Model Development for Optimization

- The methods described in the previous three lectures require an objective function as well as the constriants.
- This requires the development of a *mathematical model* for the process under consideration.

A mathematical model provides quantitative expressions that enable us to use optimization techniques to extract useful information about process design and operation. Two types of models may be developed:

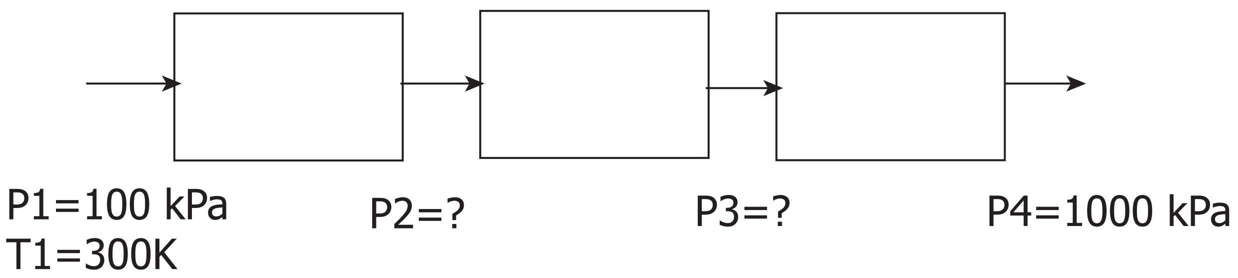
1. Fundamental Models
2. Empirical Models

Fundamental Models:

- These models are developed from fundamental principles (e.g. mass and energy balances).
- Typically *simplifying assumptions* are made to keep the size of the model small.
- Model parameters are obtained from independent experiments and are physically meaningful quantities (e.g density, viscosity).
- The model expressions have *predictive* capabilities.
- The accuracy of the model predictions depend on how good the assumptions are.

- *A lot of process experience is required to develop good models*. The challenge is to convert a *word problem* into a *mathematical description*.
- Optimization methods used on the model give the optimal solution of the *model*. Whether this is the optimal solution of the *process* depends on how accurately the model depicts the process.

Example 1:



Consider a three stage compressor with intercooling. The following process data is given:

$$P_1 = 100\ kPa \quad P_4 = 1000\ kPa \quad T_1 = 300\ K$$

Assume that the compressor is used to compress air. What should be the values of P_2 and P_3 so that the total work is minimized?

Solution:

- Assume that the flow is ideal compressible adiabatic flow.
- Since the gas is assumed to be ideal, $k = \frac{C_p}{C_v} = 1.4$ and does not change in the pressure range P_1 to P_4.
- The equation describing the work done for ideal compressible adiabatic flow can be found in standard text-books.

- The work done for each stage is given as follows:

$$\begin{aligned} W_1 &= \frac{kRT_1}{k-1}\left[\left(\frac{P_2}{P_1}\right)^{\frac{k-1}{k}} - 1\right] \\ W_2 &= \frac{kRT_1}{k-1}\left[\left(\frac{P_3}{P_2}\right)^{\frac{k-1}{k}} - 1\right] \\ W_3 &= \frac{kRT_1}{k-1}\left[\left(\frac{P_4}{P_3}\right)^{\frac{k-1}{k}} - 1\right] \end{aligned} \tag{1}$$

- The total work done W is given by:

$$\begin{aligned} W &= W_1 + W_2 + W_3 \\ &= \frac{kRT_1}{k-1}\left[\left(\frac{P_2}{P_1}\right)^{\frac{k-1}{k}} + \left(\frac{P_3}{P_2}\right)^{\frac{k-1}{k}} + \left(\frac{P_4}{P_3}\right)^{\frac{k-1}{k}} - 3\right] \end{aligned} \tag{2}$$

- The above equation gives us the objective function to minimize, as a function of P_2 and P_3.

- Clearly P_2 and P_3 will take values between $P_1 = 100\ kPa$ and $P_4 = 1000\ kPa$. We first try to find the optimal values by posing the problem as an *unconstrained* minimization problem. If the solution is not in the range $100 - 1000\ kPa$, we will add inequality constraints.

- To minimize W w.r.t. P_2 and P_3, the necessary conditions of optimality are:

$$\begin{aligned} \frac{\partial W}{\partial P_2} &= 0 \\ \frac{\partial W}{\partial P_3} &= 0 \end{aligned} \tag{3}$$

- This leads to the following algebraic equations that need to be solved simultaneously:

$$\begin{aligned} \left[(P_1)^{\frac{1-k}{k}}(P_2)^{\frac{1}{k}} - (P_3)^{\frac{k-1}{k}}(P_2)^{\frac{1-2k}{k}}\right] &= 0 \\ \left[(P_2)^{\frac{1-k}{k}}(P_3)^{\frac{1}{k}} - (P_4)^{\frac{k-1}{k}}(P_3)^{\frac{1-2k}{k}}\right] &= 0 \end{aligned} \tag{4}$$

- Substitute

$$k = 1.4 \quad P_1 = 100\ kPa \quad P_4 = 1000\ kPa$$

- Solving the two equations simultaneously for P_2 and P_3, we obtain:

$$\begin{aligned} P_2^* &= 215.44\ kPa \\ P_3^* &= 464.17\ kPa \end{aligned} \tag{5}$$

- The sufficient conditions of optimality can be checked to ensure that the solution obtained is indeed a *minimum* and not a maximum or a saddle-point.

Example 2:

Consider the following distillation problem:

The objective is to minimize Q_1 by selecting F_1, F_2, F_3, F_4, Q_1.

The feed conditions are as follows:

$$\begin{aligned}
Total\ feed &= 100 \quad lbmol/hr\ liquid \\
h_f &= 4000 \quad Btu/lbmol \\
x_1 &= 0.05 \quad (C_3H_8) \\
x_2 &= 0.15 \quad (i-C_4H_{10}) \\
x_3 &= 0.25 \quad (n-C_4H_{10}) \\
x_4 &= 0.20 \quad (i-C_5H_{12}) \\
x_5 &= 0.35 \quad (n-C_5H_{12})
\end{aligned} \tag{6}$$

The desired distillate product specifications are:

$$\begin{gathered} 10 \; lbmol/h \; liquid \\ with \; x_5 \leq 0.07 \end{gathered} \tag{7}$$

The reflux ratio used is 1.5 times the minimum reflux.

<u>Equality Constraints</u>

- Total material balances (one for each stage k, $k = 1, 2, 3, 4$)

$$F_k^L + F_k^V + V_{k-1} + L_{k+1} = V_k + L_k \tag{8}$$

- Component material balance (one for each component i for each stage k)

$$x_{i,k}^F F_k^L + y_{i,k}^F F_k^V + y_{i,k-1} V_{k-1} + x_{i,k+1} L_{k+1} = y_{i,k} V_k + x_{i,k} L_k \tag{9}$$

- Energy balance (one for each stage)

$$Q_k + h_k^F F_k + H_{k-1} V_{k-1} + h_{k+1} L_{k+1} = H_k V_k + h_k L_k \tag{10}$$

- Equilibrium relations for liquid and vapor at each stage (one for each stage)

$$y_{i,k} = K_{i,k} x_{i,k} \tag{11}$$

- Relation between equilibrium constant and p, T, x, y (one for each stage)

$$K_{i,k} = K_i(p_k, T_k, x_k, y_k) \tag{12}$$

- Relation between enthalpies and p, T, x, y (one for each stage)

$$\begin{aligned} h_k &= h(p_k, T_k, x_k) \\ H_k &= H(p_k, T_k, y_k) \end{aligned} \tag{13}$$

There are other *implicit* equalities that must be satisfied.

- Overall liquid mole fraction at each stage:

$$\sum_{i=1}^{m} x_{i,k} = 1$$
$$\sum_{i=1}^{m} y_{i,k} = 1 \tag{14}$$

- Sum of all the feeds is given in the problem statement:

$$\sum_{i=1}^{m} F_k = 100 \tag{15}$$

Inequality Constraints

$$
\begin{aligned}
Q_1 &\geq 0 \\
Q_4 &\leq 0 \\
x_{i,k} &\geq 0 \\
y_{i;k} &\geq 0 \\
F_k &\geq 0 \\
x_{5,4} &\leq 0.07 \; (\textit{given in problem statement})
\end{aligned}
\tag{16}
$$

Results of Optimization

Variable	Initial Guess	Optimal Value
F_1	25	23.7
F_2	25	0.0
F_3	25	0.0
F_4	25	76.3
Q_1	5.0×10^6	3.38×10^5

The optimal solution suggests that it is possible to use some of the cold feed as reflux in the top stage without voiding the product composition specification. This outcome is not an obvious choice for the problem specification.