla_{\boldsymbol{x}}^2 L$ is neither positive definite nor negative definite.

For the active constraint,

$$v^{\mathrm{T}} \nabla h(\boldsymbol{x}^*) = 4v_1 + 2v_2 = 0 \qquad \Rightarrow v_2 = -2v_1$$

For the inactive constraint

$$v^{\mathrm{T}} \nabla g(x^*) = v_1 + v_2 \geq 0 \qquad \Rightarrow v_1 \geq 0 \qquad \Rightarrow v_1 \leq 0$$

$$v^{\mathrm{T}} \nabla^2 L v = \begin{bmatrix} v_1 & v_2 \end{bmatrix} \begin{bmatrix} -2 & -2 \\ -2 & 0 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} > 0? \qquad \text{No.}$$

We have not been able to show that $v^{\mathrm{T}} \nabla^2 L v > 0$. Thus, $\boldsymbol{x}^*$ does not meet the sufficient conditions for a minimum.

Problem 8.15

(i) f, g and h are all twice differentiable at $\boldsymbol{x}^*$.

(ii) h is the only binding constraint, and
$\nabla h = \begin{bmatrix} 1 & -2 \end{bmatrix}^{\mathrm{T}}$ is linearly independent

(iii) The constraints are satisfied at $\boldsymbol{x}^*$.

(iv) $L=(x_1-2)^2+(x_2-1)^2+w(x_1-2x_2+1)-u(-\frac{x_1^{\;2}}{4}-x_2^{\;2}+1)$

$\partial L/\partial x_1 = 2(x_1-2)+w+ux_1/2=0$

$\partial L/\partial x_2 = 2(x_2-1)-2w+2ux_2=0$

u = 0 because g is inactive. There is no w which satisfies the above two equations at $\boldsymbol{x}^*$. Thus L is not at a stationary point.

(v) For the active constraint

$$\boldsymbol{v}^{\mathrm{T}}\begin{bmatrix}1\\-2\end{bmatrix}=0 \quad \Rightarrow \boldsymbol{v}_1=2\boldsymbol{v}_2$$

$$\boldsymbol{v}^{\mathrm{T}}\nabla^2 L\boldsymbol{v}=\begin{bmatrix}\boldsymbol{v}_1 & \boldsymbol{v}_2\end{bmatrix}\begin{bmatrix}2 & 0\\0 & 2\end{bmatrix}\begin{bmatrix}\boldsymbol{v}_1\\\boldsymbol{v}_2\end{bmatrix}=2\boldsymbol{v}_1^{\;2}+2\boldsymbol{v}_2^{\;2}\geq 0$$

(vi) For the inactive constraint

$$\boldsymbol{v}'^{\mathrm{T}}\begin{bmatrix}-0.41\\-1.82\end{bmatrix}=-\left(0.41\boldsymbol{v}'_1+1.82\boldsymbol{v}'_2\right)\geq 0,\ \text{ and } \boldsymbol{v}'_1=2\boldsymbol{v}'_2$$

$$\boldsymbol{v}'_2\leq 0;\ \ \boldsymbol{v}'_1\leq 0$$

$$\boldsymbol{v}'^{\mathrm{T}}\,\nabla^2 L\boldsymbol{v}'=2\boldsymbol{v}'^{\,2}_1+2\boldsymbol{v}'^{\,2}_2\geq 0$$

Because of (iv) the necessary conditions are not met. Because of (iv) and (vi), the sufficient conditions are not met.

Problem 8.16

(i) The functions are all twice differentiable at $\boldsymbol{x}^*$.

(ii) g_1 is the only active constraint. Its gradient $\nabla g_1=\begin{bmatrix}1 & 1\end{bmatrix}^{\mathrm{T}}$ is linearly independent.

(iii) All the constraints are satisfied, g_1 is the only active constraint, so

$u_1^{\;*}\geq 0,\ u_2^{\;*}=0,\ u_3^{\;*}=0$

(iv) $L=-ln(1+x_1)-ln(1+x_2)^2-u_1(-x_1-x_2+2)-u_2x_1-u_3x_2$

$$\nabla L = \begin{bmatrix} -1/(1+x_1)+u_1-u_2 \\ -2/(1+x_2)+u_1-u_3 \end{bmatrix} = 0$$

$$u_1 = 3/4 > 0$$

(v) Is $v^{\mathrm{T}}\nabla^2 L v \geq 0$? >0?

For the active constraints

$$v^{\mathrm{T}}\begin{bmatrix} -1 \\ -1 \end{bmatrix} = 0 \quad \Rightarrow v_1 + v_2 = 0$$

For the inactive constraints

$$v^{\mathrm{T}}\begin{bmatrix} 1 \\ 0 \end{bmatrix} \geq 0 \quad \Rightarrow v_1 \geq 0$$

$$v^{\mathrm{T}}\begin{bmatrix} 0 \\ 1 \end{bmatrix} \geq 0 \quad \Rightarrow v_2 \geq 0$$

Thus, $v_1 = v_2 = 0$

$$\nabla^2 L = \begin{bmatrix} 1/(1+x_1)^2 & 0 \\ 0 & 2/(1+x_2)^2 \end{bmatrix}$$

Thus, $\nabla^2 L$ is positive definite, but $v^{\mathrm{T}}\nabla^2 L v = 0$ as no non-zero v exists. Thus, the sufficient conditions are not met.

Problem 8.17

Solutions:

p8.4 $\quad \boldsymbol{x}^{\mathrm{T}} = \begin{bmatrix} 0.8 & 0.4 \end{bmatrix} \quad f = 0.80$

p8.8 See problem 8.8 statement for the solutions.

p8.13 $\quad \boldsymbol{x}^{\mathrm{T}} = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T \quad f = 0$

p8.24 $x_{11}^* = 120$

$x_{12}^* = x_{13}^* = x_{23}^* = x_{31}^* = x_{32}^* = 0$

$x_{21}^* = 20$

$x_{22}^* = 100$

$x_{33}^* = 170$

$f = \$2.063\text{x}10^7 \text{ / year}$

Problem 8.18

Direct substitution

From $h = x_1 + x_2 - 8 = 0$ we have $x_1 = 8 - x_2$. Substituting into *f*,

$f = 64 + 16x_2 - 2x_2^{\ 2}$

$df / dx_2 = 16 - 4x_2 = 0$ and $\Rightarrow x_2 = 4$ so that $x_1 = 4$

$d^2 f / dx_2^{\ 2} = -4 \quad \Rightarrow \begin{bmatrix} 4 & 4 \end{bmatrix}^T$ is a maximum. $f^* = 96$

Penalty function method:

(a) $P = x_1^{\ 2} + x_2^{\ 2} + 4x_1x_2 + r(x_1 + x_2 - 8)^2$

$\partial P / \partial x_1 = 2x_1 + 4x_2 + 2r(x_1 + x_2 - 8) = 0$

$\partial P / \partial x_2 = 2x_2 + 4x_1 + 2r(x_1 + x_2 - 8) = 0$

Simultaneous solution gives

$$x_1^{opt} = x_2^{opt} = \frac{16r}{6+4r}$$

(b) $$\lim_{r \to \infty} \left(\frac{16r}{6+4r} \right) = 4$$

$x_1^{opt} = x_2^{opt} = 4$

(c) $$\lim_{r \to \infty} P^{opt} = \lim_{r \to \infty} 6\left(\frac{16r}{6+4r} \right)^2 + r\left(\frac{32r}{6+4r} - 8 \right)^2 = 96 \quad = \quad f^{opt}$$

Problem 8.19

Lagrange multipliers:

$$L(x_1, x_2, w) = x_2{}^2 - x_1{}^2 + w(x_1{}^2 + x_2{}^2 - 4)$$
$$\partial L / \partial x_1 = -2x_1 + 2wx_1 = 0$$
$$\partial L / \partial x_2 = 2x_2 + 2wx_2 = 0$$
$$\partial L / \partial w = x_1{}^2 + x_2{}^2 - 4 = 0$$

Solution of these three equations gives four stationary points;

$$\begin{array}{llllll} x_1 = \ \ 2, & x_2 = \ \ 0, & w = \ \ 1, & L = f = -4 & \text{minimum} \\ x_1 = -2, & x_2 = \ \ 0, & w = \ \ 1, & L = f = -4 & \text{minimum} \\ x_1 = \ \ 0, & x_2 = \ \ 2, & w = -1, & L = f = \ \ 4 & \text{minimum} \\ x_1 = \ \ 0, & x_2 = -2, & w = -1, & L = f = \ \ 4 & \text{minimum} \end{array}$$

Penalty function method:

$$P = x_2{}^2 - x_1{}^2 + r(x_1{}^2 + x_2{}^2 - 4)^2$$
$$\partial P / \partial x_1 = -2x_1 + 4rx_1(x_1{}^2 + x_2{}^2 - 4) = 0 \qquad \text{(a)}$$
$$\partial P / \partial x_2 = 2x_2 + 4rx_2(x_1{}^2 + x_2{}^2 - 4) = 0 \qquad \text{(b)}$$

Multiply (a) by x_2 and (b) by x_1, and subtract one from the other to get

$4x_1x_2 = 0$

For $x_1 = 0$, eqn (b) gives $x_2 = \pm\sqrt{4 - (1/2r)}$

as $r \to \infty, x_2 \to \pm 2$

For $x_2 = 0$, eqn (a) gives $x_1 = \pm\sqrt{4 - (1/2r)}$

as $r \to \infty, x_1 \to \pm 2$

The minimum is $f = P = -4$ at $x_1 = \pm 2, x_2 = 0$. There is one more case: $x_1 = 0$ and $x_2 = 0$, but this is not a feasible point.

Problem 8.20

(a) $P(x, r) = x_1{}^2 + 6x_1 + x_2{}^2 + 9 + r\left(\dfrac{1}{x_1} + \dfrac{1}{x_2}\right)$

(b) Hessian matrix of P is

$$\nabla^2 P = \begin{bmatrix} 2 + \dfrac{2r}{x_1^3} & 0 \\ 0 & 2 + \dfrac{2r}{x_2^3} \end{bmatrix}$$

In general $\nabla^2 P$ is not positive definite, so P is not convex. In the region $x_1 > 0, x_2 > 0$ it always is. However, at the minimum of the original problem $\begin{bmatrix} 0 & 0 \end{bmatrix}^T, \nabla^2 P$ is not defined.

Problem 8.21

Ans: Yes

Problem 8.22

(a) Penalty function problems:

(1) min $P(\boldsymbol{x}) = 2x_1^2 - 2x_1x_2 + 2x_2^2 - 6x_1 + 6 + r(x_1 + x_2 - 2)^2$

(2) min $P(\boldsymbol{x}) = x_1^3 - 3x_1x_2 + 4 + r_1(-2x_1 + x_2^2 - 5)^2$
$+ r_2\left[\min\{0, \ (5x_1 + 2x_2 - 18\}\right]^2$

Other penalty functions are possible – see text.

(b) Augmented Lagrange problems:

(1) min $P(\boldsymbol{x}, r, w) = 2x_1^2 - 2x_1x_2 + 2x_2^2 - 6x_1 + 6$
$+ w(x_1 + x_2 - 2) + r(x_1 + x_2 - 2)^2$

(2) min $P(\boldsymbol{x}, r, w, \sigma) = x_1^3 - 3x_1x_2 + 4 + w_1(-2x_1 + x_2^2 - 5) + r_1(-2x_1 + x_2^2 - 5)^2$
$+ w_2(5x_1 + 2x_2 - 18 \ \ - \sigma^2) + r_2(5x_1 + 2x_2 + 18 - \sigma^2)^2$

Problem 8.23

(a) This formulation is called the method of moving truncations.
Advantages: (i) It will remain within the feasible region. (ii) parameter ("non parameter") adjustment is automatic.
Disadvantages: (i) An initial feasible point must be located. (ii) There is a possibility of overshooting the minimum – e.g. negating the pseudo constraint, (iii) An increased level of nonlinearity is introduced.

(b) and (c) These formulations differ only in the penalty term. We can examine the difference in terms of the value of *r* needed.

$$-r\nabla \ln g = -\frac{r}{g}\nabla g = \lambda_1 \nabla g$$
$$\nabla(r/g) = (-r/g^2)\nabla g = \lambda_2 \nabla g$$

Assume that g is a tight constraint. Because of complementary slackness, as λ_1 and λ_2 approach the optimal solution, a much smaller value of *r* is required for the ln *g* term to satisfy *g* to within a given termination criterion. For example, assume $\lambda^* = -1$, and that *g* is to be satisfied to within 10^{-6}.

$$-\lambda_1 = r/g = 1 \quad \Rightarrow r = 10^6$$
$$-\lambda_2 = r/g^2 = 1 \quad \Rightarrow r = 10^2$$

Problem 8.24

Let X_{ij} = million lb/year of DAB made by producer *i* and shipped to customer *j*: *i,j* = 1, 2, 3.

Production cost = $P_1(X_{11} + X_{12} + X_{13}) + P_2(X_{21} + X_{22} + X_{23}) + P_3(X_{31} + X_{32} + X_{33})$

where

$$P_1 = \begin{cases} 45000 - 50(\sum X_{ij} - 100 & 100 \le \sum X_{ij} \le 120 \\ 44000 + 200(\sum X_{ij} - 120) & 120 \le \sum X_{ij} \le 170 \end{cases} \qquad (\$/10^6 \text{lb})$$

$$P_2 = 50000 \qquad (\$/10^6 \text{ lb})$$

$$P_3 = \begin{cases} 39000 - 50(\sum X_{3j} - 120 & 120 \le \sum X_{3j} \le 140 \\ 46000 + 100(\sum X_{3j} - 140) & 140 \le \sum X_{3j} \le 200 \end{cases}$$

$$\text{Transportation cost} = 2000X_{11} + 7000X_{12} + 6000X_{13} + 7000X_{21} + 3000X_{22}$$
$$+8000X_{23} + 6000X_{31} + 8000X_{32} + 2000X_{33}$$

Constraints:
Capacity $100 \le X_{11} + X_{12} + X_{13} \le 170$

$$80 \le X_{21} + X_{22} + X_{23} \le 120$$
$$120 \le X_{31} + X_{32} + X_{33} \le 200$$

Demand $X_{11} + X_{21} + X_{31} = 140$

$$X_{12} + X_{22} + X_{32} = 100$$
$$X_{13} + X_{23} + X_{33} = 170$$

Non-negativity all $x_{ij} \ge 0$

Since the production cost is quadratic in the X_{ij}, we shall linearize it about some nominal set of $X^0{}_{ij}$. This gives

Production cost = $Q_1 + Q_2 + Q_3$

$$Q_1 = \begin{cases} 50000 \sum x^0{}_{ij} - 50 \sum x^0{}_{ij}{}^2 + (50000 - 100 \sum x^0{}_{ij})(\sum \Delta x_{ij}) \\ \qquad \text{for } 100 \le \sum x^0{}_{ij} \le 120 \\ 20000 \sum x^0{}_{ij} + 200 \sum x^0{}_{ij}{}^2 + (20000 - 400 \sum x^0{}_{ij})(\sum \Delta x_{ij}) \\ \qquad \text{for } 120 \le \sum x^0{}_{ij} \le 170 \end{cases}$$

$$Q_2 = 50000\left(\sum x2^0{}_j\right) + 50000\left(\sum \Delta x_{2j}\right)$$

$$Q3 = \begin{cases} 33000 \sum x^0{}_{3j} + 50 \sum x^0{}_{3j}{}^2 + (33000 + 100 \sum x^0{}_{3j})(\sum \Delta x_{3j}) \\ \qquad \text{for } 120 \le \sum x^0{}_{3j} \le 140 \\ 32000 \sum x^0{}_{3j} + 100 \sum x^0{}_{3j}{}^2 + (32000 + 200 \sum x^0{}_{3j})(\sum \Delta x_{3j}) \\ \qquad \text{for } 140 < \sum x^0{}_{3j} \le 200 \end{cases}$$

The linearized transportation cost is

$$\begin{aligned} &2000x_{11}{}^0 + 7000x_{12}{}^0 + 6000x_{13}{}^0 + 7000x_{21}{}^0 + 3000x_{22}{}^0 \\ &+8000x_{23}{}^0 + 6000x_{31}{}^0 + 8000x_{32}{}^0 + 2000x_{33}{}^0 + 2000x_{11} \\ &+7000\Delta x_{12} + 6000\Delta x_{13} + 7000x_{21} + 3000x_{22} \\ &+8000\Delta x_{23} + 6000\Delta x_{31} + 8000\Delta x_{32} + 2000x_{33} \end{aligned}$$

The linearized constraints are

$$100 - \sum x^0{}_{1j} \le \sum \Delta x_{1j} \le 170 - \sum x^0{}_{1j}$$
$$80 - \sum x^0{}_{2j} \le \sum \Delta x_{2j} \le 120 - \sum x^0{}_{2j}$$
$$120 - \sum x^0{}_{3j} \le \sum \Delta x_{3j} \le 200 - \sum x^0{}_{3j}$$

$$\sum \Delta x_{j1} = 140 - \sum x^0{}_{i1}$$
$$\sum \Delta x_{j2} = 100 - \sum x^0{}_{2j}$$
$$\sum \Delta x_{j3} = 170 - \sum x^0{}_{3j}$$

all $x^0{}_{ij} + \Delta x_{ij} \geq 0$

In addition, to maintain feasibility, we require

all $\left|\Delta x_{ij}\right| \leq h$ (some preset quantity).

We now consider the LP:

Minimize: (linearized production cost + linearized transportation cost)

Subject to: all linearized constraints are satisfied.

The solution strategy is as follows:

(1) Assume a feasible $x^0{}_{ij}$ set.

(2) Calculate numerical values for all the terms in the objective function and constraint equations which involve the $x^0{}_{ij}$'s.

(3) Solve the LP

(4) If all the Δx_{ij} are very small (with respect to some preset tolerance), then the current set $x^0{}_{ij}$ is the optimal solution. If not, go to step 5.

(5) Calculate the nominal $x^0{}_{ij}$'s for the next iteration using $(x^0{}_{ij})_{\text{new}} = (x^0{}_{ij})_{\text{old}} + (\Delta x_{ij})_{\text{opt}}$.

(6) Go back to step 2.

For example, assume

$$x^0{}_{11} = 140,\ x^0{}_{22} = 100,\ x^0{}_{33} = 170$$
$$x^0{}_{12},\ x^0{}_{13},\ x^0{}_{21},\ x^0{}_{23},\ x^0{}_{31},\ x^0{}_{32} = 0$$

The LP is then:

Minimize: $2.097\text{x}10^7 + 78000\Delta x_{11} + 83000\Delta x_{12} + 8200\Delta x_{13} + 57000\Delta x_{21} + 53000\Delta x_{22}$
$+ 58000\Delta x_{23} + 72000\Delta x_{31} + 74000\Delta x_{32} + 68000\Delta x_{33}$

Subject to: $-40 \le \sum \Delta x_{1j} \le 30$

$$-20 \le \sum \Delta x_{2j} \le 20$$
$$-50 \le \sum \Delta x_{3j} \le 30$$
$$\sum \Delta x_{j1} = 0$$
$$\sum \Delta x_{j2} = 0$$
$$\sum \Delta x_{j3} = 0$$
$$\Delta x_{11} \ge -140$$
$$x_{22} \ge -100$$
$$\Delta x_{33} \ge -170$$
$$x_{12},\ \Delta x_{13},\ \Delta x_{21},\ \Delta x_{23},\ \Delta x_{31},\ \Delta x_{32},\ \ge 0$$

all $|\Delta x_{ij}| \le 20$ (say)

The optimal solution is

$$\Delta x_{11} = -20,\ \Delta x_{21} = 20$$
$$\Delta x_{12},\ \Delta x_{13},\ \Delta x_{22},\ \Delta x_{23},\ \Delta x_{31},\ \Delta x_{32},\ \Delta x_{33} = 0$$

The new $x^0{}_{ij}$ set is

$x^0{}_{11} = 120$	$x^0{}_{12} = 0$	$x^0{}_{13} = 0$
$x^0{}_{21} = 20$	$x^0{}_{22} = 100$	$x^0{}_{23} = 0$
$x^0{}_{31} = 0$	$x^0{}_{32} = 0$	$x^0{}_{33} = 170$

This set is used to recalculate the various coefficients in the LP. Repeated application of steps 2 through 6 gives the final solution as

$x_{11}^{\text{opt}} = 120$

$x_{12}^{\text{opt}} = 0$

$x_{13}^{\text{opt}} = 0$

$x_{21}^{\text{opt}} = 20$

$x_{22}^{\text{opt}} = 100$

$x_{23}^{\text{opt}} = 0$

$x_{31}^{\text{opt}} = 0$

$x_{32}^{\text{opt}} = 0$

$x_{33}^{\text{opt}} = 170$

Cost = $\$2.063\text{x}10^7$/year.

Problem 8.25

Solution:

$$x^* = \left[0.91878, 0.39476, 0.11752, 0.99307, 0.91878, 0.39476, 0.11752, 0.99307, -0.60445\text{x}10^{-14}\right]^{\text{T}}$$

$$f^* = 0.86602$$

Problem 8.26

The known solution is at $\boldsymbol{x}^* = \begin{bmatrix} 1 & 2 & 0 \end{bmatrix}^{\text{T}}$ where $f^* = 5$.

Problem 8.27

(a) Two local minima were obtained:

(1) $\boldsymbol{x}^* = \begin{bmatrix} -0.18 & -2.43 & -2.01 \end{bmatrix}^{\text{T}}, \; f^* = -9.995$

(2) $\boldsymbol{x}^* = \begin{bmatrix} 0.16 & 2.62 & -1.47 \end{bmatrix}^{\text{T}}, \; f^* = -9.051$

n	2	4	6	8	10	-2	-4	-6	-8	-10
soln. #	2	2	1	1	1	1	2	2	2	2
f evals.	642	581	458	419	376	425	465	470	585	477
∇f evals.	514	559	501	512	440	551	452	463	187	439
h evals.	169	175	141	97	93	106	110	133	187	131
∇h evals.	64	64	51	42	34	40	42	50	68	48

(b) Six local minima were found:

(1) $f^* = 0.07877 \quad \boldsymbol{x}^* = [1.91 \;\; 1.362 \;\; 1.472 \;\; 1.635 \;\; 1.679]^{\mathrm{T}}$

(2) $f^* = 13.96 \quad \boldsymbol{x}^* = [2.717 \;\; 2.033 \;\; -0.8479 \;\; -0.4859 \;\; 0.7359]^{\mathrm{T}}$

(3) $f^* = 27.45 \quad \boldsymbol{x}^* = [-0.7661 \;\; 2.666 \;\; -0.4681 \;\; -1.619 \;\; -2.610]^{\mathrm{T}}$

(4) $f^* = 21.52 \quad \boldsymbol{x}^* = [-1.247 \;\; 2.422 \;\; 1.174 \;\; -0.2132 \;\; -1.604]^{\mathrm{T}}$

(5) $f^* = 86.52 \quad \boldsymbol{x}^* = [0.9496 \;\; -2.666 \;\; 0.5377 \;\; 3.384 \;\; 2.106]^{\mathrm{T}}$

(6) $f^* = 649.5 \quad \boldsymbol{x}^* = [-2.701 \;\; -2.989 \;\; 0.1719 \;\; 3.847 \;\; -0.7401]^{\mathrm{T}}$

n	2	4	6	8	10	-2	-4	-6	-8	-10
soln. #	1	1	1	2	1	6		4	3	4
f evals.	164	180	254	520	235	855		804	421	869
∇f evals.	106	165	427	1939	255	632		574	389	647
h evals.	67	75	101	211	82	216		267	89	253
∇h evals.	30	33	43	85	39	80		160	42	161

Problem 8.28

You must start at a feasible point. The point $\begin{bmatrix} 0 \ 1 \ 1 \end{bmatrix}^T$ satisfies h_1 and h_2 as well as $x_1, x_2, x_3 \geq 0$. Thus, it is a feasible point. Let x_3 be the independent variable, and x_1 and x_2 be the dependent variables (the choice is arbitary); $\boldsymbol{x}_D = \begin{bmatrix} x_1 \ x_2 \end{bmatrix}^T$.

Phase 1:

$$\frac{df}{dx_3} = \frac{\partial f}{\partial x_3} - \left[\frac{\partial f}{\partial \mathbf{x}_D}\right]^T \left[\frac{\partial \mathrm{h}}{\partial \mathbf{x}_D}\right]^{-1} \left(\frac{\partial h}{\partial x_3}\right)$$

$$= 2x_3 - \left[(4x_1 - 2x_2 - 4) \quad (4x_2 - 2x_1 - 6)\right] \begin{bmatrix} 1 & 1 \\ 2x_1 & 5 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$= 2 - \begin{bmatrix} -6 & -2 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 5 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 8$$

For the variable x_3, the decent direction is -8.

Phase 2:

Find the minimum of the reduced objective function by an analytical approach to get λ:

Set $\left.\frac{df}{d\lambda}\right|_{(x+\lambda\Delta)} = 0$

$$\frac{d}{d\lambda}\left\{2(0+8\lambda)^2 + 2(1+0\lambda)^2 + (1-8\lambda)^2 - 2(0+8\lambda)(1+0\lambda) - 4(0+8\lambda) - 6(1-0\lambda)\right\} = 0$$

$$384\lambda - 64 = 0$$
$$\lambda = 1/6$$
$$x_3 = 1 + \tfrac{1}{6}(-8) = -1/3$$

Since x_3 has crossed its lower bound, set $x_3 = 0$. Now h_1 and h_2 are not satisfied. So, with $x_3 = 0$, solve h_1 and h_2 for x_1 and x_2. i.e.

$$x_1 + x_2 - 2 = 0$$
$$x_1^2 + 5x_2 - 5 = 0$$

using Newton's method. The initial guess is $x_1 = 4/3$ and $x_2 = 1$. The solution is a feasible point, and is used to start the next iteration. If Newton's method does not converge to a solution, replace x_3 as the independent variable by either x_1 or x_2 and repeat.

Problem 8.29

Both are true.

Problem 8.30

(a) The solution is: $f^* = 17286.1$

$x_1^* = 3.5121$ $x_6^* = 0.6432$

$x_2^* = 4.0877$ $x_7^* = -3.4375$

$x_3^* = 2.4523$ $x_8^* = -0.1518$

$x_4^* = 4.8558$ $x_9^* = -3.9191$

$x_5^* = 1.3922$ $x_{10}^* = -3.0243$

(b) The solution is: $f^* = 12.8$

$x_1^* = 0$ $x_6^* = 0$

$x_2^* = 0$ $x_7^* = 0$

$x_3^* = 0$ $x_8^* = 0$

$x_4^* = 0$ $x_9^* = 0$

$x_5^* = 0$ $x_{10}^* = 0$

$x_{11}^* = 0$

(c) A reported solution is $f^* = 14672.826$

$x_1^* = 9.52267$ $x_4^* = -20$

$x_2^* = -6.588$ $x_5^* = 13.58267$

$x_3^* = -20$ $x_6^* = -6.51733$

(d) The solution is $f^* = 17.80$

$x_1^* = 0.4812$ $x_4^* = -0.6023$

$x_2^* = 2.4962$ $\qquad$ $x_5^* = 0.7514$

$x_3^* = 0.5263$

(e) The solution is $\quad f^* = 0 \quad x^* = \begin{bmatrix} 1\,1\,1\,1\,1 \end{bmatrix}^T$

(f) The solution is $\quad f^* = 0.2415$

$x_1^* = 1.166$ $\qquad$ $x_4^* = 1.506$

$x_2^* = 1.182$ $\qquad$ $x_5^* = 0.6109$

$x_3^* = 1.380$

(g) There are six reported solutions:

f^*	x_1^*	x_2^*	x_3^*	x_4^*	x_5^*
0.07877	1.191	1.362	1.472	1.635	1.679
13.96	2.717	2.033	-0.8479	-0.4859	0.7359
27.45	-0.7661	2.666	-0.4681	-1.619	-2.610
27.52	-1.2467	2.422	1.173	-0.2132	-1.604
86.52	0.9496	-2.266	0.5377	3.384	2.106
649.5	-2.7012	-2.989	0.1719	3.847	-0.7401

Problem 8.31

Possible ways are

(1) Minimize $\left(\sum g_i + \sum h_i^2\right)$ where g_i are the violated constraints only.

Change g_i to equality constraints

$$g_1 \to 4 - x_1^2 - x_2^2 + x_3^2 = 0$$
$$g_2 \to x_1^2 + x_2^2 - 16 + x_4^2 = 0$$

and minimize $\sum(h_i^2 + g_i^2)$

from some reasonable starting point.

Problem 8.32

Solution given in the problem.

Problem 8.33

Solution given in the problem.

Problem 8.34

The problem is

Minimize: $C = C_p AN + C_s HAN + C_f + C_d + C_b + C_L + C_x$

Subject to:

$$\frac{L}{D} = \left[\frac{1}{1 - N_{\min}/N}\right]\left(\frac{L}{D}\right)_{\min}$$

$A = K\,(\mathrm{L} + D)$

$N \geq N_{\min}$

With numerical values, this becomes ($N_{min} = 5$)

Minimize: $C = 50AN + 0.7L + 22{,}000$ (a)

Subject to:

$$L = \frac{1000\ N}{N - 5} \quad \text{(b)}$$

$$A = \frac{L + 1000}{100} \quad \text{(c)}$$

$\mathrm{N} \geq 5$ (d)

a. The variables are A, L, and N. Although N is an integer we will assume it to be a continuous variable. A and L may be eliminated using equations (b) and (c) to get a cost function in terms of N only (the independent variable):

$$C = 50N\left(\frac{10N}{N-5}+10\right)+0.7\left(\frac{1,000N}{N-5}\right)+22,000$$

$$=\frac{1,000N^2+20,200N-110,000}{N-5}$$

Thus, *N* is the independent variable, and *A* and *L* are dependent variables. To obtain the minimum,

$$\frac{dC}{dN}=\frac{1,000N^2-10,000N+9,000}{(N-5)^2}=0$$

$N = 1$ or $N = 9$

Because of constraint (d), select N = 9

$$\left.\frac{d^2C}{dN^2}\right|_{N=9}=500>0.$$ This is a minimum

b. $C^* = \$38200$
$N^* = 9$ plates
$L^* = 2250$ lb/hr
$A^* = 32.5$ ft^2

Problem 8.35

The solution is
$f* = 267.5$
$x^* = 2$
$y^* = 7.5$
$z^* = 0$

Problem 8.36

The solution is $f^* = -43.4945$

$x_1^* = 6.99958\,E-3$ $x_6^* = 4.68197\,E-4$
$x_2^* = 6.80709\,E-2$ $x_7^* = 1.75768\,E-2$
$x_3^* = 9.07223\,E-1$ $x_8^* = 2.90223\,E-3$
$x_4^* = 3.56254\,E-4$ $x_9^* = 1.51766\,E-2$

$x_5^* = 4.90799\ E-1$ $\qquad\qquad$ $x_{10}^* = 4.19451\ E-2$

Problem 8.37

The problem is

Minimize: $\quad f(\boldsymbol{a}) = \sum_{i=1}^{10}\left[P(\boldsymbol{a}, x_i) - x_i^{1/3}\right]^2$

Subject to: $\quad \begin{bmatrix}0\\0\\0\\0\end{bmatrix} \le \boldsymbol{W}_1\boldsymbol{a} \le \begin{bmatrix}5\\5\\5\\5\end{bmatrix}$

$\boldsymbol{W}_2^{\mathrm{T}}\boldsymbol{a} = 5$

where

$$\boldsymbol{W}_1 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 8 & 64 & 512 & 4096 & 32768 \\ 27 & 729 & 19683 & 531441 & 14348907 \\ 64 & 4096 & 262144 & 16777216 & 1073742824 \end{bmatrix}$$

$$\boldsymbol{W}_2^T = \begin{bmatrix} 125 & 15625 & 1953125 & 244140625 & 30517578135 \end{bmatrix}$$

The solution is $\quad f(\boldsymbol{a}) = 1.110366$

$a_1 = 0.36359\ E0$
$a_2 = -0.16220\ E-1$
$a_3 = 0.32901\ E-3$
$a_4 = -0.29062\ E-5$
$a_5 = 0.91722\ E-8$

Problem 8.38

The solution with unscaled constraints from starting points 1 and 3 is

$$f(\boldsymbol{x}^*) = 6.8408\text{x}10^{-3}$$

$x_1^* = 0.2436\text{x}10^4$ $\quad$ $x_6^* = 0.5131\text{x}10^4$

$x_2^* = 0.1788\text{x}10^4$ $\quad$ $x_7^* = 0$ lower bound

$x_3^* = 0.5795\text{x}10^2$ $\quad$ $x_8^* = 0.6019\text{x}10^4$

$x_4^* = 0.3686\text{x}10^4$ $\quad$ $x_9^* = 0.7214\text{x}10^4$

$x_5^* = 0.1328\text{x}10^3$ $\quad$ $x_{10}^* = 0.1000\text{x}10^4$ upper bound

Different codes gave slightly different results.

Problem 8.39

Case studies were used because local extrema were found. The best and second best solutions were:

Best solution:

$S_1^* = 7$	$P_{132}^* = 3$
$S_2^* = 3$	$P_{113}^* = 5$
$S_3^* = 0$	$P_{133}^* = 2$
$S_4^* = 0$	$P_{221}^* = 2$
$P_{111}^* = 1$	$P_{222}^* = 3$
$P_{121}^* = 4$	$P_{223}^* = 2$
$P_{112}^* = 4$	obj. func. = -\$11.105 MM

The second best solution is:

$S_1^* = 10$	$P_{132}^* = 3$
$S_2^* = 0$	$P_{113}^* = 5$
$S_3^* = 0$	$P_{123}^* = 2$
$S_4^* = 0$	$P_{133}^* = 2$
$P_{111}^* = 1$	$P_{122}^* = 3$
$P_{121}^* = 2$	$P_{131}^* = 4$
$P_{112}^* = 4$	obj. func. = -\$11.1031 MM

Problem 8.40

Let f_1 = tons of fuel oil to generator 1

f_2 = tons of BFG to generator 1

g_1 = tons of fuel oil to generator 2
g_2 = tons of BGF to generator 2
x_{11} = MW from generator 1 obtained using fuel oil
x_{12} = MW from generator 1 obtained using BFG
x_{21} = MW from generator 2 obtained using fuel oil
x_{22} = MW from generator 2 obtained using BFG

The NLP is

Minimize: $f_1 + g_1$

Subject to:
$$f_1 = 1.4609 + 0.15186x_{11} + 0.00145x_{11}^{\ 2}$$
$$f_2 = 1.5742 + 0.1631x_{12} + 0.001358x_{12}^{\ 2}$$
$$g_1 = 0.8008 + 0.2013x_{21} + 0.000916x_{21}^{\ 2}$$
$$g_2 = 0.7266 + 0.2556x_{22} + 0.000778x_{22}^{\ 2}$$
$$18 \le x_{11} + x_{12} \le 30$$
$$14 \le x_{21} + x_{22} \le 25$$
$$f_2 + g_2 \le 10$$
$$x_{11} + x_{12} + x_{21} + x_{22} = 50$$

Eliminate f_1, f_2, g_1 and g_2 using equality constraints. Linearizing the objective function and the constraints about some set $x_{ij}(i, j = 1, 2),$ the NLP is converted to an LP:

Minimize: $A\Delta x_{11} + B\Delta x_{21} + F$

Subject to:
$$\Delta x_{11} \quad + \Delta x_{12} \le 30 - x_{11}^{\ 0} - x_{12}^{\ 0}$$
$$\Delta x_{21} \ + \Delta x_{22} \le 25 - x_{21}^{\ 0} - x_{22}^{\ 0}$$
$$-\Delta x_{11} - \Delta x_{12} \le -18 + x_{11}^{\ 0} + x_{12}^{\ 0}$$
$$-\Delta x_{21} - \Delta x_{22} \le -14 + x_{21}^{\ 0} + x_{22}^{\ 0}$$
$$C\Delta x_{12} + D\Delta x_{22} \le E$$
$$\Delta x_{11} - \Delta x_{12} + \Delta x_{21} + \Delta x_{22} = 50 - x_{11}^{\ 0} + x_{12}^{\ 0} - x_{21}^{\ 0} - x_{22}^{\ 0}$$

where
$$A = 0.15186 + 0.0029x_{11}^{\ 0}$$
$$B = 0.2013 + 0.001832x_{21}^{\ 0}$$
$$C = 0.1631 + 0.002716x_{12}^{\ 0}$$
$$D = 0.2556 + 0.001556x_{22}^{\ 0}$$
$$E = 7.6992 - 0.1631x_{12}^{\ 0} - 0.001358x_{12}^{\ 2} - 0.2556x_{22}^{\ 0} \ -0.000778x^{0}{}_{22}{}^{2}$$
$$F = 2.2617 + 0.15186x_{11}^{\ 0} + 0.00145(x_{11}^{0})^2 + 0.2013x_{21}^{\ 0} \ +0.00916(x_{21}^{0})^2$$

Since the $\Delta x's$ are unrestricted in sign, we introduce the new variables

$$\Delta x_{11} = y_1 - y_2$$
$$\Delta x_{12} = y_3 - y_4$$
$$\Delta x_{21} = y_5 - y_6$$
$$\Delta x_{22} = y_7 - y_8$$

If we restrict the absolute values of the $\Delta x's$ to be less than, say, *h*, the LP is now

Minimize: $Ay_1 - Ay_2 + By_5 - By_6 + F$

Subject to:

$$y_1 - y_2 + y_3 - y_4 \le 30 - x_{11}{}^0 - x_{12}{}^0$$
$$y_5 - y_6 + y_7 - y_8 \le 25 - x_{21}{}^0 - x_{22}{}^0$$
$$-y_1 + y_2 - y_3 + y_4 \le -18 - x_{11}{}^0 + x_{12}{}^0$$
$$-y_5 + y_6 - y_7 + y_8 \le -14 - x_{21}{}^0 + x_{22}{}^0$$
$$Cy_3 - Cy_4 + Dy_7 - Dy_8 \le E$$
$$y_1 - y_2 + y_3 - y_4 + y_5 - y_6 + y_7 - y_8 = 50 - x_{11}{}^0 - x_{12}{}^0 - x_{21}{}^0 - x_{22}{}^0$$
$$y_1 - y_2 \le h$$
$$y_2 - y_1 \le h$$
$$y_3 - y_4 \le h$$
$$y_4 - y_3 \le h$$
$$y_5 - y_6 \le h$$
$$y_6 - y_5 \le h$$
$$y_7 - y_8 \le h$$
$$y_8 - y_7 \le h$$

and all $y_i \ge 0$

The strategy is to assume values for $x_{11}{}^0, x_{12}{}^0, x_{21}{}^0$ and $x_{22}{}^0$, and solve the LP. From the optimal solution, calculate the $\Delta x's$ and thus the new $x^0{}_{ij}'s$. Now solve the LP again using these $x^0{}_{ij}'s$. This process is repeated until the $\Delta x's$ are less than some specified tolerance. The solution is

$$x_{11}{}^* = 7.7084$$
$$x_{12}{}^* = 22.292$$
$$x_{21}{}^* = 7.2382$$
$$x_{22}{}^* = 12.762$$
$$f^* = 5.0235$$

$$f_1 = 2.718$$

$$f_2 = 5.885$$
$$g_1 = 2.306$$
$$g_2 = 4.115$$

Problem 8.41

You can use ΔT rather than log mean ΔT to simplify the problem. The equations for the heat transfer in the heat exchangers are those found in unit operations books:

$$Q = UA\Delta T_{\text{ln}} \cong UA\Delta T$$
$$Q = wC_p\Delta t$$

The solution is:

$$T_1^* = 180^0 F \qquad T_2^* = 295^0 F$$
$$A_1 + A_2 + A_3 = 7050 \text{ft}^2 \text{ (minimum total area)}$$
$$A_1 = 556 \text{ ft}^2 \quad A_2 = 1369 \text{ ft}^2 \quad A_3 = 5125 \text{ ft}^2$$

CHAPTER 9

Problem 9.1

Define the variables as y_j, $j = 1, 2, ..., 6,$ where $y_j = 1$ means the *j*th project is selected, and $y_j = 0$ means the *j*th project is omitted. The objective function to be maximized is

$$f = 100,000y_1 + 150,000y_2 + 35,000y_3 + 75,000y_4 + 125,000y_5 + 60,000y_6 \quad \text{(a)}$$

subject to the following constraints:

First year expenditure:

$$g_1 = 300,000y_1 + 100,000y_2 + 0y_3 + 50,000y_4 + 50,000y_5 + 100,000y_6 \le 450,000 \quad \text{(b)}$$

Second year expenditure:

$$g_2 = 0y_1 + 300,000y_2 + 200,000y_3 + 100,000y_4 + 300,000y_5 + 200,000y_6 \le 400,000 \quad \text{(c)}$$

Engineering hours:

$$g_3 = 4000y_1 + 7000y_2 + 2000y_3 + 6000y_4 + 3000y_5 + 600y_6 \le 10,000 \quad \text{(d)}$$

Production line is required:

$$g_4 = y_1 + y_2 \le 1 \quad \text{(e)}$$

Automation is available only with new line:

$$g_5 = y_2 - y_3 \ge 0 \quad \text{(f)}$$

Waste recovery option:

$$g_6 = y_5 + y_6 \le 1 \quad \text{(g)}$$

The branch and bound analysis begins by solving the LP problem with no integer restrictions on the variables with the following result:

$$y_1 = 0.88$$
$$y_2 = 0.12$$
$$y_3 = 0.12$$
$$y_4 = 0.40$$
$$y_5 = 1.00$$
$$y_6 = 0.00$$
$$f = \$265,200$$

Note that several variables (y_1, y_2, y_3, y_4) in this solution are not integers. The branch and bound analysis can be carried out with Excel. The final (optimal) integer solution is:

$$y_1 = 1$$
$$y_2 = 0$$
$$y_3 = 0$$
$$y_4 = 0$$
$$y_5 = 1$$
$$y_6 = 0$$
$$f = \$225,000$$

This indicates that the project 2 with the highest net present value is *not* selected because of the constraints in the problem. Note that the first noninteger solution achieves a larger value of f than the integer solution, as is expected.

Problem 9.2

An algebraic formulation follows, using GAMS-like notation:

Indices: i = generator index (i=1,2,3), t = time period index (t = 1,2)

Data: cap(i) = capacity of generator i (MW), cp(i) = operating cost of generator i ($/MW)
Cs(i) = startup cost of generator i ($), d(t) = demand for power in period t (MW)

Decision variables: x(i,t) = power generated by generator i in period t (MW)
y(i,t) = 1 if x(i,t) > 0, zero otherwise.

Constraints:

Demand must be satisfied in each period:
Sum(i,x(i,t)) >= d(t), all t

y variables turn x variables on and off:

x(i,1) <= cap(i)*y(i,1)
x(i,2) <= cap(i)*(y(i,1) + y(i,2))

The last constraint above insures that, if a generator is turned on in period 1, it stays on in period 2.

Turn each generator on at most one time per day:
Sum(t, y(i,t)) <= 1, all i

A spreadsheet model containing the optimal solution appears below. The optimal solution turns generators 1 and 2 on in period 1, and does not use generator 3. This is because generators 1 and 2 have the lowest operating costs, while 3 is much higher. Further, generator 1 is used to capacity, because it has by far the lowest operating cost, and 2 is used to satisfy the remaining demand. Even though generator 3 has the lowest startup cost, its higher operating cost excludes it.

Data

Generator	**Fixed start-up cost ($)**	**Cost per MW**	**Generator capacity in each period (MW)**	**Demand Period 1**	**Demand Period 2**
1	2800	5	1900	2500	3500
2	2000	3	1700		
3	1900	8	2900		

Model

	on-off per 1	**MW per 1**		**on-off*cap per 1**	**on-off per 2**	**MW per 2**		**sum*cap per 2**
Gen 1	1	800	<=	1900	0	1800	<=	1900
Gen 2	1	1700	<=	1700	0	1700	<=	1700
Gen 3	0	0	<=	0	0	0	<=	0
Total MW		**2500**	**>=**	**2500**		3500	>=	3500

	MW cost	**startup cost**		**sum of binarys**		
Gen 1	13000	2800		1	<=	1
Gen 2	10200	2000		1	<=	1
Gen 3	0	0	objective	0	<=	1
Total	23200	4800	28000			

Problem 9.3

DATA

Year	Minimum capacity	Cost 10 MW	Cost 50 MW	Cost 100 MW	Cost of new Generators
1	780	280	650	700	1400
2	860	230	538	771	0
3	950	188	445	640	640
4	1060	153	367	530	530
5	1180	135	300	430	430
				Total	3000
current capacity		700			

Decision on Variables and Constraints

Year	# of 10 MW	# of 50 MW	# of 100 MW	new capacity	total capacity
1	0	0	2	200	900
2	0	0	0	0	900
3	0	0	1	100	1000
4	0	0	1	100	1100
5	0	0	1	100	1200
size	10	50	100		

Comments on Solution

No 10 or 50 MW generators are installed, because their cost per MW is much higher than the 100MW. The first year two 100 MW generators are bought, because first year cost is smaller than second year. The second year nothing is bought. In years 3 to 5 only one 100 MW generator is installed. Purchases in years 3 to 5 are deferred as long as possible because costs are declining.

Problem 9.4.

A GAMS model for this problem and its solution follows.

```
 Production and Inventory Planning with Setup Costs and Times
set definitions

      Set p    products              / p1, p2 /
          t     time periods         / wk1, wk2, wk3, wk4 /   ;

model parameters
```

```
Table  pdata(*,p)  product data
                     p1        p2
setup-time           6         11
setup-cost           250       400
production-time      0.5       0.75
production-cost      9         14
holding-cost         3         3
penalty-cost         15        20
selling-price        25        35
final-inventory      0         0              ;

Table  demand(t,p)

                   p1       p2
wk1                75       20
wk2                95       30
wk3                60       45
wk4                90       30                  ;

Scalars     tavail   weekly time available(hrs) /  90 /   ;
Parameter         maxunits(p)   ;
               maxunits(p) = tavail/pdata("production-time",p);
```

Model Definition

```
Variables   prd(p,t)       units of product p produced in week t
            inv(p,t)       units of inventory of product p at end of week t
            pinv (p,t)     positive part of inventory
            ninv(p,t)      negative part of inventory
            y(p,t)         1 if product p produced in wk t else zero
            profit         objective variable ;
Positive Variables prd,pinv,ninv   ;
Binary variables   y   ;

Equations
           invbal(p,t)     inventory balance
           finalinv(p)        final inventory equal zero
           invsplit(p,t)   defines positive and negative inventory
           maxtime(t)      limit on production time
           onoff(p,t)      turn prd on or off with binary variables
           oneprod(t)      at most one product produced in any week
           objective          revenue minus all costs

  invbal(p,t)..  inv(p,t)  =e= inv(p,t-1)+prd(p,t)-demand(t,p);

  finalinv(p)..  inv(p,"wk4") =e= 0;
  invsplit(p,t)..  inv(p,t) =e= pinv(p,t)-ninv(p,t);

  maxtime(t).. sum(p, pdata("production-time",p)*prd(p,t)+
               pdata("setup-time",p)*y(p,t))=l= tavail ;
```

```
onoff(p,t).. prd(p,t) =l= maxunits(p)*y(p,t);

oneprod(t).. sum(p, y(p,t)) =l= 1;

objective..  profit =e= sum((p,t), (pdata("selling-price",p)
             -pdata("production-cost",p))*prd(p,t)
             -pdata("setup-cost",p)*y(p,t)
             -pdata("holding-cost",p)*pinv(p,t)
             -pdata("penalty-cost",p)*ninv(p,t));

Model prodplan  / all / ;
Solve prodplan using mip maximizing profit ;

MODEL STATISTICS

BLOCKS OF EQUATIONS        7     SINGLE EQUATIONS       35
BLOCKS OF VARIABLES        6     SINGLE VARIABLES       41
NON ZERO ELEMENTS        121     DISCRETE VARIABLES      8


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

     MODEL   PRODPLAN              OBJECTIVE  PROFIT
     TYPE    MIP                   DIRECTION  MAXIMIZE
     SOLVER  XPRESS                FROM LINE  83

**** SOLVER STATUS     1 NORMAL COMPLETION
**** MODEL STATUS      8 INTEGER SOLUTION
**** OBJECTIVE VALUE             5331.0000
```

This model breaks inventory into positive and negative parts as defined by the variables pinv and ninv, and the equations invsplit, because the costs for positive and negative inventory are different. The binary variables y turn the production variables prd on and off through the constraints “onoff”. They are also used to incorporate setup times into the maxtime constraints, and to include setup costs into the objective. The “oneprod” constraints insure that at most one product is produced in any week.

The optimal solution produces product 1 in weeks 1 and 3, and product 2 in weeks 2 and 4. There is unsatisfied demand for product 1 in week 2 and product 2 in week 1, because only one product can be produced in any week. This causes the penalty cost to be incurred, but the backlogged demand is satisfied in the next week (The constraint that inventory is zero at the end of week 4 insures that there is no backlogged demand after the fourth week). All of the 90 available hours are used in week one, but fewer are needed in subsequent weeks. If there are only 80 hours available per week, the problem has no feasible solution. This model can be used to determine approximately how many hours per week are needed to permit a feasible solution by solving it for different values of the parameter “tavail”.

Problem 9.5

Max sum(I,(1+r(I))*x(I))

Subject to:

Sum(I,x(I)) <= 100

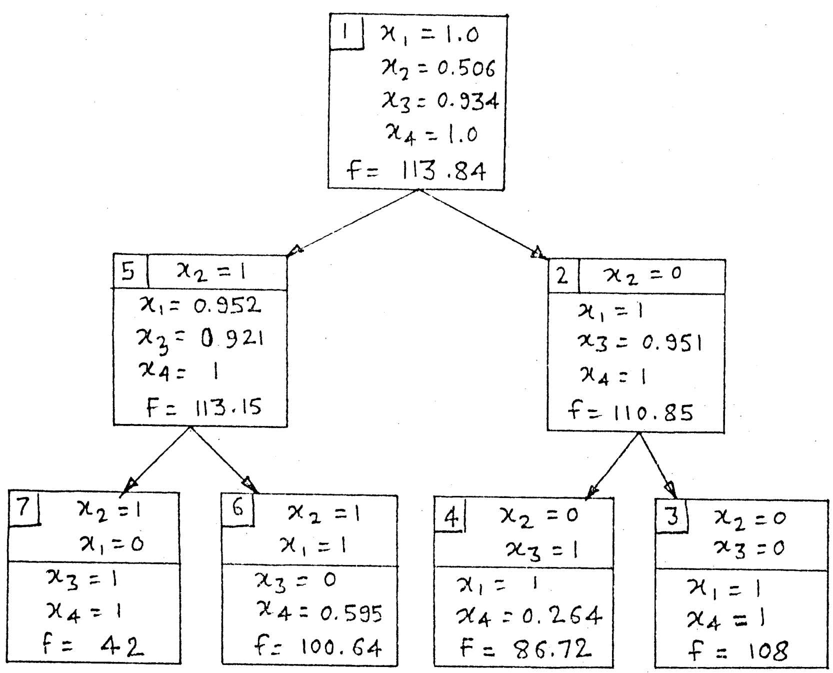
x(I) <= 20y(I) ,   all I   (1)

x(I) >= 5y(I)   all I   (2)

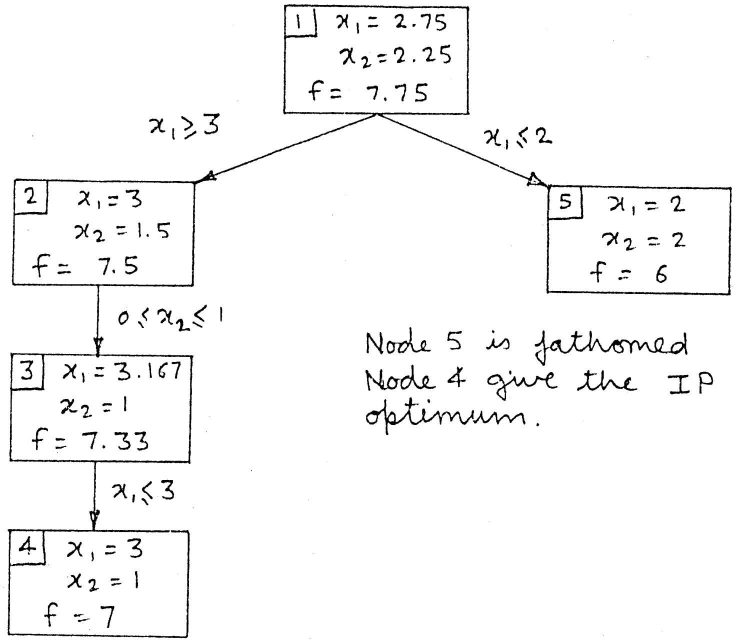
x(I) >= 0   all I

Where y(I) is a binary variable which is 1 if x(I) is positive and zero otherwise. Constraints 1 and 2 insure that y(I) = 0 if and only if x(I) = 0, and y(I) = 1 if and only if x(I) is between 5 and 20.

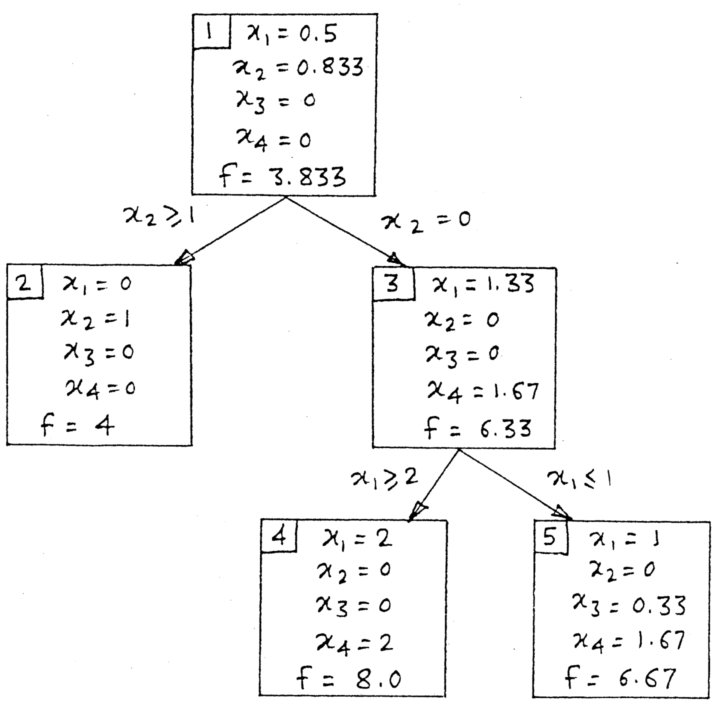
Problem 9.6



Problem 9.7



Problem 9.8



Nodes 4 and 5 are fathomed. Node 2 gives the MIP optimum.

Problem 9.9

By inspection, one can see that plant 1 has to be in operation, because plant 2 cannot satisfy the demand by itself. Thus, there are only two possibilities: $y_1 = 1,\ y_2 = 1$ and $y_1 = 1,\ y_2 = 0$. Explicit enumeration is easy in this situation.

Case I: $y_1 = 1,\ y_2 = 1$. The LP to be solved is

Minimize: $f = (3x_{11} + x_{12} + x_{22} + 2)\text{x}10^4$

Subject to:
$$x_{11} + x_{21} = 1$$
$$x_{12} + x_{22} = 1$$
$$x_{11} + x_{12} \le 2$$
$$x_{21} + x_{22} \le 1$$

The solution is $x_{11}^* = x_{22}^* = 0,\ x_{12}^* = x_{21}^* = 1,$

$f^* = 3\text{x}10^4$

Case II: $y_1 = 1,\ y_2 = 0$. The LP to be solved in this case is:

Minimize: $f = (3x_{11} + x_{12} + 1)\text{x}10^4$

Subject to:
$$x_{11} = 1$$
$$x_{12} = 1$$
$$x_{11} + x_{12} \le 2$$

The solution is $x_{11}^* = x_{12}^* = 1,\ \ x_{21}^* = x_{22}^* = 0$

$f^* = 5\text{x}10^4$

Case I gives the optimal solution to the problem.

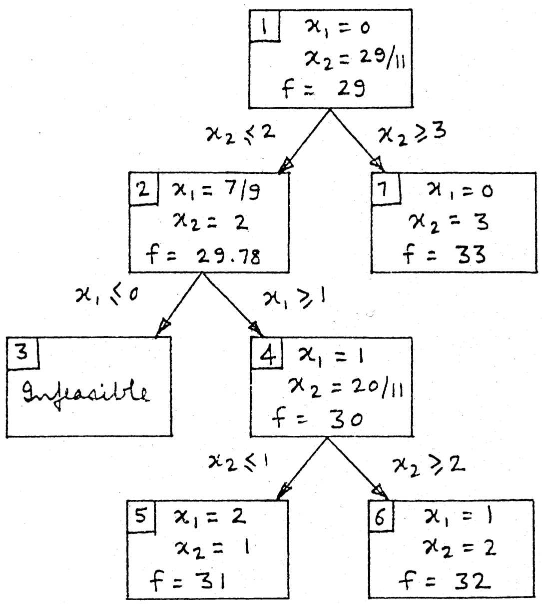
Problem 9.10

The solution can be obtained by inspection. To each extractor, assign the stream with the least cost for that extractor. The optimum pairing is

Stream	Extractor
1	4
2	2
3	3
4	1

cost = 64

Problem 9.11



Nodes 6 and 7 are fathomed. Node 5 gives the IP optimum.

Problem 9.12

$$x_1 = 0$$
$$x_3 = 0$$
$$x_2 = 1$$

$$f = 8$$

Problem 9.13

$$x = [0\ 0\ 7\ 0\ 0]^{\mathrm{T}}$$
$$f = 7$$

Problem 9.14

(a) Problem formulation:

Minimize: $\sum C_{ij} + \sum_i C_i I_i$

Subject to: for each j, $\sum_i S_{ij} \geq R_j$

for each i, $\sum_j S_{ij} \leq O_i$

and $\sum I_i \leq 1$ $I_1, I_2 \cdots I_i$ integer.

(b) Numerical solution:

Plant A	Plant B
1	0

Fixed Charge A	Fixed Charge B
700	0

A to C	A to D	B to C	B to D	Production A	Production B
200	250	0	0	450	0

Cost A to C	Cost A to D	Cost B to C	Cost B to D	C	D
200	750	0	0	200	250

Total cost
1650

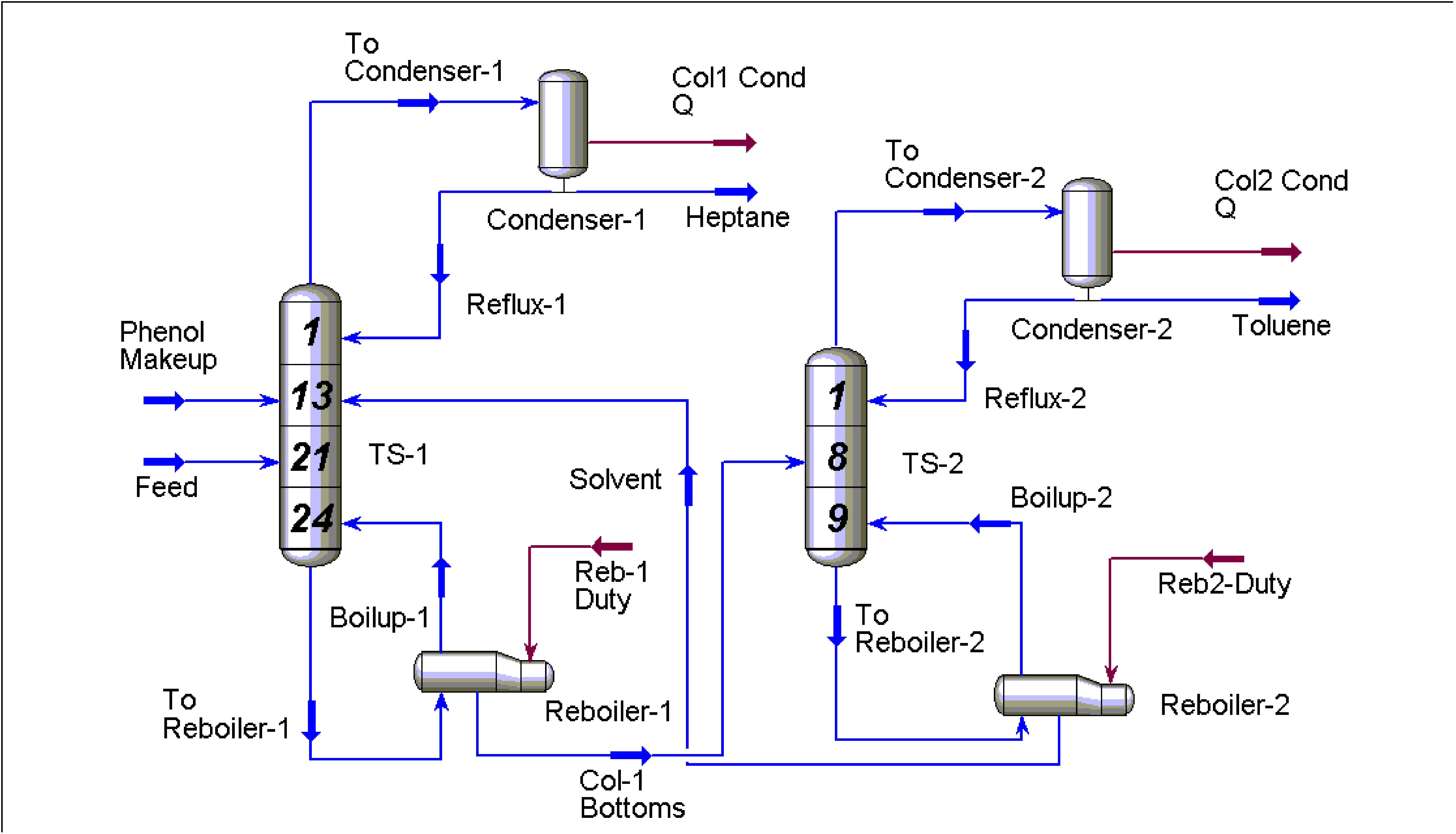
Build only plant A.

Problem 9.15

The solution is:

Refinery 1	Refinery 2	M1	M2	M3	k1	k2	k3
5000	7500	2000	5000	4000	0.08	0.06	0.04

X111	500					
X112	1500			Meet all Demand (2)	112	1
X113	1.93E-13			0 j = 1	113	1
X121	5.806898			0 j = 2		
X122	0.009896			0 j = 3	122	1
X123	0				123	1
X131	2499.993			Can't Exceed Supply (3)		
X132	0.016408			-494.1737 1 = 1	132	1
X133	0			-1005.826 1 = 2	133	1
X211	0					
X212	2.76E-13			con (4)		
X213	0			0 j = 1	C111	40
X221	494.1931			0 j = 2	C112	90
X222	1499.99			0 j = 3	C113	7.72E-15
X223	3000				C121	0.464552
X231	0			con (5)	C122	0.000594
X232	1499.984			0 j = 1	C123	0
X233	0.006911			0 j = 2	C131	199.9994
				1999.993j = 3	C132	0.000984
					C133	0
				con (6)	C211	0
				-10000 j = 1	C212	1.66E-14
		b11	500	-7000 j = 2	C213	0
		b12	1500	-9999.993 j = 3	C221	39.53545
		b13	10000		C222	89.99941
		b21	500	con (7)	C223	120
		b22	1500	0 j = 1	C231	0
		b23	10000	0 j = 2	C232	89.99902
		b31	500	0 j = 3	C233	0.000276
		b32	1500			
		b33	10000		OBJ	669.9997



To Condenser-1
Col1 Cond Q
Condenser-1
Heptane
Reflux-1
Phenol Makeup
Feed
1
13
21
24
TS-1
Solvent
Boilup-1
Reb-1 Duty
Reboiler-1
To Reboiler-1
Col-1 Bottoms
To Condenser-2
Col2 Cond Q
Condenser-2
Toluene
Reflux-2
1
8
9
TS-2
Boilup-2
Reb2-Duty
To Reboiler-2
Reboiler-2

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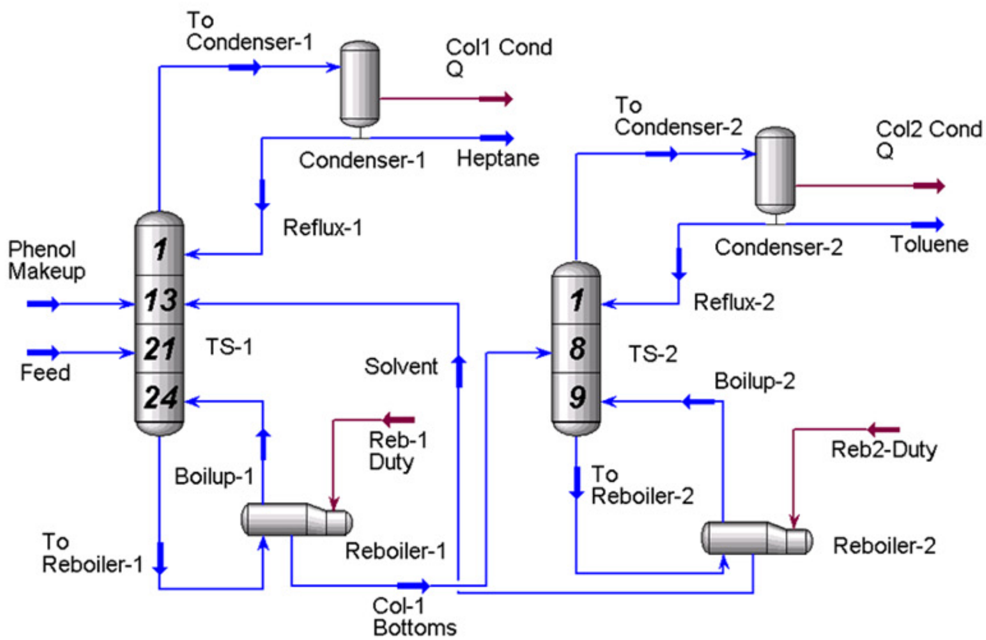
C-6 Extractive Distillation Design



C-6.1 Process Description

Using HYSYS - Conceptual Design and HYSYS.SteadyState and Dynamic Design, a two-column extractive process is modeled from conceptual design to dynamic simulation. In two distillation columns, the equimolar feed of Toluene and Heptane is separated using Phenol as a solvent. HYSYS - Conceptual Design is used to calculate the interaction parameters and carry out the preliminary design and optimization of the process. In HYSYS.SteadyState, the column is set up and optimized, using the Spreadsheet to model economic factors. Finally, controls are added and various disturbances are introduced to test the effectiveness of the design.

The objective is to maximize the purity of the Heptane and Toluene streams coming off the top of the first and second column, respectively.

Using Hyprotech's process simulation software, we can develop a conceptual design, optimize the steady-state process, and develop and test a control scheme. These are the steps:

1. Using HYSYS - Conceptual Design, calculate interaction parameters, and determine an appropriate Property Package.

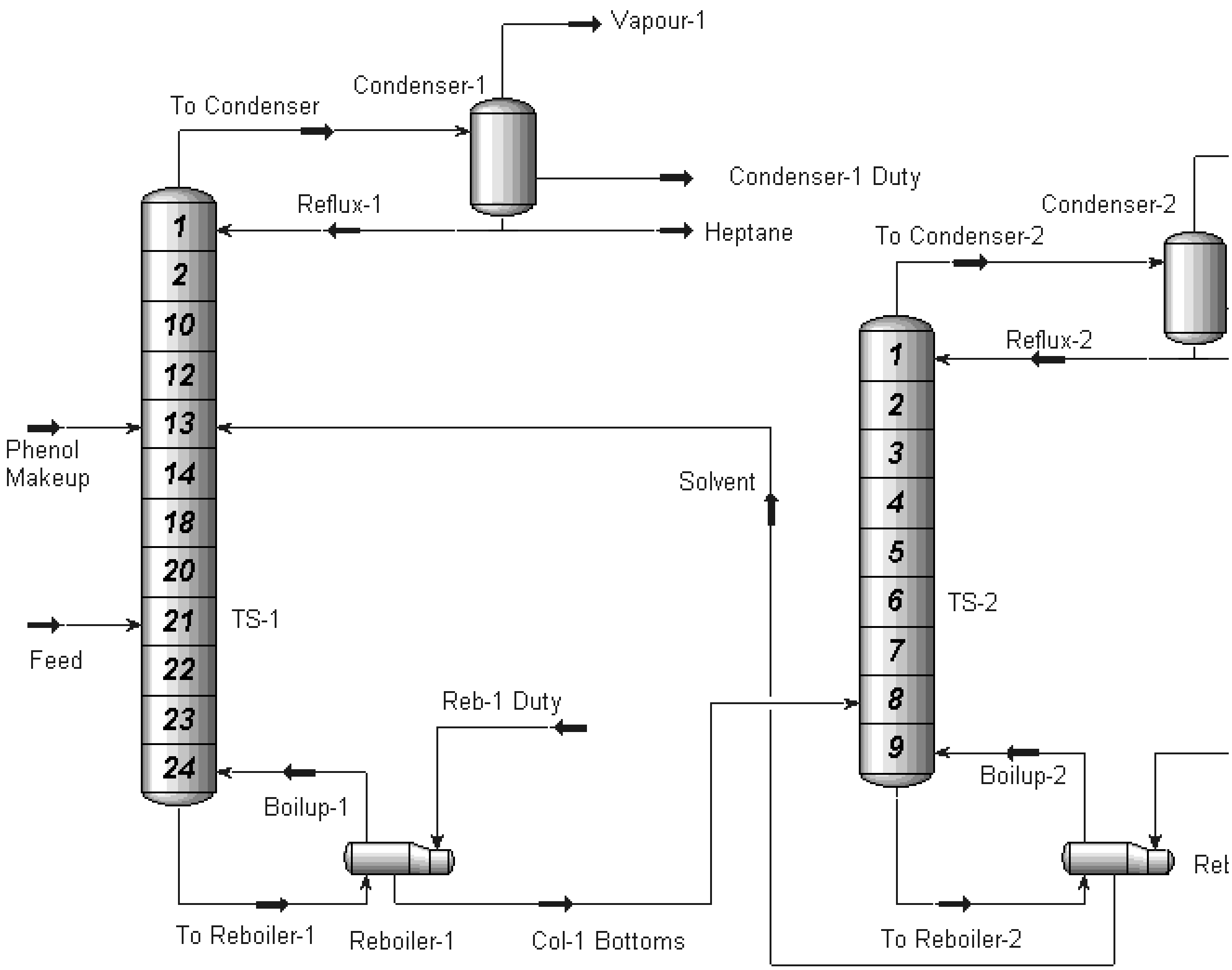
2. Using HYSYS - Conceptual Design, carry out the preliminary design and optimization, estimating/specifying key process characteristics such as Reflux Ratios, number of stages, feed location, and product purities.

3. Using HYSYS.SteadyState, set up the column configurations in a single flowsheet, using the specifications determined in the previous step.

4. Using HYSYS.SteadyState, use the Optimizer to further refine the extractive distillation process, taking into account

the basic economics.

5. Using HYSYS.Dynamics, set up a candidate control scheme and evaluate dynamic operability.



Column SubFlowsheet

C-6.2 Background

HYSYS - Conceptual Design could also be used to screen solvents based on their effect in increasing the relative volatility of n-Heptane and Toluene.

Extractive distillation is used in the petroleum industry for the separation of aromatics from non-aromatic hydrocarbons. In general, the presence of the solvent raises the vapour pressures of the key components to different degrees, so that the relative volatility between these key components is increased. The more volatile component is removed in the distillate, and the bottoms mixture (solvent and less volatile component) is separated in a second distillation column.

Toluene-"non-toluene" separation is well-documented. The non-toluene fraction is often a narrow mixture of saturated hydrocarbons, and for the purpose of this study will be represented by n-Heptane. The objective of this process, therefore, is to maximize the separation of n-Heptane and Toluene.

Reflux Ratio	No. of Stages
10	113
15	71
20	61

Reflux Ratio and number of stages for the non-extractive equimolar separation of nHeptane and Toluene, as predicted by HYSYS - Conceptual Design (NRTL-Ideal). The distillate and bottoms molar purities are 0.99.

Phenol is commonly used as the solvent, due to its effect in significantly increasing the volatility ratio of n-Heptane and Toluene. Unlike other potential solvents which can also increase the volatility ratio, phenol does not form azeotropes, and is currently inexpensive. It is not particularly dangerous, although there is some concern as to its environmental impact.

Since n-Heptane and Toluene do not form an azeotrope, the separation can theoretically be performed without the use of a solvent. However, the number of stages and reflux ratio is excessive, as shown in the side table. This is due to the fact that these components have similar volatilities.

This example is set up in five parts as outlined below. Some sections can be completed independently, without referring to previous steps. For example, if you wish to do only the Steady-State design, you need only complete steps 3 and 4, using the interaction parameters and column design as predicted in steps 1 and 2.

C-6.3

PART 1 ***Calculating Interaction Parameters***

Using experimental data from various sources, interaction parameters are generated using the NRTL and Peng Robinson Property Packages. Interaction parameters for the three binary pairs are obtained separately and combined in the binary matrix.

NRTL Interaction Parameters

> In earlier versions of HYSYS - Conceptual Design, you must have only two components in the Fluid Package in order to view binary TXY and XY plots.

In HYSYS - Conceptual Design, open the Fluid Package Manager and add a new Fluid Package. The Fluid Package is defined as follows:

¨ Property Package: **NRTL-Ideal**

¨ Components: **C7**, **Toluene**, **Phenol**

Leave all other parameters (i.e. - Binary Coefficients) at their defaults.

Now we will look at the interaction parameters for the three component pairs and if necessary, regress new parameters from experimental data.

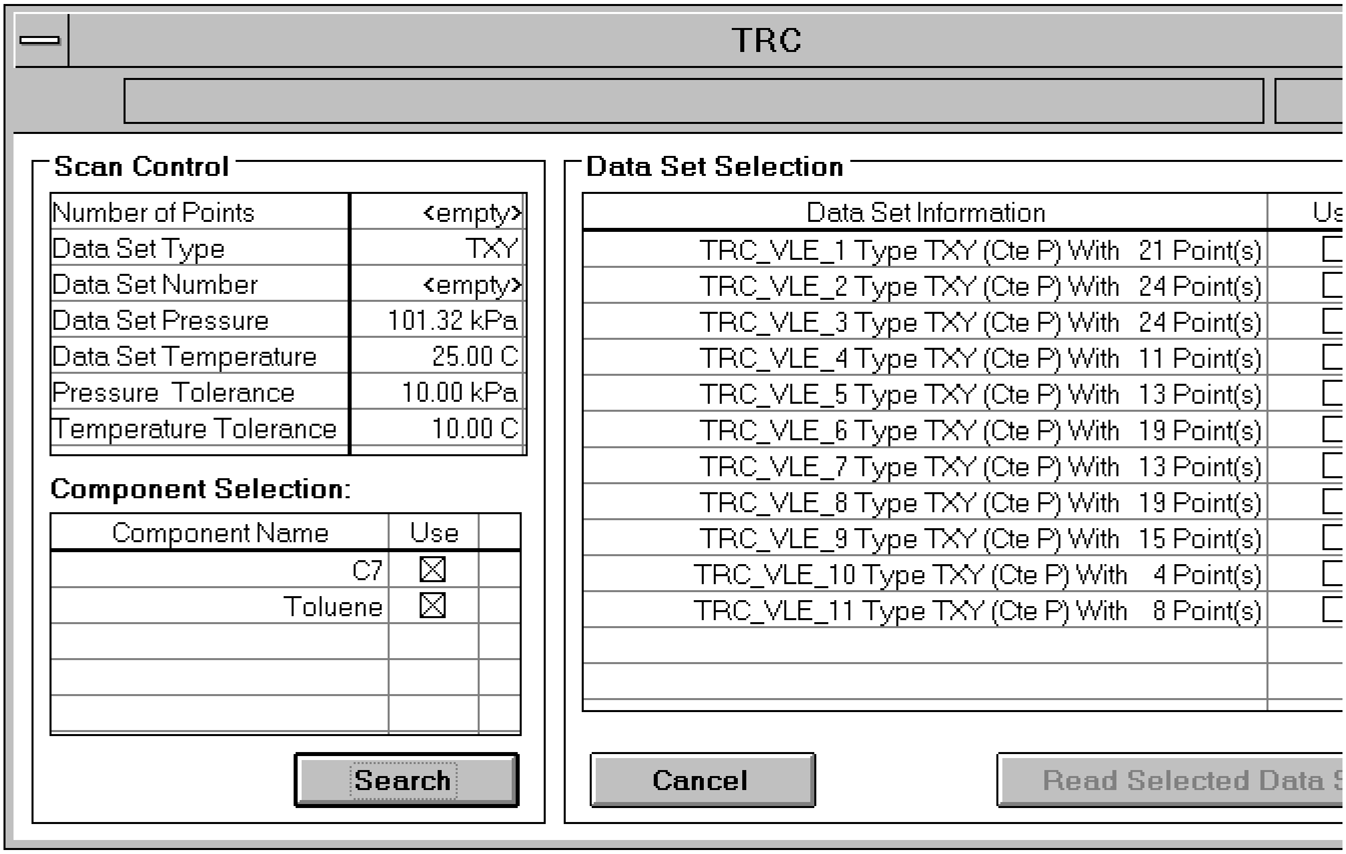
n-Heptane-Toluene Interaction Parameters

The default interaction parameters are usually reliable, although it is important to ensure that they were regressed under conditions similar to the current design. New interaction parameters can be regressed from experimental data specifically chosen for the system conditions. Data can be entered manually, or can be automatically scanned from the TRC libraries of VLE, LLE and Heats of Mixing data. The TRC database contains data for over 16000 fitted binaries.

Extensive TRC data is available for the **C7-Toluene** pair. Open a new Fluid Phase Experiment, select the ***TRC Import*** button, and specify the following Scan Control options:

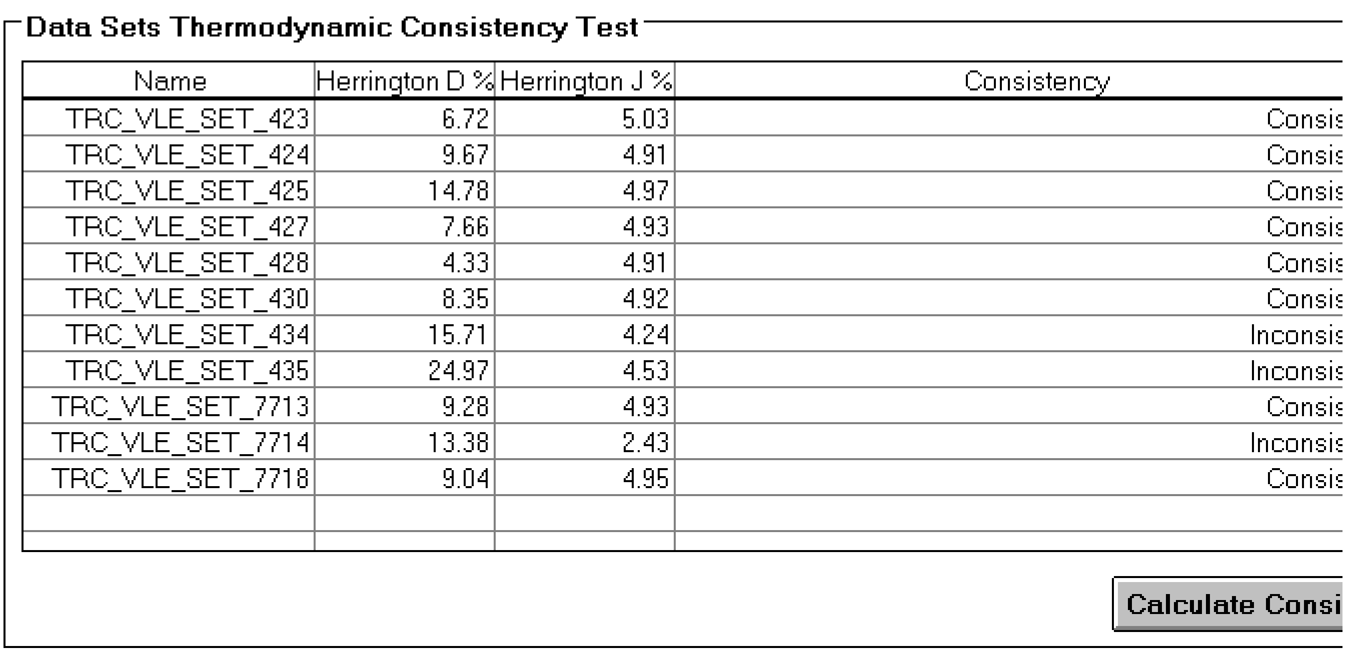
- Data Set Type — TXY
- Data Set Pressure — 101.32 kPa
- Data Set Temperature — 25 °C
- Pressure Tolerance — 10 kPa
- Temperature Tolerance — 10 °C

Search for all data sets which include the components C7 and Toluene:



For more information on the Herrington Consistency Test, see the HYSYS - Conceptual Design manual.

Check the **Use** box for each set, then select the ***Read Selected Data Sets*** button. These sets will be imported into the current Fluid Phase Experiment. Next, check the Herrington Thermodynamic Consistency for each set by selecting the Consistency page tab, and pressing the ***Calculate Consistency*** button. The Herrington parameters are calculated, and the status of each data set is displayed:


Data Sets Thermodynamic Consistency Test

Name	Herrington D %	Herrington J %	Consistency
TRC_VLE_SET_423	6.72	5.03	Consis
TRC_VLE_SET_424	9.67	4.91	Consis
TRC_VLE_SET_425	14.78	4.97	Consis
TRC_VLE_SET_427	7.66	4.93	Consis
TRC_VLE_SET_428	4.33	4.91	Consis
TRC_VLE_SET_430	8.35	4.92	Consis
TRC_VLE_SET_434	15.71	4.24	Inconsis
TRC_VLE_SET_435	24.97	4.53	Inconsis
TRC_VLE_SET_7713	9.28	4.93	Consis
TRC_VLE_SET_7714	13.38	2.43	Inconsis
TRC_VLE_SET_7718	9.04	4.95	Consis

Calculate Consi

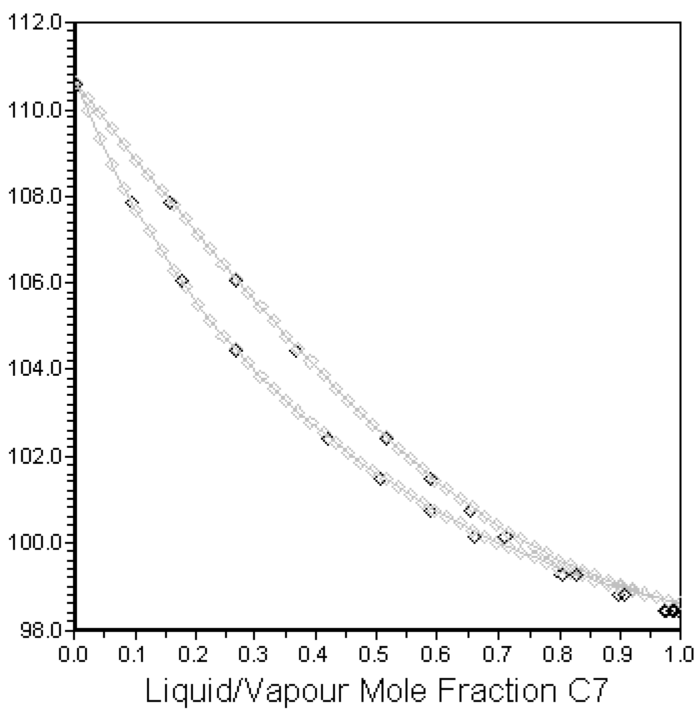
Set 428:
Rose, A.; Williams, E. T.
Ind. Eng. Chem., 1955, **47**, 1528.
P = 101 kPa
# of points = 13

Note that Set 428 has Herrington parameters of 4.33% and 4.91% for *D* and *J* respectively, which is well under the “consistency limit” for isobaric data (*D* - *J* £ 10%). This set has 13 points which is sufficient for our investigation.

If we were going to regress the interaction parameters to the experimental data, we would run the Optimizer. However, we will instead compare the experimental data to the calculated data based on the *default* interaction parameters. On the Summary page of the Fluid Phase experiment, highlight Set 428, then select the ***Edit*** button. Select the ***Calculate*** button — the XY and TXY curves will be constructed based on the default interaction parameters, and the errors will be calculated.

The calculated data in this case is the TXY or XY data calculated using the Property Package (and current interaction parameters), which is displayed graphically on the Plots page of the Data Set view.

The TXY plot appears as follows:



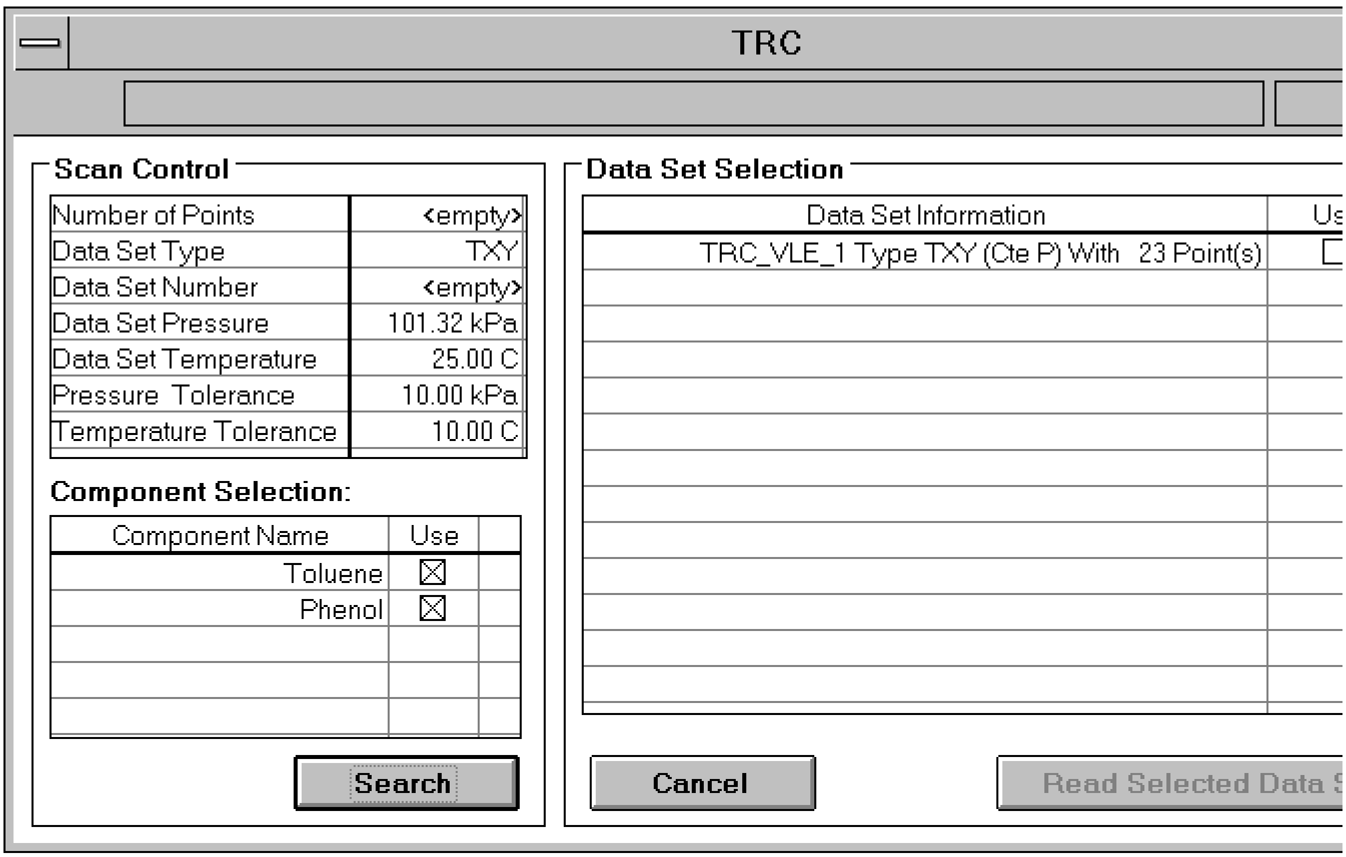
The experimental and calculated points match remarkably well, and thus it is not necessary to regress the interaction parameters for the C7-Toluene pair.

Toluene-Phenol Interaction Parameters

The amount of data available for this component pair is considerably less than what was available for C7-Toluene. We will, however, regress interaction parameters from the available TRC data set (6014).

Set 6014
Drickamer, H. G.; Brown, G.; White, R. R.
Trans. Amer. Inst. Chem. Eng., 1945, **41**, 555.
P = 101 kPa
# of points = 23
Herrington D% - 21.87
Herrington J% - 28.01

Open a new Fluid Phase Experiment, and select the ***TRC Import*** button.



There is only one data set available for the Toluene-Phenol pair. Select it by checking the **Use** box, then choose the ***Read Selected Data Sets*** button.

The Data Set Notes group box on the Summary page of the Fluid Phase Experiment displays important information related to the data set. Note that this data, obtained at 101 kPa, has 23 points.

Data Set Notes:

Drickamer, H. G.; Brown, G. G.; White, R. R.
Trans. Amer. Inst. Chem. Eng., 1945, 41, 555.
T/K - x[1] - y[1] - P/kPa = 101 N = 23

TRC Databases for Chemistry and Engineering
Copyright (c) by the Thermodynamics Research Center
of the Texas Engineering Experimental Station,

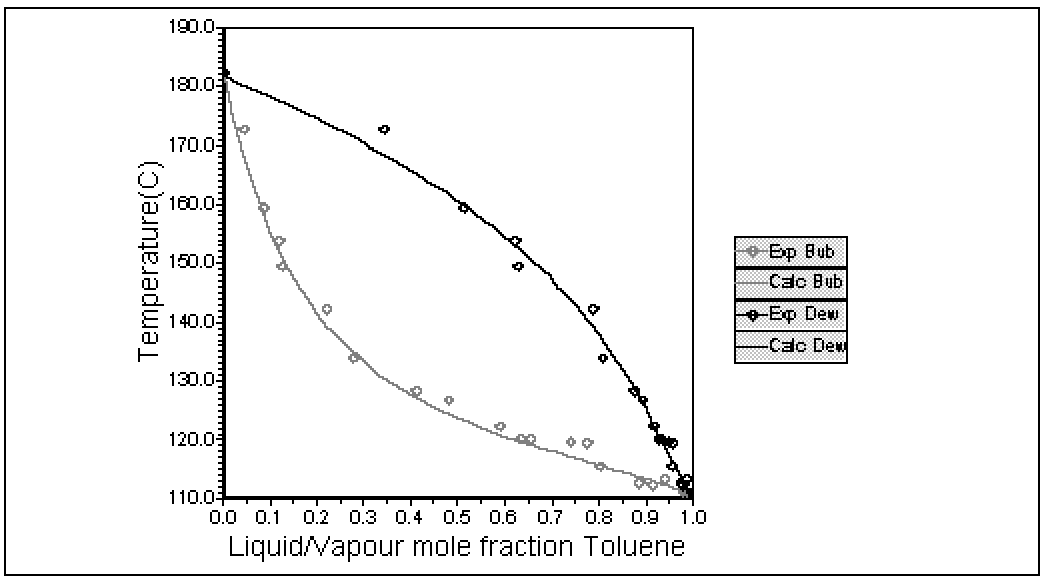
Move to the Consistency page, and calculate the Herrington Consistency as you did for the C7-Toluene data.

This data set is consistent according to the Herrington test:

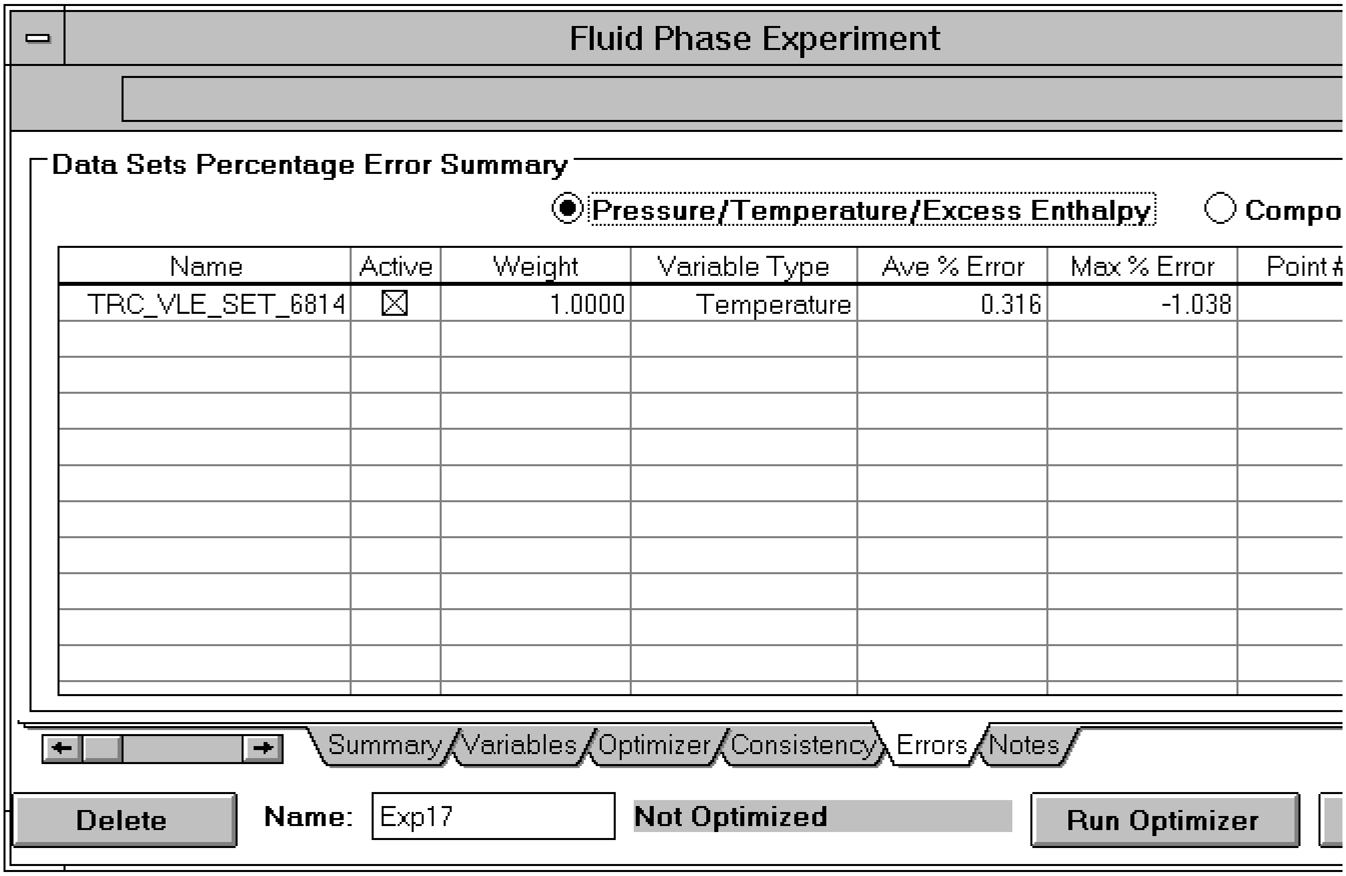
Name	Herrington D %	Herrington J %	Consistency
TRC_VLE_SET_6814	21.87	28.01	Consiste

Now we will calculate new interaction parameters based on this experimental data.

Before running the Optimizer, compare the experimental data to the predictions made using the default interaction parameters. Edit **TRC_VLE_SET_6814** and select the ***Calculate*** button. By looking at the Plots page, it appears that there is reasonably good agreement between the experimental data and calculated curves.



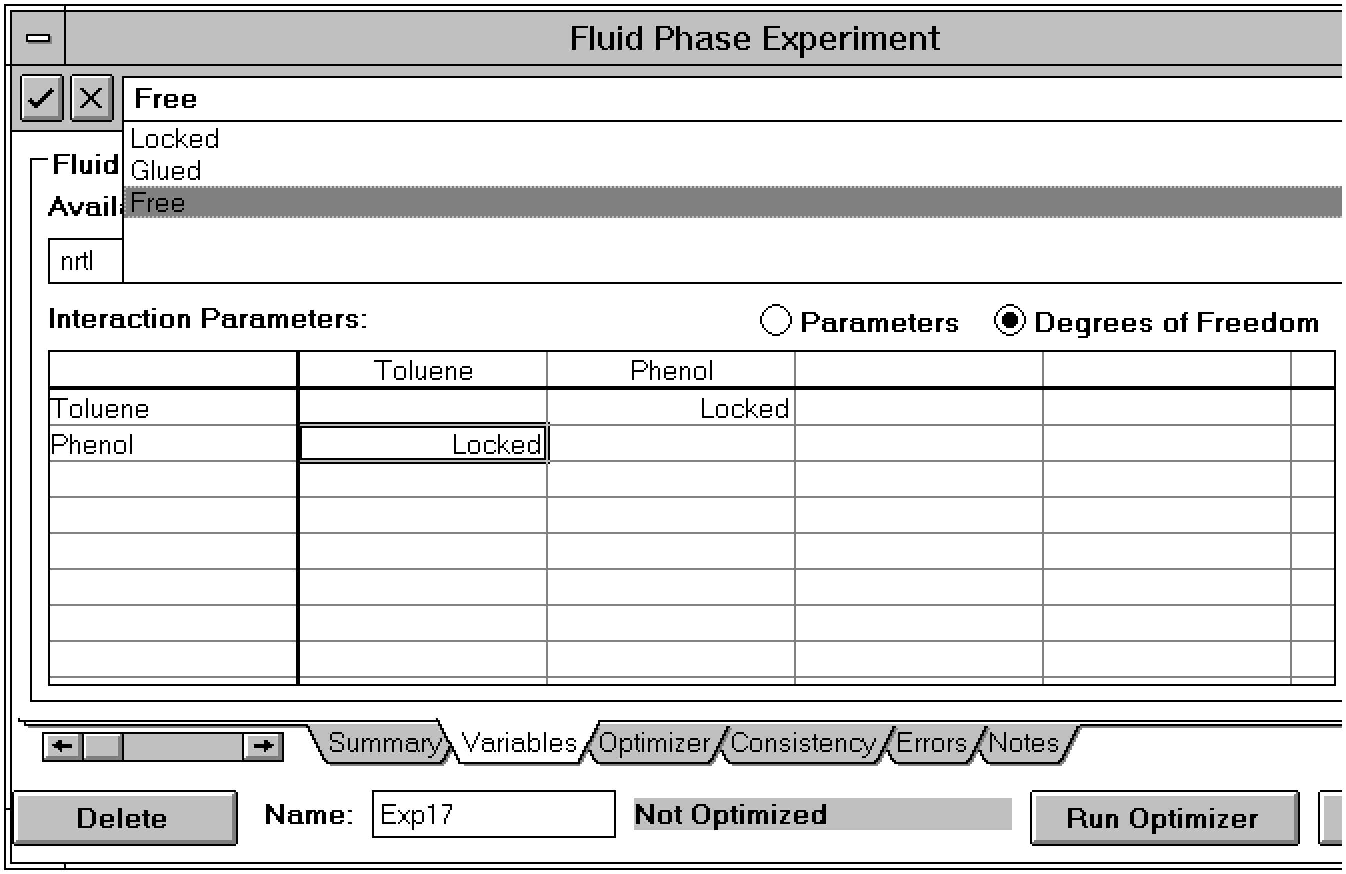
On the Errors page of the Fluid Phase Experiment view, note that the average and maximum temperature errors are 0.316% and -1.038% respectively.



Now we will run the Optimizer in order to obtain improved interaction parameters for this data set. On the Summary page of the Fluid Phase Experiment view, note that the default Objective Function is **ActivityCoeff**. Thus, the errors will be minimized with respect to the components' activity coefficients.

Type	TXY
Objective Function	ActivityCoeff
Active in Optimization	☒
Weight In Experiment	1.0000

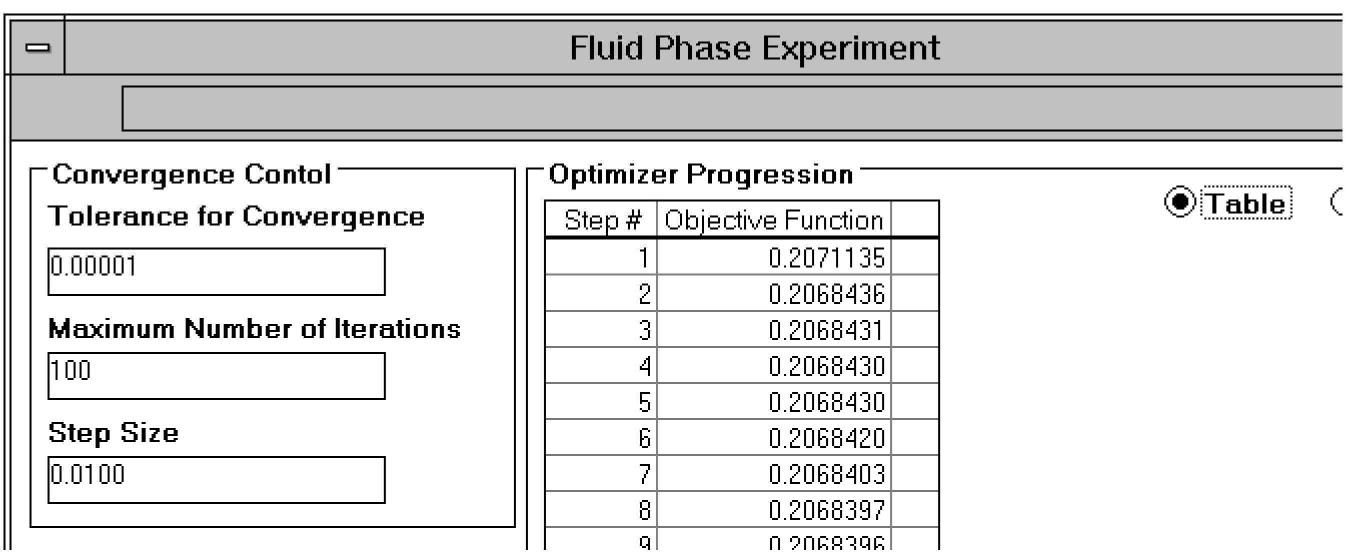
Move to the Variables page and "free" the parameters. For Matrix Pane b_{ij} (which for NRTL in HYSYS is equivalent to a_{ij} /c_{ij}), the parameters are initially locked.



To “free” the parameters, select Matrix Pane **bij** from the drop down menu, choose the **Degrees of Freedom** radio button, place the cursor on either cell containing the “Locked” message, and from the top drop down menu, select **Free**. This allows the bij parameters to vary during the optimization process. Before running the optimizer, set up the view so that you can observe the solution progress. This is best done from the Optimizer page, although you may prefer to remain on the Variables page and watch the progress of the interaction parameters (ensure that the **Parameters** radio button is selected; as well, it is probably more useful to observe the aij parameters). Once you start the optimizer you cannot change pages until the calculations are complete.

For this example, we will observe the solution progress from the Optimizer page.

Choose the Optimizer tab, then select the ***Run Optimizer*** button.



Convergence is achieved quickly, and the errors are automatically calculated once the algorithm converges; the average and maximum temperature errors are 0.313% and 1.061% respectively.

We may be able to get better results using a different Objective Function. The Maximum Likelihood function is the most rigorous from a statistical point of view, but also is the most computer intensive. The convergence time increases when we use this function, but the improved results may be worth it.

Activity Coefficients
a_{12} = 829.4
a_{21} = -60.2
$b_{12} = b_{21}$ = 0.146
Average Error = 0.313%
Maximum Error = -1.061%
Maximum Likelihood
a_{12} = 824.2
a_{21} = -188.1
$b_{12} = b_{21}$ = 0.010
Average Error = 0.251%
Maximum Error = -0.934%

Change the Objective Function to **Maximum Likelihood**, and restart the optimizer. We obtain the following interaction parameters:

	Toluene	Phenol
Toluene	0.000	-188.1
Phenol	824.2	0.000

The bij parameters are 0.01. The temperature errors are now 0.251% (average) and 0.934% (maximum). Note, however, that while the toluene composition errors decreased, the phenol composition errors increased. Nevertheless, we will use these interaction parameters for the Phenol-Toluene pair.

n-Heptane-Phenol Interaction Parameters

There is no TRC data for the **Phenol-Heptane** component pair. The following data (taken from Chang, Y.C., 1957 and Kolyuchkina et al., 1972) is used:

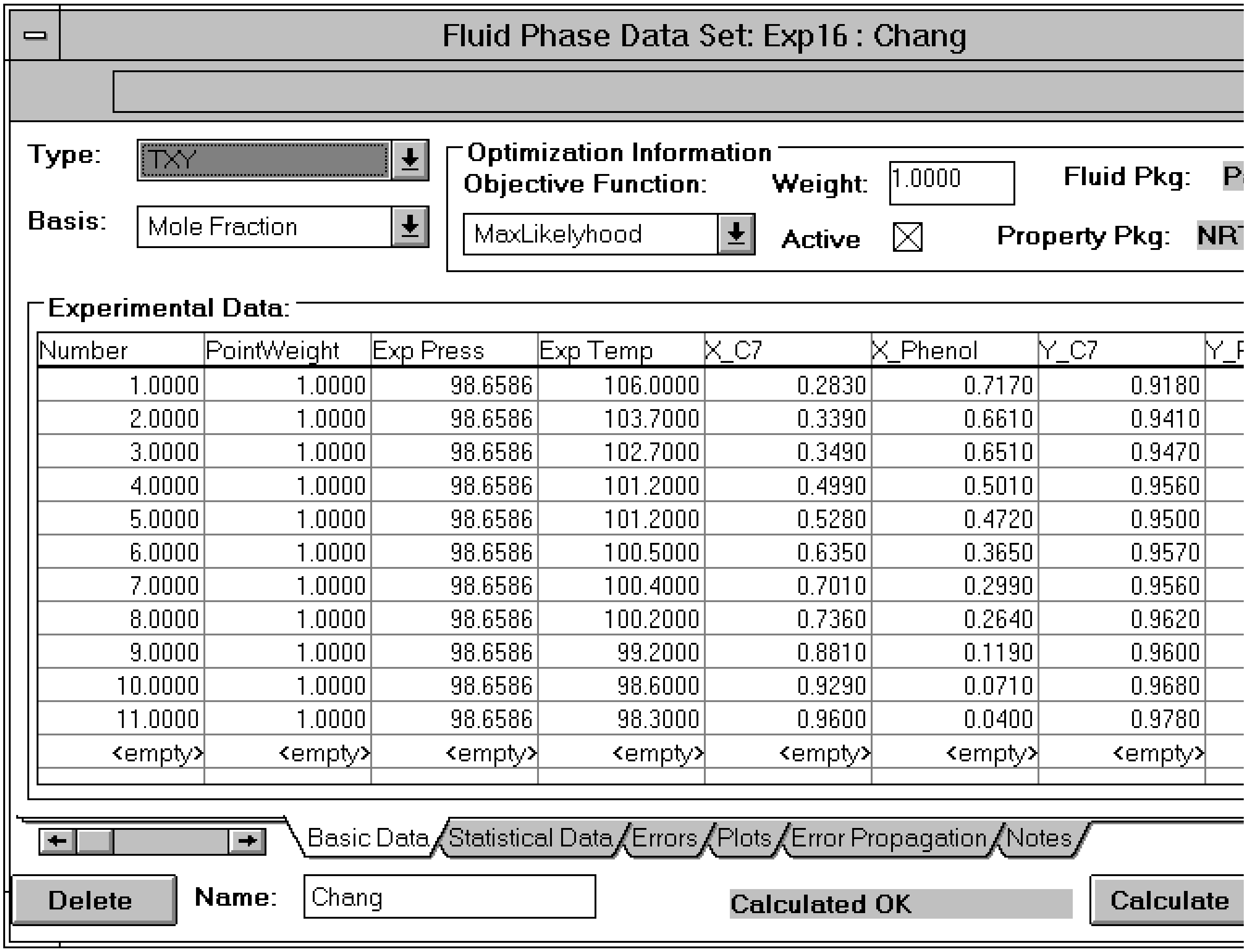
Temperature (°C)	x_1 (1 = Heptane)	y_1 (1 = Heptane)
106.0	.283	.918
103.7	.339	.941
102.7	.349	.947
101.2	.499	.956
101.2	.528	.950
100.5	.635	.957
100.4	.701	.956
100.2	.736	.962
99.2	.881	.960
98.6	.929	.968
98.3	.960	.978

TXY Data for Phenol-Heptane (Chang, 1957) Pressure = 740 mm Hg

Temperature (°C)	x_1 (1 = Heptane)	y_1 (1 = Heptane)
116.3	.090	.840
112.4	.112	.932
112.6	.120	.931
107.1	.186	.946
104.4	.233	.961
102.4	.337	.960
100.8	.535	.970
100.6	.585	.965
100.0	.720	.967
99.6	.816	.961
99.5	.837	.964
99.2	.900	.970

TXY Data for Phenol-Heptane (Kolyuchkina et al., 1972) Pressure = 760 mm Hg

Open a new Fluid Phase Experiment, select the appropriate Fluid Package (C7-Phenol), choose the ***Add*** button, and enter the data, as shown below for the first data set (Chang):



Number	PointWeight	Exp Press	Exp Temp	X_C7	X_Phenol	Y_C7
1.0000	1.0000	98.6586	106.0000	0.2830	0.7170	0.9180
2.0000	1.0000	98.6586	103.7000	0.3390	0.6610	0.9410
3.0000	1.0000	98.6586	102.7000	0.3490	0.6510	0.9470
4.0000	1.0000	98.6586	101.2000	0.4990	0.5010	0.9560
5.0000	1.0000	98.6586	101.2000	0.5280	0.4720	0.9500
6.0000	1.0000	98.6586	100.5000	0.6350	0.3650	0.9570
7.0000	1.0000	98.6586	100.4000	0.7010	0.2990	0.9560
8.0000	1.0000	98.6586	100.2000	0.7360	0.2640	0.9620
9.0000	1.0000	98.6586	99.2000	0.8810	0.1190	0.9600
10.0000	1.0000	98.6586	98.6000	0.9290	0.0710	0.9680
11.0000	1.0000	98.6586	98.3000	0.9600	0.0400	0.9780
<empty>	<empty>	<empty>	<empty>	<empty>	<empty>	<empty>

The default interaction parameters are shown here:

aij

	C7	Phenol
C7	0.000	701.706
Phenol	1120.082	0.000

bij

	C7	Phenol
C7	0.000	0.293
Phenol	0.293	0.000

The interaction parameters are written as follows:
1 = C7
2 = Phenol
a_{12} = 1120.082
a_{21} = 701.706
$b_{12} = b_{21}$ = 0.293

Various methods are possible for regressing the interaction parameters. In this example, the following schemes will be used:

1. With only the first data set active, optimize using the Activity Coefficients Objective Function.
2. With only the first data set active, optimize using the Maximum Likelihood Objective Function.
3. With only the second data set active, optimize using the Activity Coefficients Objective Function.
4. With only the second data set active, optimize using the Maximum Likelihood Objective Function.
5. With both data sets active, optimize using the Objective Function which results in the smallest error.

Scheme 5 uses the Maximum Likelihood Objective Function.

The following table outlines the results of this analysis. In all cases, using the Maximum Likelihood Objective function rather than the Activity Coefficients Objective function resulted in significantly smaller temperature errors, while in most cases the composition errors increased slightly. In some instances, the average or maximum composition decreased when the Maximum Likelihood Objective function was used (see *Ave C7* and *Max Phenol* for Schemes *3* and *4*). Therefore, we conclude that the Maximum Likelihood Objective function results in a better fit.

	Interaction Parameters			**Errors**					
Scheme	a_{12}	a_{21}	b_{12}	**Avg T**	**Max T**	**Ave C7**	**Max C7**	**Ave Phenol**	**Max Phenol**
Default	1120	701.7	.293	C=.157 K =.868	C=-.489 K=2.32	C=.713 K=1.87	C=2.83 K=-5.34	C=14.6 K=35.3	C=-31.7 K=73.2
Scheme 1	1672	1580	.528	C=.169	C=.329	C=.456	C=1.98	C=8.24	C=-22.1
Scheme 2	1362	1001	.490	C=.068	C=.245	C=.540	C=2.40	C=10.6	C=-26.9
Scheme 3	2052	1125	.509	K=.581	K=1.32	K=1.75	K=-4.12	K=29.8	K=68. 9
Scheme 4	1438	1172	.460	K=.125	K=.199	K=1.73	K=6.41	K=30.2	K=58.4
Scheme 5	1539	1328	.508	C=.149 K=.192	C=-.480 K=.502	C=.471 K=1.82	C=2.44 K=6.59	C=8.05 K=31.3	C=-27.3 K=65.4

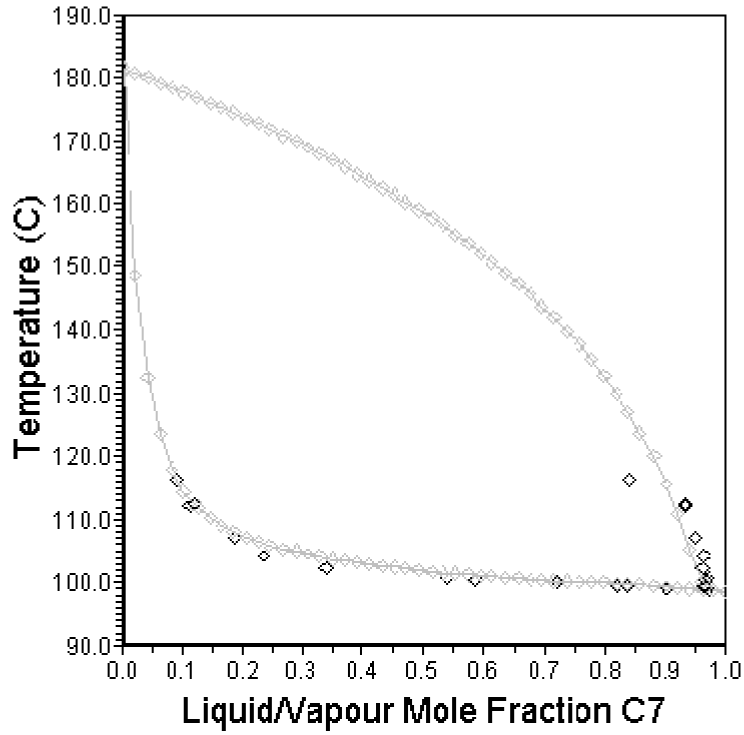
We will use the interaction parameters obtained using Scheme *5*.

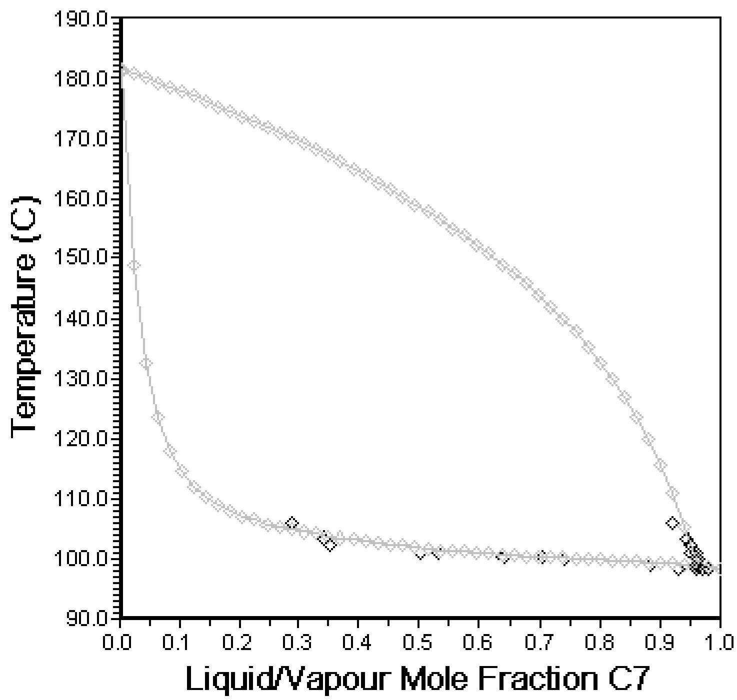
For this component set, there is no liquid-liquid region. If a liquid-liquid region were predicted, then the Property Package and/or interaction parameters would be unacceptable, because they predict physically incorrect behaviour. A liquid-liquid region is not predicted with our interaction parameters.

Although we can be reasonably confident of these results, it is wise to regard the following:

1. Consider defining a weight of zero for outliers (data points which deviate significantly from the regressed curve).
2. Check the prediction of liquid-liquid regions.

The plots shown below are the TXY diagrams for Phenol-Heptane, comparing the experimental data to the points calculated from the Property Package. The figure on the left plots the Kolyuchkina experimental data, while the figure on the right plots the Chang experimental data.





We can check the prediction of liquid-liquid regions from the Binary Coefficients page of the appropriate Fluid Package view (ensure that you have entered the interaction parameters as shown below):

aij

	C7	Toluene	Phenol
C7	0.000	425.193	1328.000
Toluene	-160.034	0.000	-188.100
Phenol	1539.000	824.200	0.000

bij

	C7	Toluene	Phenol
C7	0.000	0.302	0.508
Toluene	0.302	0.000	0.010
Phenol	0.508	0.010	0.000

You can see the LLE ternary plot on the **Binary Coeffs** page of the Fluid Package view. This requires you to enter a temperature and a pressure. You can see the VLLE ternary plot on the **Setup** page of the Ternary Distillation Experiment view. Here, you only enter a pressure.

Select the **Ternary plot** radio button, transfer the three components to the **Selected Components** group, and enter a temperature and pressure. Over a range of temperature and pressures, no liquid-liquid region is predicted.

Peng Robinson Interaction Parameters

Default interaction parameters are available only for the C7-Toluene pair (0.006). Unlike the NRTL interaction parameters, only one PR interaction parameter matrix pane is available; as well, binaries are constructed such that $a_{ij} = a_{ji}$.

Open the Fluid Package Manager and add a new Fluid Package:

- Property Package: **PR**
- Components: **C7**, **Toluene**, **Phenol**

Leave all other parameters at their defaults. As we did in the previous section, we will determine the Interaction Parameters based on TRC and literature experimental data. The procedure is essentially the same, and is concisely summarized below.

n-Heptane-Toluene Interaction Parameters

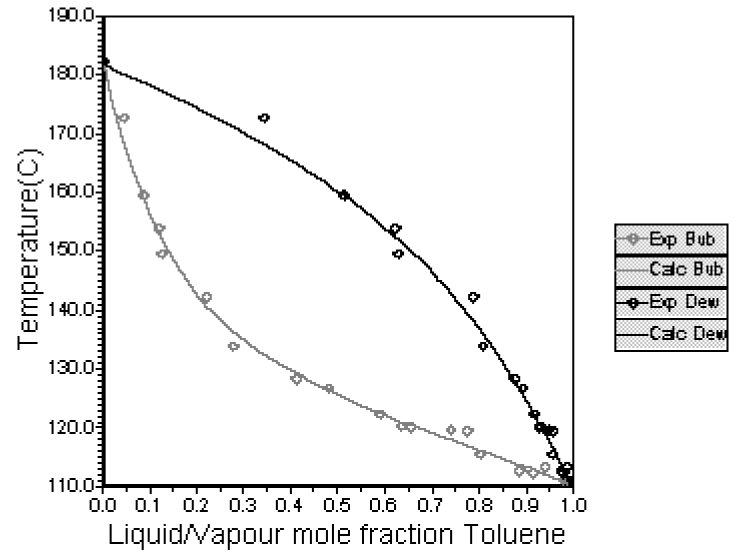
We will use the default interaction parameter $a_{ij} = a_{ji} = 0.006$.

Toluene-Phenol Interaction Parameters

Recall that only one TRC data set is available for this binary (Data Set #6814).

The **Activity Coefficient** Objective Function should not generally be used for Equations of State as results tend to be mediocre for highly polar systems. When we use the **Bubble Temperature** or **Maximum Likelihood** Objective Functions, we obtain an interaction parameter of $a_{ij} = a_{ji} = 0.014$. Note that you may have to decrease the tolerance or step size in order to obtain adequate convergence in this order of magnitude.

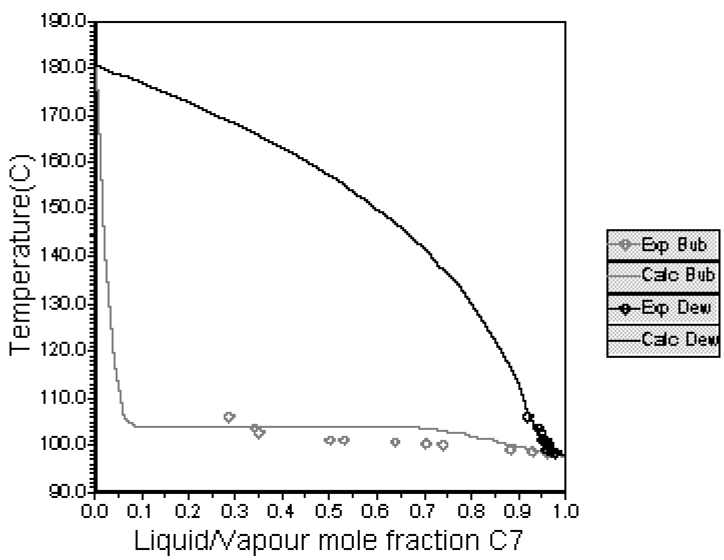
The TXY plot (using this interaction parameter) is shown below, displaying a reasonably good fit.

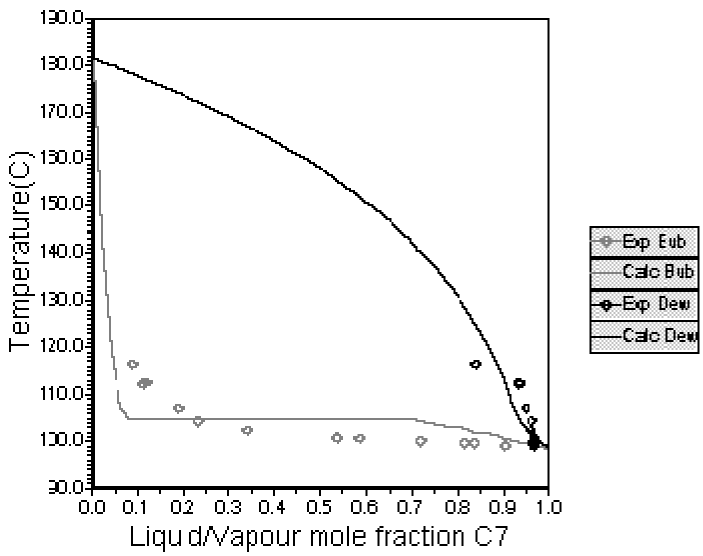


***n*-Heptane-Phenol Interaction Parameters**

As before, we will use the data of Chang and Kolyuchkina et al.

The interaction parameters predicted using the Chang data is very different from the Kolyuchkina data. Chang predicts a_{ij} = 0.045 (Maximum Likelihood), and Kolyuchkina et al. predicts a_{ij} = 0.010. When we combine both data sets, we obtain a_{ij} = 0.03. The TXY plots (using an interaction parameter of 0.03) are below:



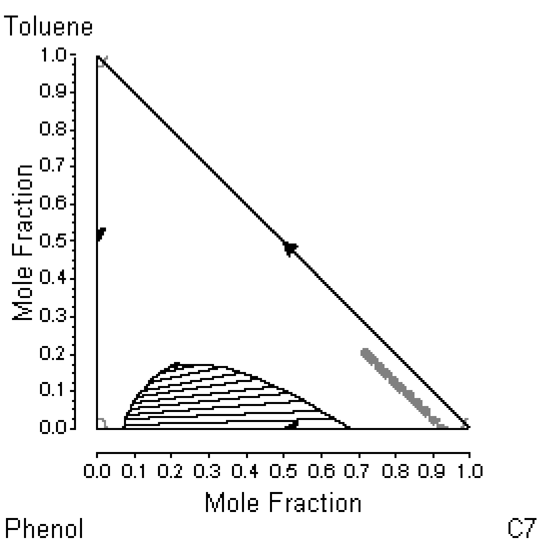


The figure on the left plots the Chang data and the figure on the right plots the Kolyuchkina data.

These plots show that the dew point curve does not match the experimental data very well, and they also indicate a liquid-liquid region. This can be confirmed by looking at the ternary LLE or VLLE plot.

You can see the ternary LLE plot on the **Binary Coeffs** page of the Fluid Package view. This requires you to enter a temperature and a pressure. You can see the VLLE plot on the **Setup** page of the Ternary Distillation Experiment view. Here, you only enter a pressure.

The VLLE plot at a pressure of 18 psia is shown below.



We can avoid the prediction of a liquid-liquid region by setting the n-Heptane-Phenol interaction parameter to 0.007 or less. However, the calculated curve still does not fit the experimental data very well, and we conclude that the Peng-Robinson Property Package is not acceptable for this example.

Note that using the PRSV Property Package results in a better fit, although a two-liquid-phase region is incorrectly predicted under certain conditions.

Prediction of Azeotropes using NRTL

At 18 psia, NRTL does not predict any azeotropes. However, at higher pressures, an azeotrope between n-Heptane and Phenol is predicted, as shown in the following table:

Pressure (psia)	Azeotropic Composition
23	No azeotropes
24	C7=0.9993
30	C7=0.9923
40	C7=0.9825

It is important to remember that activity models generally do not extrapolate well with respect to pressure, so we should therefore regard these results with caution. The point is that we should not allow the pressure to fluctuate excessively, so that incorrect predictions/azeotrope formation will not be a problem.

Parameters used in this Example

For this example, we will use the NRTL Property Package with the following interaction parameters:

aij

	C7	Toluene	Phenol
C7	0.000	425.193	1328.000
Toluene	-160.034	0.000	-188.100
Phenol	1539.000	824.200	0.000

bij

	C7	Toluene	Phenol
C7	0.000	0.302	0.508
Toluene	0.302	0.000	0.010
Phenol	0.508	0.010	0.000

C-6.4

PART 2 ***Ternary Distillation Design (NRTL)***

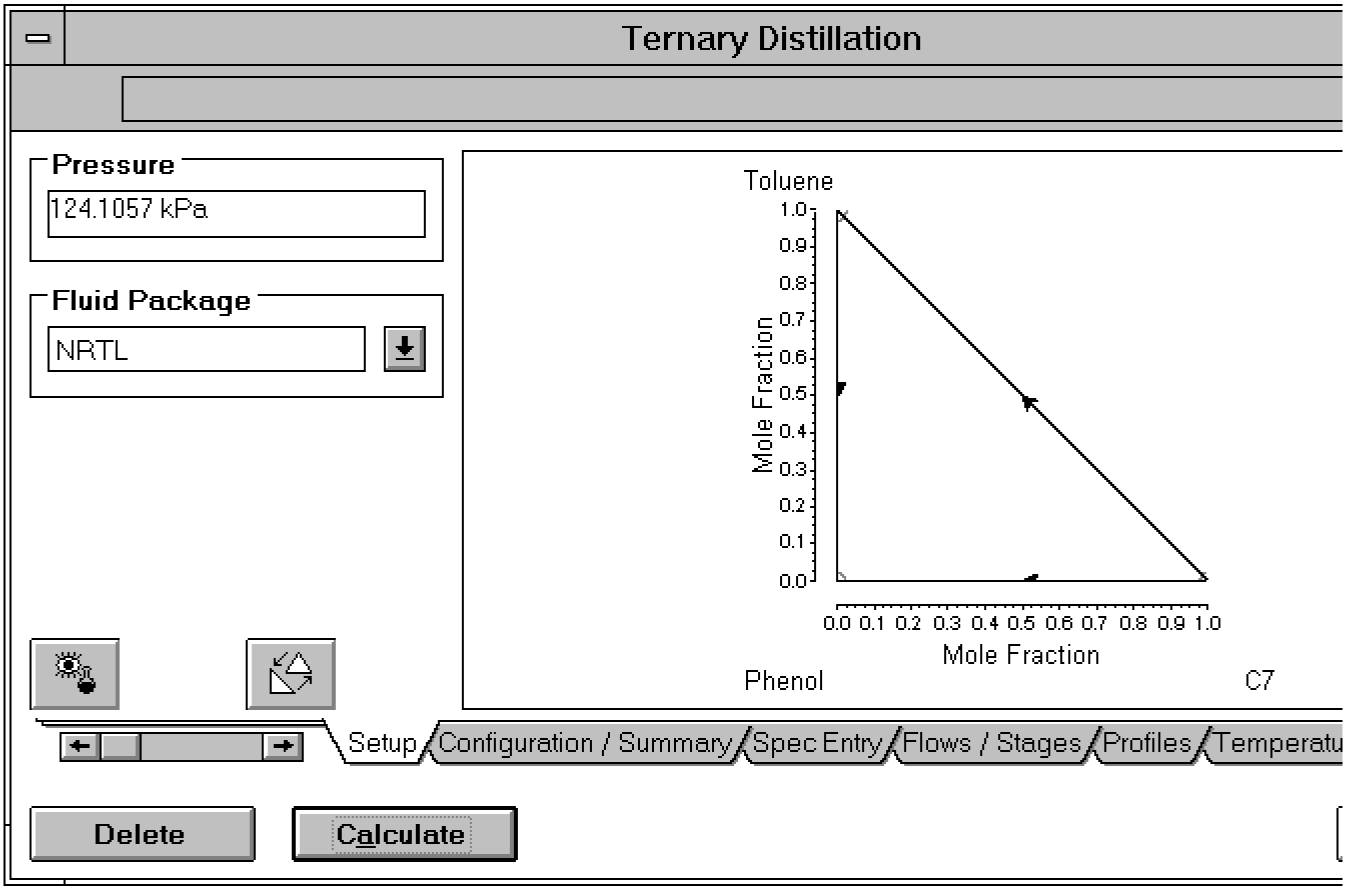
First Column

> HYSYS - Conceptual Design allows for single-column design. For the ternary distillation experiment, the column can have two feeds, a sidestream, condenser, reboiler and decanter.

We will use the NRTL Property Package, and the Interaction Parameters as defined in the previous section.

A trial-and-error type of procedure is required, as we must cycle between the two columns until the connecting streams have roughly the same compositions and flowrates. The bottoms stream of the first column feeds the second column, and the bottoms stream of the second column is the upper feed to the first column.

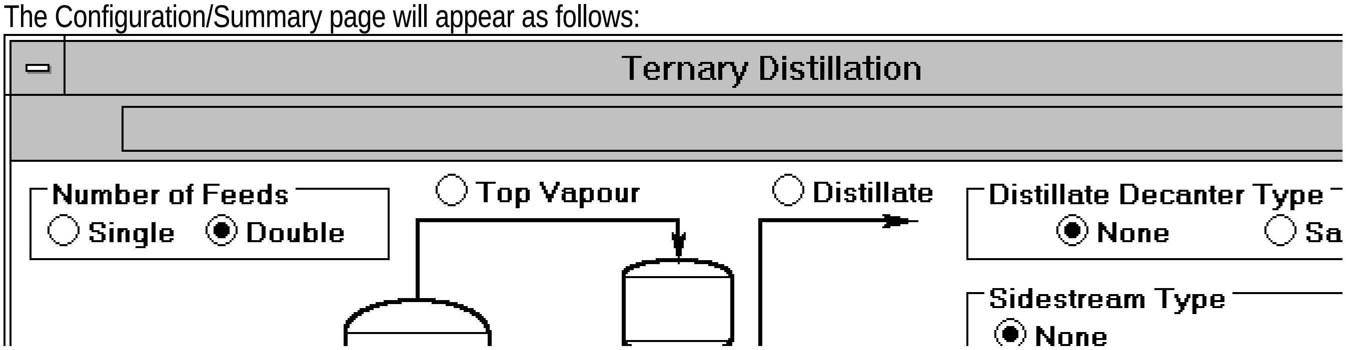
Open a Ternary Distillation Experiment, set a pressure of 18 psia (the average of the top and bottom pressures in the column, 16 and 20 psia), and select the appropriate Fluid Package from the drop down list. The program will then determine if there are any azeotropes or two-liquid regions:



There are no azeotropes or liquid-liquid regions at this pressure, as predicted by the NRTL Property Package (using our new interaction parameters).

The first column (extractive distillation) has two feeds to it, the process feed (50% Toluene, 50% n-Heptane on a molar basis), and the recycle stream from the second column. There is no decanter or sidestream.

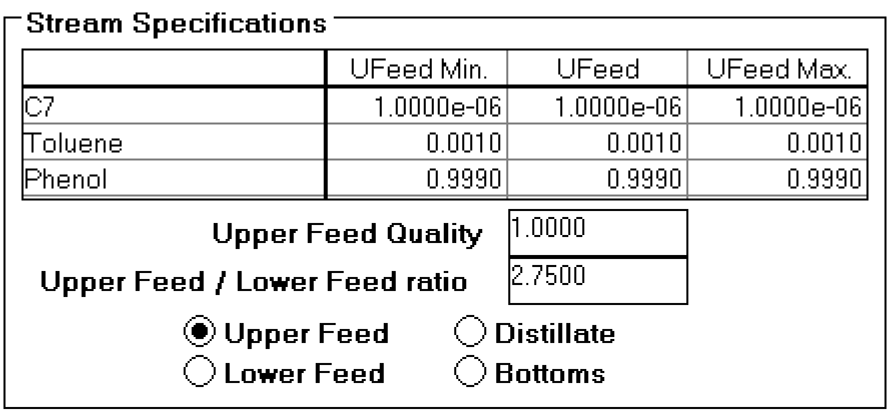
The Configuration/Summary page will appear as follows:



Note that we have entered the specifications for the process feed stream (Lower Feed). The molar flow of the process feed stream is 400 lbmole/hr. For the remaining streams, we will enter the specifications on the Spec Entry page.

Before entering the specifications, set the Reflux Ratio to be 5. Later, we will do a sensitivity analysis in order to estimate an optimum Reflux Ratio.

We know that the upper feed is primarily phenol. As an initial estimate, we will use the following specifications:

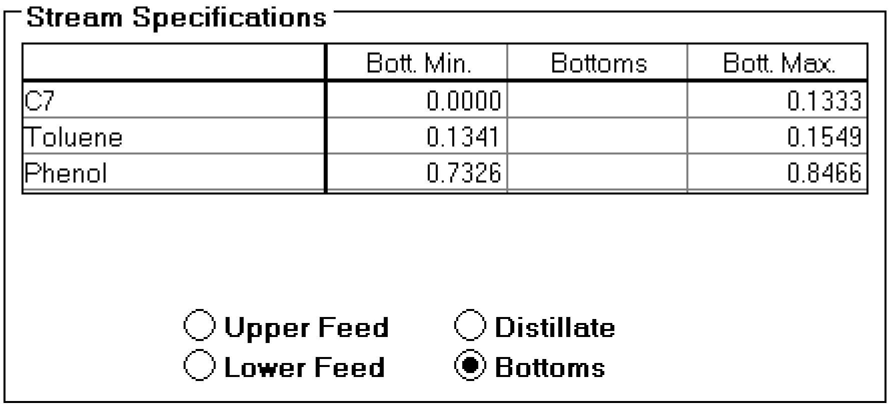


	UFeed Min.	UFeed	UFeed Max.
C7	1.0000e-06	1.0000e-06	1.0000e-06
Toluene	0.0010	0.0010	0.0010
Phenol	0.9990	0.9990	0.9990

We have specified the C7 and Phenol mole fractions to be 1E-06 and 0.9990 respectively. With an Upper Feed/Lower Feed ratio of 2.75, the Upper Feed flowrate is 1100 lbmole/hr. Note that at this point, we do not know if this is the optimum Upper Feed/Lower Feed ratio.

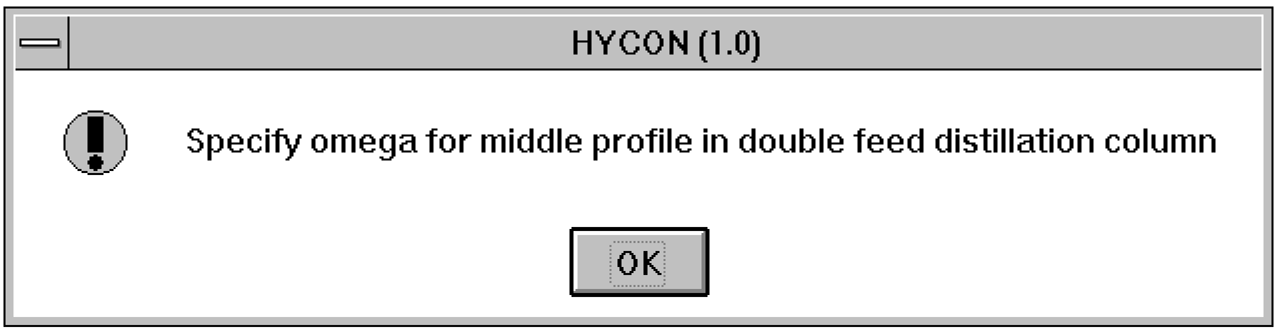
Next, specify a Distillate C7 mole fraction of 0.990. This restricts our range of choice for the remaining specifications.

Select the **Bottoms** radio button. You will see the following:



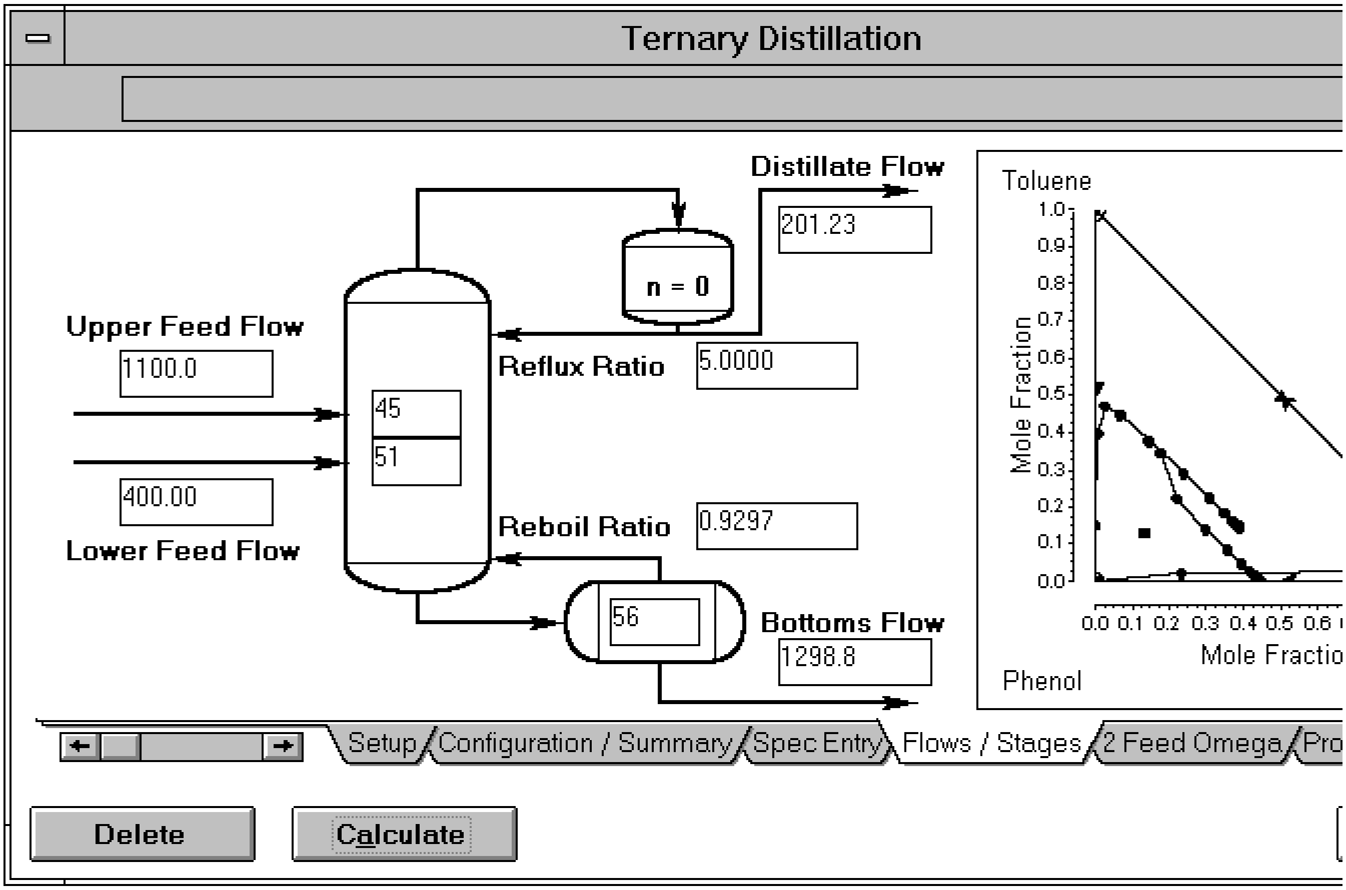
It would be advantageous to maximize the phenol in the bottoms stream. Set the Phenol fraction to be 0.846. This constrains the C7 mole fraction from 0 to 0.0007. Specify the C7 fraction to be 0.0006. The remaining mole fractions will be calculated based on the overall mole balance. At this point, all that is left is to specify a reflux ratio. As an initial estimate, set the reflux ratio to be 5.

Select the ***Calculate*** button. You will see the following message:



The optimum value for *Omega* (that which results in the lowest number of total stages) is automatically calculated; if you simply press the ***Calculate*** button again, the number of stages will be determined using this optimum value. Alternatively, you could set Omega to any value you wanted on the 2 Feed Omega page. We will always use the optimum value in this example.

After you select the ***Calculate*** button, move to the Flows / Stages page:



The total number of stages is excessively high. We could specify a lower heptane fraction in the bottoms — if we define it to be 0.0001 for instance, 29 stages are required. As well, if we respecify the bottoms composition so that the phenol fraction is lower, we will require less stages in this column.

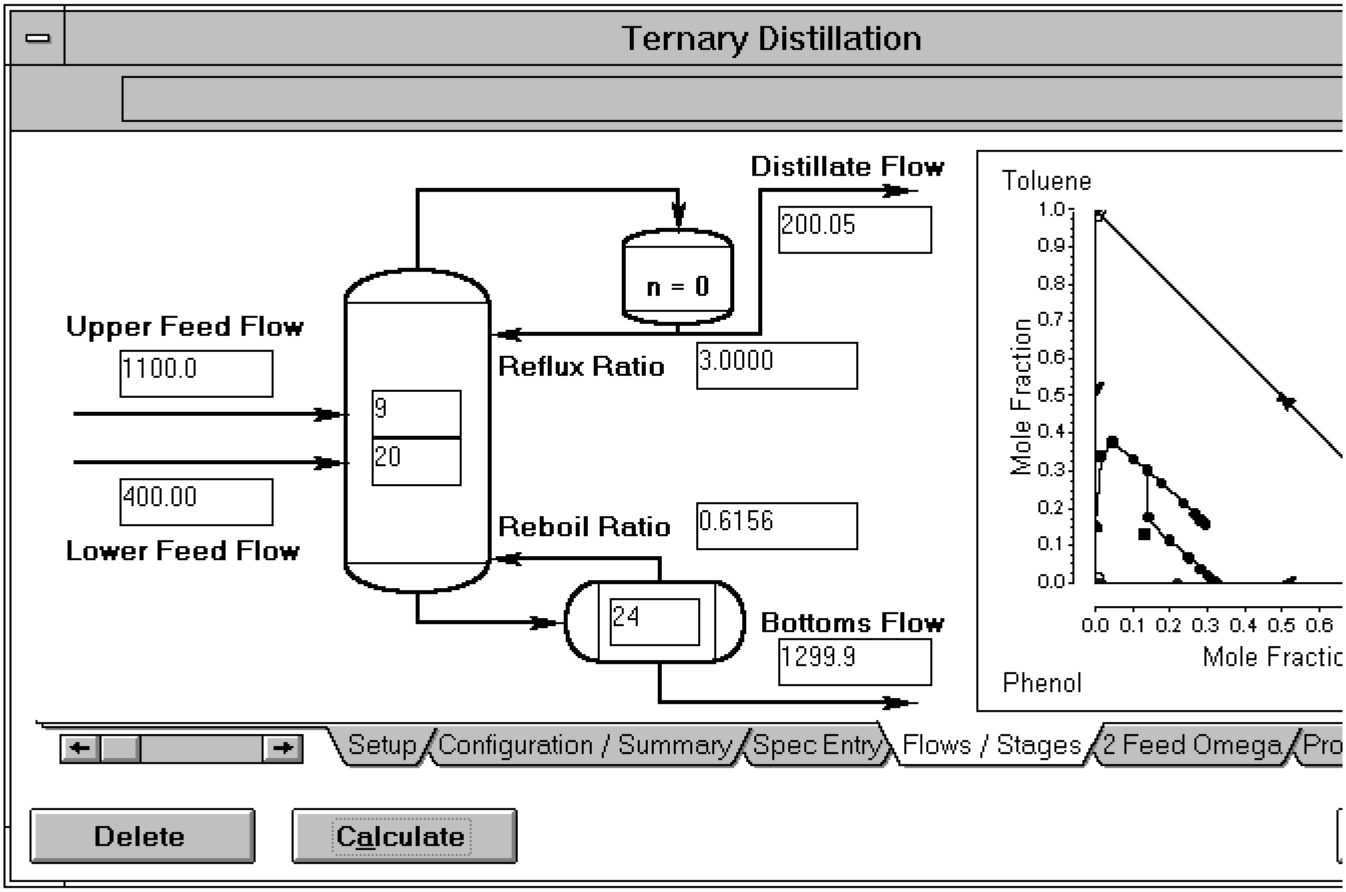
Because we want to take relatively pure toluene off the top of the second column and relatively pure phenol off the bottom, the heptane fraction in the bottoms coming off the first column must be small. Note that as we decrease the phenol composition, we must increase the C7 composition. Also, below a certain point (phenol composition » 0.836), the column profiles will not converge.

If we were to specify the heptane and phenol compositions to be 0.0065 and 0.84 respectively, 20 stages would be required to achieve these bottom compositions.

Note that most of the toluene and heptane in the bottoms stream will exit in the distillate stream of the second column. The toluene composition would be (1 - 0.84 - 0.0065) = 0.1535, and the toluene to heptane ratio about 24, which means that if most of the toluene and heptane were to exit in the distillate stream of the second column, the best purity we could obtain would be about 0.96. This is not adequate; therefore, the heptane composition must be even lower.

Specify the heptane and phenol compositions to be 0.0015 and 0.844. The Heptane to Toluene ratio is now 103, which should allow the Toluene fraction off the top of the second tower to be about 0.99.

The results are shown here:



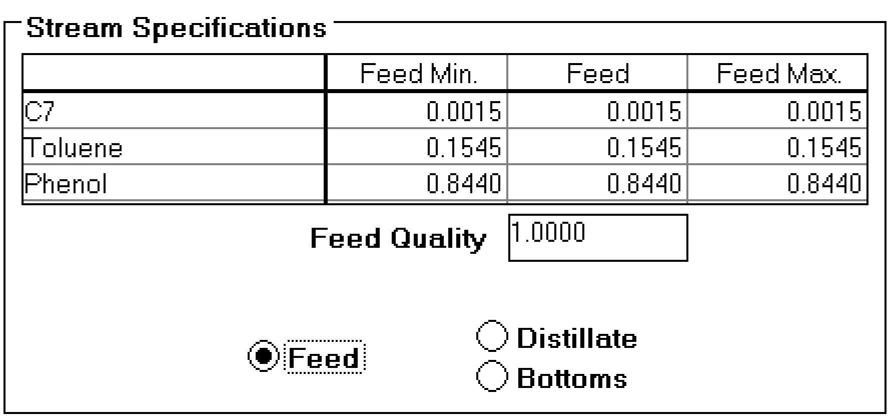
We will now create a new ternary distillation experiment, transferring the bottoms specifications for the first column to the feed for the second column.

Second Column

As before, set the pressure to 18 psia, and select the appropriate Fluid Package. Leave the settings on the Configuration/Settings page at their defaults (Single Feed, No Decanter, No Sidestream).

The Reflux Ratio for the second column will initially be set at 5.

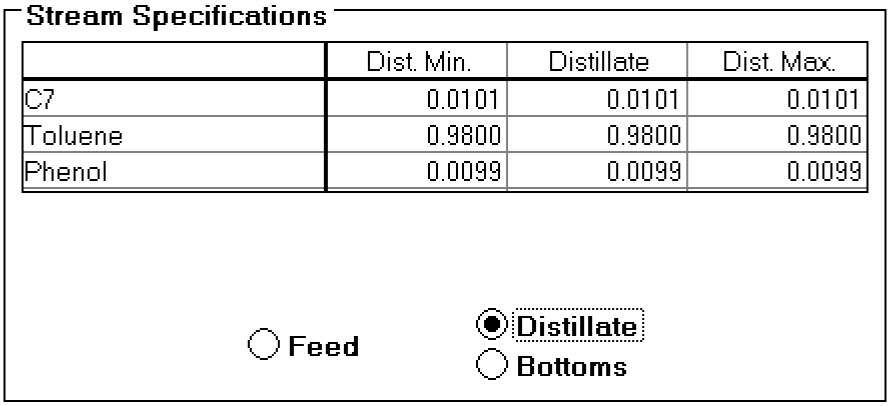
The Feed specifications, taken from the bottoms stream off the first column, are shown here:


Stream Specifications

	Feed Min.	Feed	Feed Max.
C7	0.0015	0.0015	0.0015
Toluene	0.1545	0.1545	0.1545
Phenol	0.8440	0.8440	0.8440

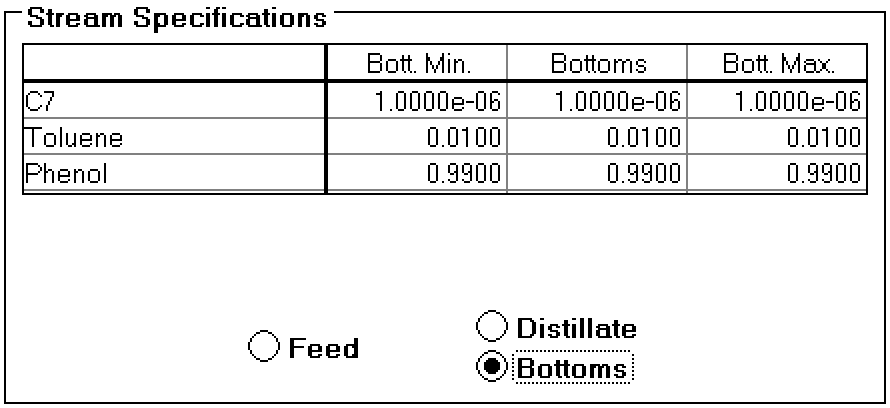
At this point, it may take some experimentation to see what stream specifications will result in a converged column.

The following specifications work for the distillate and bottoms:



Stream Specifications

	Dist. Min.	Distillate	Dist. Max.
C7	0.0101	0.0101	0.0101
Toluene	0.9800	0.9800	0.9800
Phenol	0.0099	0.0099	0.0099



Stream Specifications

	Bott. Min.	Bottoms	Bott. Max.
C7	1.0000e-06	1.0000e-06	1.0000e-06
Toluene	0.0100	0.0100	0.0100
Phenol	0.9900	0.9900	0.9900

Note that we should be able to obtain a higher toluene purity. As well, the phenol composition off the bottoms had to be adjusted to 0.99 (initially we had set the phenol composition in the recycle to 0.999).

At this step, 6 stages are required for the second column (where the sixth “stage” is the reboiler); the feed enters on the fourth stage.

At this point, we must return to the first column, using the new recycle stream specs. In other words, we must use the Bottoms specifications obtained here for the Top Feed of the first column.

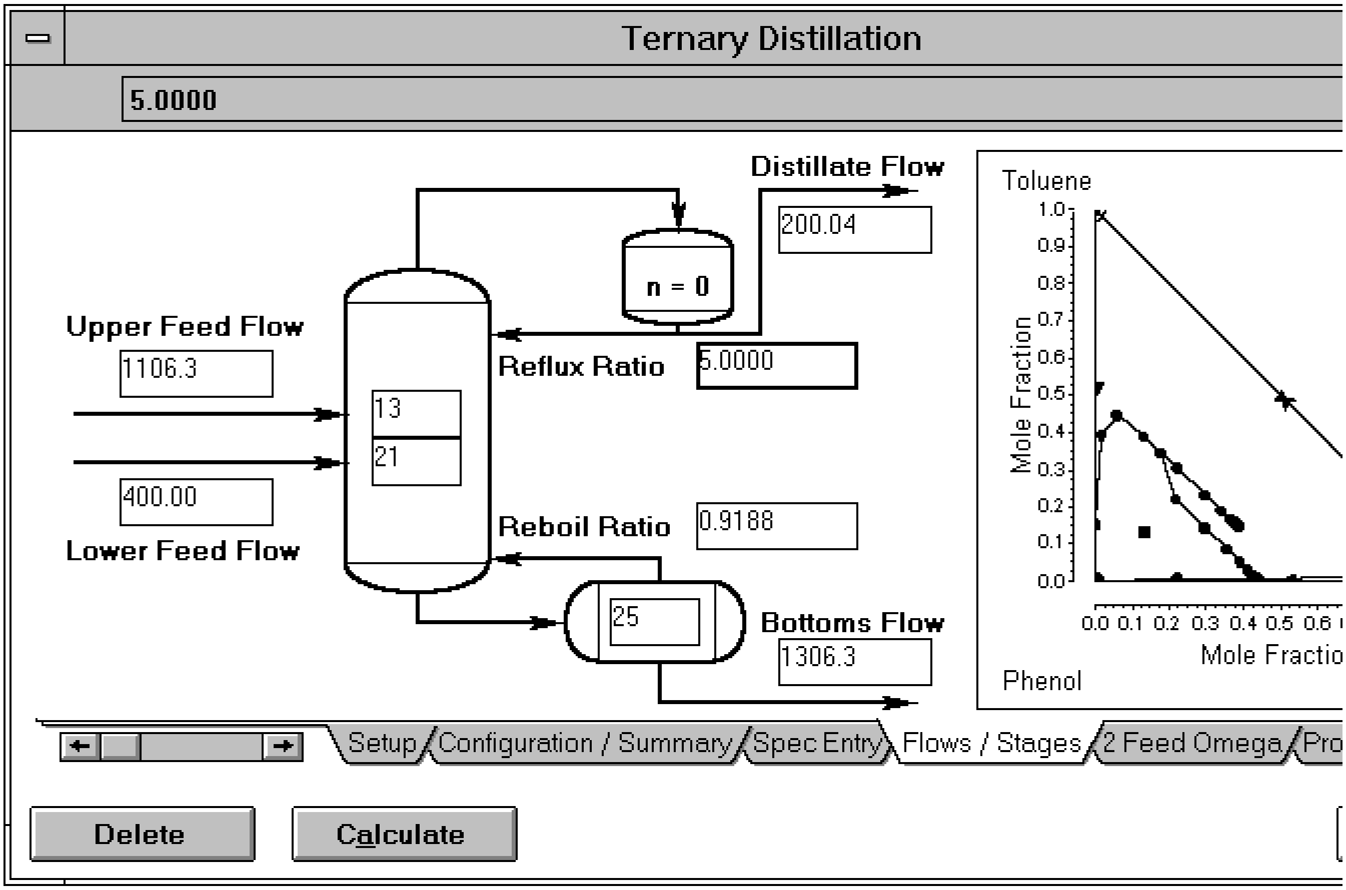
First Column: Second Pass

The recycle stream flow (upper feed) is now 1106.3, which gives us a feed ratio of 2.766. If we keep the recycle compositions as they are, the minimum number of stages required to obtain a heptane composition of 0.99 in the distillate is high (about 29). Thus we will have to increase the phenol composition to compensate.

We now have the following composition specifications:

Component	**Mixed Feed**	**Solvent Feed**	**Distillate**	**Bottoms**
C7	**0.5000**	**1e-6**	**0.99**	**0.0015**
Toluene	**0.5000**	0.0050	0.0055	0.1565
Phenol	0.0000	**0.9950**	0.0045	**0.8420**

Component fractions in boldface are specified; all other component fractions are calculated. The Flows/Stages page is shown below:

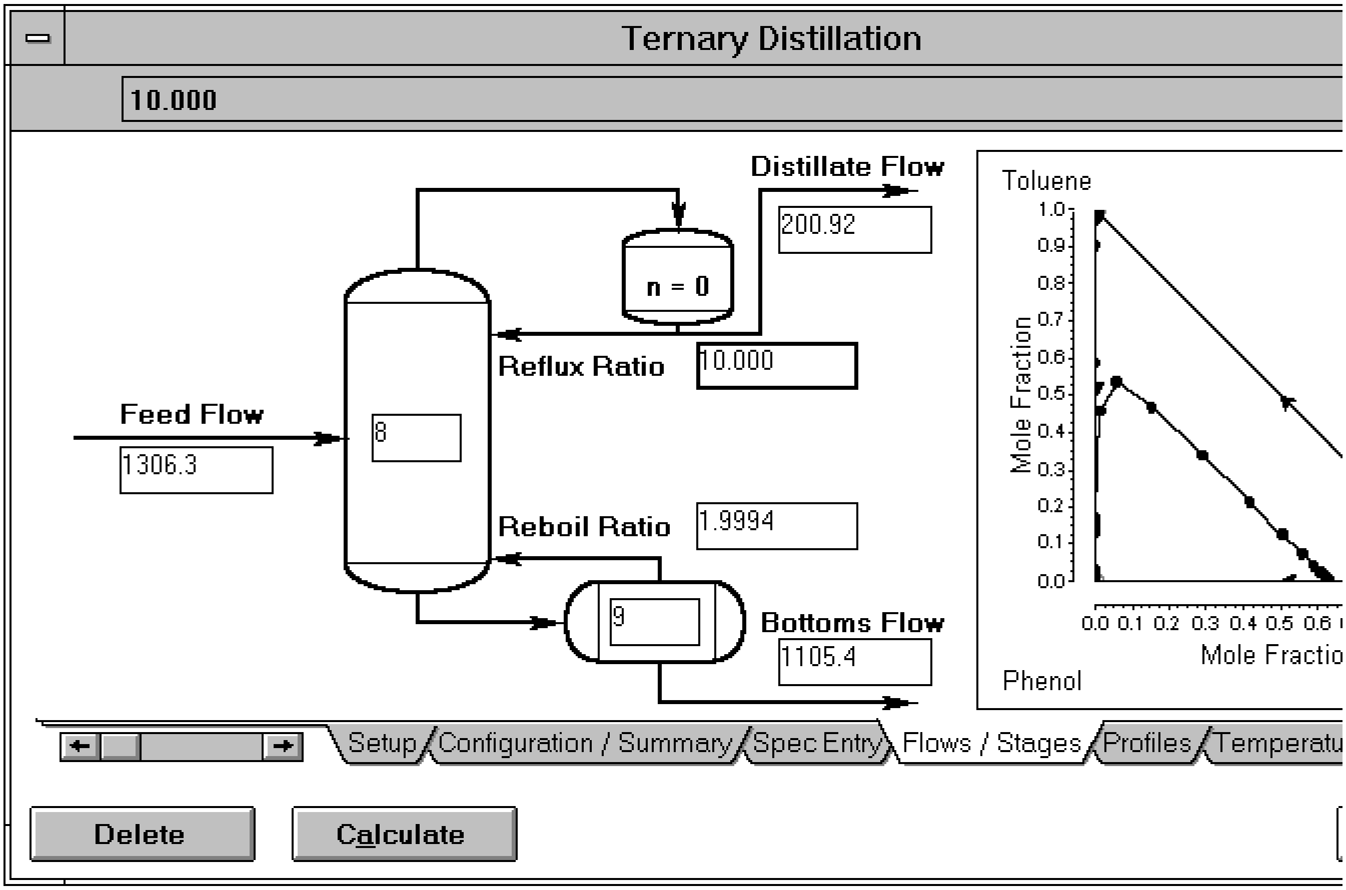


Second Column: Second Pass

At this point, the solvent feed stream to the first column has the same composition as the bottoms stream of the second column, and the feed to the second column has the same composition as the bottoms stream of the first column. The specifications are shown below:

Component	Feed	Distillate	Bottoms
C7	**0.0015**	0.0097	**1e-6**
Toluene	0.1565	**0.9900**	0.0050
Phenol	**0.8420**	0.0003	**0.9950**

The Flows/Stages page is shown below:



Note that the flows between the columns do not match precisely, but this is acceptable considering that this is a preliminary approximation. As well, there are inherent simplifications, such as the assumption of constant molal overflow. Thus, the results obtained here will not exactly match those determined in HYSYS.SteadyState. Using these results as a base case, the reflux ratio and product purities are now adjusted in order to determine an optimum configuration.

Effect of Reflux Ratio, Reboil Ratio and Purities

We will adjust the Reflux Ratio and Purities, observing their effect on other column variables such as the Reboil Ratio and the Number of Stages. Two configurations will be proposed, one which has lower purities (0.985/0.985), and one with higher purities (0.99/0.99), at the expense of a higher number of stages and/or higher Reflux/Reboil ratios.

Higher purities (0.99 / 0.99)

The *Base Case* constants and variables are tabulated below:

Constant	
Recycle Composition	1e-6 Toluene / 0.005 Heptane/ 0.995 Phenol
Lower Feed Composition	0.5 Toluene / 0.5 Heptane / 0 Phenol
Variable	
Reflux Ratio, Column 1	5
Reboil Ratio, Column 1	0.9188
Upper Feed Stage, Column 1	13
Lower Feed Stage, Column 1	21
Number of Stages, Column 1	25
Heptane Fraction, Column 1 Distillate	0.99
Reflux Ratio, Column 2	5
Reboil Ratio, Column 2	1.0906
Feed Stage, Column 2	8
Number of Stages, Column 2	10
Toluene Fraction, Column 2 Distillate	0.99

Reflux Ratio (Reboil Ratio) Column 1

Keeping other variables constant, the reflux ratio is adjusted. As shown in the table below, increasing the reflux ratio above 5 gives no improvement in the number of stages required for the separation. Decreasing the reflux ratio below five causes the number of stages to increase. We therefore conclude that a reflux ratio of 5 is optimum for the first column.

Reflux Ratio	**3**	**4**	**5**	**10**	**20**
Upper Feed Stage	18	15	13	11	10
Lower Feed Stage	26	24	21	20	20
Number of Stages	**30**	**28**	**25**	**24**	**25**
Reboil Ratio	0.6126	0.7657	0.9188	1.6846	3.2160

Heptane Fraction Column 1

As we increase the Heptane fraction in the distillate, the number of stages also increases. Although we would like a high purity, the number of stages increases substantially as we increase the Heptane Fraction above 0.990. At a Heptane fraction of 0.994, the number of stages is 58 which is much too high to be viable. We will go with a Heptane fraction of 0.990, at the expense of some extra stages.

Heptane Fraction	**0.985**	**0.989**	**0.990**	**0.991**	**0.992**	**0.994**
Upper Feed Stage	7	11	13	16	20	46
Lower Feed Stage	15	19	21	24	28	54
Number of Stages	**19**	**24**	**25**	**28**	**32**	**58**
Reflux Ratio (spec.)	5	5	5	5	5	5
Reboil Ratio	0.9242	0.9199	0.9188	0.9178	0.9167	0.9146

Reflux Ratio (Reboil Ratio) Column 2

The number of stages in the second column is only somewhat sensitive to the reflux ratio, as shown below. A reflux ratio of 5 is selected as the optimum. Decreasing the ratio to 4 is done at a cost of two extra stages, while increasing the ratio to 10 reduces the number of stages by one.

Reflux Ratio	**4**	**5**	**10**	**20**
Feed Stage	10	8	8	8
Number of Stages	**12**	**10**	**9**	**9**
Reboil Ratio	0.9088	1.0906	1.9994	3.8171

Toluene Fraction Column 1

With this configuration, we cannot predict toluene fractions above 0.99. We will keep the toluene fraction of 0.990, even though more stages are required.

Toluene Fraction	**0.985**	**0.989**	**0.990**
Feed Stage	6	7	8
Number of Stages	**8**	**9**	**10**
Reflux Ratio (spec.)	5	5	5
Reboil Ratio	1.0972	1.0919	1.0906

Upper/Lower Feed Ratio

Finally, the Upper/Lower Feed ratio was varied, and the effect on the number of stages in the first column observed:

U/L Ratio	**2**	**2.5**	**2.7**	**3**	**4**
Upper Feed Stage	23	13	13	11	10
Lower Feed Stage	30	22	21	20	20
Number of Stages	**35**	**26**	**25**	**24**	**23**

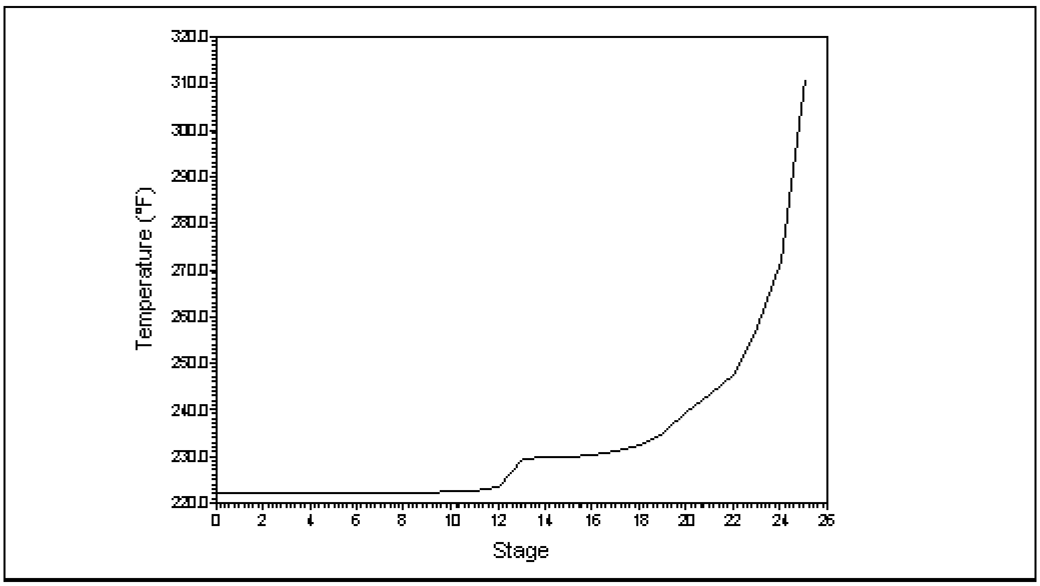
It appears that the U/L ratio that we used, 2.7, is reasonable in this case. Any increase in the ratio does not decrease the number of stages significantly.

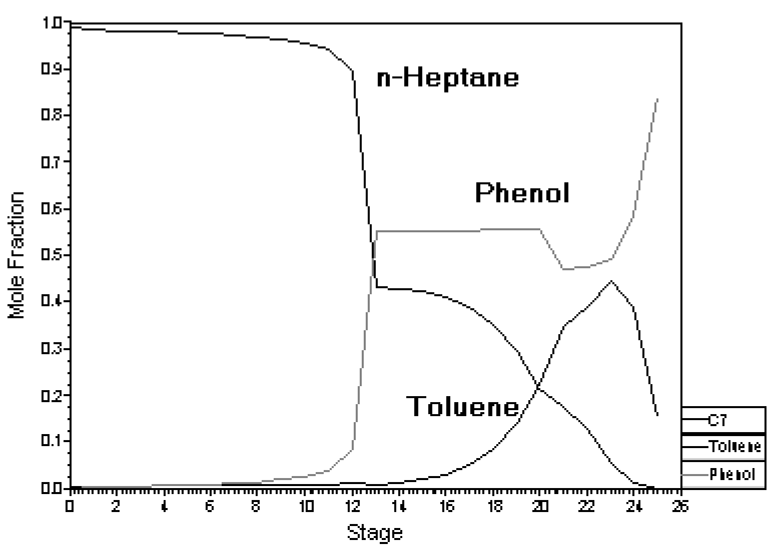
Results Using Optimized Values

These are the specs for the first (high purity) column configuration:

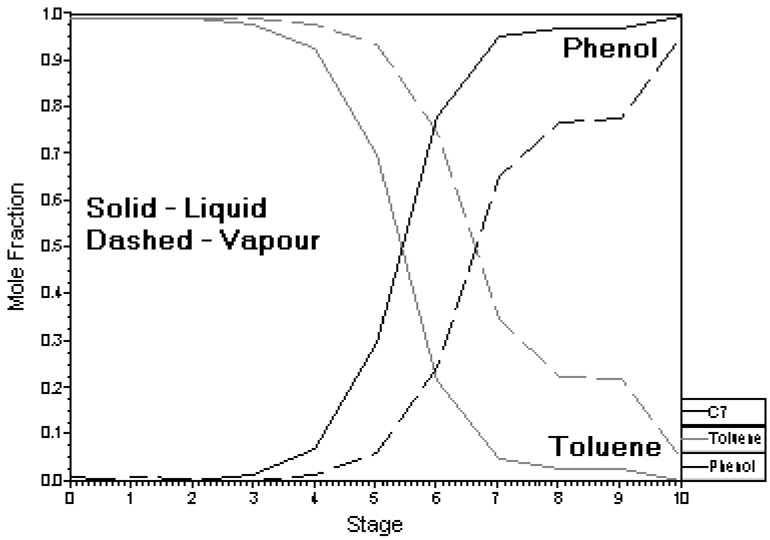
Reflux Ratio, Column 1	**5**
Reboil Ratio, Column 1	0.9188
Upper Feed Stage, Column 1	13
Lower Feed Stage, Column 1	21
Number of Stages, Column 1	25
Heptane Fraction, Column 1 Distillate	**0.99**
Reflux Ratio, Column 2	**5**
Reboil Ratio, Column 2	1.0906
Feed Stage, Column 2	8
Number of Stages, Column 2	10
Toluene Fraction, Column 2 Distillate	**0.99**

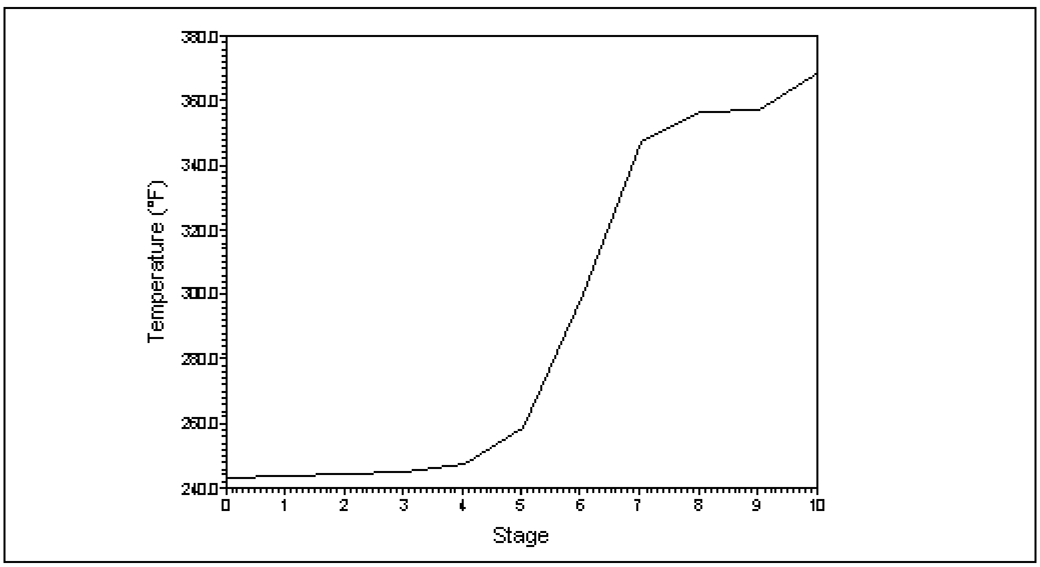
The temperature and liquid composition profiles for the first column are displayed below. Note that there are feed streams at stages 13 and 21.





The temperature and liquid/vapour composition profiles for the second column are shown below:





Lower purities (0.985 / 0.985)

With lower purities, we require a smaller phenol fraction in the Recycle (0.993); as well, we have set the upper/lower feed ratio to 2.75. As with the high purity case, we will start with a Reflux Ratio of 5 for both columns.

The *Base Case* constants and variables are tabulated below:

Constant	
Recycle Composition	1e-6 Toluene / 0.007 Heptane/ 0.993 Phenol
Lower Feed Composition	0.5 Toluene / 0.5 Heptane / 0 Phenol

Variable	
Reflux Ratio, Column 1	5
Reboil Ratio, Column 1	0.9231
Upper Feed Stage, Column 1	7
Lower Feed Stage, Column 1	17
Number of Stages, Column 1	20
Heptane Fraction, Column 1 Distillate	0.985
Reflux Ratio, Column 2	5
Reboil Ratio, Column 2	1.1015
Feed Stage, Column 2	8
Number of Stages, Column 2	10
Toluene Fraction, Column 2 Distillate	0.985

We will optimize only the reflux ratios, leaving the purities at 0.985 for both columns.

Reflux Ratio (Reboil Ratio) Column 1

As before, we adjust the reflux ratio, and observe the effect on the number of stages. When we increase the reflux ratio above 5, there is no improvement in the number of stages required for the separation. Decreasing the reflux ratio below five causes the number of stages to increase. We therefore conclude that a reflux ratio of 5 is optimum for the first column.

Reflux Ratio	**4**	**5**	**10**	**20**
Upper Feed Stage	8	7	7	6
Lower Feed Stage	19	17	17	19
Number of Stages	**23**	**20**	**21**	**20**
Reboil Ratio	0.7693	0.9231	1.6924	3.2310

Reflux Ratio (Reboil Ratio) Column 2

The number of stages in the second column is only somewhat sensitive to the reflux ratio, as shown below. A reflux ratio of 4 is selected as the optimum.

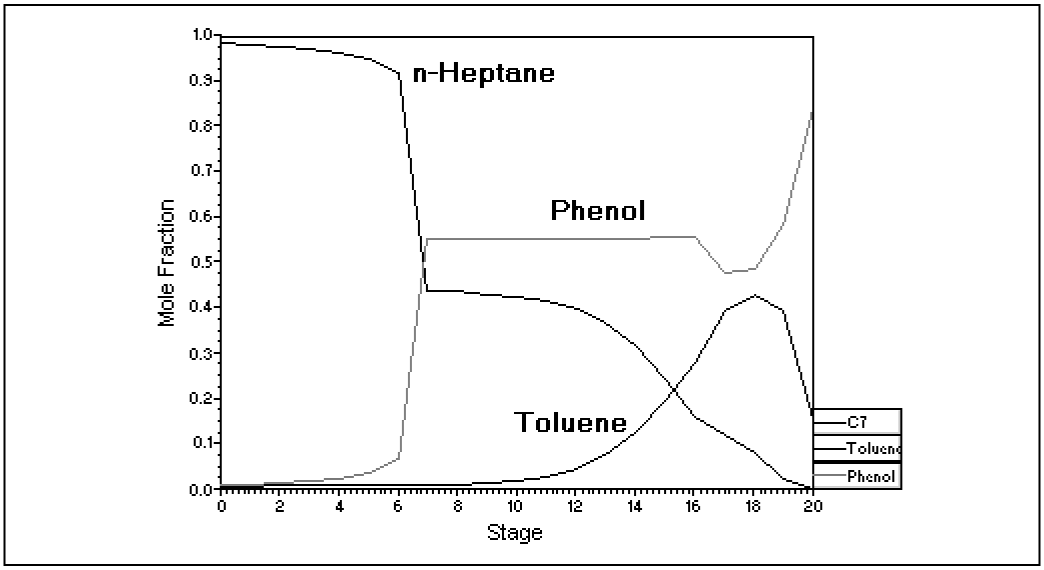
Reflux Ratio	**3**	**4**	**5**	**10**	**20**
Feed Stage	9	8	8	7	8
Number of Stages	**11**	**10**	**10**	**9**	**9**

Results Using Optimized Values

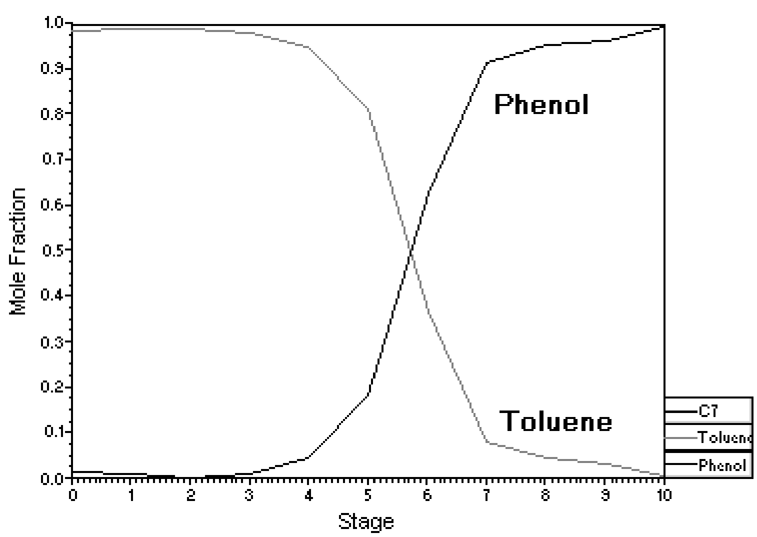
These are the specs for the second (lower purity) column configuration:

Reflux Ratio, Column 1	**5**
Reboil Ratio, Column 1	0.9231
Upper Feed Stage, Column 1	7
Lower Feed Stage, Column 1	17
Number of Stages, Column 1	20
Heptane Fraction, Column 1 Distillate	**0.985**
Reflux Ratio, Column 2	**4**
Reboil Ratio, Column 2	0.9187
Feed Stage, Column 2	8
Number of Stages, Column 2	10
Toluene Fraction, Column 2 Distillate	**0.985**

The Stage Liquid Compositions are shown here for the first column:



Also, the Liquid composition profiles for the second column are shown:



C-6.5

PART 3 *Building the Columns in HYSYS*

In this section, we will construct the columns in HYSYS.SteadyState, and obtain a steady-state solution for both column configurations.

> Note that the interaction parameters for the NRTL package can be exported from HYSYS - Conceptual Design to HYSYS.SteadyStateor HYSIM using the ***Export to HYSIM*** button in the HYSYS - Conceptual Design Fluid Package.

Define the Fluid Package as follows:

- Property Package — **NRTL**
- Components — **n-Heptane**, **Toluene**, **Phenol**

> In HYSYS.SteadyState, the c term is the alpha term.
> In HYSYS - Conceptual De-sign, the b term is the alpha term.

Change the Interaction Parameters to match the regressed parameters obtained in Part 1 (or copy the .dat and .idx files which you created in HYSYS - Conceptual Design to the Support directory).

Activity Model Interaction Parameters

Coeff Matrix To View: (●) Aij ( ) Bij ( ) Alphaij / Cij

	n-Heptane	Toluene	Phenol			
n-Heptane	—	425.193	1328.000			
Toluene	-160.034	—	-188.100			
Phenol	1539.000	824.200	—			

Activity Model Interaction Parameters

Coeff Matrix To View: ( ) Aij ( ) Bij (●) Alphaij / Cij

	n-Heptane	Toluene	Phenol			
n-Heptane	—	0.302	0.508			
Toluene	0.302	—	0.010			
Phenol	0.508	0.010	—			

> We require the phenol stream to “make up” for phenol lost in the toluene and heptane product streams.

In the Main Environment WorkSheet, specify the Feed and phenol makeup streams as follows:

Name	**Feed**	**phenol makeup**
Vapour Frac	0.0000	0.0000
Temperature [F]	**220.0000**	**220.0000**
Pressure [psia]	**20.0000**	**20.0000**
Molar Flow [lbmole/hr]	**400.0000**	**1.2000**
Mass Flow [lb/hr]	38469.1605	94.1128
Liq Vol Flow [barrel/day]	3448.3151	6.1028
Heat Flow [Btu/hr]	-1.5788e+07	-60190.9080
Comp Mole Frac [n-Heptane]	**0.5000**	**0.0000**
Comp Mole Frac [Toluene]	**0.5000**	**0.0000**
Comp Mole Frac [Phenol]	**0.0000**	**1.0000**

High Purity Configuration

In HYSYS - Conceptual Design, the number of trays includes the reboiler. In HYSYS.SteadyState, the number of trays does not include the reboiler. Therefore the number of trays in each column are 24 and 9, not 25 and 10, as predicted in part 2. The Feed locations remain the same.

In the SubFlowsheet, add the Tray Sections, Reboilers and Condensers for the high purity setup:

TRAY SECTION	TS-1
CONNECTIONS	
Number of Trays Feeds (Stage) Liquid Inlet Vapour Inlet Liquid Outlet Vapour Outlet	24 Feed (21) Solvent (13) Phenol Makeup (13) Reflux-1 Boilup-1 To Reboiler 1 To Condenser-1
PARAMETERS	
Tray Section Type	Standard

TRAY SECTION	TS-2
CONNECTIONS	
Number of Trays Feeds (Stage) Liquid Inlet Vapour Inlet Liquid Outlet Vapour Outlet	9 COL1 Bottoms (8) Reflux-2 Boilup-2 To Reboiler-2 To Condenser-2
PARAMETERS	
Tray Section Type	Standard

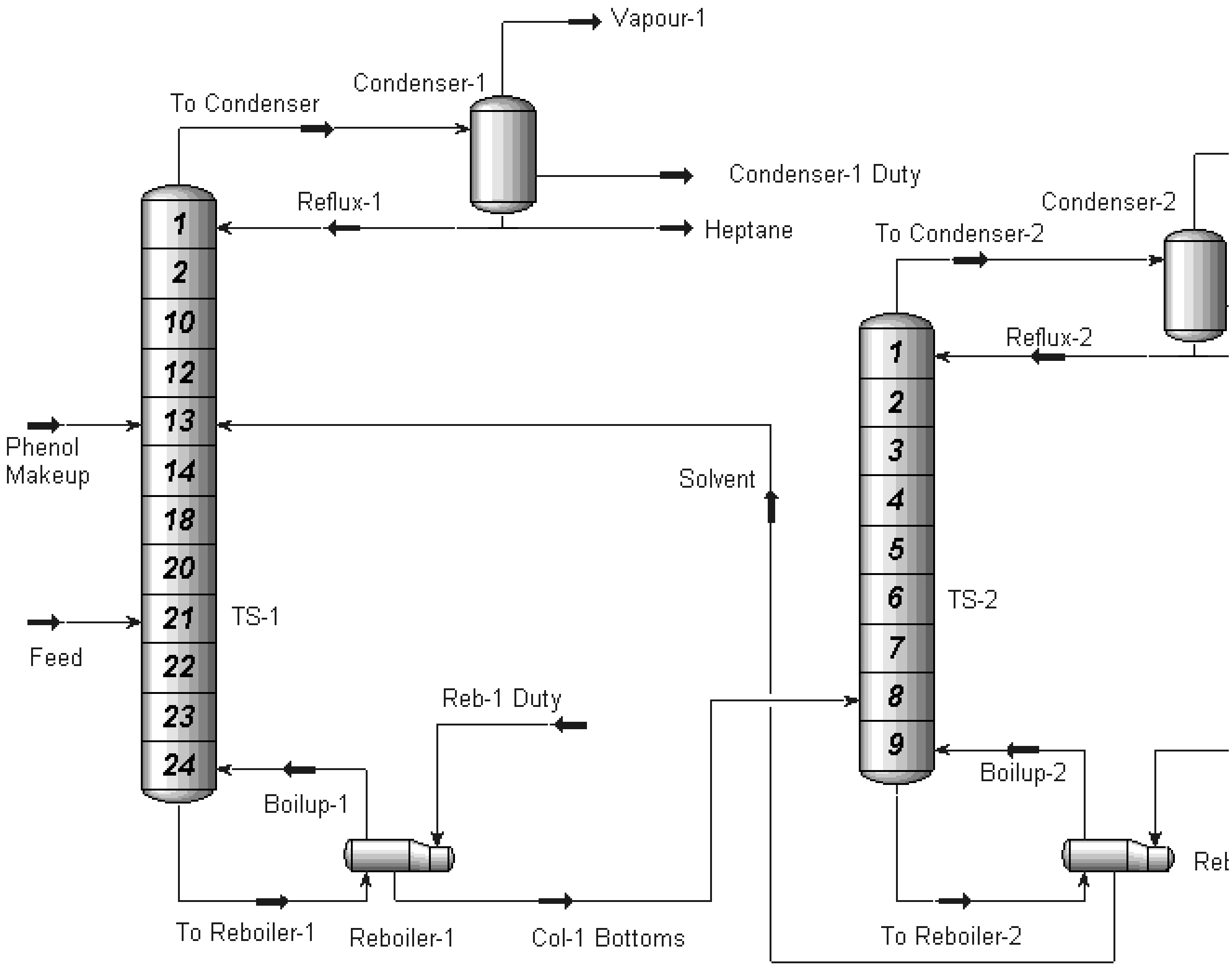
TOTAL CONDENSER	Condenser-1
CONNECTIONS	
Feed Distillate Reflux Energy	To Condenser-1 Heptane Reflux-1 COL1 Cond Q
PARAMETERS	
Pressure Drop	0 psi

TOTAL CONDENSER	Condenser-2
CONNECTIONS	
Feed Distillate Reflux Energy	To Condenser-2 Toluene Reflux-2 COL2 Cond Q
PARAMETERS	
Pressure Drop	0 psi

REBOILER	Reboiler-1
CONNECTIONS	
Feed Boilup Bottoms Product Energy	To Reboiler-1 Boilup-1 COL1 Bottoms COL1 Reb Q
PARAMETERS	
Pressure Drop	0 psi

REBOILER	Reboiler-2
CONNECTIONS	
Feed Boilup Bottoms Product Energy	To Reboiler-2 Boilup-2 Solvent COL2 Reb Q
PARAMETERS	
Pressure Drop	0 psi

The PFD will appear as follows:



Return to the Main Flowsheet, bring up the Column view, and enter the following specifications:

Pressures

- Condenser-2 — 16 psia
- Reboiler-2 — 20 psia
- Condenser-1 — 16 psia
- Reboiler-1 — 20 psia

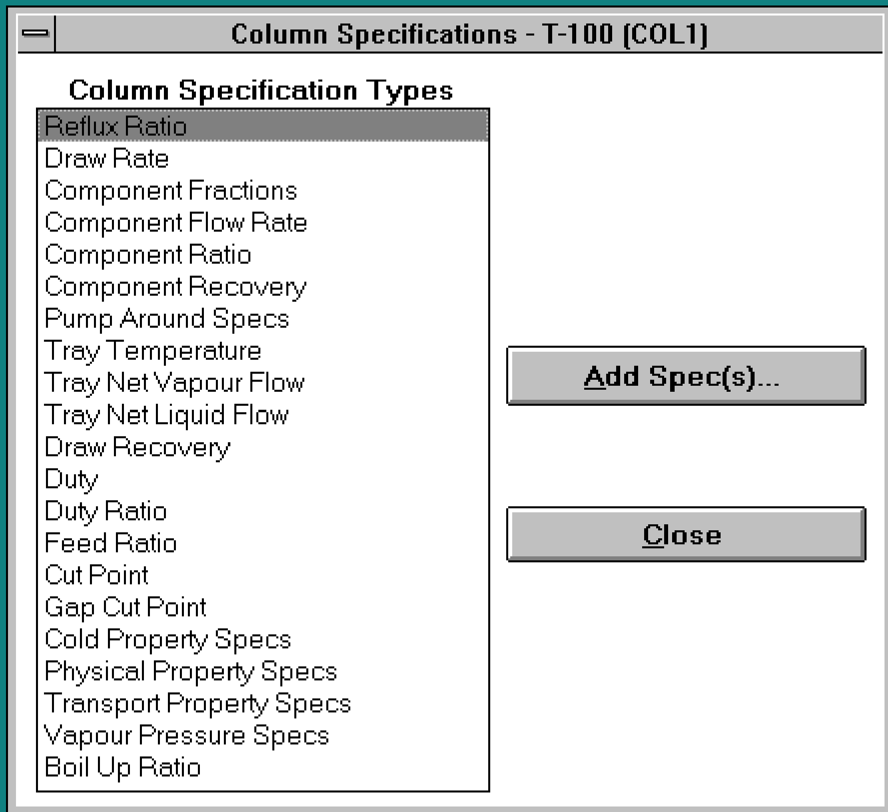
Temperature Estimates

- Temperature Estimate Condenser-1 — 220 F
- Temperature Estimate Condenser-2 — 240 F

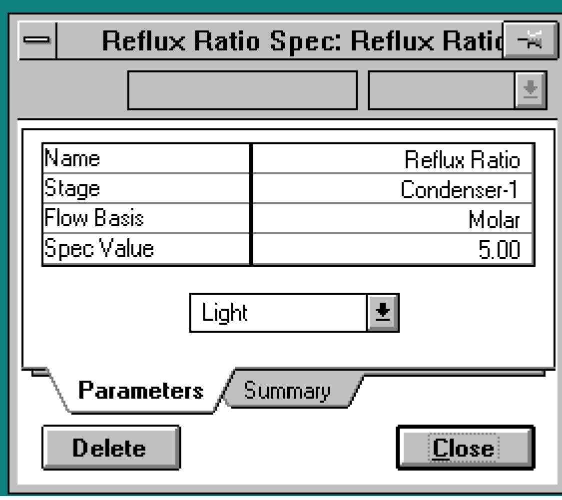
Solving the Column

Next, we will add the specifications.

To add a specification, select the ***Add*** button on the Specs Page, then select a specification from the list:



As an example, the Reflux Ratio spec is shown here:



We want to solve to the following specifications:

- Reflux Ratio = 5 (Reflux Ratio-1, Condenser-1, Molar, 5)
- Reflux Ratio2 = 5 (Reflux Ratio-2, Condenser-2, Molar, 5)
- Heptane Frac = 0.99 (Heptane Frac, Condenser-1, Mole Fraction, Liquid, 0.99, Heptane)
- Toluene Frac = 0.99 (Toluene Frac, Condenser-2, Mole Fraction, Liquid, 0.99, Toluene)

It may not be possible to immediately solve to these specifications. There are several alternative methods you can use to obtain a solution; the following two methods may work:

1. Add the following Flow Spec:

- Toluene Flow = 200 lbmole/hr (Toluene Flow, Toluene, Molar, 200 lbmole/hr)

Activate the Reflux Ratio specs, the Toluene Frac spec and the Toluene Flow spec. Run the column. Once it solves, replace the Toluene Flow spec with the Heptane Frac spec. Re-run the column (do not reset).

2. Add the following Toluene Recovery Spec:

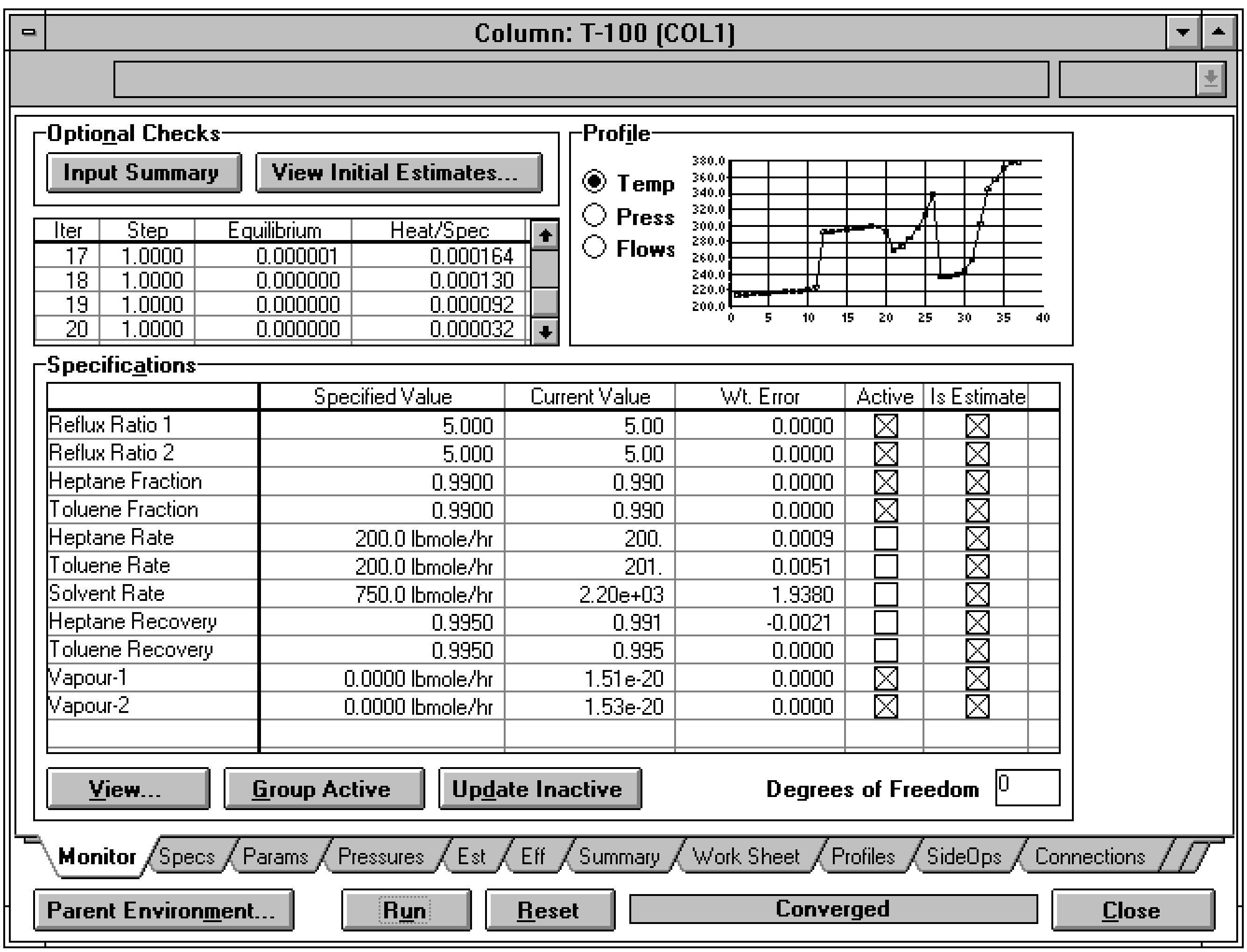
- Toluene Recovery = 0.995 (Toluene Recovery, Toluene, Molar, 0.995)

Activate the Reflux Ratio specs, the Heptane Frac spec and the Toluene Recovery spec. Run the column. Once it solves, replace the Toluene Recovery spec with the Toluene Frac spec. Re-run the column.

> Whether a certain set of specifications will solve depends in part on the solution history, even if you have ***Reset*** the solution.

You may have to "approach" a spec by choosing a conservative value for the specification, then successively approaching the actual specification. ***Run*** (but do not ***Reset***) the column after each change.

In any case, once you have converged, you will see a view similar to the following:



Note the similarities in the temperature profile shown here with the profiles obtained using HYSYS - Conceptual Design.

We obtain the following Condenser and Reboiler duties:

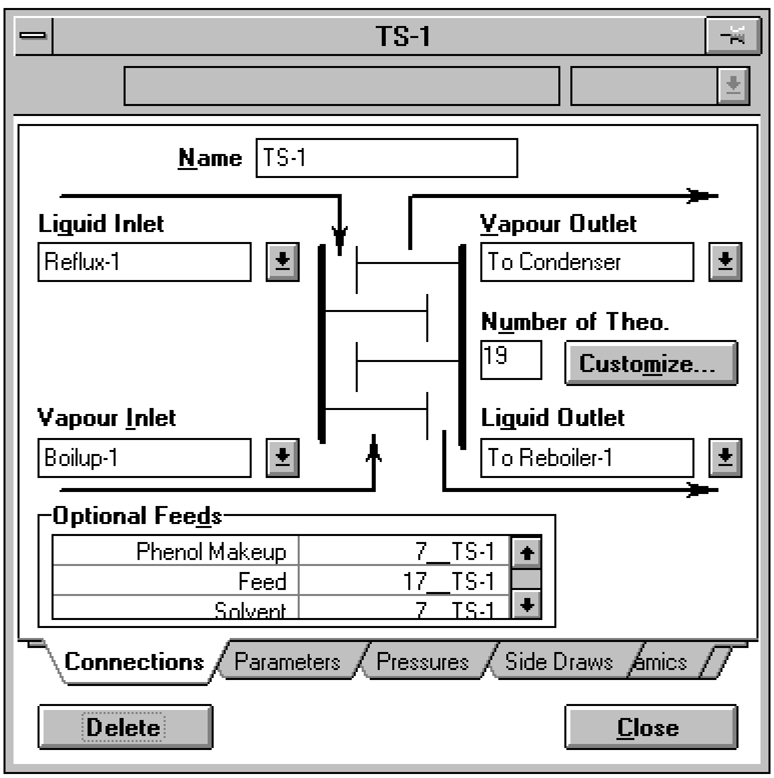
- Column 1 Condenser — 1.64e+07 Btu/hr
- Column 2 Condenser — 1.72e+07 Btu/hr
- Column 1 Reboiler — 1.32e+07 Btu/hr
- Column 2 Reboiler — 2.04e+07 Btu/hr

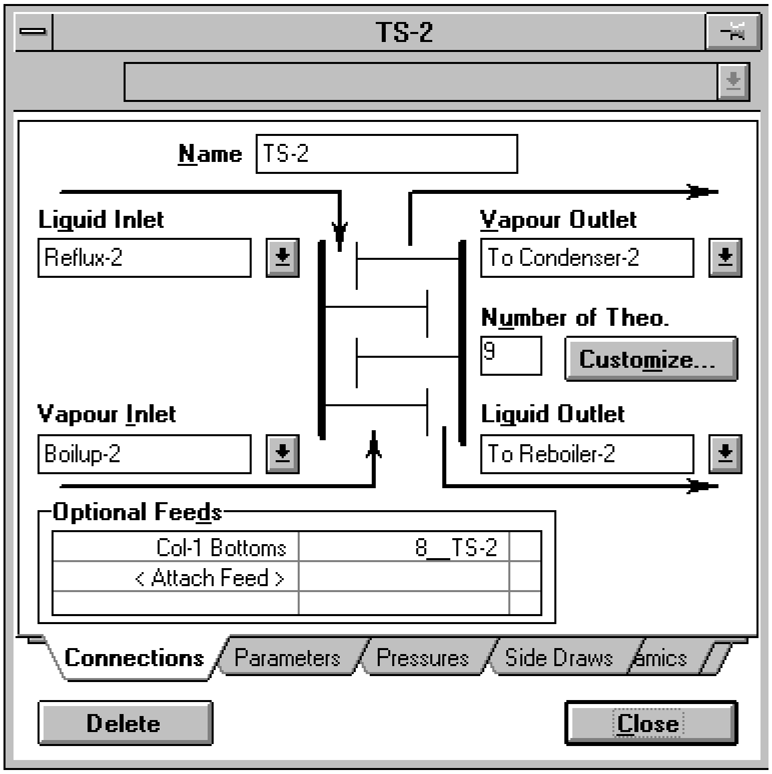
Note that we can further increase the distillate compositions to 0.994 and 0.993 (Toluene and Heptane, respectively). This is an improvement over the specifications estimated using HYSYS - Conceptual Design.

At this point, you may want to save the first configuration in a separate file.

Low Purity Configuration

Rather than reinstalling the Tray Sections, Reboilers and Condensers, simply adjust the number of stages and feed locations as follows:





Ensure that you are in the Main Flowsheet, then bring up the column view. The pressures and temperature estimates will be defined as before:

Pressures

- Condenser-2 — 16 psia
- Reboiler-2 — 20 psia
- Condenser-1 — 16 psia
- Reboiler-1 — 20 psia

Temperature Estimates

- Temperature Estimate Condenser-1 — 220 F
- Temperature Estimate Condenser-2 — 240 F

The types of specifications are the same as before; therefore it is not necessary to add new specs. Simply change the Heptane and Toluene Fracs to 0.985.

Solving the Column

We want to solve to the following specifications:

- Reflux Ratio = 5 (Reflux Ratio-1, Condenser-1, Molar, 5)
- Reflux Ratio2 = 5 (Reflux Ratio-2, Condenser-2, Molar, 5)
- Heptane Frac = **0.985** (Heptane Frac, Condenser-1, Mole Fraction, Liquid, 0.985, Heptane)
- Toluene Frac = **0.985** (Toluene Frac, Condenser-2, Mole Fraction, Liquid, 0.985, Toluene)

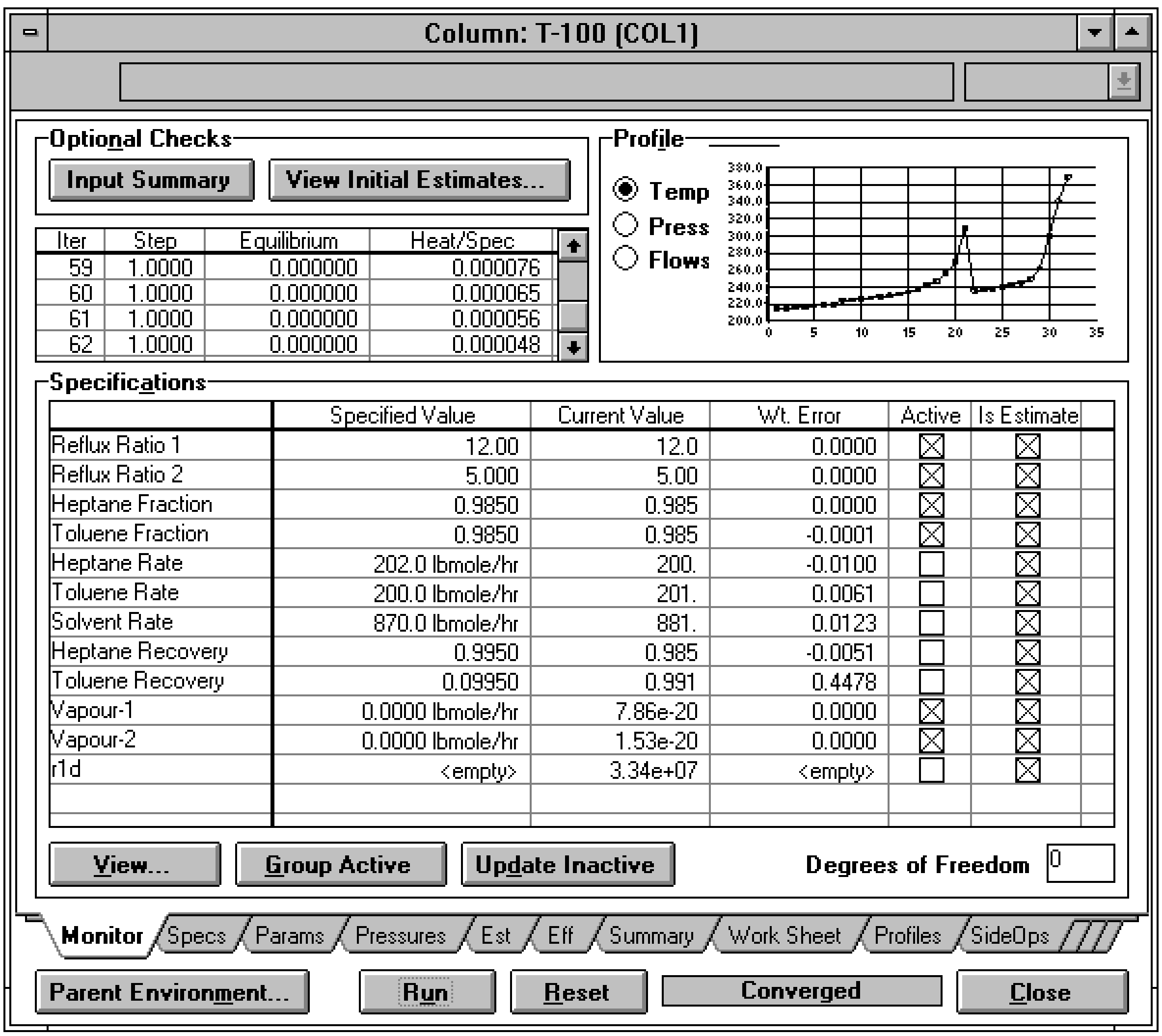
In this case, it is not possible to meet the specifications predicted by HYSYS - Conceptual Design. The following configurations for the low purity case are possible:

- Heptane Fraction 0.985
- Toluene Fraction 0.985
- Reflux Ratio Column 1 = 12
- Reflux Ratio Column 2 = 4

or

- Heptane Fraction = 0.970
- Toluene Fraction = 0.985
- Reflux Ratio Column 1 = 5
- Reflux Ratio Column 2 = 4

The first configuration maintains the purity specs, while the second maintains the reflux ratio specs. The first configuration is more desirable despite the high Reflux Ratio; the solved column using these specifications appears as follows:



Although less stages are required for this configuration, the Condenser and Reboiler duties are much higher, and it is unlikely that the reduced capital cost will compensate for the increased utility cost. This will be confirmed in the next section.

We obtain the following Condenser and Reboiler duties:

- Column 1 Condenser — 3.54e+07 Btu/hr
- Column 2 Condenser — 1.72e+07 Btu/hr
- Column 1 Reboiler — 3.34e+07 Btu/hr
- Column 2 Reboiler — 1.92e+07 Btu/hr

C-6.6 Optimization

PART 4 ***Economics: Background***

A Spreadsheet will now be set up in HYSYS.SteadyState to calculate the economics of the process. The methods used here to calculate capital costs, expenses and revenue are relatively simple, but are sufficient to provide a preliminary estimate. The benefit of these methods is that they are easy to implement, and as they are formula-based, can be used in the optimization calculations.

This section is divided into the following parts:

- **Raw Data** — Data which is used in the calculation of capital costs, expenses, revenue and net present worth.
- **Capital Cost** — Initial equipment and related costs associated with the construction of the process, incurred at time zero.
- **Annual Expenses** — Expenses associated with the operation of the plant, incurred at the end of each year.
- **Revenue** — Income obtained from the sale of the process products, namely Toluene and Heptane; incurred at the end of each year.
- **Net Present Worth** — Economic calculation taking into account the Capital Cost and Gross Income, used to obtain the net present worth.
- **Nomenclature and Constants** — A list of the nomenclature and constants used in the various expressions in this section.

Raw Data

Some of the Economic, Material and Utility costs that are used in this simulation are shown below:

Economic	
Cost Index 1996 to 1990	1.07
Tax Rate	28%
Interest minus Inflation	7%
Working Days/Year	300

Raw Material, Product and Utility Costs	
Toluene ($/gal)	0.76
Heptane ($ /gal)	0.74
Feedstock ($/gal)	0.58
Phenol ($/lb)	0.41
Water ($/1000 gal)	0.25
Natural Gas ($/1E6 Btu)	3.20

In addition to these, the following variables are required from the Steady-State solution, and will be imported into the Spreadsheet.

First Condenser Duty	Second Condenser Duty	First Reboiler Duty
Second Reboiler Duty	Phenol Mass Flow	Toluene Mass Flow
Heptane Mass Flow	Feed Flow	TS 1 Liquid Mass Flow
TS 2 Liquid Mass Flow	Feed Standard Density	Toluene Standard Density
Heptane Standard Density	Number of Trays, Column 1	Number of Trays, Column 2

Capital Cost

A *percentage of delivered-equipment cost* method is used to determine the total capital investment. That is, the equipment (column tray sections, reboilers and condensers) are sized and priced; all additional costs, such as piping, construction and so on are calculated as a percentage of the equipment cost.

Equipment Cost

Equipment	Cost	Reference
First Column Condenser	$12.75 \times \frac{Q_{COND_1}}{9000} + 9300$	1-373
Second Column Condenser	$12.75 \times \frac{Q_{COND_2}}{9000} + 9300$	1-373
First Column Reboiler	$19.5 \times \frac{Q_{REB_1}}{5300} + 15000$	1-373
Second Column Reboiler	$19.5 \times \frac{Q_{REB_2}}{5300} + 15000$	1-373
First Column Tray Section	$\exp\left(0.958 \times \ln\left(D_{TRAY1} \times 12\right) + 4.44\right) \times N_{TRAY1}$ $D_{TRAY1} = \sqrt{\frac{F_{TRAY1} \times (1/120)}{0.25\,\pi \times (1/6) \times \rho}}$	1-712
Second Column Tray Section	$\exp\left(0.958 \times \ln\left(D_{TRAY2} \times 12\right) + 4.44\right) \times N_{TRAY2}$ $D_{TRAY2} = \sqrt{\frac{F_{TRAY2} \times (1/120)}{0.25\,\pi \times (1/6) \times \rho}}$	1-712

All expressions here are derived from a graph or table. The Reboiler and Condenser expressions are regressed linearly, while the Tray Section expression assumes a linear relationship on a log-log scale.

The sum of the costs of these six items is the Equipment cost (based on 1990 prices).

Direct and Indirect Costs

The costs of each item below is estimated as the Equipment cost multiplied by the respective Factor for that item. Direct costs include Installation, Instrumentation, Piping, Electrical, New Building, Yard, Service and Land. Indirect costs include Engineering /Supervision and Construction.

Item	Factor	Reference
Installation	0.40	1 (171)
Instrumentation	0.18	1 (172); 1 (183)
Piping	0.60	1 (173)
Electrical	0.10	1 (174)
New Building	0.20	1 (175)
Yard	0.10	1 (182)
Service	0.70	1 (182)
Land	0.06	1 (182)
Engineering / Supervision	0.33	1 (182)
Construction	0.30	1 (182)

Contracting and Contingency

These are applied based on the Equipment, Direct and Indirect Costs. Contracting is estimated to be 5% of the sum of all Equipment, Direct and Indirect Costs, and Contingency (unforeseen events) is estimated as 10% of the sum of these costs.

Item	Factor	Reference
Contracting	0.05	1 (182)
Contingency	0.10	1 (182)

The total Fixed Capital Investment (FCI) is the sum of all Equipment, Direct, Indirect, Contracting and Contingency costs, multiplied by the cost index factor of 1.07.

Working Capital

The working capital is estimated to be 15% of the Fixed Capital Investment.

Annual Expenses

The following table lists the expenses which are considered in the economic analysis of this plant.

Expense	Annual Cost	Reference
Cost of Phenol	$F_{PH} \times C_{PH} \times 24N$	1 (197); 1 (816)
Cost of Feedstock	$\frac{F_F \times C_F \times 7.481 \times 24 \times N}{\rho_{F,STD}}$	1 (197)
Labour*	$\exp\left(0.219 \times \ln\left(\left(\frac{F_{TOL} \times 24}{2000}\right) + 2.844\right)\right) \times L_{COST} \times N$	1 (198)
Supervision and Clerical	Labour Cost x 15%	1 (202)
Maintenance and Repairs	FCI x 6%	1 (203)
Operating Supplies	Maintenance x 15%	1 (204)
Lab Charges	Labour Cost x 15%	1 (204)
Condenser 1 Cooling Water	$\frac{Q_{COND_1} \times 24 \times N \times 7.481 \times C_{H_2O}}{70 \times 62.4 \times 1000 \times C_p^{H_2O}}$	1 (815)
Condenser 2 Cooling Water	$\frac{Q_{COND_2} \times 24 \times N \times 7.481 \times C_{H_2O}}{70 \times 62.4 \times 1000 \times C_p^{H_2O}}$	1 (815)
Reboiler 1 Natural Gas	$\frac{Q_{REB_1} \times 24 \times N \times C_{GAS}}{1E6}$	1 (815)
Reboiler 2 Natural Gas	$\frac{Q_{REB_2} \times 24 \times N \times C_{GAS}}{1E6}$	1 (815)
Depreciation	FCI x 10%	1 (205)
Local Taxes	FCI x 2%	1 (205)
Insurance	FCI x 1%	1 (205)
Plant Overhead	(Labour Cost + Supervision and Clerical Cost + Maintenance and Repairs Cost) x 60%	1 (205)
Administrative	Labour Cost x 20%	1 (206)
Distribution	Gross Income x 4%	1 (207)
Research and Development	Gross Income x 4%	1 (207)

* Linearly Regressed from Graph

The individual expenses are totalled, and multiplied by a cost index factor (1.07) to account for 1990 to 1996 inflation.

Revenue

Revenue	Annual Cost	Reference
Toluene	$\frac{C_{TOL} \times 24 \times N \times 7.481 \times F_{TOL} \times x_T}{\rho_{T,STD}}$	1 (816)
Heptane	$\frac{C_{HEP} \times 24 \times N \times 7.481 \times F_{HEP} \times x_H}{\rho_{H,STD}}$	1 (816)

The total gross revenue is the sum of the amount obtained from selling the products, multiplied by the cost index factor (1.07).

Calculation of Net Present Worth

The following points outline the simplified calculation for net present worth:

- The total capital investment is the Fixed Capital Investment plus the Working Capital. This expenditure is the total cash flow for year zero.
- It is assumed that the life of the process is five years. The revenue and expenses are applied at the end of each year, from years one to five.
- The Annual Operating Income is the Annual Income minus the Annual Costs.
- The Income after tax is the Annual Operating Income multiplied by one minus the tax rate.
- The Annual Cash Income is the Income after tax plus the Depreciation Expense, which was earlier discounted as an annual expense.
- It is assumed that there is no salvage value; the Annual Cash Income is exactly the same for years one to five.
- The Net Present Worth *of the Annual Cash Income* is determined using the following formula:

$$PW = \left(\frac{1}{1+i} + \frac{1}{(1+i)^2} + \ldots + \frac{1}{(1+i)^n} \right) \times \textit{Annual Income}$$

This expression simplifies to:

$$PW = \left(\frac{\left(1 - \left(\frac{1}{(1+i)^n}\right)\right)}{i} \right) \times \textit{Annual Income}$$

- The Total Net Present Worth is the total capital investment (negative cash flow) plus the Net Present Worth of the Annual Cash Income.

Nomenclature and Constants used in Economic Analysis

Nomenclature
$r_{F,STD}$ = Standard Density of Feedstock (lb/ft^3)
$r_{H,STD}$ = Standard Density of Heptane (lb/ft^3)
$r_{T,STD}$ = Standard Density of Toluene (lb/ft^3)
C_F = Cost of Feedstock ($/gal)
C_{GAS} = Cost of natural gas ($/1E6 Btu)
C_{H2O} = Cost of water ($/1000 gal)
C_{HEP} = Cost of Heptane ($/gal)
C_{PH} = Cost of Phenol ($/lb)
C_p^{H2O} = Heat Capacity of water (1 Btu/lb F)
C_{TOL} = Cost of Toluene ($/gal)
D_{TRAY1} = Diameter of First Tray Section (ft)
D_{TRAY2} = Diameter of Second Tray Section (ft)
F_{FOL} = Feed Flow (lb/hr)
F_{PH} = Phenol Flow (lb/hr)
F_{TOL} = Toluene Flow (lb/hr)
$F_{TRAY1,}$ = Liquid Mass Flowrate for First Tray Section, from Stage 20 (lb/h)
$F_{TRAY2,}$ = Liquid Mass Flowrate for Second Tray Section, Stage 1 (lb/h)
i = Annual rate of interest (in this case, interest minus inflation)
N = Number of working days/yr
N_{TRAY1} = Number of Trays in First Tray Section
N_{TRAY2} = Number of Trays in Second Tray Section
n = Life of project (y)
Q_{COND1} = Duty, Column 1 Condenser (Btu/hr)
Q_{COND2} = Duty, Column 2 Condenser (Btu/hr)
Q_{REB1} = Duty, Column 1 Reboiler (Btu/hr)
Q_{REB2} = Duty, Column 2 Reboiler (Btu/hr)
x_H = Mole Fraction of Heptane in Heptane Product
x_T = Mole Fraction of Toluene in Toluene Product

Constant Used in Expression	Unit
24	hours/day
7.481	gal/ft^3
2000	lb/ton
0.219	Constant in Labour Cost Expression
2.844	Constant in Labour Cost Expression
70	F (DT Cooling Water)
62.4	lb/ft^3 (Density of water)
1000	No units (Cost = $/1000 gal)
1E6	No units (Cost = $/1E6 Btu)
0.25	No units (Portion of formula for area)
1/6	ft (Height of weir - 2”)
1/120	hr (Residence time on tray - 1/2 minute)

Setting up the Spreadsheet

Note that the Spreadsheet we are constructing contains some information which is not used in this example, but which may be of generic use.

Note that the Spreadsheet we are constructing contains some information which is not used in this example, but which may be of generic use.

If you want to use this Spreadsheet as a template for other processes, it is a good idea to set it up as a template file, then insert it as subflowsheet in the appropriate case. These are the steps:

1. Create a new template and enter Fluid Package data.
2. Add a Spreadsheet and enter the following information:

Note that the Spreadsheet we are constructing contains some information which is not used in this example, but which may be of generic use.

- Simulation Data
- Economic Data
- Capital Cost Data
- Expense and Revenue Data
- Capital Cost Calculation
- Expense and Revenue Calculation
- Net Present Worth Calculation

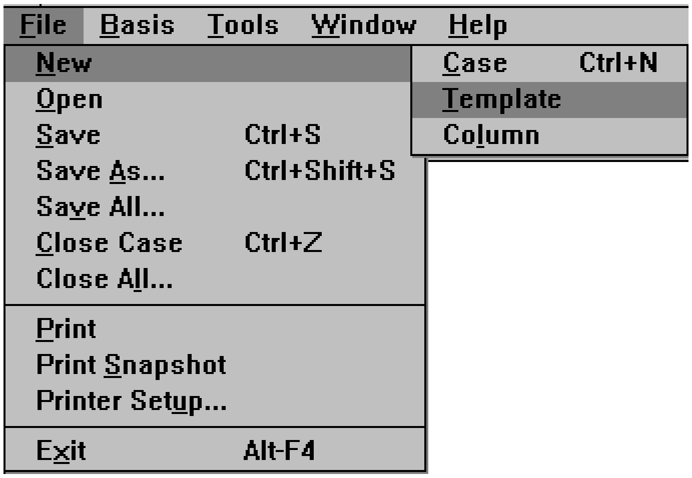
3. Save the template.

4. Retrieve the process case, and add a subflowsheet, using the previously created file as a template.

5. Import data links into Spreadsheet.

Creating a New Template

From the file menu, select **New Template**.



As with creating a Case, it is necessary to define a Fluid Package. Select NRTL with components n-Heptane, Toluene and Phenol. Enter the Main Environment.

Adding the Spreadsheet

Simulation Data

Column *A* lists the headings, while column *B* will contain the data imported from the case file, or the appropriate formula. When we load this template into the case, we will then import the appropriate variables into this Spreadsheet.

Enter the headings as shown below.

	A	B
1	SIMULATION DATA	
2	Condenser Duty	
3	Condenser 2 Duty	
4	Reboiler Duty	
5	Reboiler 2 Duty	
6	COL1 Bottoms Flow	
7	COL1 Bot Density	
8	Solvent Flow	
9	Solvent Density	
10	Phenol Flow	
11	Toluene Flow	
12	Heptane Flow	
13	# Trays COL1	
14	# Trays COL2	
15	Feed Flow	
16	Feed StdDensity	<empty>
17	CC CALC	
18	C1 Duty	<empty>
19	C2 Duty	<empty>
20	R1 Duty	<empty>
21	R2 Duty	<empty>
22	Tray Section 1 D	<empty>
23	Tray Section 2 D	<empty>
24		
25	Flow TS 1	
26	Flow TS 2	

The formulae for cells B16 - B23 (excluding B17) are:

B16	+((b15*24)/(b17*5.615))/c17*b17
B18	+b2
B19	+b3
B20	+b4
B21	+b5
B22	+((b25)/(5*3.1415*b7))^.5
B23	+((b26)/(5*3.1415*h16))^.5

Although the Feed Standard Density could also be imported in HYSYS.SteadyState, HYSYS - Dynamic Design does not accept the import, and it is necessary to enter the formula as shown in cell B16.

Economic and Annual Data

The Economic, Annual Expense and Revenue Data is shown below:

	C	D	E	F
1	ECONOMIC DATA		DP COST DATA	
2	Cost Index/1990	1.07	Phenol ($/lb)	0.41
3	Tax Rate	0.28	Feedstock ($/gal)	0.58
4	Interest-Inflation	0.07	Ave. Labor ($/hr)	20
5	Working Days/Year	300	Sup/Cl - % of Op Lab	15
6			Maint - % of FCI	6
7	FIXED CHARGES		Supplies - % of Maint	15
8	Dep (% of FCI)	10	Lab - % of Op Lab	15
9	Local Tax (% of FCI)	2	C H2O ($/1000 gal)	0.25
10	Insurance (% of FCI)	1	Gas ($/1e6 Btu)	3.2
11				
12	PLANT OVHD		GENERAL DATA	
13	% of Labor & Main.	60	Admin (% Op Lab)	20
14			Distribution (% G Inc)	4
15	Toluene ($/gal)	0.76	R&D (% of Gross Inc)	4
16	Heptane ($/gal)	0.74		
17				

Enter all data exactly as shown. There are no formulae on this page.

Capital Cost Data

	G	H
1	CAP COST DATA	
2	Install Factor	0.4
3	Instrument. Factor	0.18
4	Piping Factor	0.6
5	Electrical Factor	0.1
6	New Building Factor	0.2
7	Yard Factor	0.1
8	Service Factor	0.7
9	Land Factor	0.06
10	Eng/Sup Factor	0.33
11	Construction Factor	0.3
12	Contracting Factor	0.05
13	Contingency Factor	0.1
14	Work Cap (% of FCI)	15
15		
16	Toluene Density	
17	Heptane Density	
18	Toluene StdDensity	<empty>
19	Heptane StdDensity	<empty>

The Capital Cost Data is set up in columns G and H. There is also some additional Simulation Data in this area (H16 - H19). The Toluene Density and Heptane Density will be imported into cells H16 and H17, respectively. Although the Standard Densities could also be imported in HYSYS.SteadyState, HYSYS - Dynamic Design does not accept the import, and we must use the following formulae:

H18	+((b11*24)/(h16*5.615))/i6*h16
H19	+((b12*24)/(h17*5.615))/i7*h17

Capital Cost Calculation

The Capital Cost Calculation is performed in cells C18 - D30. Note that cells A18 - B26 have already been completed.

	A	B	C	D
18	C1 Duty	<empty>	Condenser 1 Cost	<empty>
19	C2 Duty	<empty>	Condenser 2 Cost	<empty>
20	R1 Duty	<empty>	Reboiler 1 Cost	<empty>
21	R2 Duty	<empty>	Reboiler 2 Cost	<empty>
22	Tray Section 1 D	<empty>	TS 1 Cost	<empty>
23	Tray Section 2 D	<empty>	TS 2 Cost	<empty>
24			SUBTOTAL	<empty>
25	Flow TS 1		D&I Factors	3.02
26	Flow TS 2		SUBTOTAL	<empty>
27			C&C Factors	0.15
28			TOTAL FCI	<empty>
29			Adjusted FCI	<empty>
30			TOTAL WCP	<empty>

All of the cells in column D shown here are formulae **- do not** enter the values *3.02* and *0.15*!

The formulae are listed below:

D18	+12.75*b18/9000+9300
D19	+12.75*b19/9000+9300
D20	+b20*19.5/5300+15000
D21	+b21*19.5/5300+15000
D22	@exp(.958*@ln(b22*12)+4.44)*b13
D23	@exp(.958*@ln(b23*12)+4.44)*b14
D24	+d18+d19+d20+d21+d22+d23
D25	+h2+h3+h4+h5+h6+h7+h8+h9+h10+h11+h12
D26	+d24*(1+d25)
D27	+h12+h13
D28	+d26*(1+d27)
D29	+d2*d28
D30	+d29*h14/100

Expense Calculation

The Total Expenses and Adjusted Expense (incorporating Cost Index Factor) are displayed in cells B50 and D50, respectively.

The Expenses are listed in column B, rows 32-49.

	A	B	C	D
31	Ann. PROD COSTS			
32	Phenol	<empty>		
33	Feedstock	<empty>		
34	Labor	<empty>		
35	Super/Clerical	<empty>		
36	Maintenance	<empty>		
37	Operating	<empty>		
38	Lab	<empty>		
39	C1 Cooling Water	<empty>		
40	C2 Cooling Water	<empty>		
41	Reboiler 1 Nat. Gas	<empty>		
42	Reboiler 2 Nat. Gas	<empty>		
43	Depreciation	<empty>		
44	Local Taxes	<empty>		
45	Insurance	<empty>		
46	Plant Overhead	<empty>		
47	Administrative	<empty>		
48	Distribution	<empty>		
49	R&D	<empty>		
50	TOTAL EXPENSES	<empty>	Adjusted Expense	<empty>

These are the formulae used:

B32	+b10*f2*24*d5
B33	+b15*f3*24*7.481*d5/b16
B34	+(@exp(.219*@ln(b11*24/2000)+2.844))*f4*d5
B35	+f5*b34/100
B36	+f6*d29/100
B37	+f7*b36/100
B38	+f8*b34/100
B39	+b2*24*d5*7.481*f9/(70*62.4*1000)
B40	+b3*24*d5*7.481*f9/(70*62.4*1000)
B41	+b4*24*d5*f10/(1e6)
B42	+b5*24*d5*f10/(1e6)
B43	+d28*d8/100
B44	+d28*d9/100
B45	+d28*d10/100
B46	+d13*(b34+b35+b36)/100
B47	+f13*b34/100
B48	+f14*(e33+e34)/100
B49	+f15*(e33+e34)/100
B50	+b32+b33+b34+b35+b36+b37+b38+b39+b40+b41+b42+b43+b44+b45+b46+b47+b48+b49
D50	+b50*d2

Revenue Calculation

The calculation of Revenue is shown below; the purities of the Toluene and Heptane in the respective distillates will be imported to cells D33 and D34.

	C	D	E	F
32	INCOME	Purity	Annual Income	Adjusted Income
33	Toluene		<empty>	<empty>
34	Heptane		<empty>	<empty>
35			TOTAL	<empty>

E33	+d15*24*d5*7.48*b11*d33^1/h18
E34	+d16*24*d5*7.48*b12*d34^1/h19
F33	+d2*e33
F34	+d2*e34
F35	+f33+f34

Calculation of Net Worth

This is determined in cells E37 - F50, as shown below.

	E	F
37	FCI	<empty>
38	WC	<empty>
39	Capital Investment	<empty>
40		
41	Annual Income	<empty>
42	Annual Cost	<empty>
43	Annual Op Income	<empty>
44	Income after tax	<empty>
45	Annual Cash Income	<empty>
46		
47	LIFE OF PROJECT	5
48	Capital Investment	<empty>
49	Total Present Value	<empty>
50	NET Present Worth	<empty>

Note that cell F47 contains the constant *5*, indicating the life of the project.

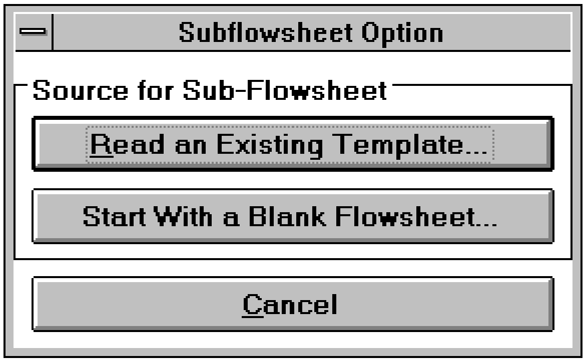
The formulae are listed below:

F37	+d29
F38	+d30
F39	+f37+f38
F41	+f35
F42	+d50
F43	+f41-f42
F44	+(1-d3)*f43
F45	+b43+f44
F48	+f39
F49	+((1-(1/(1+d4)^f47))/d4)*f45
F50	+f49-f48

The template is now complete. Save it (e.g. - ECONANAL.TPL), and load the HYSYS case.

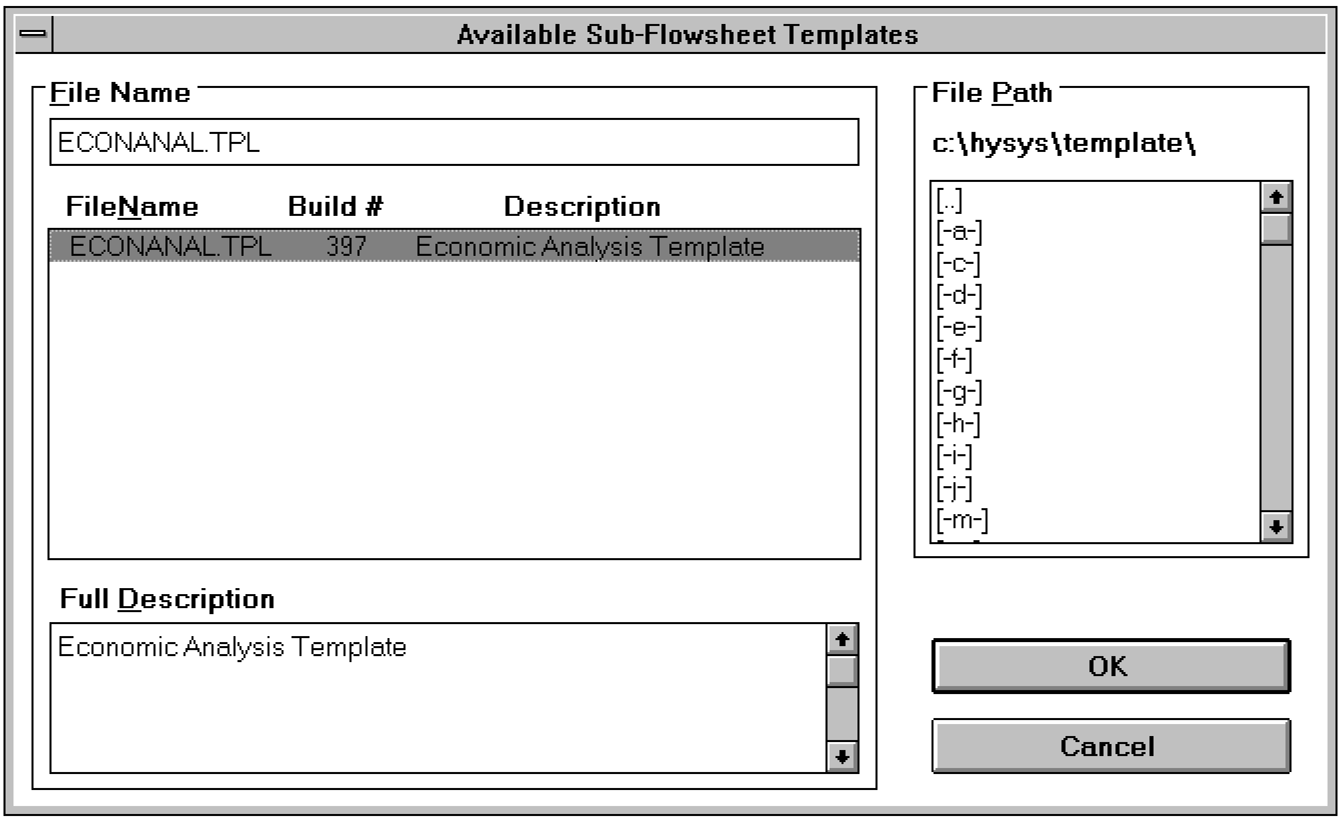
Importing Variables into Spreadsheet

First, add the subflowsheet; select the ***Read an Existing Template*** button when prompted to select the source for the sub-flowsheet.



Select the template from the list (in this case, we have called the template ECONANAL.TPL, and saved it in the c:\hysys\template directory).

HYSYS will create a new subflowsheet with the Spreadsheet you set up when you created the template.



There are a large number of variables to import into the Spreadsheet. They are all listed below:

Imported Variables

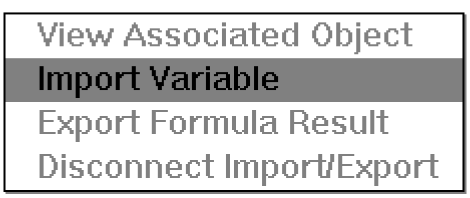
Cell	Object	Variable Description
B2	Condenser-1 Duty	Heat Flow
B3	Condenser-2 Duty	Heat Flow
B4	Reb-1 Duty	Heat Flow
B5	Reb-2 Duty	Heat Flow
B6	Col-1 Bottoms	Mass Flow
B7	Col-1 Bottoms	Mass Density
B8	Solvent	Mass Flow
B9	Solvent	Mass Density
B10	Phenol Makeup	Mass Flow
B11	Toluene	Mass Flow
B12	Heptane	Mass Flow
B15	Feed	Mass Flow
B17	Feed	Mass Density
B25	TS-1	Stage Liq Net Mass Flow (20__TS-1)
B26	TS-2	Stage Liq Net Mass Flow (1__TS-2)
C17	Feed	Liquid Volume Flow
D33	Toluene	Comp Mole Frac (Toluene)
D34	Heptane	Comp Mole Frac (n-Heptane)
H16	Toluene	Mass Density
H17	Heptane	Mass Density
I16	Toluene	Liquid Volume Flow
I17	Heptane	Liquid Volume Flow

There are two ways to import the variables to the Spreadsheet:

1. Importing From the Connections Page

To add an import, select the ***Add Import*** button, and choose the variable using the Variable Navigator (For more information, see HYSYS Reference, **Chapter 4 - Navigation**). In the **Cell** column, type or select from the drop down list the Spreadsheet cell to be connected to that variable. When you move to the Spreadsheet page, that variable will appear in the cell you specified.

2. Importing Variables from the Spreadsheet Page (Browsing)



You may also import a variable by positioning the cursor in an empty field of the Spreadsheet and clicking the right mouse button. You will see the menu shown to the right. Choose **Import Variable**, and using the Variable Navigator (see HYSYS Reference, **Chapter 4 - Navigation**) select the flowsheet variable you wish to import to the Spreadsheet.

Note that you may also drag variables into the Spreadsheet.

Once you have imported all the variables, ensure that you are in the Main Flowsheet and that your column is solved. Make sure that no cells read **<empty>**. If Cell *F50* (Net Present Worth) has calculated, then your Spreadsheet is complete.

For the high purity configuration (RR1 = 5, RR2 = 5, Heptane Purity = 0.99, Toluene Purity = 0.99), the Net Present Worth is $3.84 Million.

Comparison of Configurations

"Heptane Purity" refers to the Heptane composition in the first column distillate stream (**Heptane**). "Toluene Purity" refers to the Toluene composition in the second column distillate stream (**Toluene**).

Recall that we could improve the Toluene Purity and Heptane Purity to 0.994 and 0.993 respectively. The Net Present Worth increases to $4.41 Million.

First, we have the High Purity Configuration with the following specifications:

- Column 1 Solvent Stage = 13
- Column 1 Feed Stage = 21
- Column 1 Number of Stages = 24
- Column 2 Feed Stage = 8
- Column 2 Number of Stages = 9
- Reflux Ratio 1 = 5
- Reflux Ratio 2 = 5
- Heptane Purity = 0.99
- Toluene Purity = 0.99

The Net Present Worth is $3.84 Million.

For the Low Purity Configuration specify the following:

- Column 1 Solvent Stage = 7
- Column 1 Feed Stage = 17
- Column 1 Number of Stages = 19
- Column 2 Feed Stage = 8
- Column 2 Number of Stages = 9
- Reflux Ratio 1 = 12
- Reflux Ratio 2 = 4
- Heptane Purity = 0.985
- Toluene Purity = 0.985
- In the Spreadsheet, set the number of stages in cells B13 and B14 to 19 and 9, respectively. Also, change the first column stage on which the tray liquid molar flow is being measured to *16* (Cell B5).

The Net Present Worth is $1.72 Million.

Even though we could improve this figure, it is safe to say that the first configuration (high purity) is economically superior. All further analysis will consider only the first configuration.

Optimization

We will use the following procedure in determining the optimum location of the feed streams:

1. Set the location of the feed stream.

2. Solve the column to the following specifications:

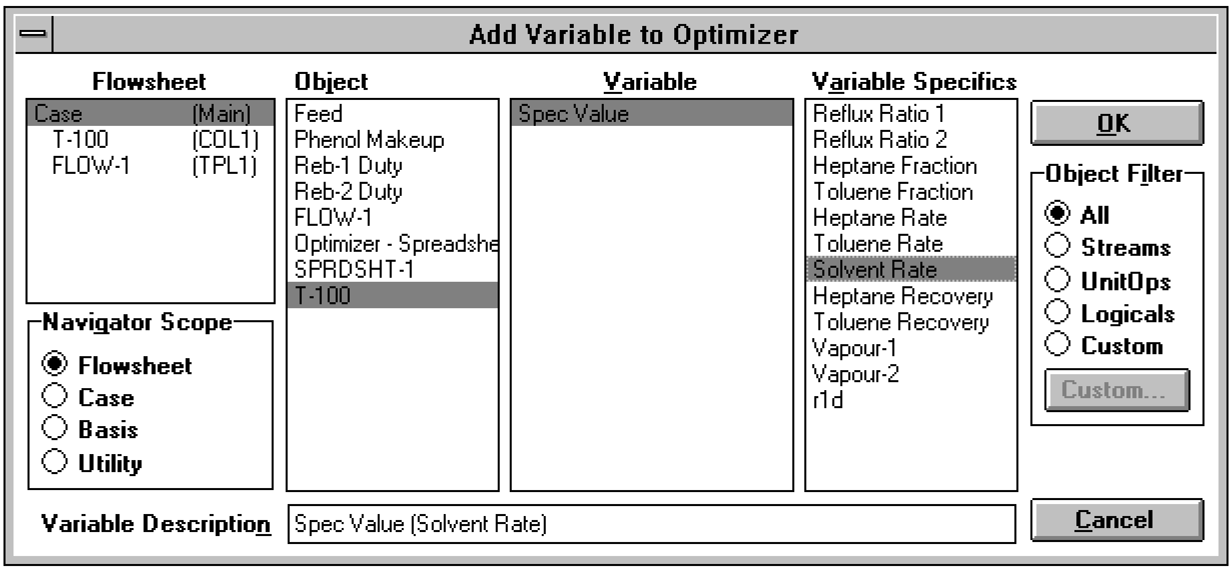
- First Column Reflux Ratio = 5
- Second Column Reflux Ratio = 5
- Toluene Purity = 0.99
- Heptane Purity = 0.99

3. After the column solves, replace the First Column Reflux Ratio specification with the following spec:

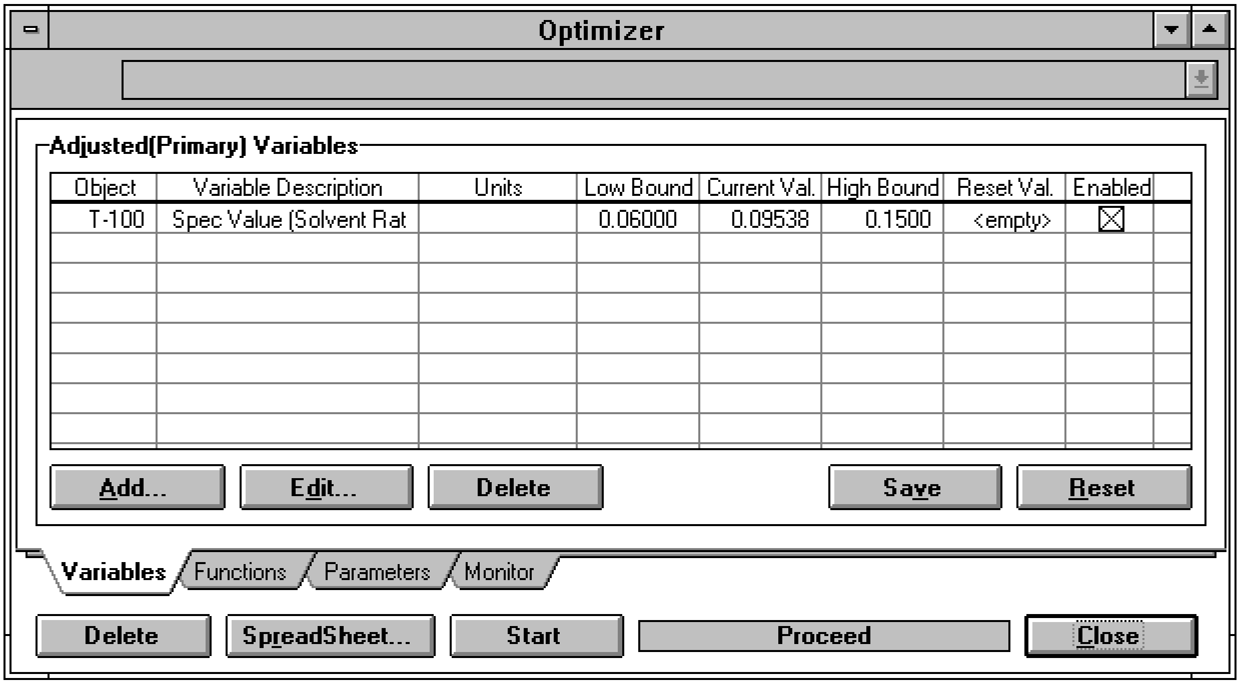
- Solvent Rate = *Current Value*

4. Set up the Optimizer to Maximize the Net Worth by adjusting the Solvent Rate specification:

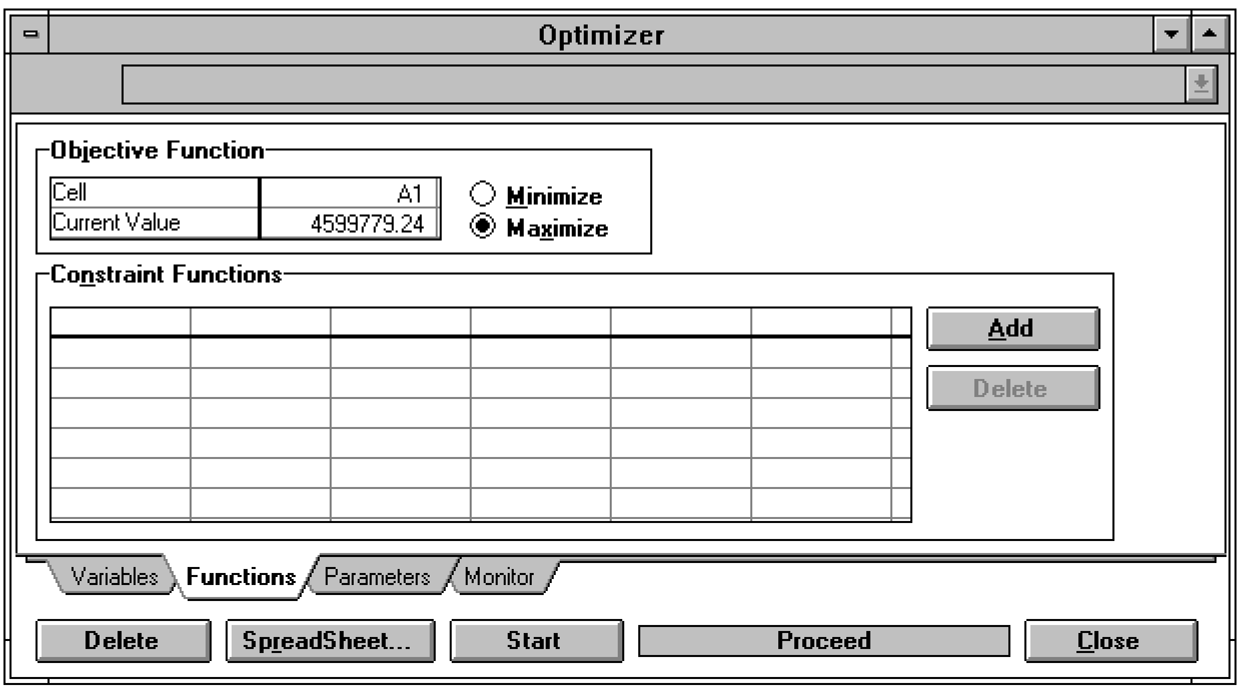
- On the Variables Page of the Optimizer, add the Solvent Rate specification as a Primary Variable:



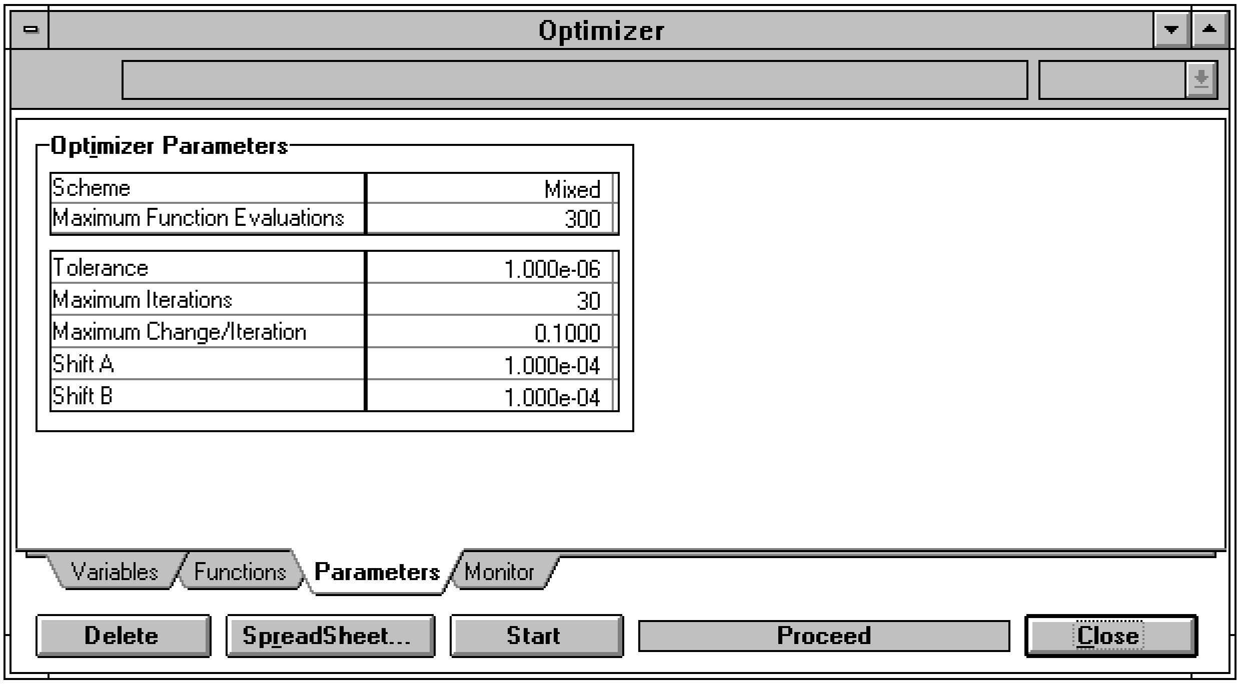
Set low and high bounds of 0.06 and 0.150:



- Import the Net Worth from the Case Spreadsheet into Cell A1 of the Optimizer Spreadsheet.
- On the Functions page of the Optimizer, specify the Objective Function Cell as *A1* and select the **Maximize** radio button:



- On the Parameters page, select the **Mixed** scheme, set the tolerance to 1e06, and reduce the Maximum Change/Iteration to 0.1000:



5. Select the ***Start*** button, allowing HYSYS to adjust the Solvent stream in order to Maximize the Net Worth of the process.

Location of Feed Stream

We adjust the Solvent Rate for two reasons:

1. It is a stable specification to adjust; that is, the Column will solve over an extensive range of Solvent Rates.
2. There is a point somewhere in the middle of the range of Solvent Rates where the Net Present Worth is maximized. If, for example, we were to adjust a Reflux Ratio, the Net Present Worth would be maximized close to the minimum Reflux Ratio for which the column solves, making that method inherently unstable. Similar logic applies for the Toluene and Heptane Fractions.

First, adjust the location of the Solvent feed to the first column, using the Optimizer to maximize the Net Worth for each feed configuration. The results are tabulated below.

Stage	RR1	RR2	Toluene	Heptane	Solvent Flow	Net Worth
13	3.939	5	0.99	0.99	880	$4.69 M
12	3.776	5	0.99	0.99	807	$4.79 M
11	**3.641**	**5**	**0.99**	**0.99**	**777**	**$4.86 M**
10	3.819	5	0.99	0.99	677	$4.83 M

From this point on, we will feed the solvent recycle on stage 11.

Next, we will adjust the location of the Mixed Feed to the first column:

Stage	RR1	RR2	Toluene	Heptane	Solvent Flow
21	3.641	5	0.99	0.99	777
20	**3.414**	**5**	**0.99**	**0.99**	**741**
19	3.429	5	0.99	0.99	764

From this point on, we will feed the process feed to stage 20 (minimum Reflux Ratio).

Finally, we adjust the location of the Feed to the second column:

Stage	RR1	RR2	Toluene	Heptane	Solvent Flow	Net Worth
8	3.438	5	0.99	0.99	716	$4.73 M
7	**3.350**	**5**	**0.99**	**0.99**	**713**	**$4.765 M**
6	3.370	5	0.99	0.99	698	$4.761 M

For the rest of the optimization, we will feed the solvent recycle to stage 11 of the first column, the process feed to stage 20 of the first column, and the first column bottoms to stage 7 of the second column.

Optimization of Purities and Reflux Ratios

Several variations of the reflux ratios and purities are now tested, with the following results:

Case Description	**Reflux Ratio 1**	**Reflux Ratio 2**	**Heptane Purity**	**Toluene Purity**	**Solvent Rate (lbmole/hr)**	**Capital Investment**	**Annual Income**	**Net Present Worth**
Base Case I	5	5	0.99	0.99	2203	3.60 M	1.75 M	3.60 M
Maximize Net Present Worth by adjusting the Solvent Rate and allowing the Reflux Ratio for Column 1 to vary.	3.350	5	0.99	0.99	713	2.98 M	1.89 M	4.77 M
Maximize Net Present Worth by adjusting the Solvent Rate and allowing the Reflux Ratio for Column 2 to vary.	5	1.347	0.99	0.99	648	2.71 M	2.03 M	5.60 M
Maximize the Heptane Purity, which in turn maximizes the Net Present Worth.	5	5	0.994	0.99	1401	3.39 M	1.82 M	4.08 M
Maximize the Toluene Purity, which in turn maximizes the Net Present Worth.	5	5	0.99	0.996	2120	3.58 M	1.81 M	3.86 M
Maximize the								

Heptane Purity, then maximize the Net Present worth by adjusting the Solvent Flow and allowing Reflux Ratio 2 to vary.	5	4.038	0.994	0.99	1068	3.19 M	1.89 M	4.57 M
Maximize the Toluene purity, then maximize the Net Present Worth by adjusting the Solvent Flow and allowing Reflux Ratio 2 to vary.	5	1.570	0.99	0.996	782	2.78 M	2.07 M	5.70 M

The last results (bottom row of table) are the best up to this point. The search for the optimum result has gone to the point where we have to include more primary variables and allow HYSYS to find the appropriate solution. The danger with this approach is that we cannot simply input the maximum purities as the high limit and the minimum reflux ratios as the low limit. There would be many combinations in this range which would not solve, due to the fact that we are pushing the limits on the column feasibility. We therefore have to be cautious when we select the primary variable ranges, and/or provide a small value for the Maximum Change/Iteration.

The Optimizer is set up as follows:

Primary Variable 1:

- Source — **T-100**
- Variable — **T-100**, **Spec Value**, **Solvent Rate**
- Low Bound — 0.08
- High Bound — 0.12

Primary Variable 2:

- Source — **T-100**
- Variable — **T-100**, **Spec Value**, **Heptane Fraction**
- Low Bound — 0.985
- High Bound — 0.994

Primary Variable 3:

- Source — **T-100**
- Variable — **T-100**, **Spec Value**, **Toluene Fraction**
- Low Bound — 0.985
- High Bound — 0.996 (set at the maximum)

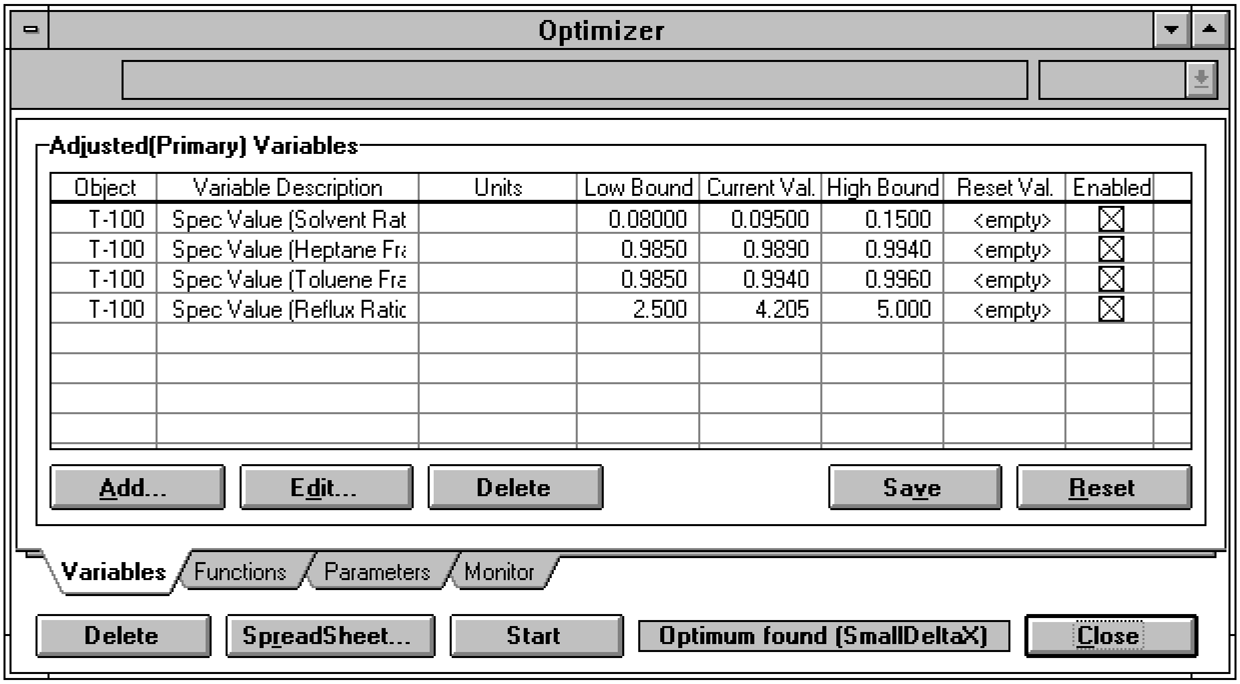
Primary Variable 4:

- Source — **T-100**
- Variable — **T-100**, **Spec Value**, **Reflux Ratio 1**

- Low Bound — 2.50
- High Bound — 5.00

It is important to ensure that the current (starting) values of these variables are within the bounds.

The Reflux Ratio for the second column will be allowed to vary while we attempt to find the maximum Net Worth. The Optimizer Variables page is shown below, after an Optimum is found:



Note that none of the Actual Values are at the Boundary limits. This is significant, as it means that a true maximum has been found, rather than a maximum imposed by a boundary constraint.

The results are tabulated below:

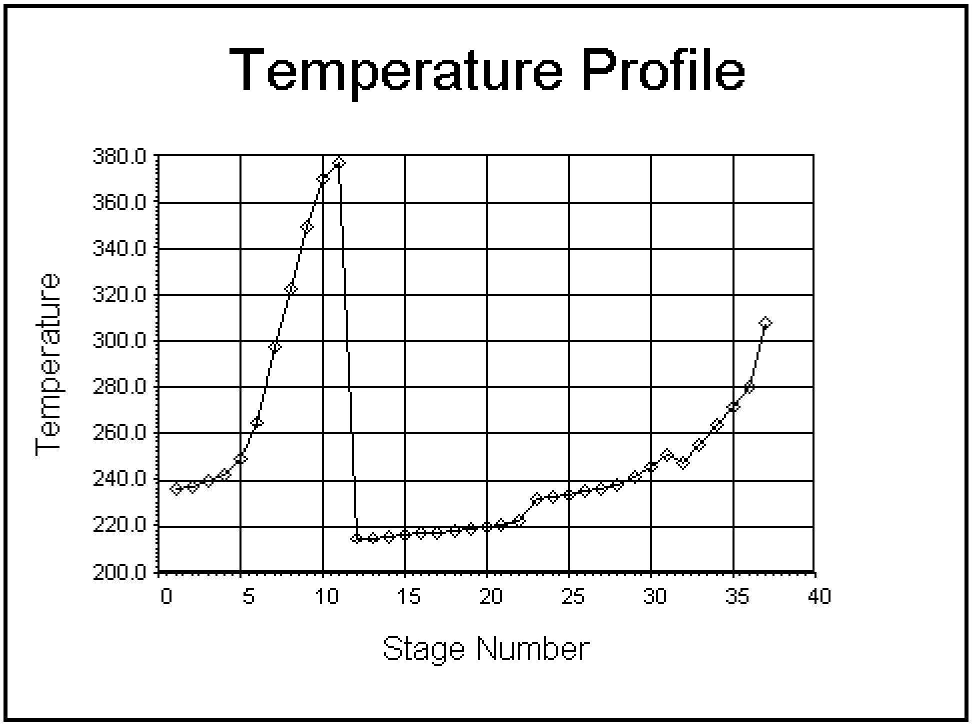
Reflux Ratio 1	4.205	**Solvent Rate**	757 lbmole/hr
Reflux Ratio 2	1.593	**Capital Investment**	$2.65 M
Heptane Purity	0.989	**Annual Income**	$2.09 M
Toluene Purity	0.994	**Net Present Worth**	$5.93 M

It is important to note that although this appears to be the optimum steady-state solution, it does not mean that this configuration is controllable in dynamics. In the next section, we will study the dynamics of the process. The column configuration is summarized below:

First Column	**Second Column**
Number of Stages — 24	Number of Stages — 9
Process Feed Stage — 20	Feed Stage (from Column 1 Bottoms) — 7
Solvent Recycle Stage — 11	
Reflux Ratio — 4.2	Reflux Ratio — 1.6
Heptane Fraction — 0.989	Toluene Fraction — 0.994

Note that the temperature profile for the second column is shown first.

The Results are shown here:



Temperature Profile, Column 2 (1-11) and Column 1 (12-37)

	n-Heptane	Toluene	Phenol
Condenser-2	0.005	0.994	9.665e-04
1__TS-2	0.003	0.993	0.005
2__TS-2	0.002	0.983	0.015
3__TS-2	0.001	0.952	0.047
4__TS-2	0.001	0.858	0.141
5__TS-2	5.544e-04	0.590	0.410
6__TS-2	1.859e-04	0.251	0.749
7__TS-2	1.085e-04	0.133	0.867
8__TS-2	8.570e-06	0.057	0.943
9__TS-2	4.959e-07	0.018	0.982
Reboiler-2	2.387e-08	0.004	0.996

Component Summary, Column 2

Name	Reflux-1	Boilup-1	To Condenser	To Reboiler-1
Vapour Fraction	0.0000	1.0000	1.0000	0.0000
Temperature [F]	214.8621	308.5018	214.8807	280.9955
Pressure [psia]	16.0000	20.0000	16.0000	20.0000
Molar Flow [lbmole/hr]	845.7788	668.7166	1046.8953	1625.7845
Mass Flow [lb/hr]	84687.6284	62049.0837	104825.3814	151728.8834
Liquid Volume Flow [barrel/day]	8420.0689	4681.5682	10422.2653	10758.5323
Heat Flow [Btu/hr]	-7.4108e+07	7.0283e+06	-7.7486e+07	-4.3766e+07
Comp Mole Frac (n-Heptane)	0.9894	0.0170	0.9894	0.0076
Comp Mole Frac (Toluene)	0.0055	0.7242	0.0055	0.4222
Comp Mole Frac (Phenol)	0.0050	0.2588	0.0050	0.5702

Name	Phenol Makeup	Solvent	Col-1 Bottoms	Reb-1 Duty
Vapour Fraction	0.0000	0.0000	0.0000	<empty>
Temperature [F]	220.0000	377.1493	308.5018	<empty>
Pressure [psia]	20.0000	20.0000	20.0000	<empty>
Molar Flow [lbmole/hr]	1.2000	756.9845	957.0679	<empty>
Mass Flow [lb/hr]	112.9354	71235.4568	89679.7997	<empty>
Liquid Volume Flow [barrel/day]	7.3234	4623.5221	6076.9642	<empty>
Heat Flow [Btu/hr]	-71120.6617	-3.8729e+07	-3.8480e+07	1.2314e+07
Comp Mole Frac (n-Heptane)	0.0000	2.3868e-08	0.0011	<empty>
Comp Mole Frac (Toluene)	0.0000	0.0043	0.2112	<empty>
Comp Mole Frac (Phenol)	1.0000	0.9957	0.7877	<empty>

Column Worksheet

	n-Heptane	Toluene	Phenol
Condenser-1	0.989	0.006	0.005
1__TS-1	0.988	0.006	0.006
2__TS-1	0.986	0.007	0.008
3__TS-1	0.983	0.007	0.009
4__TS-1	0.981	0.008	0.011
5__TS-1	0.978	0.008	0.014
6__TS-1	0.974	0.009	0.017
7__TS-1	0.970	0.010	0.021
8__TS-1	0.962	0.010	0.027
9__TS-1	0.948	0.011	0.040
10__TS-1	0.908	0.013	0.079
11__TS-1	0.313	0.010	0.677
12__TS-1	0.310	0.014	0.676
13__TS-1	0.304	0.019	0.676
14__TS-1	0.295	0.029	0.677
15__TS-1	0.278	0.044	0.677
16__TS-1	0.253	0.068	0.679
17__TS-1	0.215	0.102	0.682
18__TS-1	0.171	0.147	0.682
19__TS-1	0.139	0.200	0.661
20__TS-1	0.176	0.326	0.497
21__TS-1	0.111	0.390	0.498
22__TS-1	0.057	0.445	0.498

Component Summary, Column 1

Name	Heptane	Reflux-2	Boilup-2	To Condenser-2
Vapour Fraction	0.0000	0.0000	1.0000	1.0000
Temperature [F]	214.8441	236.3411	377.1493	236.6788
Pressure [psia]	16.0000	16.0000	20.0000	16.0000
Molar Flow [lbmole/hr]	201.1166	318.6492	467.6184	518.7327
Mass Flow [lb/hr]	20137.7529	29374.1238	43972.1588	47818.4666
Liquid Volume Flow [barrel/day]	2002.1964	2314.7253	2875.1941	3768.1673
Heat Flow [Btu/hr]	-1.7622e+07	3.5957e+06	-1.3849e+07	1.3236e+07
Comp Mole Frac (n-Heptane)	0.9894	0.0050	1.2600e-06	0.0050
Comp Mole Frac (Toluene)	0.0055	0.9940	0.0398	0.9940
Comp Mole Frac (Phenol)	0.0050	0.0010	0.9602	0.0010
Name	Condenser-2 Duty	Toluene	Reboiler-2 Duty	Vapour-1
Vapour Fraction	<empty>	0.0000	<empty>	1.0000
Temperature [F]	<empty>	236.3231	<empty>	214.8801
Pressure [psia]	<empty>	16.0000	<empty>	16.0000
Molar Flow [lbmole/hr]	<empty>	200.0834	<empty>	8.4578e-20
Mass Flow [lb/hr]	<empty>	18444.3429	<empty>	8.4696e-18
Liquid Volume Flow [barrel/day]	<empty>	1453.4420	<empty>	8.4245e-19
Heat Flow [Btu/hr]	7.3830e+06	2.2576e+06	9.3915e+06	-6.2677e-15
Comp Mole Frac (n-Heptane)	<empty>	0.0050	<empty>	0.9909
Comp Mole Frac (Toluene)	<empty>	0.9940	<empty>	0.0050
Comp Mole Frac (Phenol)	<empty>	0.0010	<empty>	0.0040

Column Worksheet

As a point of interest, an attempt was made to reproduce the process as set up in the original HYSYS Reference Manual (page 463). As in the example, the Peng Robinson Property Package was used (earlier shown to be unacceptable) with the following results:

First Column	**Second Column**
Number of Stages — 20	Number of Stages — 10
Process Feed Stage — 13	Feed Stage (from Column 1 Bottoms) — 10
Solvent Recycle Stage — 6	
Reflux Ratio — 3.8	Reflux Ratio — 12
Heptane Fraction — 0.99	Toluene Fraction — 0.985

- Solvent Rate = 1145 lbmole/hr
- Capital Investment = $4.04 M, Annual Income = $1.34 M
- **Net Present Worth = $1.44 M**

However, when the NRTL Property Package with the updated interaction parameters is used, the same specifications could not be met. The Reflux Ratio for Column 1 was relaxed to 10, and the Heptane fraction was relaxed to 0.97. This is clearly an unacceptable option, but the best possible using the same configuration. Nevertheless, the results are shown below:

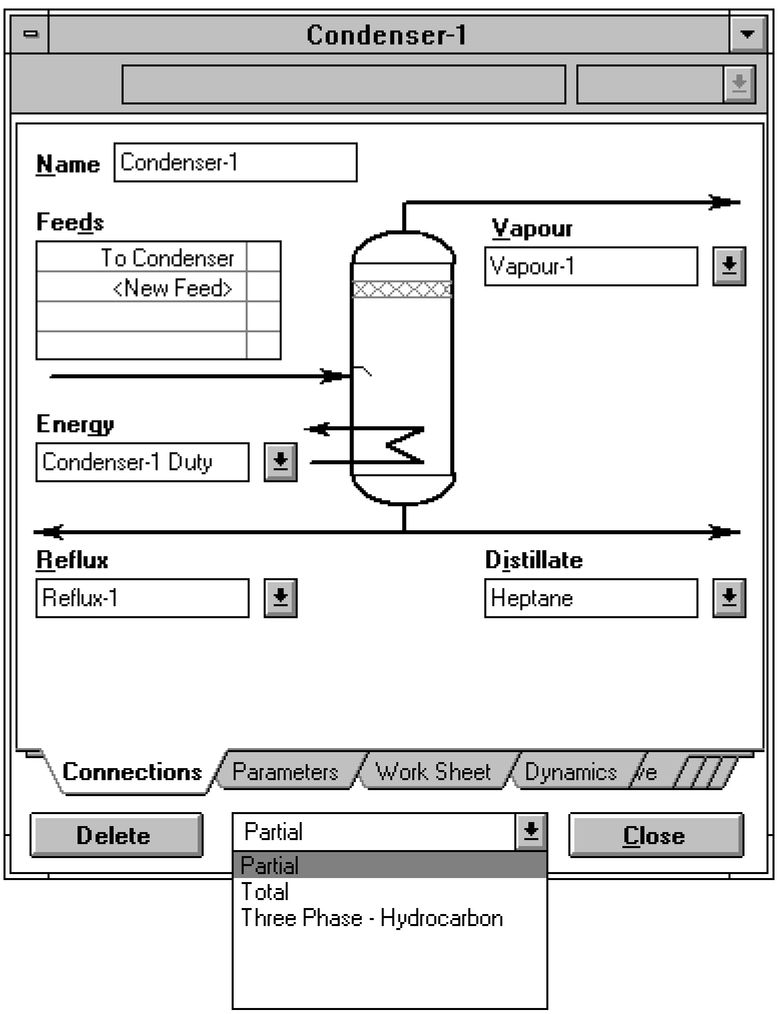
First Column	Second Column
Number of Stages — 20	Number of Stages — 10
Process Feed Stage — 13	Feed Stage (from Column 1 Bottoms) — 10
Solvent Recycle Stage — 6	
Reflux Ratio — 10	Reflux Ratio — 12
Heptane Fraction — 0.97	Toluene Fraction — 0.99

- Solvent Rate = 337 lbmole/hr
- Capital Investment = $4.50 M, Annual Income = $0.69 M
- **Net Present Worth = ($1.65 M)**

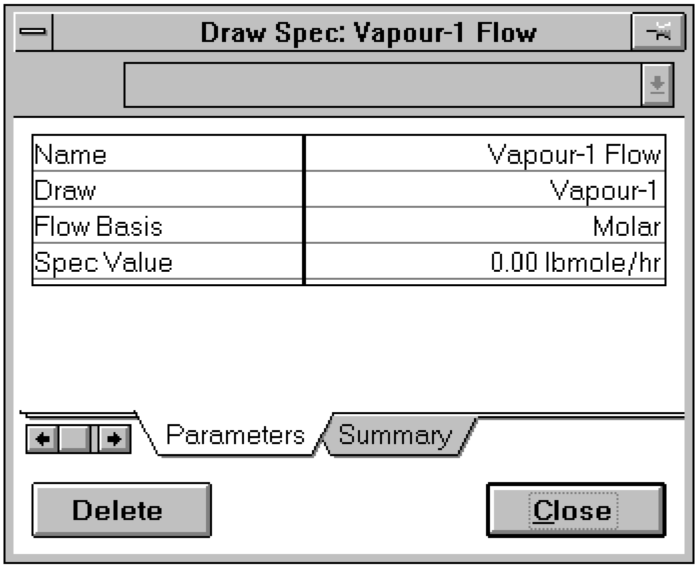
C-6.7

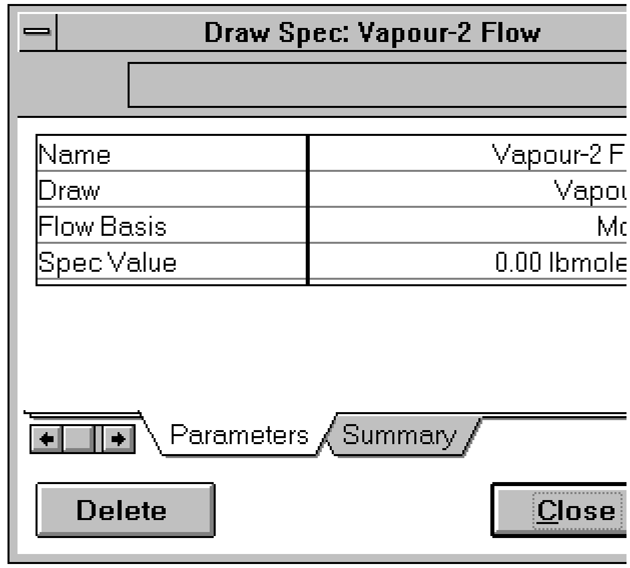
PART 5 ***Dynamics***

In Dynamics, we require that Partial Condensers be used. If you installed your Condensers as Total Condensers, change them to Partial Condensers as shown below:



Call the Vapour streams **Vapour 1** and **Vapour 2**. We will now have to provide two additional columns specifications. We do not want any vapour flow off the condensers, so the specifications will be as shown:





Overview

Before we can run the process dynamically, there are several important steps:

- **Sizing the Vessels** — The Tray Sections, Condensers, and Reboilers must be appropriately sized based on their respective liquid flowrates. Note that we already did some sizing calculations in the Steady-State portion of this simulation.
- **Adding the Controls** — We require at least ten controllers, for both columns' Reflux, Distillate, Bottoms, Condenser Duty and Reboiler Duty. The control scheme (selection of Process Variable) and Tuning are very important in ensuring a stable control configuration.
- **Sizing the Valves** — All of the valves must be sized, typically to span twice the steady-state value.
- **Setting up the Strip Charts** — We will track key variables while we run the simulation.

Setting the Dynamic Property Model Parameters — The proper choice of these parameters will ensure numeric stability and accurate extrapolation.

Once we have completed these steps, we can run the process dynamically, introducing various upsets to the system to ensure that our control system can adequately handle them.

Sizing the Vessels

It is important to correctly size the vessels in order to ensure a reasonable dynamic response. It is also imperative that the Cooling Volume and Tower Volume (set in the Condenser) are accurate.

Tray Sections

In the economic analysis, we estimated the diameter of the first tray section as follows:

$$D_{TRAY} = \sqrt{\frac{F_{TRAY} \times (1/120)}{0.25\,\pi \times (1/6) \times \rho}}$$

where F_{TRAY1} is the liquid volume flowrate on stage 20 of the first tray section.

The volume of the first tray section is:

$$V_{TRAY} = \frac{F_{TRAY} \times (1/120)}{\rho}$$

The factor (1/120) is the residence time, 1/120th of an hour or half a minute.

Using the Steady-State values, we have:

$$V_{TRAY1} = \frac{(1.526E5\ lb\ /\ hr)(1\ /\ 120\ hr)}{56.22\ lb\ /\ ft^3}$$

$$V_{TRAY1} = 22.6\ ft^3$$

When you enter this value on the Dynamics page of the Tray Section, the diameter is calculated to be 13.24 ft (assuming a weir height of 0.16 ft).

For the second tray section, we have:

$$V_{TRAY1} = \frac{(2.906E4\ lb\ /\ hr)(1\ /\ 120\ hr)}{48.48\ lb\ /\ ft^3}$$

$$V_{TRAY1} = 5.00\ ft^3$$

The diameter is calculated to be 6.23 ft.

Condensers

The volume of the condensers are calculated as follows:

$$\text{Volume} = \frac{\text{Holdup Time} \times \text{Flowrate}}{\text{SP(\% Full)}}$$

For the first condenser:

$$\text{Volume} = \frac{(1/6\ \text{hour}) \times (104825\ \text{lb}/\text{hr})}{(38.06\ \text{lb}/\text{ft}^3) \times (50\%)}$$

$$\text{Volume} = 920\ \text{ft}^3$$

For the second condenser:

$$\text{Volume} = \frac{(1/6\ \text{hour}) \times (47818\ \text{lb/hr})}{(48.48\ \text{lb/ft}^3) \times (50\%)}$$

$$\text{Volume} = 330\ \text{ft}^3$$

The tower volume and cooling volumes are estimated as follows:

$$\text{Vapour Volume / Tray} = (\text{Liquid Volume / Tray}) \times 10$$
$$\text{Tower Volume} = (\text{Vapour Volume / Tray}) \times (\text{Number of Trays})$$
$$\text{Cooling Volume} = \text{Condenser Volume} \times 30\%$$

For the first column:

$$\text{Vapour Volume / Tray} = 22.6\ \text{ft}^3 \times 10 = 226\ \text{ft}^3$$
$$\text{Tower Volume} = 226\ \text{ft}^3 \times 24 = 5424\ \text{ft}^3$$
$$\text{Cooling Volume} = 920\ \text{ft}^3 \times 30\% = 276\ \text{ft}^3$$

For the second column:

$$\text{Vapour Volume / Tray} = 5\ \text{ft}^3 \times 10 = 50\ \text{ft}^3$$
$$\text{Tower Volume} = 50\ \text{ft}^3 \times 9 = 450\ \text{ft}^3$$
$$\text{Cooling Volume} = 330\ \text{ft}^3 \times 30\% = 99\ \text{ft}^3$$

Reboilers

The volumes of the reboilers are calculated as follows:

$$\text{Volume} = \frac{\text{Holdup Time} \times \text{Flowrate}}{\text{SP}(\%\ \text{Full})}$$

For the first reboiler:

$$\text{Volume} = \frac{(1/6\ \text{hour}) \times (151729\ \text{lb/hr})}{(54.07\ \text{lb/ft}^3) \times (50\%)}$$

$$\text{Volume} = 935\ \text{ft}^3$$

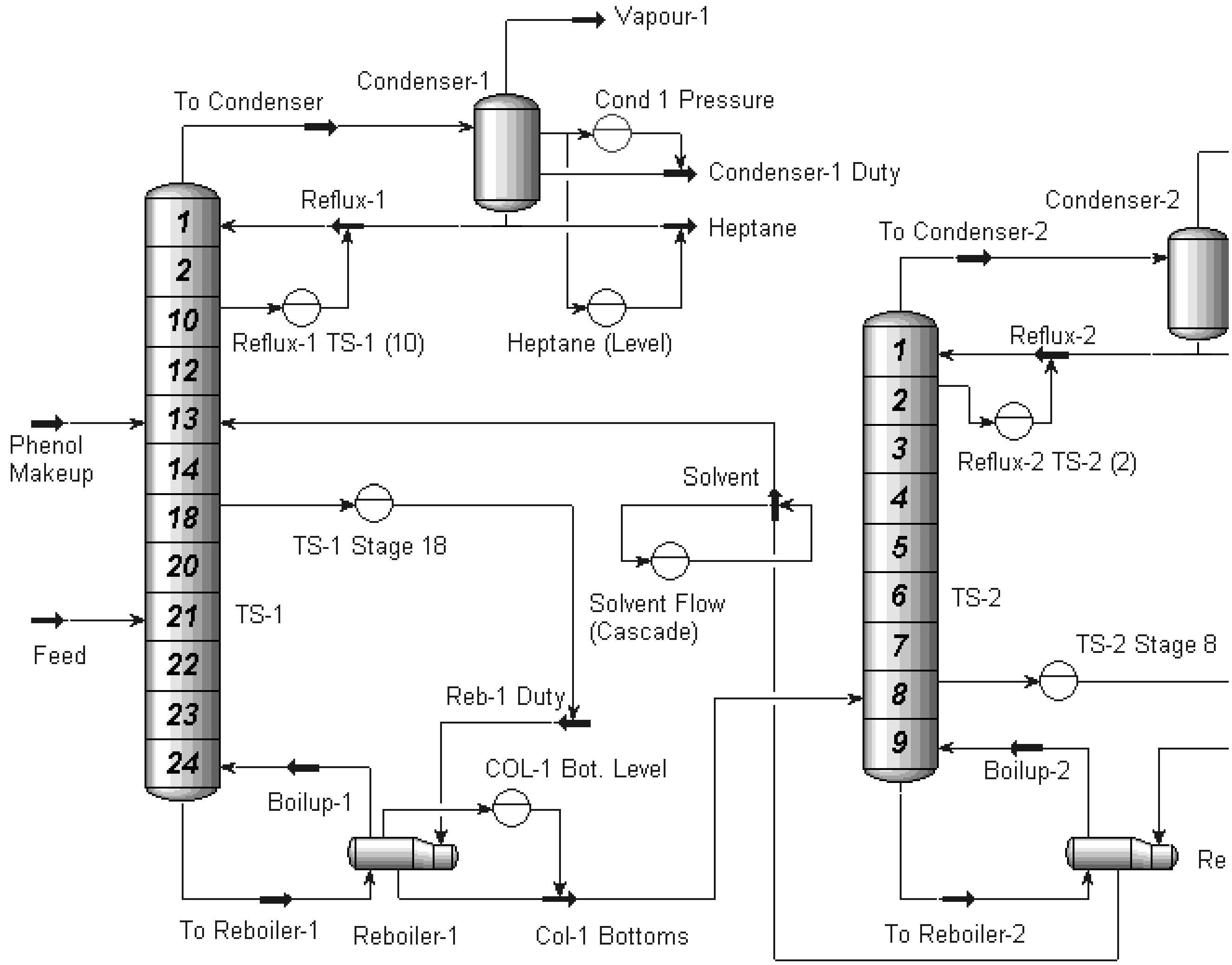
For the second reboiler:

$$\text{Volume} = \frac{(1/6\ \text{hour}) \times (115207\ \text{lb/hr})}{(56.78\ \text{lb/ft}^3) \times (50\%)}$$

$$\text{Volume} = 676\ \text{ft}^3$$

Adding the Controls and Sizing the Valves

Various approaches could be taken in the development of the control scheme. The control scheme which we will be using is outlined here:



Control Scheme

One benefit of using HYSYS to develop a control scheme is that several different schemes could be considered, set up and dynamically tested. Therefore, if you decided, for instance, that you did not want dual-point temperature control on the two distillation columns but instead wanted ratio controllers to manipulate the reboiler duties, it would be fairly straightforward to set it up. However, the comparison and fine-tuning of different control schemes is beyond the scope of this paper; therefore, the control scheme as shown in this figure will be used. Note that fairly conservative tuning parameters have been chosen for the controllers. As shown later, the dynamic response is reasonable, therefore no effort is made to fine-tune the parameters.

Condenser Duty Controllers

For each column, we will have a Pressure Controller maintaining the Partial Condenser pressure by manipulating the Condenser duty. The pressure of the condenser determines the pressure profile of the column, and it is therefore important to closely control the condenser pressure. As noted in other examples, the tray temperature (PV of the Reboiler Duty Controllers) and condenser pressure are interacting variables. We must ensure that the controllers are tuned such that any adverse interaction is minimized. The Controller parameters are displayed below:

CONTROLLER	Cond 1 Pressure
CONNECTIONS	
PV Object PV OP Object	Condenser-1 Vessel Pressure Condenser-1 Duty
Control Valve	
Duty Source	From Utility Fluid
Min Flow	0 lbmole/hr
Max Flow	10000 lbmole/hr
PARAMETERS	
PV Min & Max	10 & 20 psia
Action	Direct
Controller Mode	Auto
SP	16.0000 psia
TUNING	
Kp	0.8
Ti	15
Td	<empty>

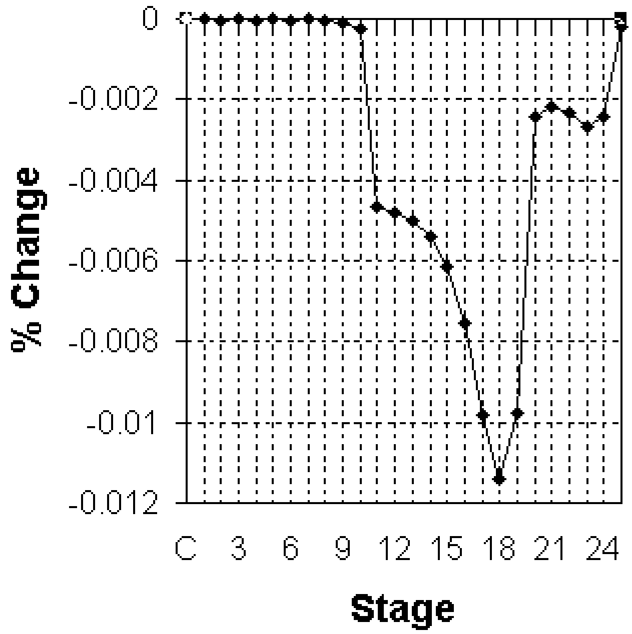
CONTROLLER	Cond 2 Pressure
CONNECTIONS	
PV Object PV OP Object	Condenser-2 Vessel Pressure Condenser-2 Duty
Control Valve	
Duty Source	From Utility Fluid
Min Flow	0 lbmole/hr
Max Flow	10000 lbmole/hr
PARAMETERS	
PV Min & Max	10 & 20 psia
Action	Direct
Controller Mode	Auto
SP	16.0000 psia
TUNING	
Kp	0.8
Ti	15
Td	<empty>

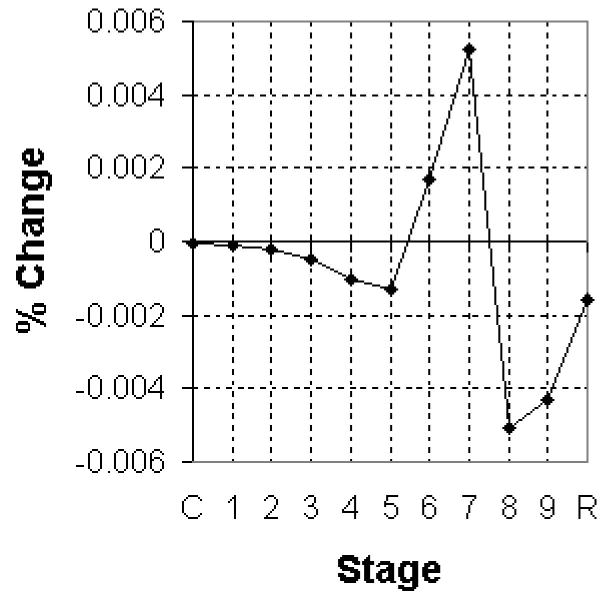
For the Utility Fluid, set the Minimum and Maximum Flow to 0 and 10000 lbmole/hr. Note that when you enter Dynamic Mode, the utility fluid flowrate for each condenser duty stream will be calculated and displayed.

Reboiler Duty Controllers

By manipulating the reboiler duty, temperature control is achieved, which ultimately implies composition control. Generally, we want to control the temperature of the tray where the temperature sensitivity is the highest.

To determine which tray has the highest sensitivity to temperature, we will do a steady-state sensitivity analysis which varies the reboiler duty by a small amount, so that we can see where the change in temperature is the greatest:





The Case Study tool can be used to produce these plots.

As is apparent from the graphs, the greatest change in temperature in the first column occurs on Stage 18. We will use the Stage 18 Temperature as the Process Variable for the first column. For the second column, we will use the Stage 8 Temperature as the PV. Although Stage 7 has a large *% Change* (roughly equal and opposite to Stage 8), it is not a recommended practice to have a feed stage as the process variable for a controller.

CONTROLLER	TS-1 Stage 18
CONNECTIONS	
PV Object PV OP Object	TS-1 Stage 18 Temp. Reboiler-1 Duty
Control Valve	
Duty Source	Direct Q
Min Available	0 Btu/hr
Max Available	2.0e+07 Btu/hr
PARAMETERS	
PV Min & Max	200 & 300 F
Action	Reverse
Controller Mode	Auto
SP	241.9 F
TUNING	
Kp	0.8
Ti	15
Td	<empty>

CONTROLLER	TS-2 Stage 8
CONNECTIONS	
PV Object PV OP Object	TS-2 Stage 8 Temp. Reboiler-2 Duty
Control Valve	
Duty Source	Direct Q
Min Available	0 Btu/hr
Max Available	2.0e+07 Btu/hr
PARAMETERS	
PV Min & Max	300 & 400 F
Action	Reverse
Controller Mode	Auto
SP	347.6
TUNING	
Kp	0.8
Ti	15
Td	<empty>

Column 1 Material Stream Controllers

The parameters for the Material Stream Controllers in the first column are displayed below:

CONTROLLER	Reflux 1 TS-1(10)
CONNECTIONS	
PV Object PV OP Object	TS-1 Stage 10 Temp. Reflux-1
Control Valve	
Flow Type	Molar Flow
Min Flow	0 lbmole/hr
Max Flow	1600 lbmole/hr
PARAMETERS	
PV Min & Max	200 & 300 F
Action	Direct
Controller Mode	Auto
SP	221.7 F
TUNING	
Kp	0.4
Ti	20
Td	<empty>

CONTROLLER	Heptane (Level))
CONNECTIONS	
PV Object PV OP Object	Condenser-1 Liquid Level Heptane
Control Valve	
Flow Type	Molar Flow
Min Flow	0 lbmole/hr
Max Flow	400 lbmole/hr
PARAMETERS	
PV Min & Max	40 & 60%
Action	Direct
Controller Mode	Auto
SP	50%
TUNING	
Kp	1.8
Ti	<empty>
Td	<empty>

CONTROLLER	COL1 Bott. Level
CONNECTIONS	
PV Object PV OP Object	Reboiler-1 Liquid Level Col-1 Bottoms
Control Valve	
Flow Type	Molar Flow
Min Flow	0 lbmole/hr
Max Flow	2000 lbmole/hr
PARAMETERS	
PV Min & Max	40 & 60%
Action	Direct
Controller Mode	Auto
SP	50%
TUNING	
Kp	1.8
Ti	<empty>
Td	<empty>

For the Reflux Stream, we use the temperature for Stage 10 (TS-1) as the Process Variable. This Stage is especially sensitive to variations in the feed flowrate. Set the Control Valve range from 0 to 1600 lbmole/hr.

The Heptane stream will be set on Level control, so that the first Condenser is 50% full. We want the flowrate of this stream to vary with changes to the Feed flowrate and composition. The Minimum and Maximum Flow are set at 0 and 400 lbmole/hr.

The bottoms stream also has Level control; the first Reboiler's setpoint is a 50% Liquid Level. The Minimum and Maximum Flow are set at 0 and 2000 lbmole/hr.

Column 2 Material Stream Controllers

The parameters for the Material Stream Controllers in the second column are displayed below:

CONTROLLER	Reflux 2 TS-2(2)
CONNECTIONS	
PV Object PV OP Object	TS-2 Stage 2 Temp. Reflux-2
Control Valve	
Flow Type	Molar Flow
Min Flow	0 lbmole/hr
Max Flow	800 lbmole/hr
PARAMETERS	
PV Min & Max	200 & 300 F
Action	Direct
Controller Mode	Auto
SP	239.9 F
TUNING	
Kp	0.8
Ti	15
Td	<empty>

CONTROLLER	Toluene (Level))
CONNECTIONS	
PV Object PV OP Object	Condenser-2 Liquid Level Toluene
Control Valve	
Flow Type	Molar Flow
Min Flow	0 lbmole/hr
Max Flow	400 lbmole/hr
PARAMETERS	
PV Min & Max	40 & 60%
Action	Direct
Controller Mode	Auto
SP	50%
TUNING	
Kp	1.8
Ti	<empty>
Td	<empty>

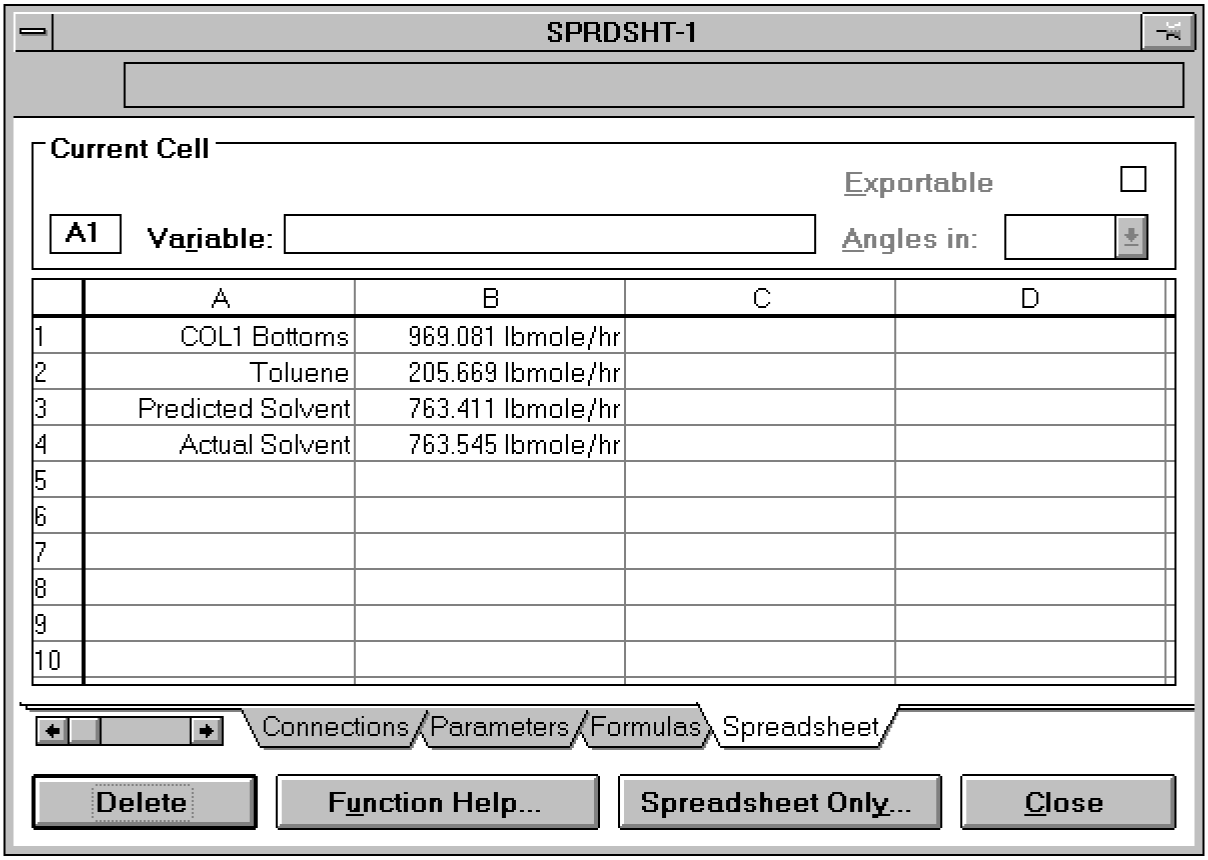
CONTROLLER	Solvent Flow
CONNECTIONS	
PV Object PV OP Object Cascaded SP Source Spreadsheet Cell	Solvent Molar Flow Solvent SPRDSHT-1 B3: Calculated Solvent
Control Valve	
Flow Type	Molar Flow
Min Flow	0 lbmole/hr
Max Flow	1500 lbmole/hr
PARAMETERS	
PV Min & Max	0 & 1500 lbmole/hr
Action	Reverse
Controller Mode	Cascaded SP
TUNING	
Kp	0.8
Ti	15
Td	<empty>

Similar to the first Reflux control, we use the temperature for Stage 2 (TS-2) as the Process Variable for the second Reflux control. This Stage is especially sensitive to variations in the feed flowrate. Set the Control Valve range from 0 to 800 lbmole/hr.

The Toluene stream will be set on Level control, so that the second Condenser is 50% full. We want the flowrate of this stream to vary with changes to the Feed flowrate and composition. The Minimum and Maximum Flow are set at 0 and 400 lbmole/hr.

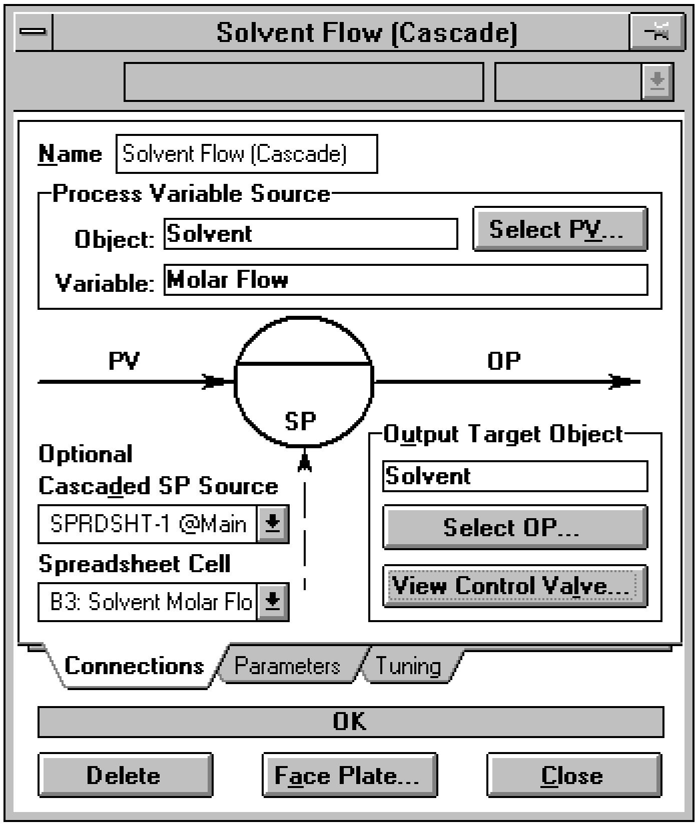
Finally, the bottoms stream (**Solvent**) has a cascaded set point. The Flowrate is chosen as the Process Variable, but the “Calculated” rate of the Solvent will be the Set Point for this control. The Calculated Solvent rate is simply the Column 1 Bottoms Flowrate minus the Toluene (Distillate) flowrate. Note that we must select Spreadsheet Cell B3 when setting up the Cascaded Control.

Create a new Spreadsheet in the Main Flowsheet and set it up as follows:



- Import the Column 1 Bottoms Molar Flow into cell *B1.*
- Import the Toluene Molar Flow into cell *B2*.
- Enter the formula *+B1-B2* into cell *B3*.
- Import the Solvent Molar Flow into cell *B4*. In Steady-State, cell *B3* will always equal cell *B4*. However, in Dynamics, these cells will not necessarily be the same.

On the Parameters page, you may wish to enter a Variable Name for cell *B3* so that it will be recognizable when you set up your controller, which will be set up as follows:

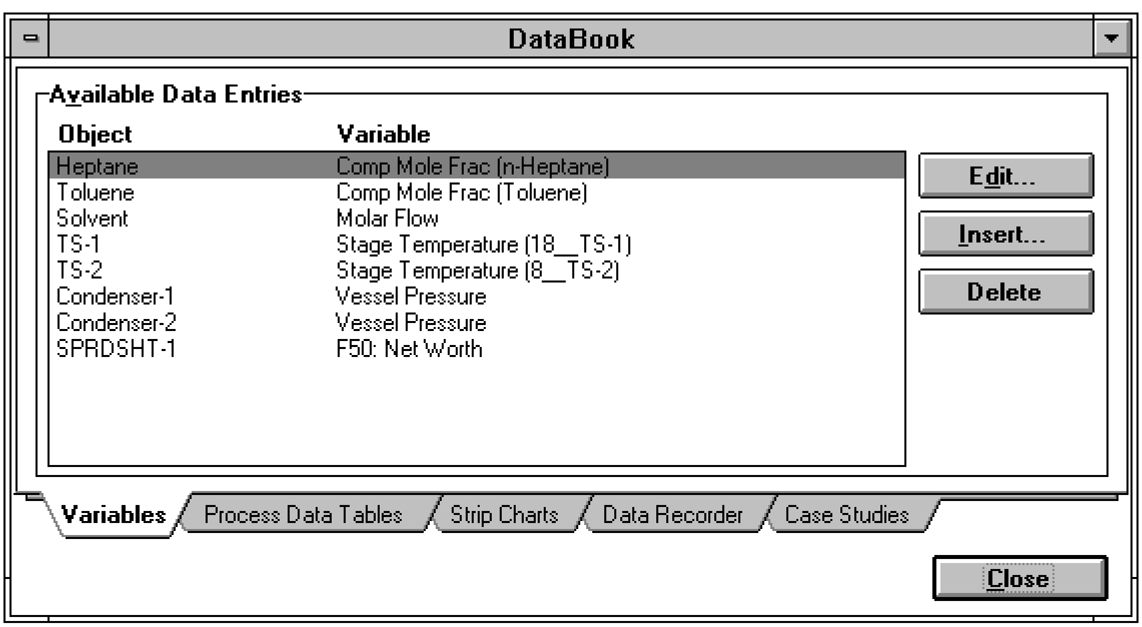


Feed Stream Controllers

If you wish, you may put Manual controllers on the Feed and Phenol streams. However, flowrates and compositions may also be adjusted from the WorkSheet, so they are not crucial to the simulation.

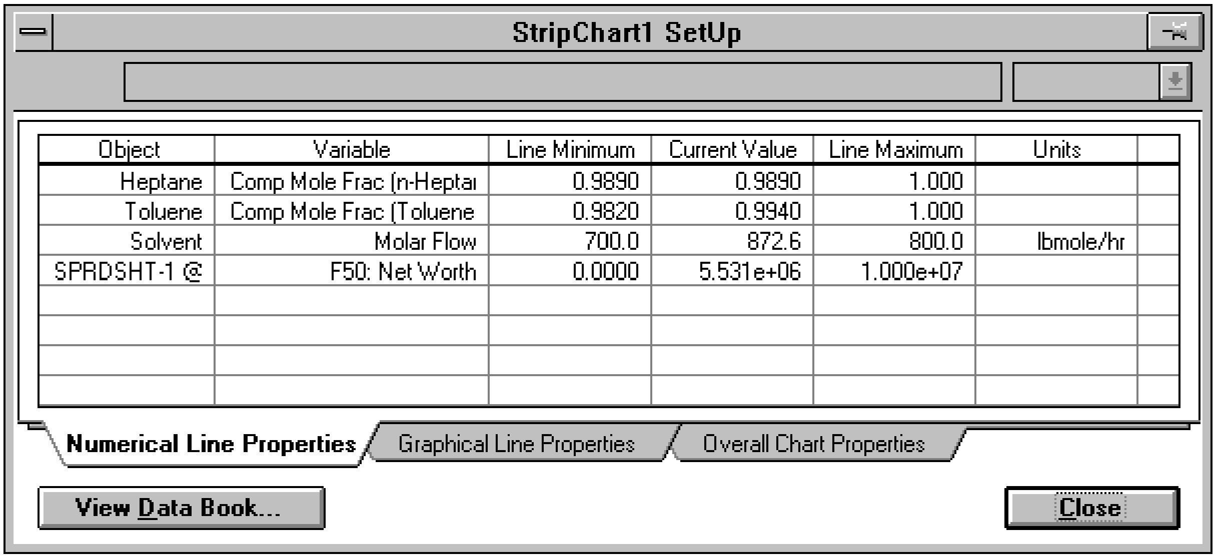
Setting up the Strip Charts

Enter the following variables in the DataBook:



We will be setting up two Strip Charts, each having four variables.

The first Strip Chart will plot the Heptane and Toluene Molar Fractions, the Solvent Molar Flow rate, and the “Net Worth”. Although the concept of an *instantaneous* Net Worth is of no practical use, it will be useful to see the effect of certain variables on the bottom line.



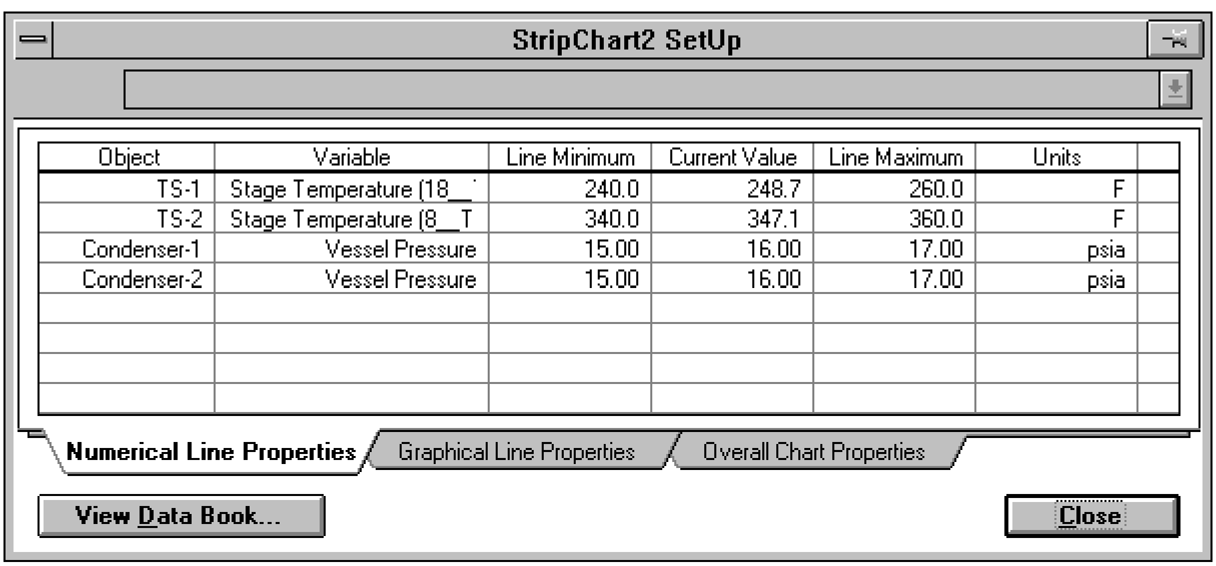
Object	Variable	Line Minimum	Current Value	Line Maximum	Units
Heptane	Comp Mole Frac (n-Heptai	0.9890	0.9890	1.000	
Toluene	Comp Mole Frac (Toluene	0.9820	0.9940	1.000	
Solvent	Molar Flow	700.0	872.6	800.0	lbmole/hr
SPRDSHT-1 @	F50: Net Worth	0.0000	5.531e+06	1.000e+07	

In the Net Worth Analysis, certain variables such as the column diameter were dependent on key flowrates. In Dynamics, you need to ensure that the initial capital cost does not fluctuate when there are changes in process variables.

Change cell *D29* to the figure that is currently being displayed (2.3042e+06).

All that is required is to replace the formula in the cell which calculates the Adjusted FCI with the actual figure in that cell, so that the FCI will not change as the simulation progresses.

The second Strip Chart contains the following variables:



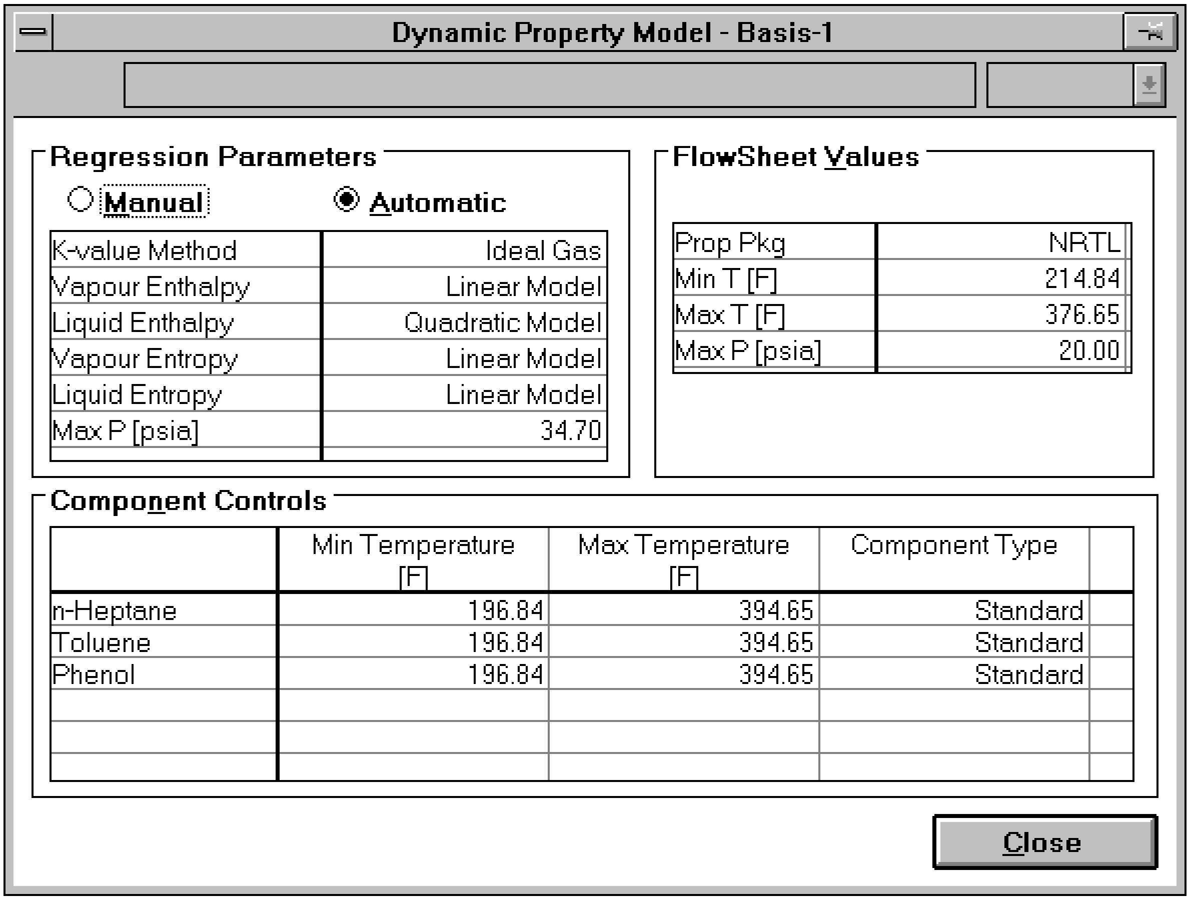
Object	Variable	Line Minimum	Current Value	Line Maximum	Units
TS-1	Stage Temperature (18__	240.0	248.7	260.0	F
TS-2	Stage Temperature (8__T	340.0	347.1	360.0	F
Condenser-1	Vessel Pressure	15.00	16.00	17.00	psia
Condenser-2	Vessel Pressure	15.00	16.00	17.00	psia

The temperatures of the stages which are used as the Process Variables in the Reboiler Duty controllers are plotted, along with the Condenser Pressures.

Setting the Dynamic Property Model Parameters

It is always important to ensure that appropriate parameters are used for the Dynamic Property Model.

In this case, the default parameters are sufficient:

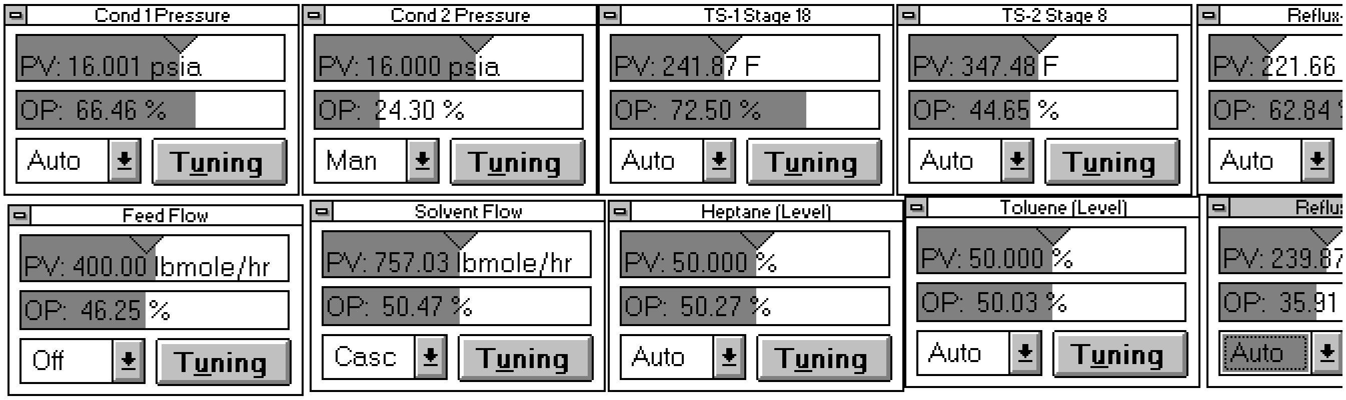


If you were concerned that you were not achieving proper accuracy over a range of temperatures and pressures, you might want to use the Property Package Method or Local Model in calculating the K-values, Enthalpies or Entropies. However, this causes the integration to proceed at a much slower rate, and in this case, switching models does not seem to be justified.

Dynamic Simulation

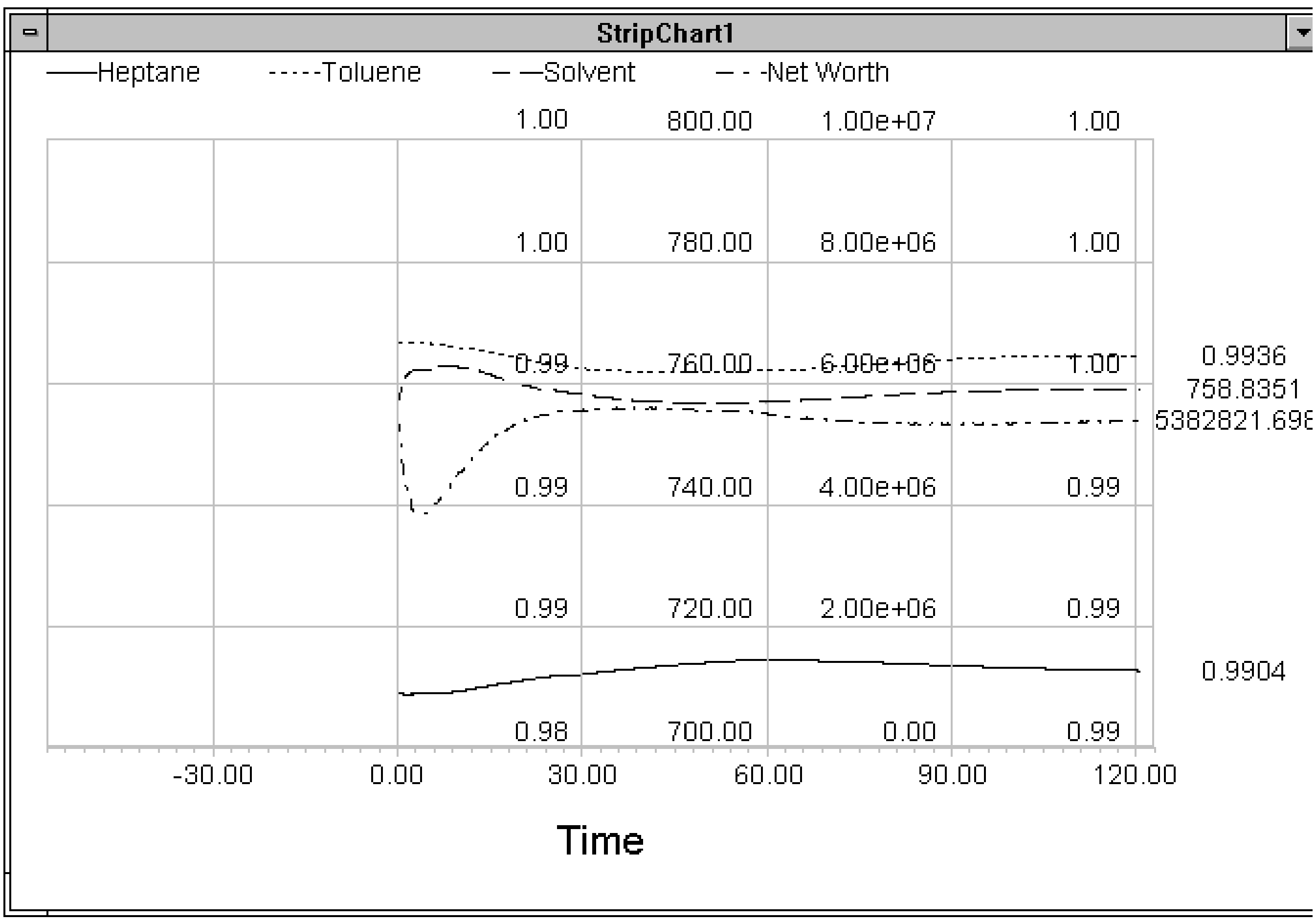
After switching to dynamics, and before running the integrator, ensure that the starting point of each controller is correct, in order to avoid a large “bump” as soon as you start the integrator. This can be achieved by resetting each controller by turning it off, then “on” again (to *Auto* or *Cascade* control, whichever is appropriate for that control).

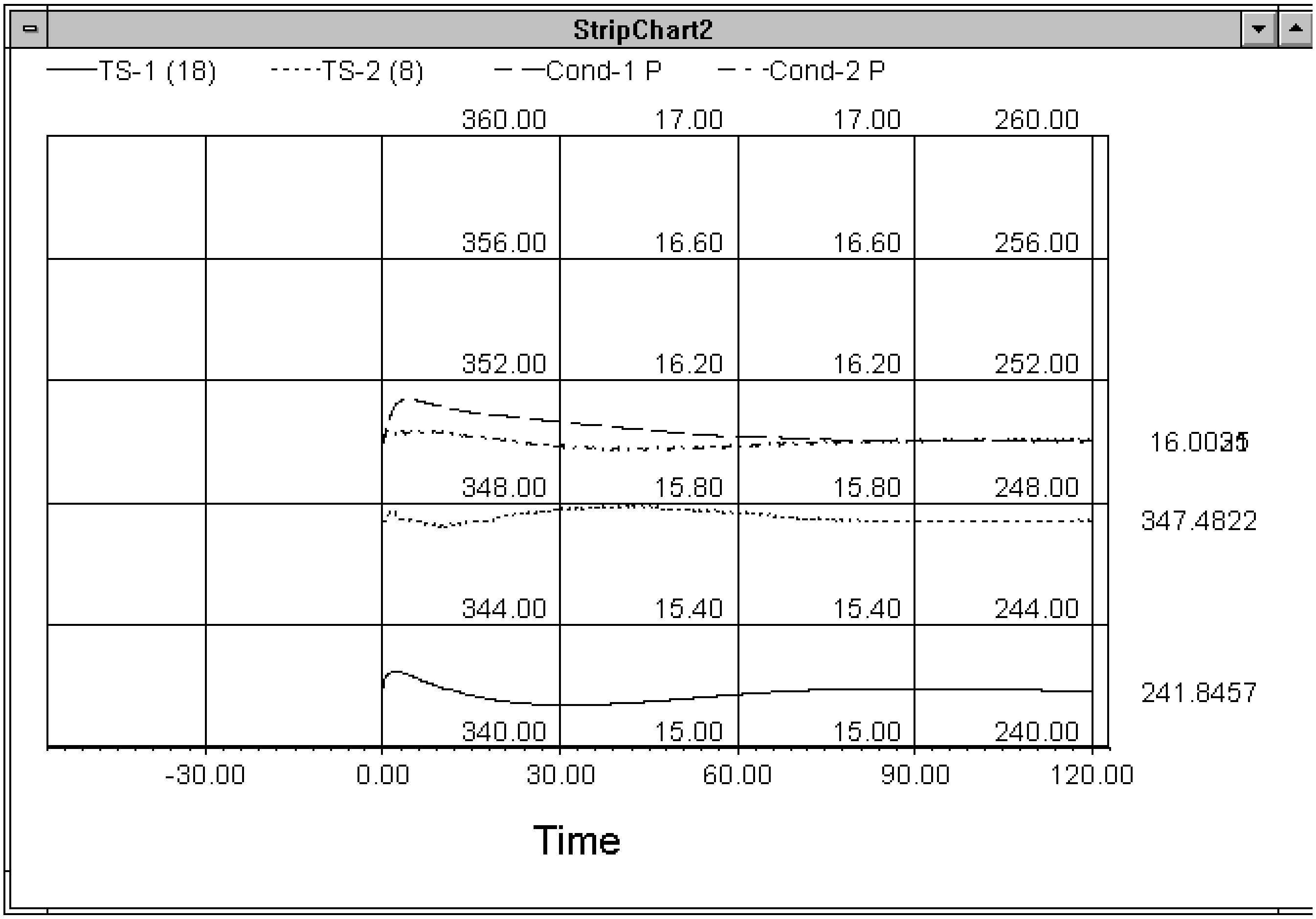
The control FacePlates appear as follows:



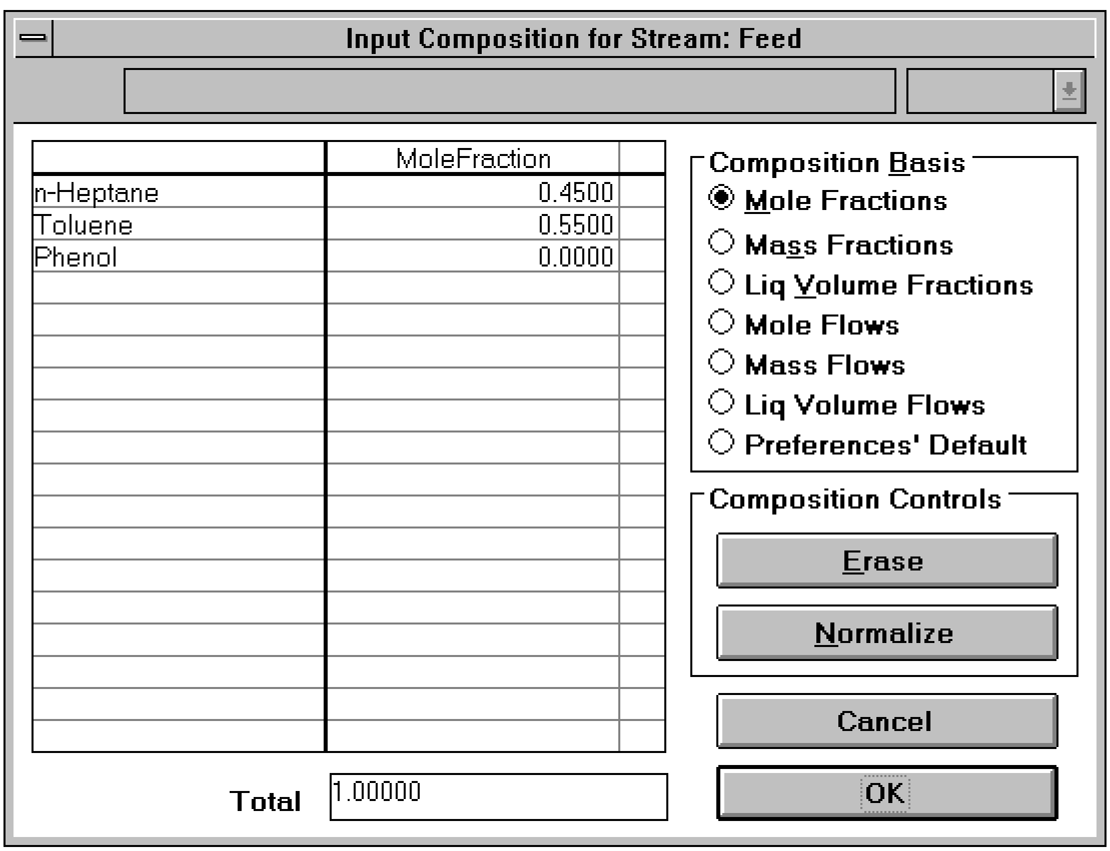
Note that we have included a Feed Flow and Phenol Flow controller; however, these are turned off, and we will instead be making changes from the WorkSheet.

Run the integrator. After a period of time, the process variables will line out:

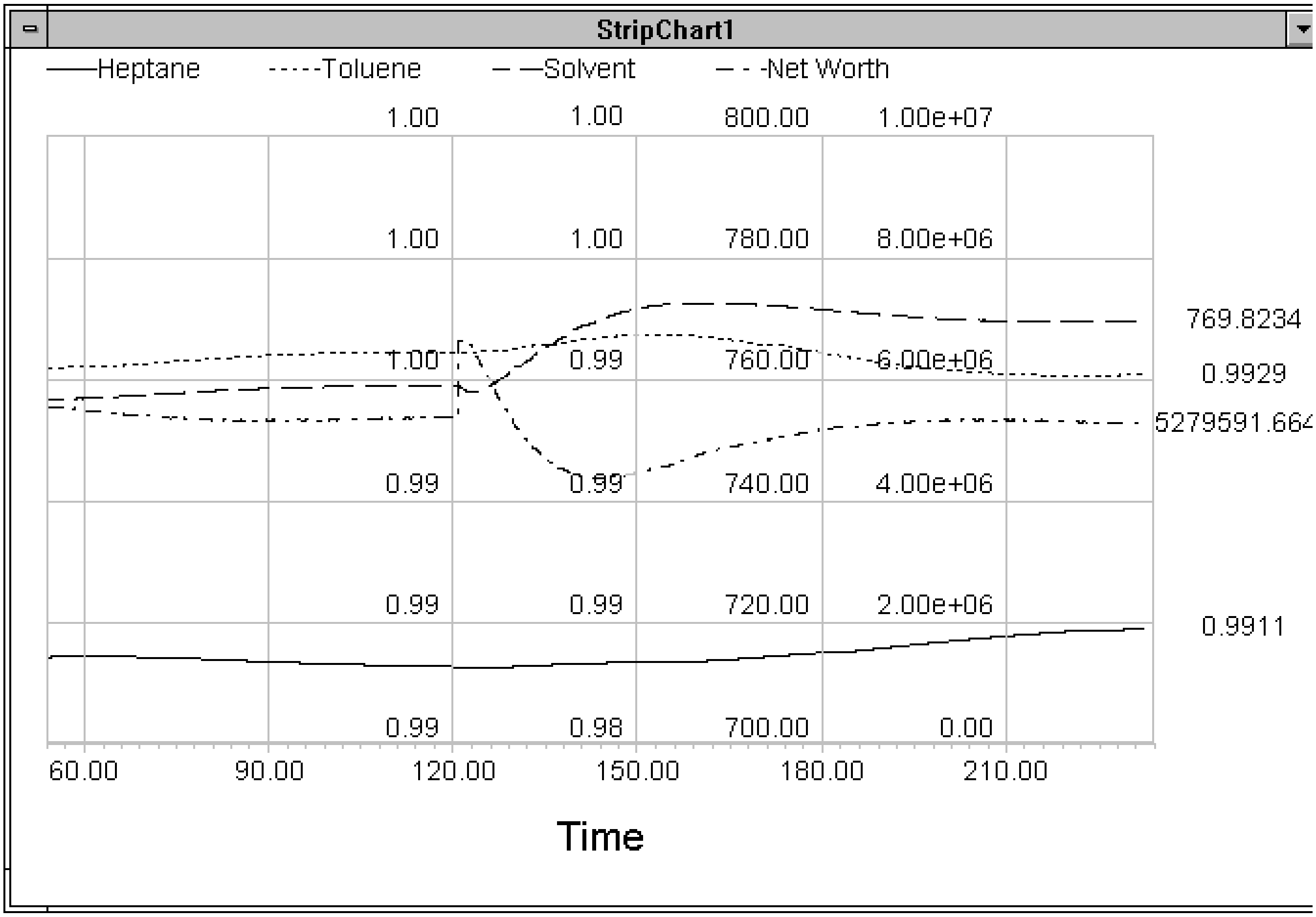


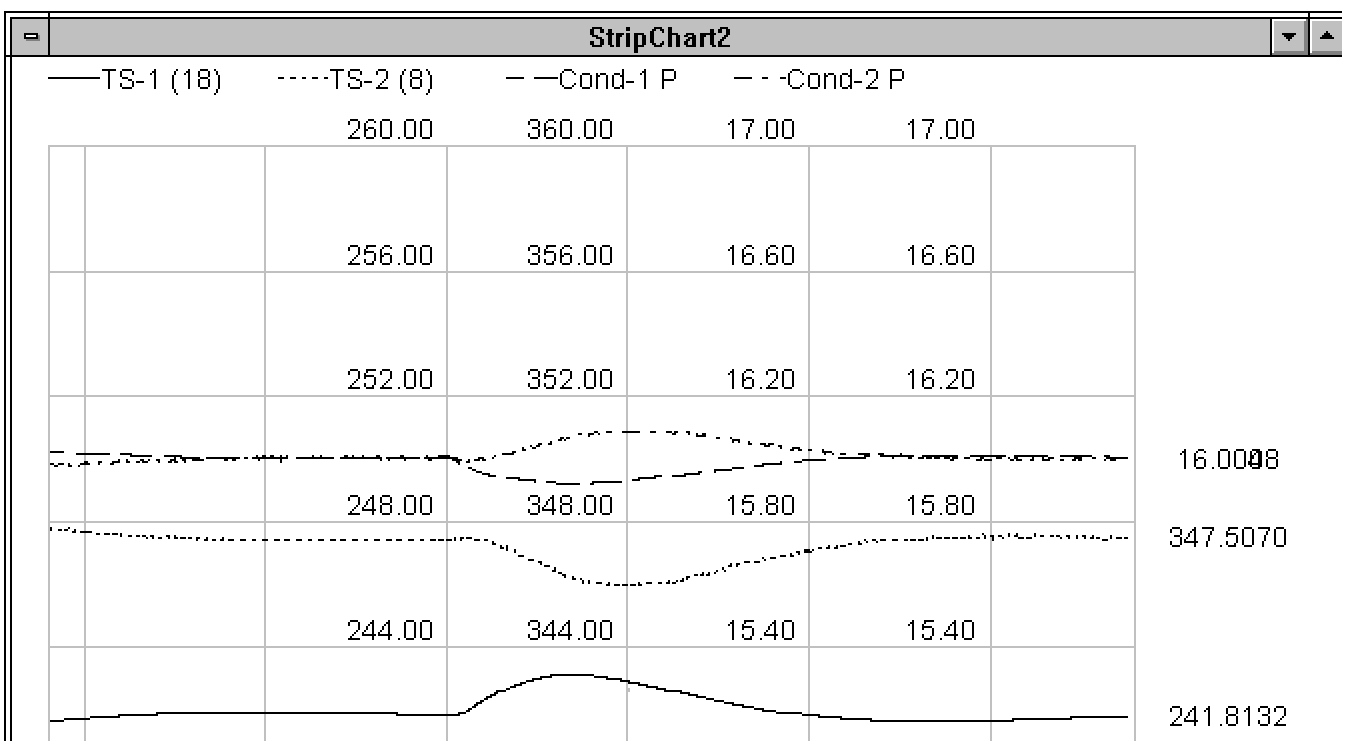


Now introduce a feed composition upset as shown below:

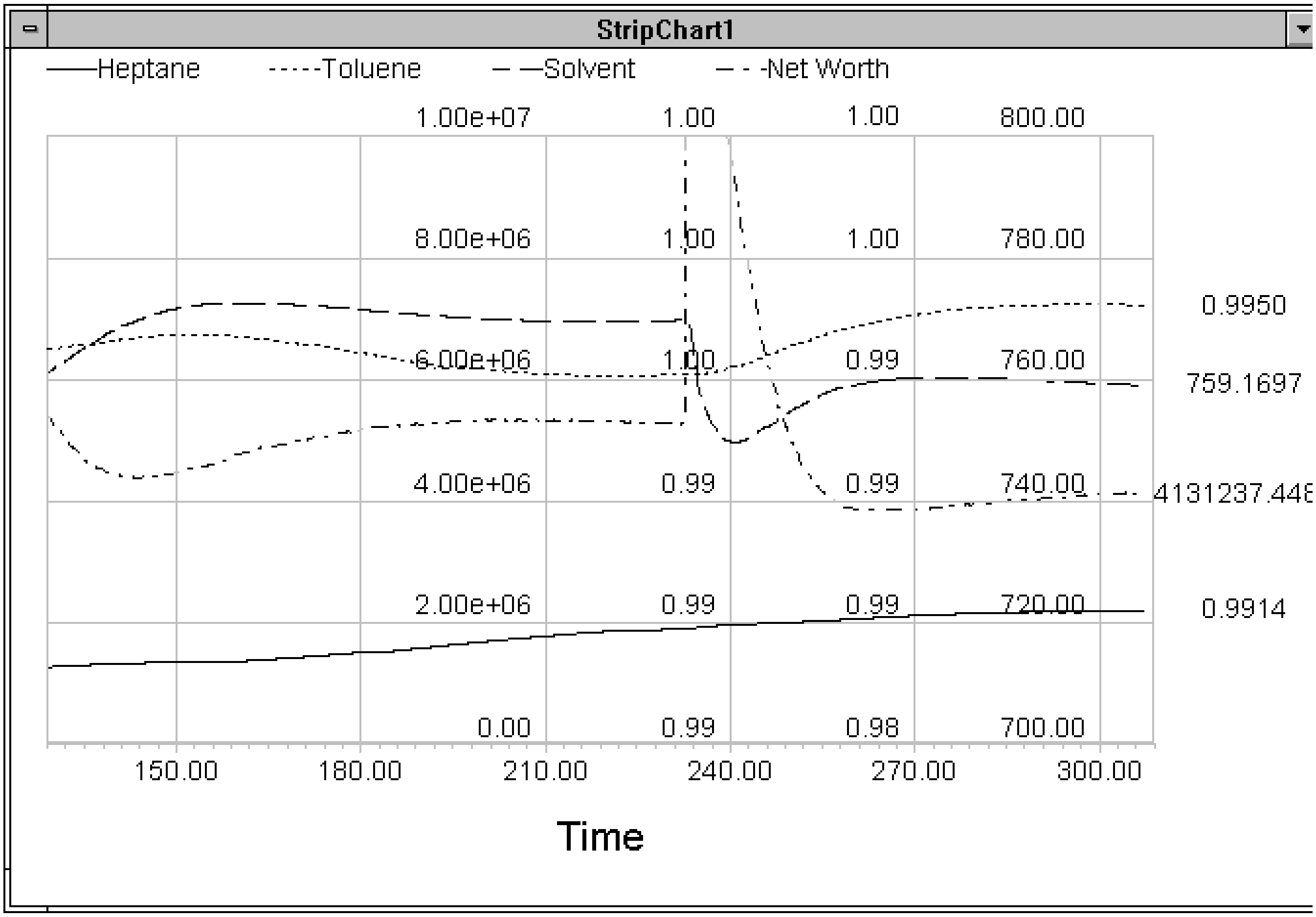


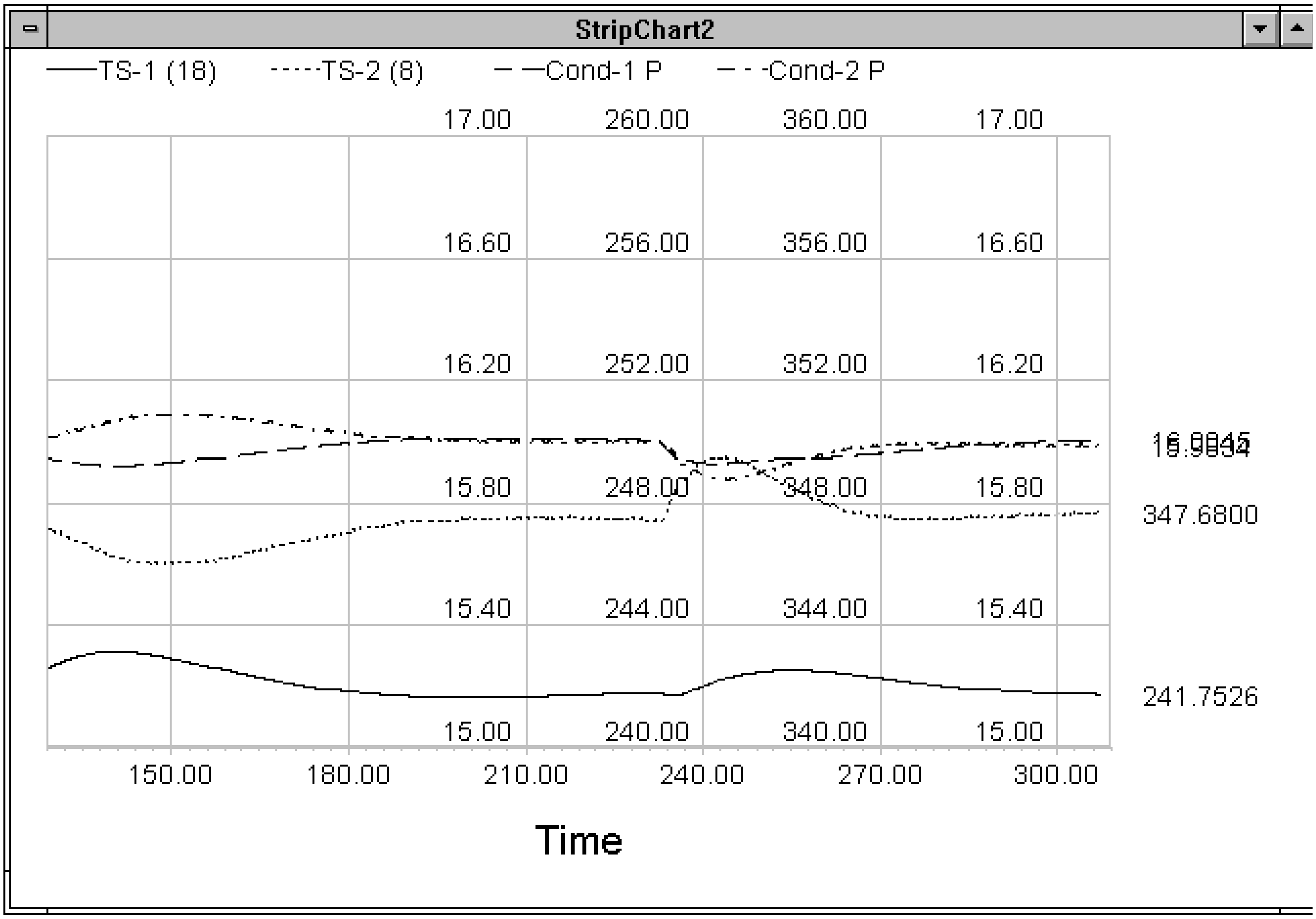
As shown in the Strip Charts, the pressures and temperatures shift somewhat from their Set Points but eventually return. The purities line out at different values, which is expected, since we have changed the composition of the feedstock. As well, the Solvent Molar Flow lines out at a higher value.





Next, we will introduce a Feed Molar Flow upset. Change the Molar Flow of stream **Feed** from 400 to 360 lbmole/hr. The Strip Charts are shown here:





At this point, we can safely conclude that our control scheme is reasonable. However, there is no doubt that the scheme could be refined further. We also may be able to achieve better control with a different scheme.

Note that the Net Worth spikes as soon as we add the upset; this is because the cost of the Feed decreases suddenly, drastically increasing the overall Net Worth. This is an example where this instantaneous Net Worth function is certainly not realistic. However, the lined-out value is valuable. It is interesting to note that even though the purities on the output stream increased, the Net Worth has actually decreased.

C-6.8 Summary and Conclusions

The use of HYSYS - Conceptual Design was crucial to this simulation, in that we could be confident that the predicted VLE would closely match experimental behaviour. Without this assurance, one would probably end up designing either an inefficient or an impossible column configuration.

HYSYS - Conceptual Design was used to estimate interaction parameters for the NRTL and Peng-Robinson Property Packages. A good fit was obtained for the NRTL property package, but not for the Peng-Robinson and PRSV Property Packages. Both Equation of State models incorrectly predicted liquid-liquid behaviour. Therefore, NRTL was used for this simulation, applying the new interaction parameters regressed from experimental data.

HYSYS - Conceptual Design was used to obtain low-purity and high-purity column configurations. This step was important, as it gave a fundamental understanding of the separation process, allowing us to see the process limitations and perimeters. The high purity configuration (0.99 Heptane, 0.99 Toluene) required more stages than the low purity configuration (0.985 Heptane, 0.985 Toluene), but the Reflux Ratios were roughly the same.

HYSYS.SteadyState was used to build the two column configurations. For the high purity configuration, even higher purities were possible than what was predicted using HYSYS - Conceptual Design (0.993, 0.994). For the low purity configuration, the specifications could not be met, and one of the Reflux Ratios had to be increased in order to obtain a solution.

The results were very similar between HYSYS - Conceptual Design and Steady State, and any differences could be attributed to the fact that an approximate solution was obtained in HYSYS - Conceptual Design (i.e. - a solution in which the passed streams between the two columns were similar, but not exactly the same; also, additional assumptions were made, such as constant molal overflow).

The feed locations for both columns, the solvent feed location, the reflux ratios and product purities were all varied in an effort to maximize the Present Net Worth.

An Economic Analysis Spreadsheet was set up in HYSYS.SteadyState, which calculated the Present Net Worth by incorporating the Fixed Capital Cost, Annual Expenses, Annual Revenues and Economic and Plant Data. The high purity configuration was shown to be superior (in terms of the Present Net Worth) to the low purity configuration.

The Optimizer was used to further refine the high purity configuration. Based on the preliminary economic data, it was possible to obtain a Net Worth of $5.93 Million, with a $2.65 Million Capital Investment, indicating that this is an economically viable process.

Finally, the process was set up in HYSYS.Dynamics. The vessels were sized, controllers were added, tuning parameters were defined, valves were sized, strip charts were set up, and Dynamic Model parameters were checked.

The process was run dynamically. Feed composition and feed flow upsets were individually introduced, and key variables were observed to ensure that the control system was adequate. The system responded reasonably to these upsets, indicating that the control scheme was satisfactory, although it is acknowledged that further improvements are certainly possible.

Perhaps most importantly, the setup of this process, from the definition of property package interaction parameters to the dynamic system response were carried out entirely using HYSYS - Conceptual Design and HYSYS.SteadyState and dynamics.

C-6.9 Bibliography

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