Chapter 14
Process Optimization

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The Base Case

For any optimization, we need a starting point – this is our <u>base case</u>

- The base case may be any technically feasible process
- The further the base case is from optimum, the more optimization must be done
- An objective function based (OF) on operating and capital investment, *e.g*., EAOC or NPV should be chosen with the aim of minimizing or maximizing the function – other OFs are possible, *e.g*., maximize production of chemical B from the plant, etc.
- A *Pareto* analysis (80-20 rule) is often helpful to focus attention on what should be looked at first
- Overall material balance tells us how efficiently raw materials are being used – even though these costs are high, it may not be possible to reduce them significantly.

Key Decision Variables

Even simple processes have tens if not hundreds of potential decision variables. Therefore, it is important to identify which of these has a significant effect on the *OF*.

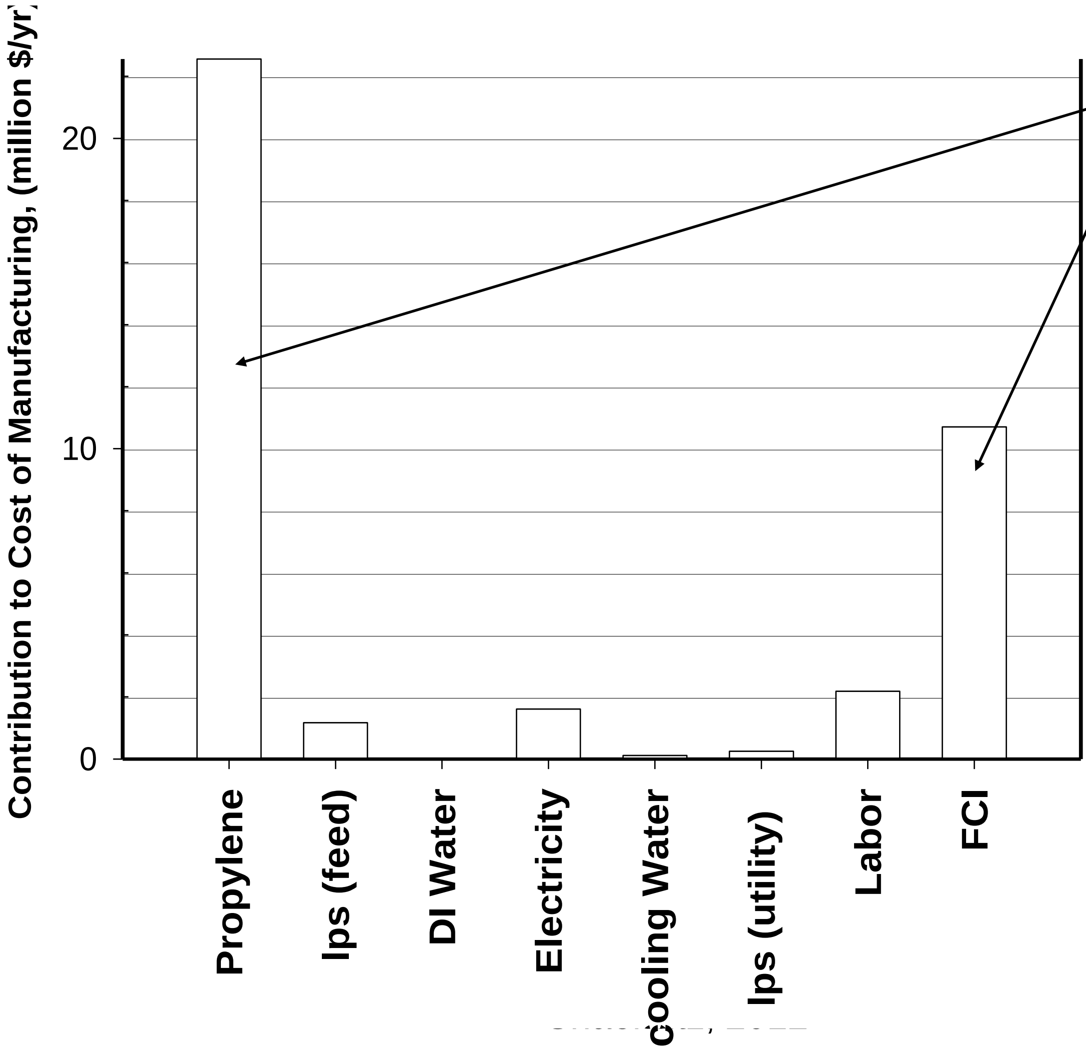
- A *Pareto* analysis will identify the major costs, but how those costs are affected by changes in operating variables needs some preliminary investigation.
- Usually, the single-pass conversion in the reactor is an important decision variable since recycle rates are influenced directly.
    - It is easy to mask the effect of conversion using different variables such as reactor temperature and pressure.
    - Interpreting results in terms of conversion is usually more straight forward than *T* and *P* – but *T* and *P* may be easier to set in the simulation.

Key Decision Variables

- If unreacted material leaves the process, then decision variables that reduce these streams by better recovery in the separations sections (and higher conversion) should be considered.
- High utility costs (steam and electricity) warrant decision variables that focus on recovering heat and work. Also, there is heat integration.

Key Decision Variables

Costs associated with the production of a new facility to produce acrylic acid via the partial oxidation of propylene



Largest improvements may not be associated with the largest costs

$$C_3H_6 + \frac{3}{2}O_2 \rightarrow C_3H_4O_2 + H_2O$$

acrylic acid

$$C_3H_6 + \frac{5}{2}O_2 \rightarrow C_2H_4O_2 + H_2O + CO_2$$

acetic acid

$$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3H_2O + 3CO_2$$

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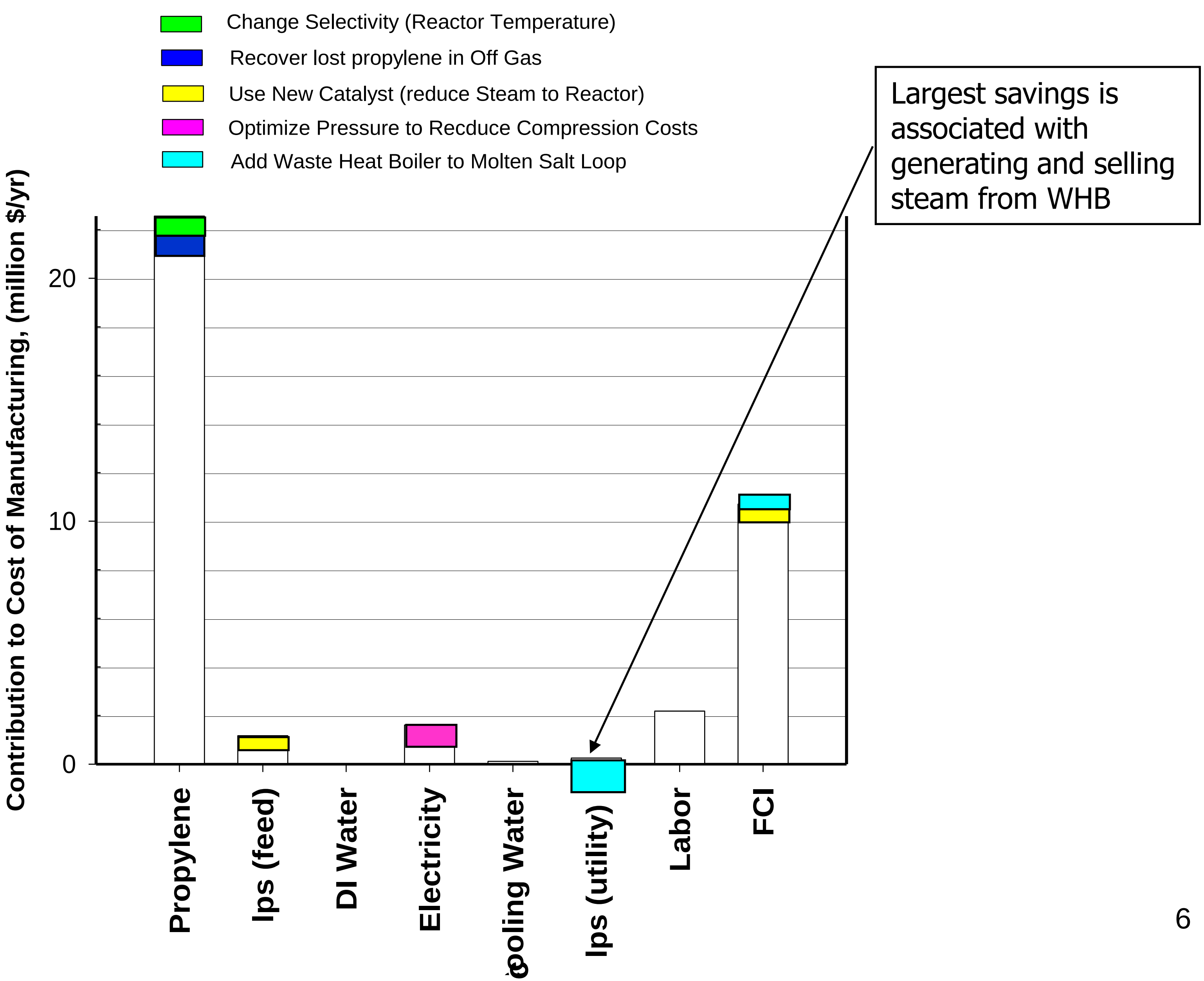


Topological vs. Parametric Optimization

Topological Optimization involves changes in the arrangement (topology) of process equipment. Questions that should be addressed include:

- Can unwanted by-products be eliminated?
- Can equipment be eliminated or rearranged?
- Can alternative separation methods or reactor configurations be employed?
- Can heat integration be improved?

Often, topological changes lead to large improvements in the *OF* and are considered early on in the design phase.

Many of the more common topological changes were considered in Chapter 2 – *Structure and synthesis of process flow diagrams*

Topological vs. Parametric Optimization

Parametric Optimization involves the manipulation of process variables such as single-pass conversion, reflux ratio, product purity and yield, operating pressure, etc. Parametric optimizations may lead to changes in the topology of the process. For example, by increasing the single-pass conversion, it may be possible to eliminate a separation unit and the recycle of unused reactant.

Parametric Optimization – 1 variable

Parametric Optimization – Case Study No .1

Optimum reflux in a distillation column

For a fixed feed, operating pressure, and product yields and purities – the size (diameter and height) of a distillation tower is fixed based on the reflux ratio, *R* (assuming % flood, tray design, etc., are fixed)

As *R* increases

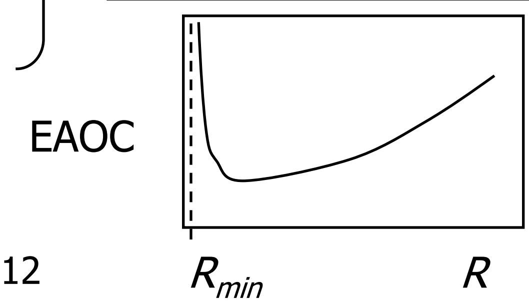
Reboiler duty, size, and utility costs increase

Condenser duty, size, and utility costs increase

Tower Diameter increases

Number of stages + tower height decreases

Formulate costs in terms of EAOC or NPV and optimize

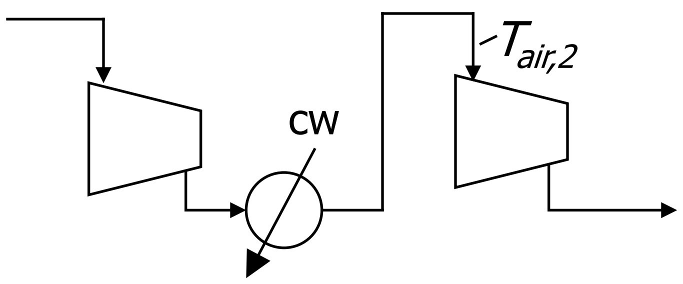


Parametric Optimization – 1 variable

Parametric Optimization – Case Study No .2

Consider the compression of feed air into a process that produces maleic anhydride.

The air (10 kg/s) enters the process at atmospheric pressure and 25°C and is compressed to 3 atm in the first compressor. The compression is 65% efficient based on a reversible adiabatic process. Prior to entering the second stage of compression (where the air is compressed to 9 atm at the same efficiency) the air flows through a water-cooled heat exchanger where the temperature is cooled. What is the optimum size of the heat exchanger?



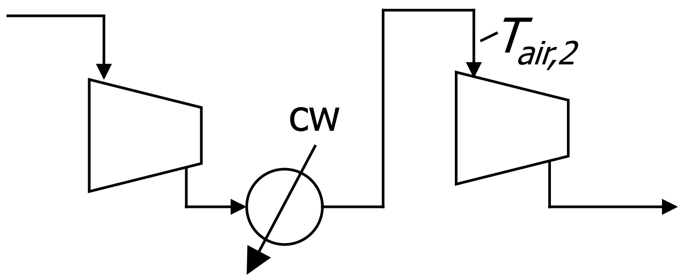
Assume: ignore pressure drop in pipe and exch,

U = 42 W/m^2°C, $T_{cw,in}$ = 30°C and $T_{cw,out}$ = 40°C

Problem is specified by choosing $T_{air,2}$

Parametric Optimization – 1 variable

Parametric Optimization – Case Study No .2



As $T_{air,2}$ decreases

C_{exch}

C_{cw}

C_{power}

C_{comp}

Formulate total cost as EAOC and minimize

Parametric Optimization – 1 variable

Parametric Optimization – Case Study No .3

Look at the distillation of light (volatile) materials, *e.g.*, propane from butane, in a depropanizer and consider the column pressure as the decision variable.

General trends as P ↑

Separation becomes harder – equilibrium curve moves closer to $x = y$ line

Column has more stages and a smaller diameter

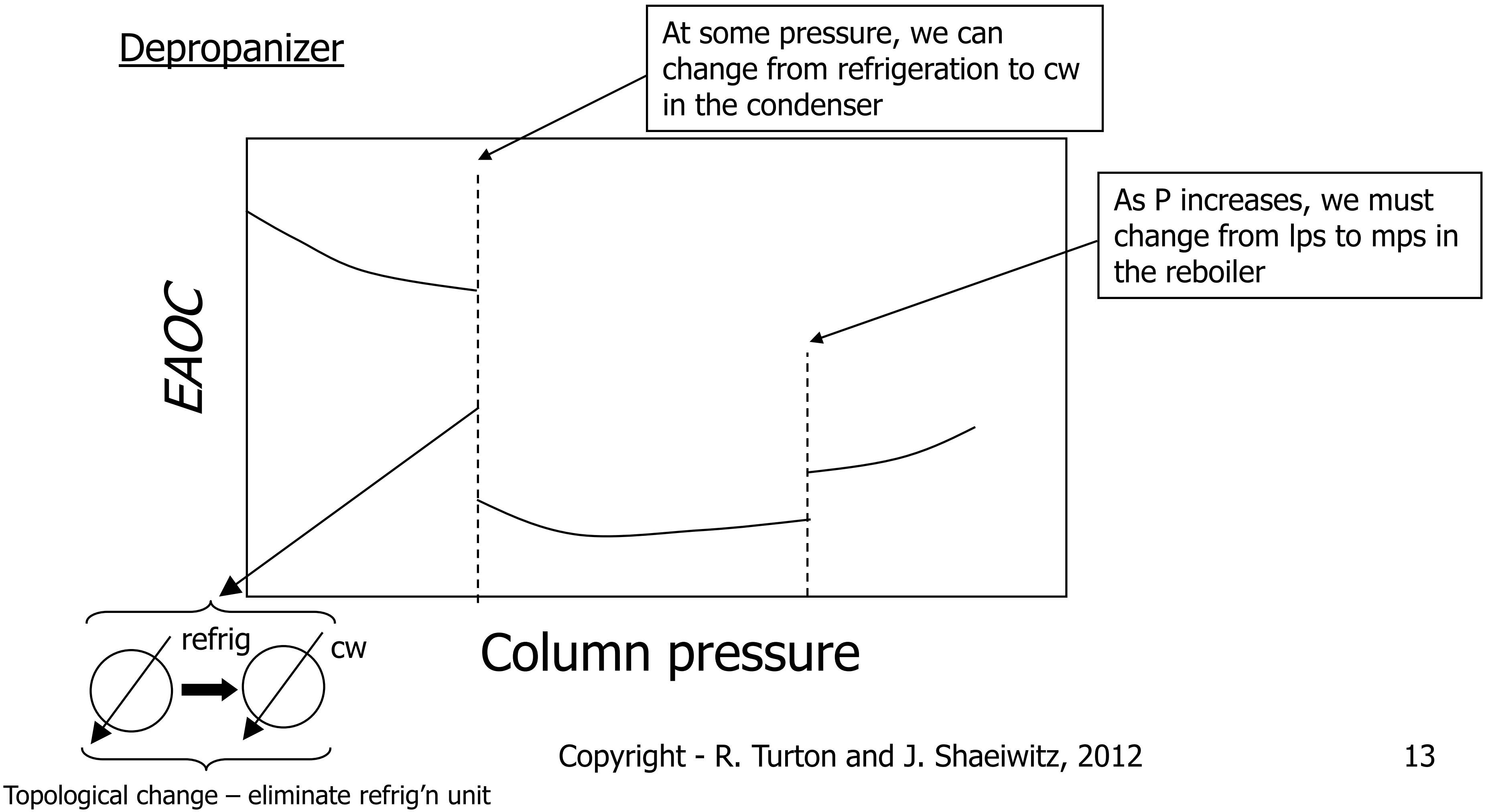
Column temperature increases (top and bottom)

Objective function, OF = $EAOC = \left\{ \left[\frac{A}{P}, i, n \right] \sum_{\substack{tower \\ reboiler \\ condenser, etc}} \mathrm{FCI} \right\} + \text{utility costs (reboiler, condenser, pumps)}$

Parametric Optimization – 1 variable

Parametric Optimization – Case Study No .3

Depropanizer



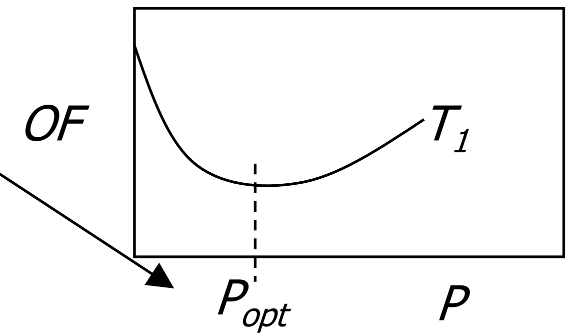
Parametric Optimization – Multivariable

<u>Parametric Optimization – multivariable</u>

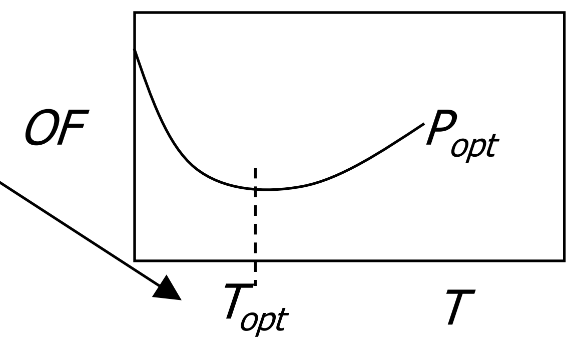
When considering multivariable problems **<u>it is tempting to</u>** change one variable at a time and proceed in a stepwise manner.

For example: Consider an *OF* and two variables *T* and *P*

First hold *T* constant at T_1 and vary *P* to get



Then using P_{opt}, we vary *T* to get

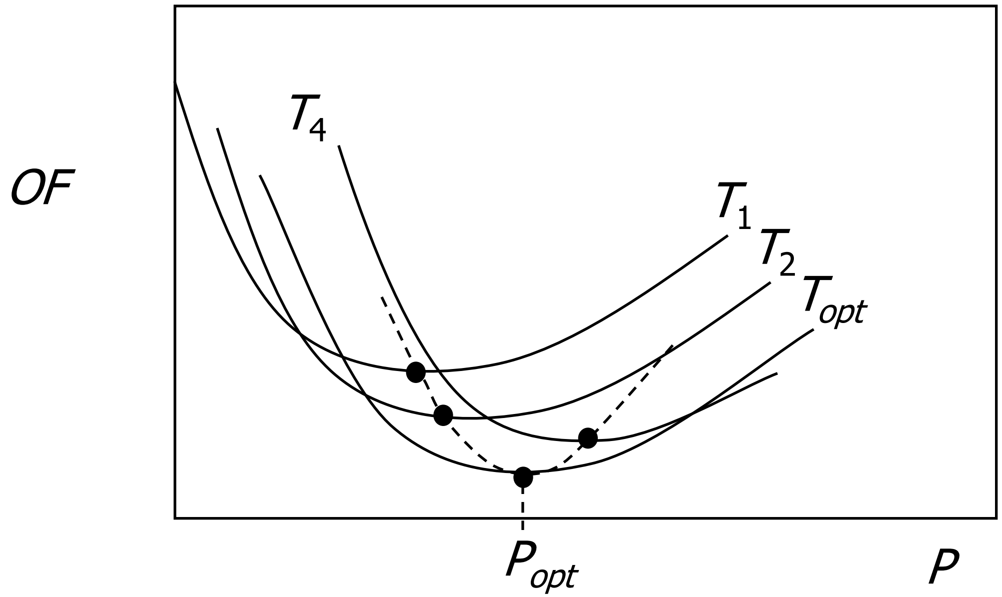


However T_{opt}, P_{opt} is not the "global" optimum

Parametric Optimization – Multivariable

Parametric Optimization – multivariable

What should be done is:

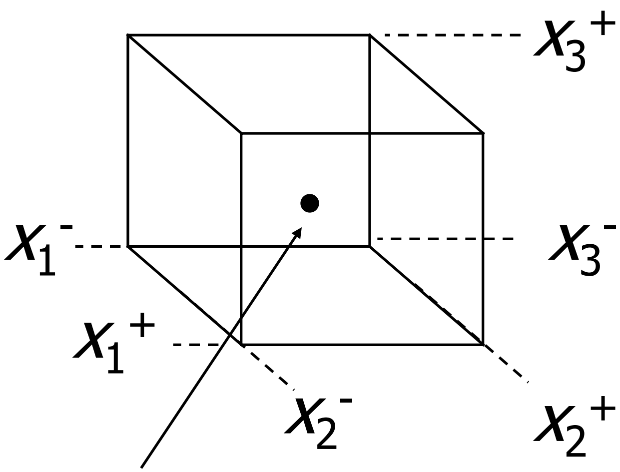


Parametric Optimization – Multivariable

Parametric Optimization – multivariable

For more than 2 variables, the previous approach becomes very tedious, so try a DOE (design of experiments or lattice approach).

Consider the simulation and associated cost analysis that provides the *OF* as the result of a single "experiment." Choose values of decision variables in a reasonable range and pick the end points of the range as independent variables. Thus, for three decision variables there are $2^3=8$ "experiments."



May include a "base case" or center point

$$OF_1 = f(x_1^-, x_2^-, x_3^-)$$

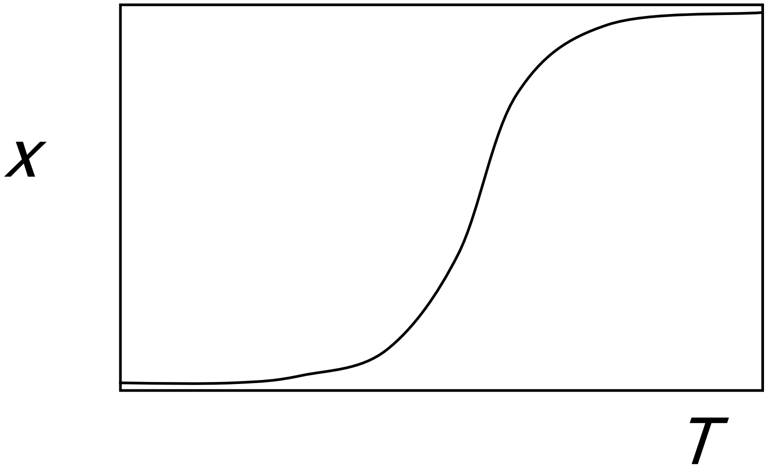
$$OF_2 = f(x_1^-, x_2^-, x_3^+)$$

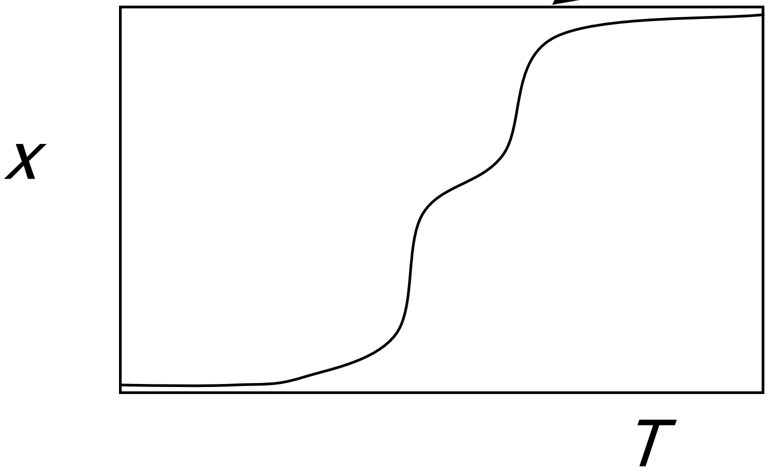
$$\vdots$$

Find best *OF* and then refine the grid or use linear regression techniques to fit the data and predict optimum *OF*

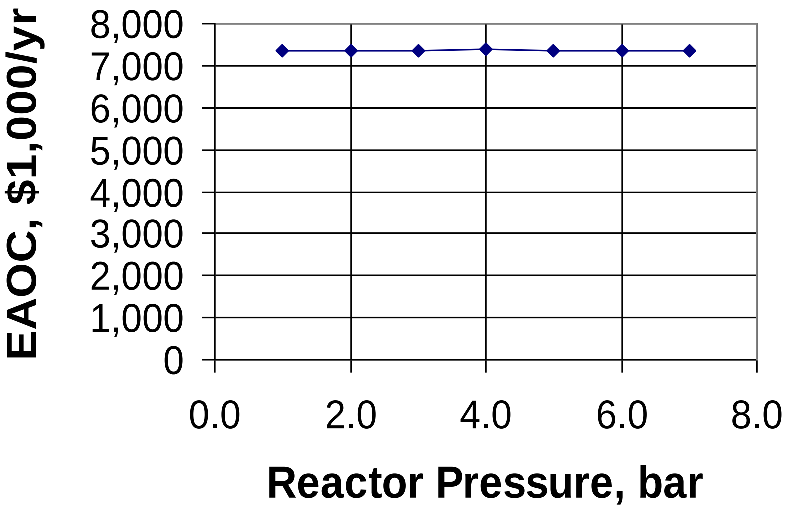
Presentation of Optimization Results

In general, when plotting optimization results the curves should be <u>smooth</u> if all the variables are continuous. For example, if plot conversion as a function of reactor temperature then should get something <u>like this</u> **not this**

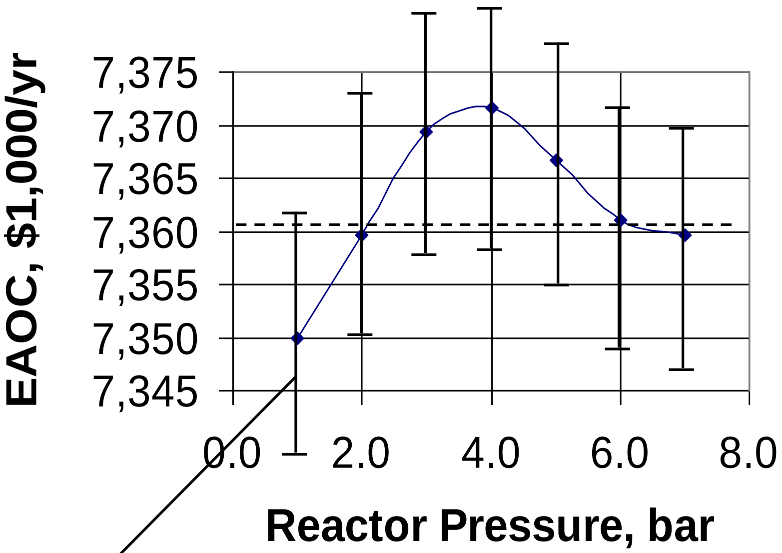




Presentation of Optimization Results



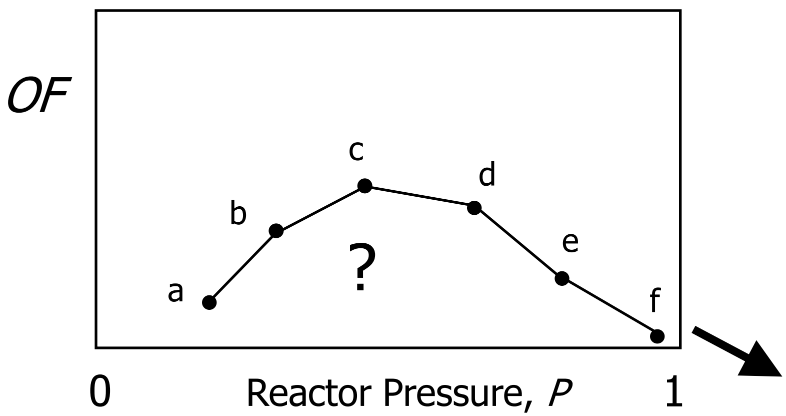
Beware of expanding the *y*-axis



Be aware of the accuracy of
your estimates

Presentation of Optimization Results

Understand the main effects



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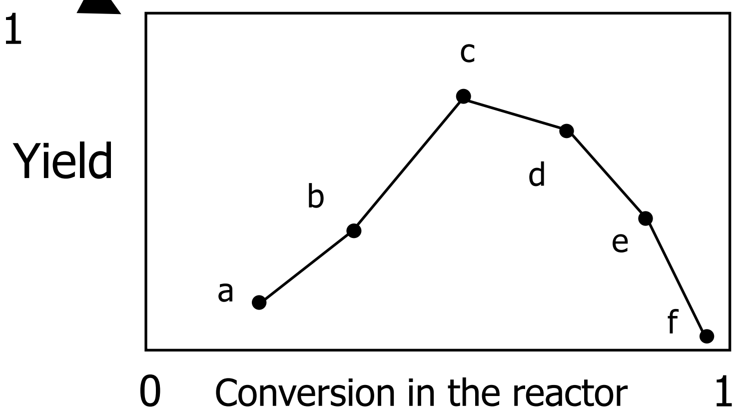


Optimization Examples

Example – 1 for Class

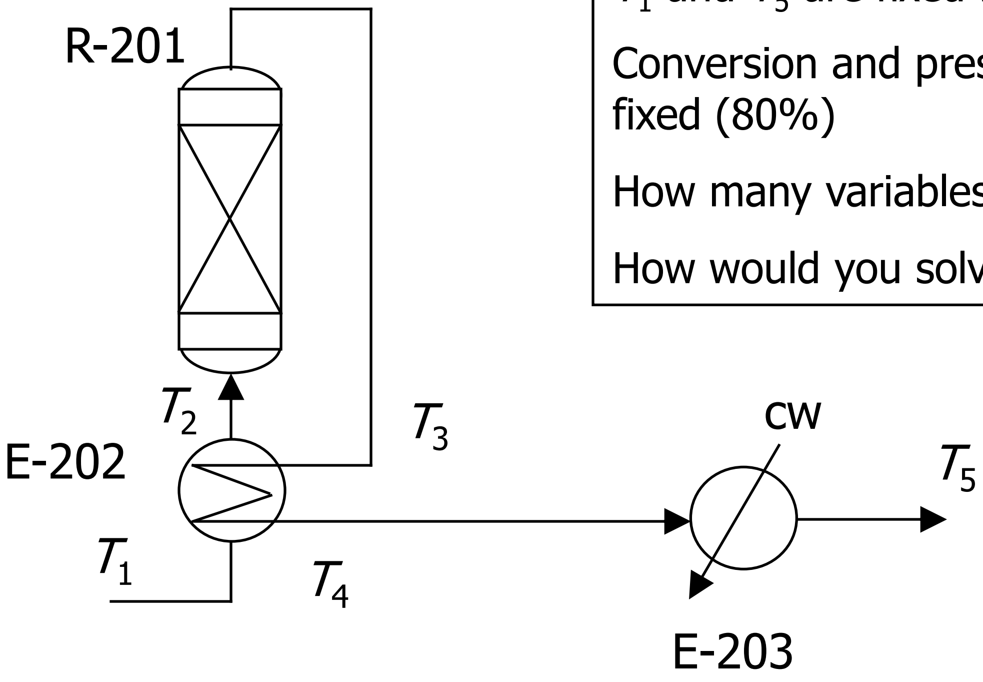
Consider the reactor preheat exchanger for the DME process given in Appendix 1.

T_1 and T_5 are fixed by process

Conversion and pressure in the adiabatic reactor are fixed (80%)

How many variables are there in this optimization?

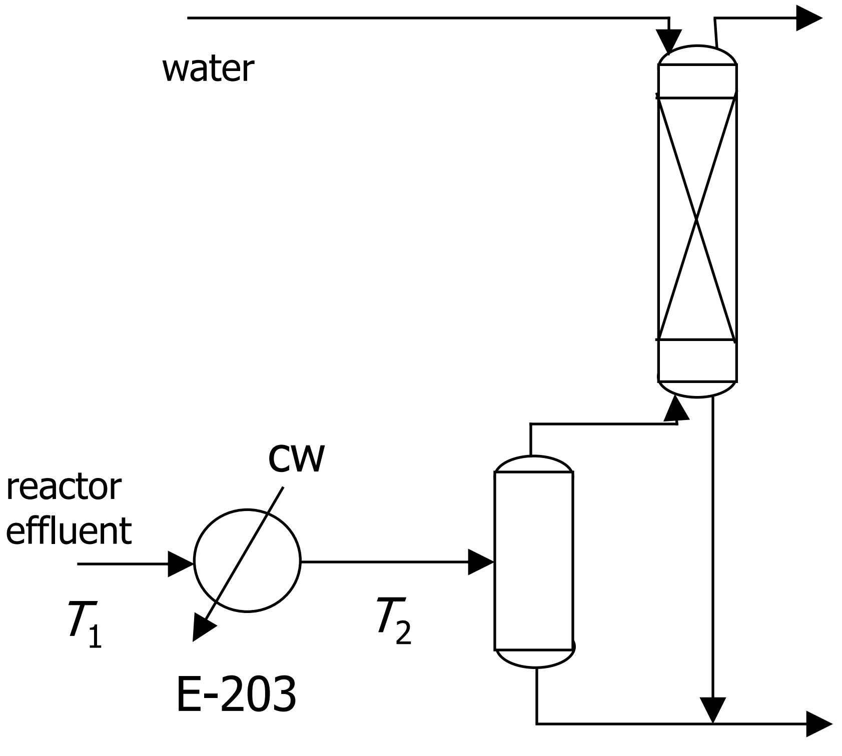
How would you solve this problem?



Optimization Examples

Example - 2 for Class

Consider the recovery of acetone from the reactor effluent



T_1 and composition are fixed by process

Reactor effluent contains acetone, IPA, and hydrogen.

What are the key decision variables in this optimization?

How would you solve this problem?