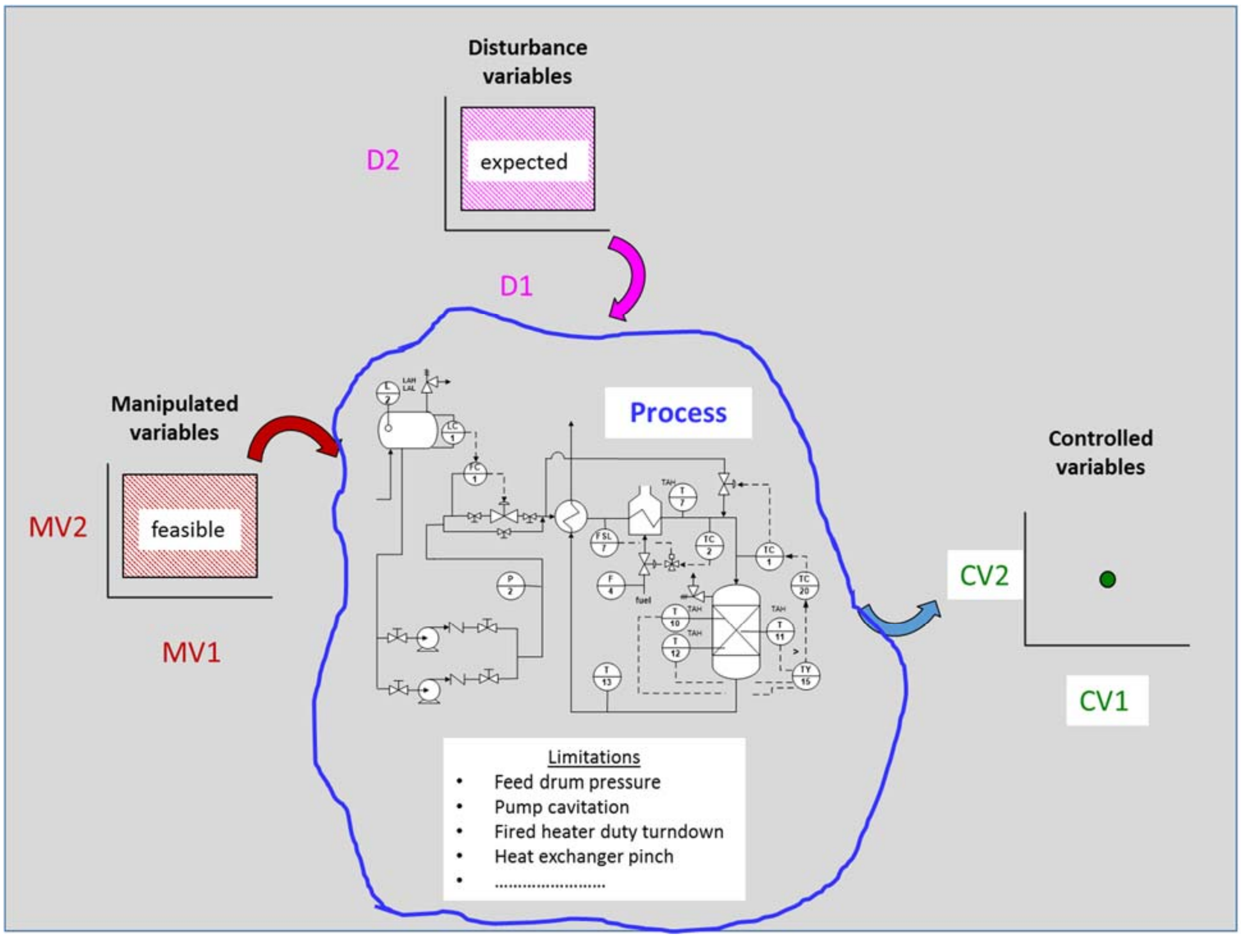
Operability in Process Design: Achieving Safe, Profitable, and Robust Process Operations

Chapter 2. Operating Window



Thomas Marlin

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This material is provided to promote education in the general field of "process operability" via the Internet site www.pc-education.mcmaster.ca . It is one of the chapters of an integrated presentation of selected operability topics. The author would like to hear from readers on how they are using this material. In addition, he would appreciate suggestions for improvements and extensions. He can be contacted at marlint@mcmaster.ca .

Acknowledgements

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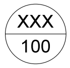
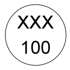
Symbols



CONTROL ROOM BOARD MOUNTED INSTRUMENT

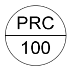


LOCAL BOARD MOUNTED INSTRUMENT

MEASURED VARIABLE:
L: LEVEL
P: PRESSURE
A: ANALYZER
F: FLOW
T: TEMPERATURE

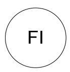
FUNCTIONS:
I: INDICATOR
C: CONTROLLER
A: ALARM
(H =HIGH, L=LOW)

EXAMPLES:

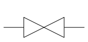


PRESSURE RECORDER CONTROLLER: I.D. NUMBER 100, MOUNTED IN CENTRAL CONTROL ROOM.

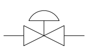
TAH TEMPERATURE ALARM: ACTIVATED AT HIGH TEMPERATURE.



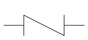
LOCAL FLOW INDICATOR



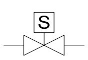
VALVE



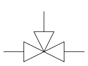
DIAPHRAGM VALVE: CONTROLLED BY AIR LINE



CHECK (ONE-WAY) VALVE

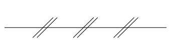


SOLENOID VALVE CONTROLLED BY ELECTRICAL SIGNAL



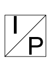
THREE-WAY VALVE

SPRING LOADED SAFETY VALVE

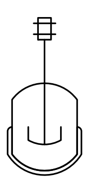


AIR LINE

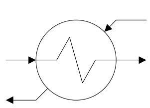
ELECTRICAL SIGNAL



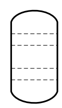
ELECTRICAL (CURRENT) TO PNEUMATIC SIGNAL CONVERTER



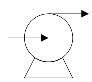
STIRRED TANK



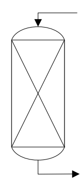
SHELL AND TUBE HEAT EXCHANGER



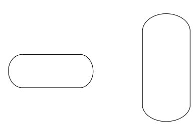
TRAYED COLUMN



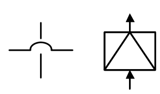
CENTRIFUGAL PUMP



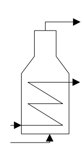
PACKED TOWER OR PROCESS VESSEL (SUCH AS A REACTOR).



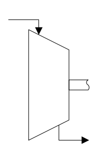
GENERIC TOWER OR PROCESS VESSEL (SUCH AS A REACTOR).



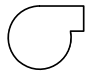
RUPTURE DISK, BURST DIAPHRAGM



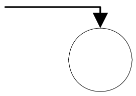
FIRED HEATER (FURNACE)



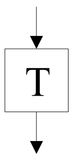
AXIAL COMPRESSOR



CENTRIFUGAL FAN

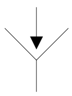


HEADER (STEAM OR CONDENSATE)

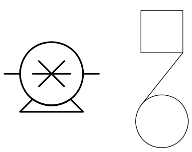


STEAM TRAP

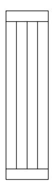
MOTOR



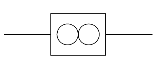
DRAIN TO SEWER



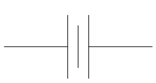
POSITIVE DISPLACEMENT PUMP



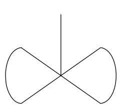
CONDENSER



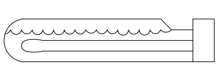
TURBINE FLOW METER



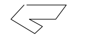
ORIFICE PLATE



IMPELLER

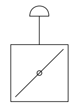


VAPORIZER OR REBOILER

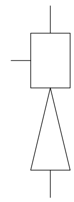


FILTER AND DRAIN

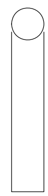
CYCLONE



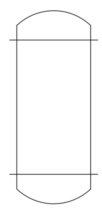
DAMPER OR BUTTERFLY VALVE



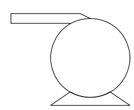
STEAM EJECTOR



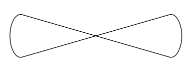
FLARE STACK



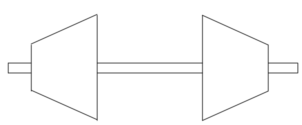
SHELL AND TUBE HEAT EXCHANGER



FAN OR BLOWER



FAN



TURBINE USED TO PROVIDE WORK TO DRIVE COMPRESSOR

Nomenclature

a	Coefficient in cooling coil heat transfer model
A	Linear model coefficients in equation (2.1)
B	Linear model coefficients in equation (2.1)
c	Linear model coefficients in equation (2.1)
C_A	Molar concentration of component A in reactor
C_{A0}	Molar concentration of component A in feed
C_p	Heat capacity
CV	Controlled output variables (non-linear model)
d	Disturbance input variables (linear model)
D	Disturbance input variables (non-linear model)
E	Activation energy for Arrhenius temperature dependence
F	Volumetric flow rate
F_c	Coolant flow rate
FV	Reboiled vapor flow rate
FR	Reflux flow rate
ΔH_{rxn}	Heat of reaction
k_0	Frequency factor in reaction kinetic expression
L_i	Liquid flow rate from tray i
m	Number of manipulated input variables
MV	Manipulated input variables (non-linear model)
n	Number of controlled output variables
P	Pressure
P_{vp}	Vapor pressure (or bubble point for multicomponent)
q	Fraction liquid in the distillation feed
Q	Heat transfer duty
R	Gas constant
t	time
T	Temperature
T_{cin}	Inlet coolant temperature
u	Manipulated input variables (linear model)
x	Volume fraction
x_B	Bottoms product light key mole fraction
x_D	Top product light key mole fraction
x_n	Mole fraction of component n in the liquid phase
V	Reactor volume
y	Controlled output variables (linear model)
y_n	Mole fraction of component n in vapor phase
z	Feed light key mole fraction
z	Height (equation (2.1)
Greek symbols	
α	Relative volatility
β	Conversion from pressure units to head
ρ	Density

Chapter 2. Operating Window

2.0 To the Student

Imagine that you attempted to make a call with your mobile phone, and it did not function. You investigated and determined that the phone only functioned properly when the temperature was 20°C (68°F); you found that even variation to 15°C or 25°C would result in unreliable phone performance. You would find this situation unacceptable because you (and everyone else) will use the phone in various conditions, including a range of temperatures. Being a reasonable person, you would not expect the phone to function at temperature extremes, such as -50°C or 150°C, although this large range could be possible at a much higher manufacturing (and purchase) cost. Therefore, the design engineer and the customer must agree on a range of key variables for which the phone will work reliably and safely; we will term this range of variables an "operating window".

2.1 Introduction – What is the operating window

After the process chemistry and flow structure have been decided, the first detailed design calculations typically involve a steady-state simulation of the material and energy balances for the integrated plant. We will term this calculation the "flowsheet". The values that define the operation, including raw material composition, production rate, product purities, and so forth, are taken to be the most likely conditions at which the plant will operate. We call these conditions the "base case" operation. It is reasonable to begin our analysis of the design using the base case operation. However, the design should not be completed using only this limited information; the engineer needs to ensure that the process has the capacity to function well over a range of conditions.

> A model of a process at a single, base case operation is an important starting point for design; however, a design based only on the single point is likely to be deficient. We must consider a range of conditions.

Process conditions will vary because of factors introduced in Chapter 1 and briefly discussed in the following.

- **Deliberate changes** – While the design point is the expected condition, process management must make changes based on economics, product demand, feed availability, and other factors. For example, the production rate must be adjusted to satisfy the demands of the customers. We would like to sell the maximum capacity of the plant, but the market decides the actual sales, which must be satisfied.
- **Disturbances** – Variability is introduced by external factors that influence plant operation but cannot be controlled by the plant personnel. Perhaps, the most significant factor is raw material composition. The raw material for many processes involve a complex mixture of components, such as crude oil, tree pulp, and iron ore, that varies even when supposedly

supplied from the same source. Other external sources include the weather (cooling water temperature) and utilities provided from other plants (steam, hydrogen, oxygen, etc.).

- **Model mismatch** – Naturally, we predict the future behavior of the process using mathematical models of the process, and decades of engineering development have resulted in an extensive library of very good models. However, no model is perfect, so the engineer should understand the possible mismatch between predictions and actual process behavior. We expect material and energy balances to be exact, but physical properties and equipment parameters like heat transfer coefficients are not known exactly. Also, reaction kinetics and complex hydrodynamics can lead to significant mismatch.
- **Equipment performance** – Even if we could predict the behavior of equipment at plant start-up, we would still need to model the changes in performance during months of plant operation. For example, over a period of months, the following changes typically occur; catalyst activity decreases, heat exchangers foul, and steam turbine efficiency decreases.
- **Human error** – We have already noted that personnel change conditions to match market needs. Occasionally, a person makes an error when changing plant operation, which can lead to hazards and equipment damage. This source of variability will not be addressed in this chapter, but it is addressed in the chapters on reliability and safety.

Is it likely that much variability will occur in a specific process? Let us recall that (1) a process starts up for one to three years after the design has been completed and (2) a typical process operates for decades after start up. Clearly, the delay from analysis to start up and the long time in operation makes large variations a near certainty.

The previous discussion demonstrates the ubiquity of variation in process operation. To maintain high quality products at desired production rates safely and without damaging equipment, the operating conditions of the process must be adjusted in response to this variability. Failure to respond to variability could lead to hazards, long-term equipment damage, and low quality products, and we do not want any of those outcomes! To enable a process to respond to variability, the process equipment must have sufficient capacity and flexibility. This chapter addresses capacity, and the next chapter addresses flexibility.

We will use the concept of the "operating window" when evaluating operability. The following statements define the operating window and its use in evaluating operability.

- An **operating window** defines the achievable operation of a flexible process when considering ranges of input variables and design parameters that change over the operating life of the process.

- A process has an **acceptable operating window** when all desired set point values can be achieved and all expected disturbances can be compensated by manipulated variable adjustments.

Our goal is to learn how to (1) define a reasonable range of variability, (2) design equipment with the proper capacity to satisfy this range of variability, and (3) design equipment that has the flexibility to change operation through automated or manual commands. The first two of these goals are addressed in this chapter, while the third goal is addressed in the next chapter.

It seems as though an engineer could always design equipment to have large capacity, for example, a heat exchanger with a large area or a pump with a large maximum flow rate. Would such deliberate "overdesign" provide acceptable performance? The answer is a resounding "No" because excessive overdesign would have very undesirable consequences, a few of which are discussed in the following.

- **Capital cost** – Overdesign results in higher capital costs for essentially all equipment.
- **Reliability** – When operating large equipment at low flow rates. i.e., that is far from the best operation due to overdesign, the equipment can experience long-term damage. An example is a centrifugal pump that can experience damage due to cavitation at low flows.
- **Operating cost** – Some equipment have a narrow range of acceptable operation, so that recycle around the equipment is required during low production rates, which would increase operating cost.
- **Efficiency** – The efficiency of equipment can depend on the production rate. For example, a boiler thermal efficiency is highest near its design steam production rate, and it decreases as the production rate is decreased.
- **Lack of precise operation** – Some large equipment cannot be adjusted accurately enough to achieve precise operation at low rates. For an example, a large control valve cannot be adjusted to closely achieve a very small flow rate.

Then, what is the design goal with respect to the operating window?

The engineer should seek a design with the smallest capital and operating cost (i.e., the highest profitability) that satisfies all operating conditions anticipated to occur during the process operation.

To achieve this design goal, the engineer should conscientiously define expected variability, understand equipment performance, and performance analysis to size equipment with the smallest capacities that achieve all expected conditions. To emphasize, the goal is not overdesign; the goal is the smallest investment yielding a process that will function properly in the future.

To design an appropriate operating window, the engineer must anticipate the variability experienced in the process. Therefore, the next section discusses sources of variability and gives process examples.

2.2 Defining variability

When performing design, we must "look into a crystal ball" and predict the future. We can always be safe by defining a very large variability, but responding to large variability will require expensive capital investments. In contrast, allowing for (unrealistic) little or no variability will result in a low capital investment but low operating profits. Clearly, this challenging task requires considerable experience with similar equipment. Therefore, our learning objective will not be to provide a detailed variability checklist, because variability will be different for the same equipment in different processes, process structures and environments. Our learning objective is to gain some initial experience with sources of variability.

2.2.1 External variation – Many factors that influence a process are external to the process equipment. Some of these are listed below

i. Raw material composition
ii. Raw material availability
  - If the desired raw materials is not available in sufficient quantity, other raw material might be processed
iii. Raw material prices
iv. Product specifications
  - Some processes produce multiple products with the same equipment in "blocked" operation, i.e., producing one set of products at a time
v. Product demand
vi. Product prices
vii. Prices of resources like electricity and fuel
vi. Weather (for example, affecting cooling water temperature)

2.2.2 Equipment Performance – Excellent models for process equipment are available in flowsheeting software. For these models, the engineer must define input variables (perhaps, from integrated model results) and parameters (like heat transfer coefficients). When the model has been fully specified, the resulting output represents a "single-point" process operation. The following list gives some variability in the parameters that will require extending analysis from a single point to a variability range.

i. Heat exchanger
  - Heat transfer coefficients change over processing time due to surface fouling.
  - Input variables like cooling water temperatures vary (from day to night and over seasons)
ii. Chemical reaction rate
  - Catalyst activity decreases over processing time
  - By-product (coke) buildup in a tubular reactor can reduce selectivity, for example, high-temperature pyrolysis reactions of hydrocarbons to product olefins
  - Feed impurity concentrations strongly effects desired reaction rates
iii. Compressor
  - Blade fouling that reduces efficiency

Many of the causes for performance variability involve changes over time. The equipment is initially placed in service in a "clean" condition, and its performance degrades over time. The clean condition is termed "start-of-run" (SOR), and the degraded condition when the equipment is removed from service for maintenance is termed "end-of-run" (EOR). For commonly occurring equipment, the performance at both conditions can be modeled; for example, fouling heat transfer resistances are available in the literature. Typically, equipment is designed to operate well (high quality products, design production rate, etc.) at the end-of-run (EOR) conditions.

In this section, we have learned that a process experiences many sources of variability. In your process control course, you learned that selected variables (called manipulated variables) can be adjusted in response to variability. However, processes are not infinitely "elastic"; there are limits to achievable adjustments. The limits are addressed in the next section.

2.3 Bounds on equipment operation

Essentially all process equipment has limitations in their performance. Naturally, these limits are important in determining the operating windows of a process because they establish the frame of the window. These limitations can be due to materials of construction, material design parameters (e.g., pressure limits), and performance limits (e.g., low limits). While upper limitations are more obvious, the engineer must also consider lower limits in process conditions. Some examples are listed in the following.

i. Pump and piping
  - Maximum flow rate due to pump outlet pressure matching flow resistance at higher flow rates
  - Minimum controllable flow rates due to either (1) control valve opening imprecision or (2) poor flow sensor reproducibility

ii. Heat exchanger
  - Maximum heat transfer due to temperature pinch
  - Minimum duty for steam heated exchanger

iii. Compressor
  - Maximum flow rate due to stonewall at higher flow rates
  - Minimum flow rate due to surge

iv. Distillation
  - Maximum reboiler duty
  - Maximum condenser duty

v. All closed vessels
  - Maximum vessel pressure
  - Minimum vessel pressure for vessels that cannot sustain a significant vacuum

2.3.1 Special bounds on equipment

Some equipment bounds occur in process equipment that are not as obvious as the examples mentioned above. A few examples of these special bonds are given in the following.

i. Since several bounds involve cavitation, we begin by explaining this phenomenon.

Cavitation is the process of vaporization and subsequent collapse of vapor. Vaporization occurs through nucleation when the pressure of a liquid is reduced below the liquid vapor pressure. When the pressure subsequently increases, the bubbles collapse, and bubble collapse is a particularly important subject because of the noise and material damage that can be caused by the high velocities, pressures, and temperatures that may result from that collapse. (Encyclopedia Britannica, 2019)

a. **Pump cavitation**: As fluid proceeds through a centrifugal pump, it pressure first decreases (because the fluid velocity is increased) and finally increases above its initial pressure (when the velocity is returned to the inlet value). This behavior is expected and often does not cause special issues. However, if the pressure in the pump falls below the fluid vapor pressure, nucleation occurs, and when the fluid slows, the bubbles collapse. The bubble collapse causes significant damage to the pump impeller and walls. Therefore, conditions leading to cavitation must be avoided during the design.

The situation leading to cavitation in a centrifugal pump is shown in Figure 2.1a. The pressure is above the liquid vapor pressure at the pump inlet. As the fluid flows into the pump, the pressure deceases because of frictional loses and more importantly, the increase in velocity of the fluid according to Bernoulli's principle. In Figure 2.1a, the pressure at the pump eye (entering at the impeller) is below the vapor pressure; therefore, vapor forms in the pump. As the liquid slows in the pump, the bubbles collapse, which causes damage to the pump.

The most obvious solution is to increase the pump suction pressure without changing the liquid vapor pressure. The situation with a higher suction pressure is shown in Figure 2.1b; the pressure at the eye is above the bubble point, so cavitation does not occur. This situation occurs when the liquid entering the pump is near its bubble point; is this common in process plants? The answer is, "Yes!" Liquids are boiled and vapors condensed in many equipment, including boilers, reboilers, condensers, and evaporators. So, we must take care to prevent cavitation by ensuring that the pump suction pressure is high enough, where "high enough" is greater than the pressure drop from the suction to the eye. The pressure drop inside the pump depends upon the pump design, so the pump manufacturer provides this information, which is called the "required net positive suction head ($NPSH_r$)" reported in height of fluid column. The available NPSH ($NPSH_a$) is defined in the following equation (Fernandez, et.al., 2002).

$$NPSH_a = \beta(P_1 - P_{vp} - \Delta P_f) + \Delta z \tag{2.1}$$

The symbol β converts pressure to head units, and ΔP_f is the flow pressure drop due to friction in the pipe. $NPSH_a$ must be greater than the required ($NPSH_r$) to prevent cavitation. The common solution is shown in Figure 2.2, in which the pump is located below the source of the liquid in the process so that the head increases the pump suction pressure. Note that this is a costly design modification because a large structure's height is increased, but the cost is required for reliable operation.

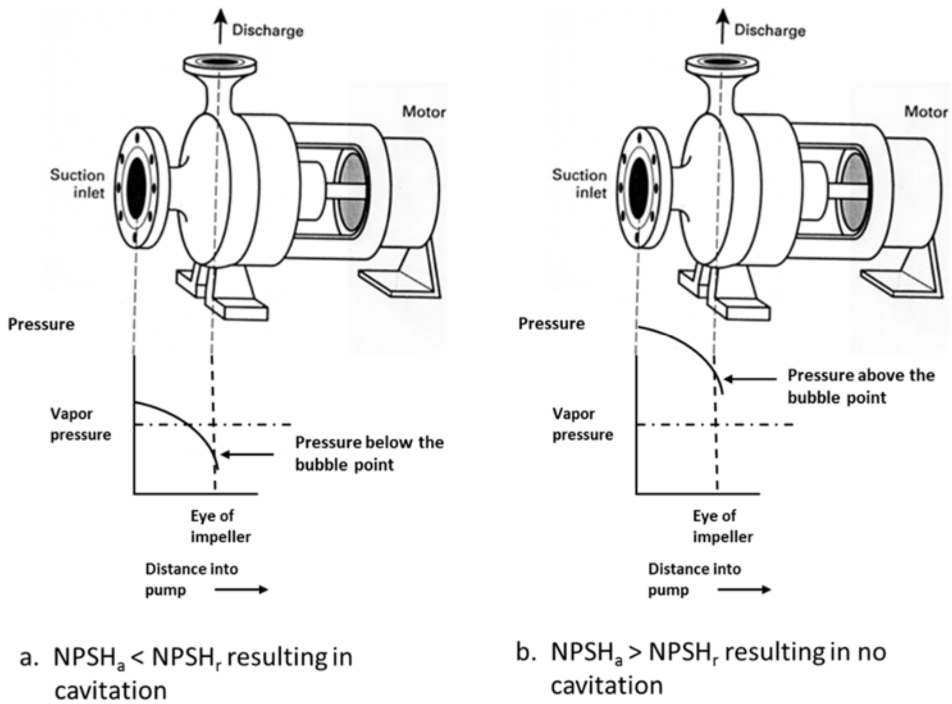


Figure 2.1 Pump cavitation (based on Figure 2-37 in Woods, 1995)

b. **Flow meter cavitation**: Flow through an orifice meter accelerates as the cross sectional area of the streamlines decreases; the smallest cross sectional area occurs at the vena contracta. Thereafter, the velocity increases as the streamlines reach the pipe cross sectional area. If the entering fluid is near its bubble point, cavitation can occur in the meter, which will confound the measurement accuracy and cause damage to the equipment. This situation is shown in Figure 2.3 In which the fluid is a liquid before and after the orifice plate; however, immediately after the orifice, the pressure decreases below the bubble point, and the fluid is partially vaporized. Cavitation occurs as the pressure increases.

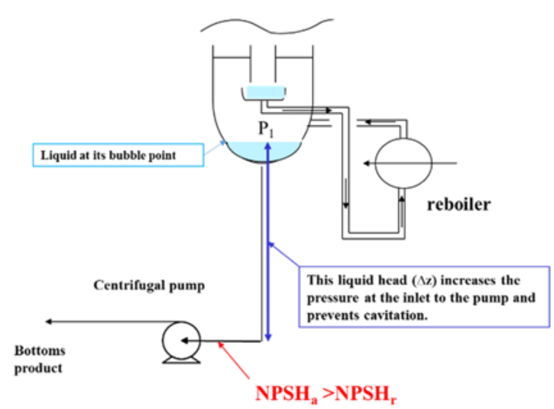


Figure 2.2. Providing the required head to prevent pump cavitation.

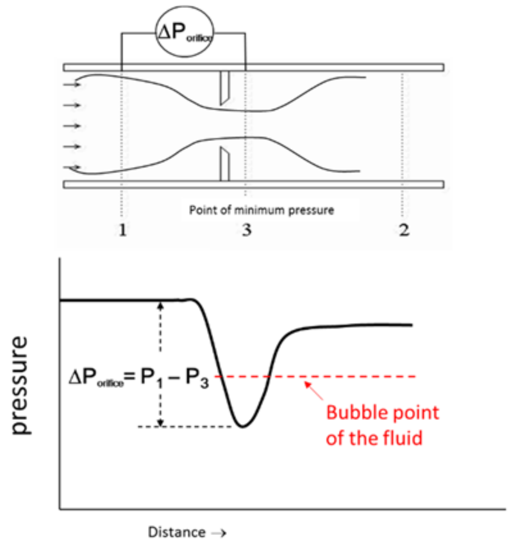


Figure 2.3 Pressure drop in an orifice meter can lead to cavitation.

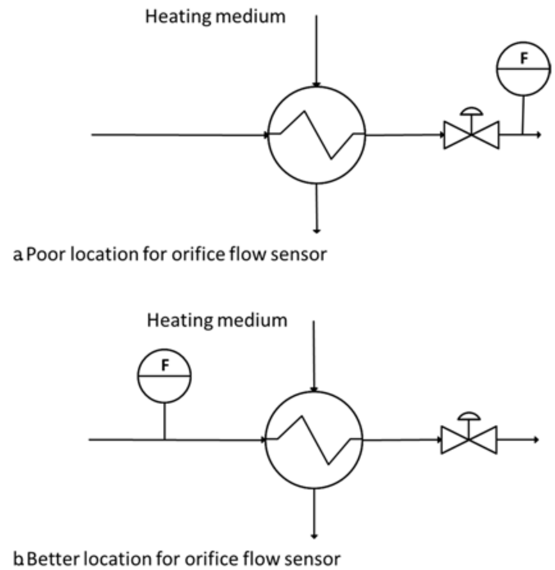


Figure 2.4 Locations for orifice flow sensor.

Therefore, the general rule is to locate such a flow meter at the highest pressure and lowest temperature possible. For example, the location of the flow sensor in Figure 2.4a is poor because the lowest pressure occurs at the highest temperature and lowest pressure, which can lead to cavitation ; the location of the flow sensor in Figure 2.4b is better.

ii. Some bounds on operation are due to internal hydraulics.

a. One common example of hydraulic bounds occurs in distillation. The flows on a distillation tray are shown in Figure 2.5, where the liquid flows across a tray and exits over the weir and flows down the downcomer to the next lower tray. The vapor flows up through the openings in the tray, contacts the liquid on the tray and disengages to continue to flow to the next upper tray. This equipment provides good liquid-vapor contact over a limited range of flow rates; some bounds are shown in the schematic in Figure 2.6 and discussed briefly in the following.

- Too low a vapor flow allows liquid to flow through the tray openings; this is termed weeping.
- Too high a vapor flow rate results in liquid being entrained with the rising vapor.
- Too high a liquid flow rate requires a high liquid head in the downcomer; at some point, the liquid fills the downcomer and trays begin to over-fill.
- Too small a liquid rate relative to the vapor rate leads to coning results in pushing of the liquid away from the tray openings

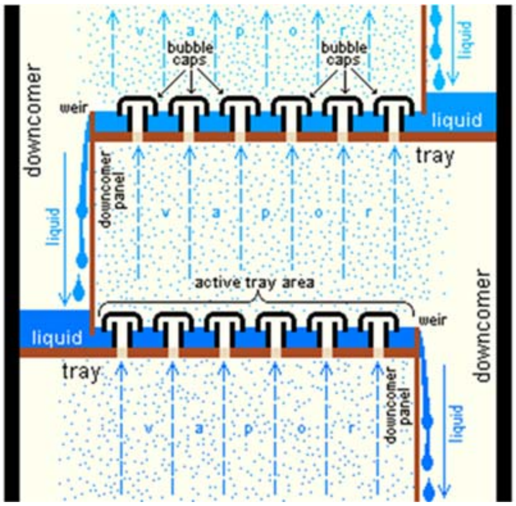


Figure 2.5. Liquid and vapor flows in a distillation tower (Padleckis, 2006A)

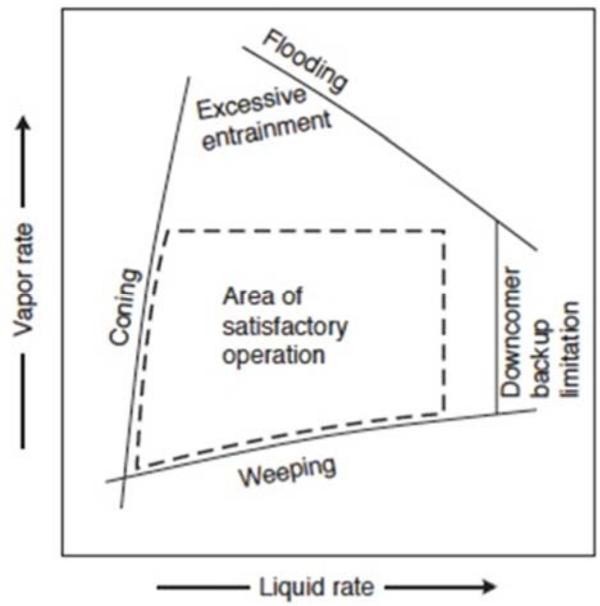


Figure 2.6 Distillation tray operating window (Pickerton et.al., 2014)

iii. Heat exchangers requires good heat transfer between the exchanger walls and the fluids. For boiling applications, the wall temperature must be higher than the bubble point of the fluid; however, very high wall temperatures should be avoided. A moderate temperature difference results in bubbles that disengage from the wall surface; this "nucleate boiling" gives high heat transfer. A higher temperature difference leads to film boiling, where the vapor blankets the surface and surprisingly, the heat transfer coefficient decreases significantly. This effect is shown in Figure 2.7. This effect is especially important when designing distillation reboilers (Hagan and Kruglov, 2010).

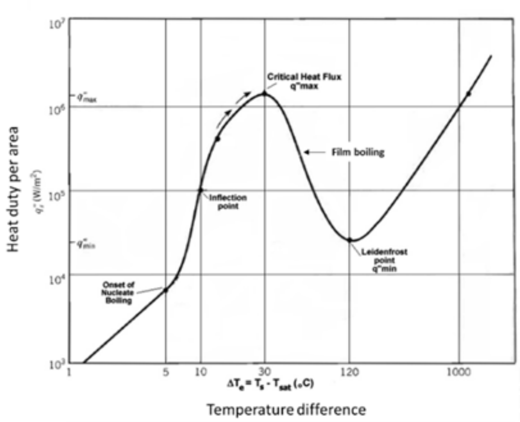


Figure 2.7 Heat transfer showing the nucleate and film boiling. (Wikipedia, 2019)

iv. Many bounds are required to satisfy process chemistry requirements. Generally, engineers prevent the mixing of oxygen with hydrocarbons in process equipment to avoid explosions. However, the feed to a packed bed reactor to produce maleic anhydride considers of oxygen and n-butane. To operate the process safety, the feed mixture must avoid mixtures in the range that will support combustion. The limits for n-butane are 1.6-8.4 volume % butane; therefore, the butane concentration must be maintained below 1.6 volume %.

v. Often, a process functions well within a range of variables, but it fails to operate well outside of this range. For example, the Unipol polyethylene reactor involves a fluid bed of polymer particles. If the reactor temperature exceeds the melting temperature of the polymer (around 400 K) the polymer particles can aggregate, forming a solid mass in the reactor (Ali et.al., 1998). Therefore, the reactor temperature must never exceed a maximum limit.

2.3.2 Bounds due to the Integrity Operating Window

When determining bounds for processes, we need to consider both long and short-term consequences of variability conditions. Some important variables can experience a large range without causing immediate operation that is hazardous, damages equipment or results in unacceptable product properties. However, operation near the limits of the large range can result in long-term costs, often due to damage to equipment that occurs over time. The American Petroleum Institute (API RP 584) has developed the Integrity Operating Window concept to include the longer-term factors when determining the allowable range of operation (Davis, 2017). The Integrity Operating Window is shown schematically in Figure 2.8.

When a variable reaches its critical limit, immediate and strong actions must be taken, which might involve process shutdown. When a variable exceeds its standard level, the process will degrade; therefore, timely alterations to process conditions are required. Operation within the standard levels does not result in hazards or excessive equipment degradation. Operation within the target range and near the optimal target results in high quality products and high profit.

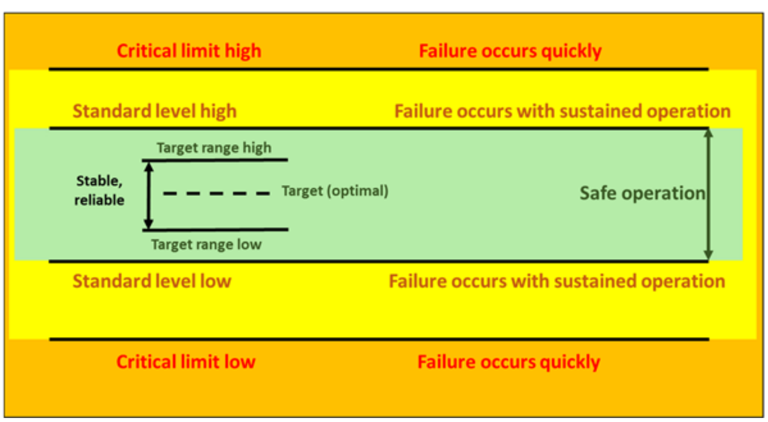


Figure 2.8 Integrity Operating Window

Longer-term considerations are important for much of the equipment in a process plant. A few examples are given in the following.

i. Water cooled heat exchanger
- If the cooling water exit temperature is about 50°C, the water-side surface will foul rapidly, reducing time between shutdown for cleaning

ii. Steam turbine
- If the steam temperature is too high, the life of the turbine blades will be reduced

iii. Fired heater
- If the tube metal temperature of the pipe containing the heated fluid is too high, the life of the pipes decreases

iv. Pump
- If the flow through a centrifugal pump is much lower than the best efficiency point, the pump life will be shortened by cavitation

2.3.3 Production capacity high and low limits

Production flow rates can change over a wide range because of variability in market demands. Therefore, we are concerned with both a maximum and a minimum flow rate through each process, which we describe with the term “turndown ratio”.

Turndown ratio is the normal maximum value of a variable divided by the normal minimum valve of the variable. The modifier “normal” is included to limit the range of the variable to values that can be sustained over a long time reliably without hazard or damage to equipment.

Naturally, the capacity of the process is important. We will apply the following definition of a process capacity.

Capacity is the maximum sustainable, average production that satisfies the all constraints, such as, (1) sales, (2) equipment, (3) personnel, and (4) safety.

Since a plant usually involves a network of integrated processes, determining the total plant capacity requires the analysis of the network. A hypothetical plant consisting of a series of processes is shown in Figure 2.9 with the maximum and minimum production for each. The maximum and minimum production for the series plant is not necessarily determined by any individual process, and typically, the range of achievable production is smaller for the plant than for any one individual process.

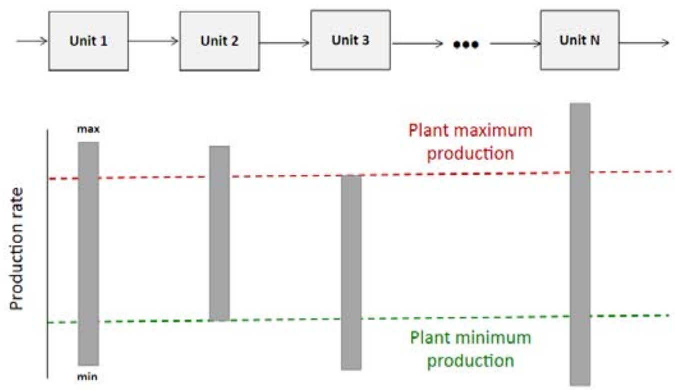


Figure 2.9 Plant capacity for a series of units

Typical turndown ratio values for some process equipment are given in Table 2.1. These values are "typical; the engineer should determine the turndown ratios for the equipment and supplier for a specific process.

Table 2.1 Typical turndown ratios

Equipment	Turndown ratio	Comment	Reference
Valve	20:1	Globe valve	Liptak (1999)
	50:1	Butterfly valve	
	10:1	Gate valve	
	5:1	Pinch valve	
Flow sensor	3:1	Orifice, Venturi	Liptak (2003)
	10:1	Turbine	
	100:1	Coriolis	
Distillation trays	10:1	Bubble cap trays have very large liquid rate turndown	Bander (2019)
	2:1	Sieve trays	
	4:1	Valve trays	
Fired heater	2:1	Burners have much larger turndown ration	
Centrifugal compressor	2:1	Flow reduction below lower limit causes immediate damage; automated "antisurge" recycle is required to maintain flow above the lower limit.	Typical compressor maps
Constant speed centrifugal pump	3:1 Intermittent 1.5:1 Sustained	Operation far from the best efficiency point (BEP) for extended time can cause damage. Providing multiple pumps in series enables operation near BEP for wide range of flow rates. Alternative is to provide recirculation piping and valves.	Ferman (2012)
Positive displacement pump	Large	Can operate over a very large range without damage or significant loss of efficiency.	
Gas Fired boiler	5:1 to 10:1	Thermal efficiency generally decreases at low turndown operation.	Thorncock and Clark (2002)
Gas turbine	2:1	Significant loss of efficiency and increased NOx generation occur at lower than 50% capacity	Wartsila (2019)

In this section, we have learned that limitations exist for the maximum and minimum values for many process variables. This should not be surprising; we would not expect a process design to be able to achieve any range of operating conditions. The importance of these equipment limits on design decisions provides motivation for engineers to "dig into" the details of equipment in the processes to "know how things work". In the next section, we combine variability and bounds to formulate a simulation model to determine the operating window.

2.4 Determining the operating window

In this section, we will develop a method for determining the operating window. Before an engineer applies this method, the following information is required.

- Process structure
- Flowsheet solution for the base case operation with most likely values of all inputs
- Estimate of the variability in variables and parameters. If the variabilities are independent, they define a hyper-cube; if the variabilities are correlated, they define an ellipsoid. The two possibilities are shown in Figure 2.10. The method described in this chapter is applicable to both, while the solved examples all consider independent variation.
- Estimate of the bounds for the equipment in the process. It is especially important to know the reasons for the bounds, while the limiting values can be adjusted during the method to achieve an acceptable operating window.

The approach for evaluating an operating window is shown schematically in Figure 2.11. Three sets of variables are highlighted; adjustable manipulated variables (MV), disturbance variables (D), and controlled variables (CV). Note that the arrows in the figure represent causality in the physical world, not a sequence of model solution. With some restrictions (addressed later in the chapter), we can define values for two of the variables sets in Figure 2.11 and solve for the values of the third variable set. To evaluate an operating window resulting from variability, many problems can be solved; the choice of problem type depends on the information needed for the design. Three typical problem types are defined in Table 2.2.

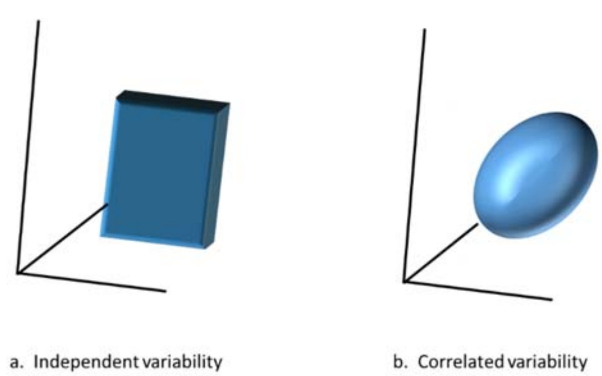


Figure 2.10. Independent (uncorrelated) and correlated variability in three dimensions

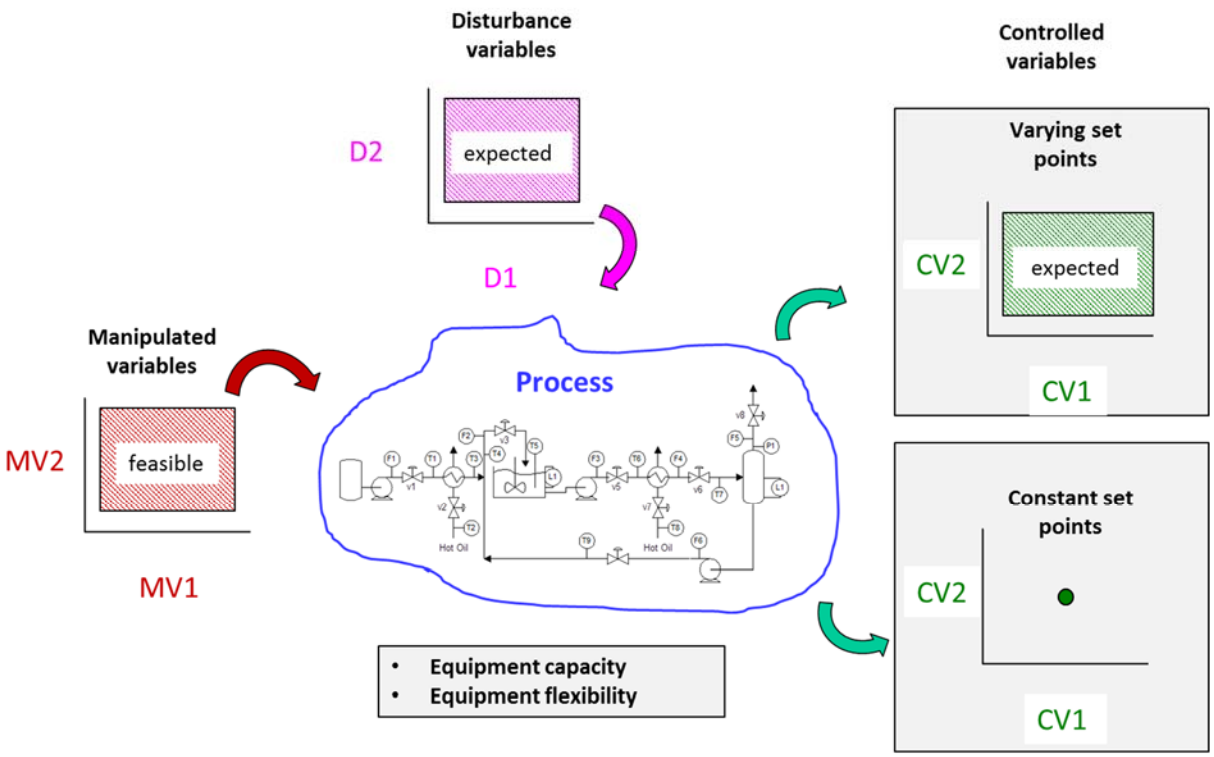


Figure 2.11 Schematic of the relationships among manipulated, disturbance and controlled variables.

Table 2.2 Problem Types for Analyzing the Operating Window

Problem	Specified values*	Value solved for	Importance for process design
I	y, d, a to c	u	Values of the manipulated variable (u) that yield desired y (controlled variable) for range of disturbances (d) and parameters (a to c)
II	y, u, a to c	d	Values of the disturbance (d) that can be corrected by the manipulated variable (u) to yield the desired value for the controlled variable y
III	u	y	Values for the achievable set points without disturbances or parameter variability

* these values can be the known (constant) values or samples from a variability distribution

To introduce the method, we will consider the following simple linear model so that the modelling calculations can be easily understood.

$$y = A * u + B * d + c \tag{2.2}$$

with
y = vector of dependent variables (i.e., controlled variables)
u = vector of adjustable independent variables (i.e., a manipulated variables)
d = vector of independent variables that cannot be directly adjusted (i.e., a disturbances)
A, B, c = parameters, vector or matrix as appropriate

The dependent variable (y) is a controlled variable or a variable that is not controlled but is required to remain within some region to achieve acceptable operation. The manipulated variable (u) can be adjusted to achieve desired performance by (1) maintaining a controlled variable at its set point or (2) to keep an uncontrolled variable within required bounds. Uncertainty can exist in the disturbance variable (d) and the parameters, (A, B, and c).

For the present, we will concentrate on uncertainty in the variables in equation (2.2). For the variables that are uncertain, we can select a sample of values within the uncertainty region, for example within the bounds if the value has hard bounds or within a specific confidence interval for values that are defined by a probability distribution. Then, the problem can be solved for the unknown variables for each sample of the known sampled values of the variables. Let's consider examples of this approach applied to equation (2.2) with the values given in Table 2.3. When evaluating operating windows, values of specified variables will be allowed to vary around their base case values, and the effects of this variation is determined using the model in equation (2.2).

Table 2.3. Model parameters for case studies using the linear model in equation (2.2)

$A = \begin{bmatrix} 1 & 0.5 \\ 0.3 & 0.9 \end{bmatrix}$	$B = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$		$c = \begin{bmatrix} 37.5 \\ 8.5 \end{bmatrix}$
	Output variables	Manipulated variables	Disturbances variables
Base case	$y = \begin{bmatrix} 80 \\ 40 \end{bmatrix}$	$u = \begin{bmatrix} 30 \\ 25 \end{bmatrix}$	$d = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$
Problem III	Evaluated using model	Allowed to take values within variability ranges	$d = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$
Problem I	$y = \begin{bmatrix} 80 \\ 40 \end{bmatrix}$	Evaluated using model	Allowed to take values within variability ranges

Problem Type III

```
Input data, define variation ranges, size arrays

for jj = 1 : ncase

    % Select a value for the first variable from its range
     u(1)  = u1min  + (u1max-u1min)   * (jj-1)/(ncase-1) ;

    for kk = 1 : ncase

        % select a value for the second variable from its range
          u(2) = u2min + (u2max-u2min)* (kk-1)/(ncase-1)     ;

        %  Solve the model for the unknown variables

        y = A*u + B*d +c ;

        % increment the case number counter
        count = count + 1   ;

        % save results for scatter plot display

         y1store (count) = y (1);
         y2store (count) = y (2);

         u1store (count) = u (1);
         u2store (count) = u (2);

         d1store (count) = d (1);
         d2store (count) = d (2);


    end

end


Plot results
```

Problem Type I

```
Input data, define variation ranges, size arrays

for jj = 1 : ncase

   % Select a value for the first variable from its range
    d(1)  = d1min  + (d1max-d1min)   * (jj-1)/(ncase-1) ;

   for kk = 1 : ncase

       % select a value for the second variable from its range
         d(2) = d2min + (d2max-d2min)* (kk-1)/(ncase-1)     ;

       %  Solve the model for the unknown variables

       u = inv(A)*y - inv(A)*B*d -inv(A)*c ;

       % increment the case number counter
       count = count + 1   ;

       % save results for scatter plot display

        y1store (count) = y (1);
        y2store (count) = y (2);

        u1store (count) = u (1);
        u2store (count) = u (2);

        d1store (count) = d (1);
        d2store (count) = d (2);


   end

end


Plot results
```

Figure 2.12 Pseudo-code for solution of operating windows for the linear model in equation (2.2) with results plotted in Figures 2.13 and 2.14.

We will start by solving Problem Type III, in which the manipulated variables can take values within a specified range; the disturbances are constant; and the range of output variables is determined. This problem determines the range of controlled variables that can be achieved by adjusting the manipulated variables without disturbances occurring. This is an important issue in process design; if the required range of controlled variables cannot be achieved, the equipment capacities must be altered. If the range is much larger than needed, the engineer can consider reducing the capacity of some equipment, contingent upon the analysis of Problem Type I.

The ranges and values for the parameters and variables are given in Table 2.3. The pseudo code for solving the problem is given in Figure 2.12. The results are displayed in Figure 2.13; we observe that the range of output variables is not defined by a rectangle because of the interaction in the process; interaction exists because both manipulated variables affect both controlled variables.

Next, we analyze the same model and parameter values to solve Problem Type I. This problem determines the necessary range for the manipulated variables to maintain the controlled variables are their constant set points, which is an important issue in process design for continuous plants that operate with constant set points. If the controlled variables cannot be maintained at their set points for the expected range of disturbances, the engineer must increase the capacity of some equipment (or enhance the design with additional manipulated variables).

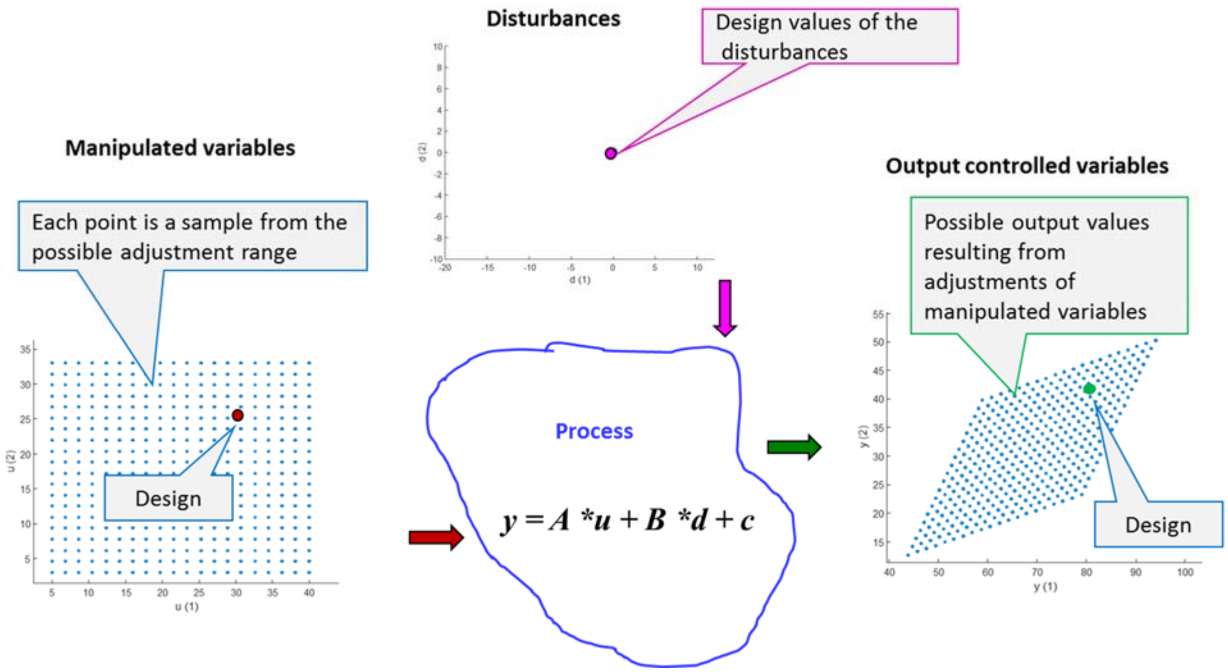


Figure 2.13. Results for Problem Type III for the linear process model in equation (2.2) Arrows indicate the calculation sequence, which in this case is the same as causality.

The ranges and values for the parameters and variables are given in Table 2.3. The pseudo code for solving the problem is given in Figure 2.12. We first note that the solution to this problem requires the inverse of the parameters matrix A, as seen in the code in Figure 2.12; the matrix is invertible, as can be confirmed by evaluating its determinant, which is not zero.. The inverse is required because the equation (2.2) is formulated to calculate the output variables (y) based on values of the input variables (u and d). However, Problem Type I evaluates of the input manipulated variables (u) based on values of the outputs (y) and inputs (d). The results are displayed in Figure 2.14; we note that the required range for the second manipulated variable (u(2)) is much larger than for the first manipulated variable (u(1)).

We could continue with linear models of the form of equation (2.2); however, we are interested in large changes in operating conditions when we evaluate the operating window. Therefore, we will use non-linear models to provide good accuracy. The more complex models can be solved by (1) commercial flowsheeting software or (2) a user-written numerical solution of the appropriate modeling equations. Naturally, the flowsheeting approach is more efficient and likely more accurate, if the models are available. Let’s continue with some process examples.

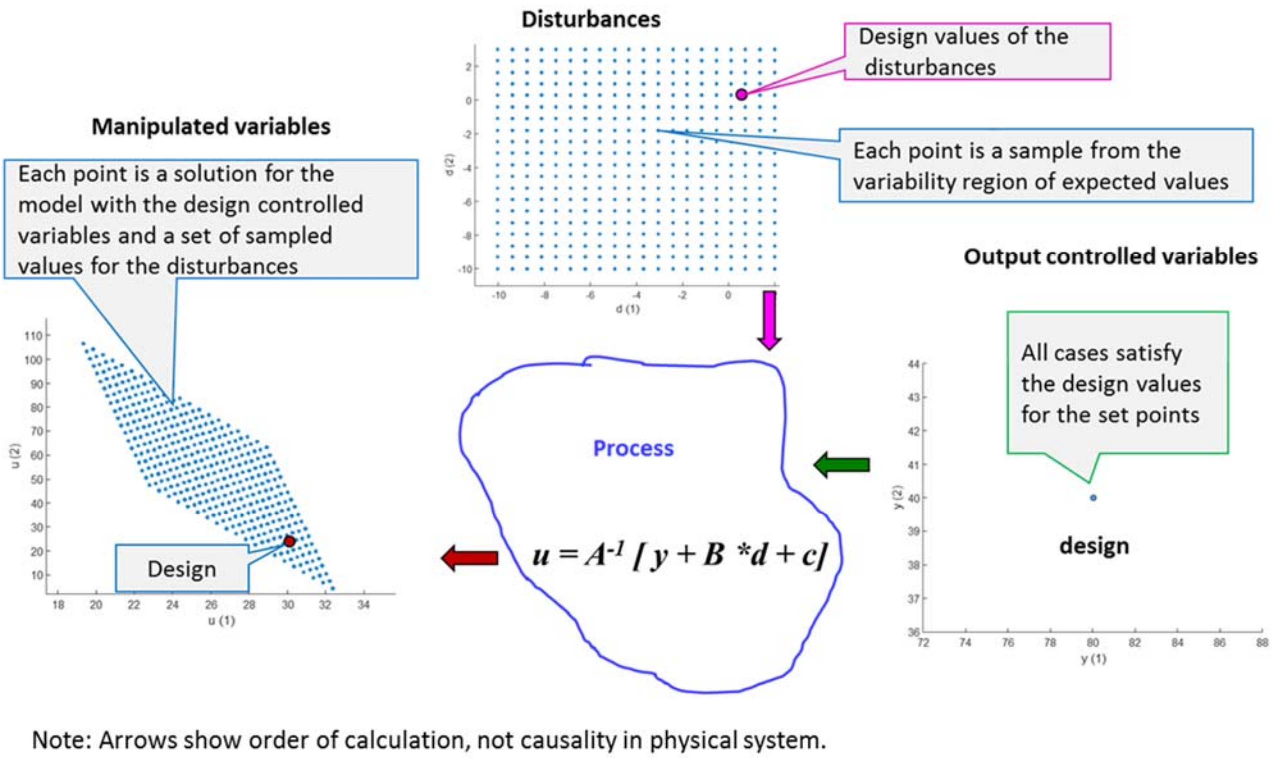


Figure 2.14. Results for Problem Type I for the linear process model in equation (2.2) Arrows indicate the calculation sequence, which in this case is not the same as causality

Example 2.1 A simple, blending process shown in Figure 2.15. The model for the process is shown in the following.

$$F_A + F_S = F_M$$

$$F_A x_A + F_S x_{AS} = F_M x_{AM}$$

Each inlet flow rate can vary between zero and its maximum value. Determine the achievable range of controlled variables, total flow rate (F_M) and mixed stream composition (x_{AM}). To answer this question, we need to solve Problem Type III from Table 2.2. The outputs (F_M and x_{AM}) are calculated for numerous sample values of the inputs (F_A and F_S). The flowchart of a computer program to perform the calculations are given in Figure. The results of the calculations are shown in Figure 2.16. We note that the feasible operating window is not a rectangle; a mixed flow rate of 77 m^3/h can be achieved, but only if the mixed composition is between approximately 0.20 and 0.40 weight fraction.

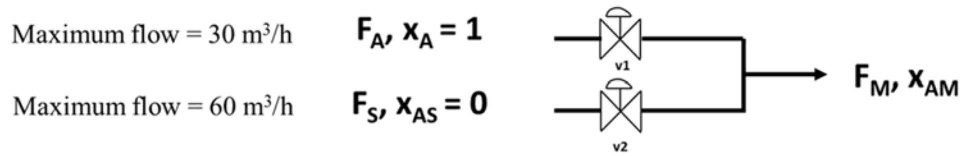


Figure 2.15 Blending process considered in Example 2.1.

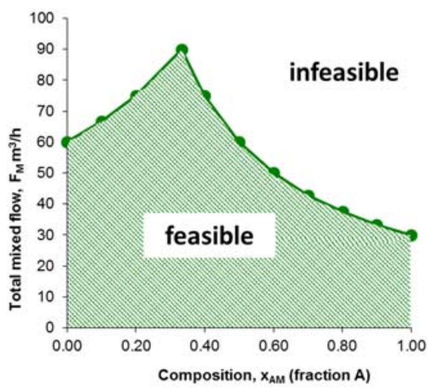


Figure 2.16 Operating window for the blending process in Example 2.1.

Example 2.2 We want to determine important operating window parameters for the non-isothermal CSTR in Figure 2.17. The controlled variables, reactant effluent concentration and reactor temperature, need to maintained at their design values in spite of disturbances in the coolant temperature and the total feed flow rate. A number of manipulated variables are possible; in this example, the reactant feed concentration and the coolant flow rate are selected. In this example, we will determine the required range for these manipulated variables for a specified variation in the disturbance variables. The model for this process is given in Marlin (2000) and summarized in Appendix A of this chapter.

The calculations for this example involve setting the disturbance variables to sample values selected from their allowable ranges; this is Problem Type I. For all cases, the dependent controlled variables are set equal to their set points. For each set of sample disturbance values, the values for the manipulated variables are determined using the model. Since the model is complex, each solution involves an iterative numerical method to solve the non-linear equations describing the material and energy balances and heat transfer for the CSTR process.

The results of the calculations are shown in Figure 2.17. The original design range for the manipulated variables is shown with a purple dot-dash box; we conclude that the manipulated variable range is too small. A new range based on this analysis that satisfies the operating window requirement is shown in the red dashed box. We observe that the expanded range for the manipulated variables can satisfy all cases, including maximum capacity for the most demanding cases and large enough turn-down ratio to operate when the demands on the manipulated variables are small.

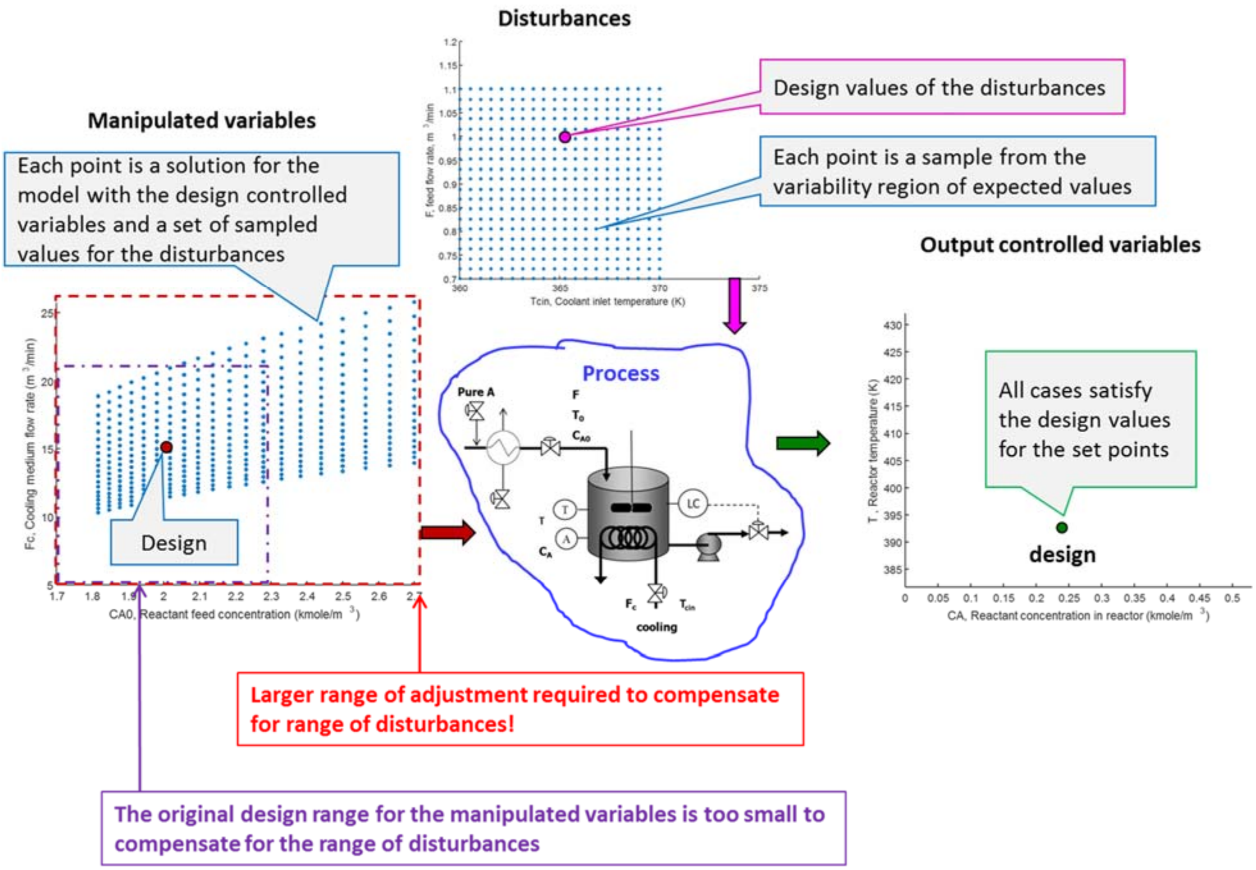


Figure 2.17 Results for Problem Type I for the CSTR process in Example 2.2.

Example 2.3. We want to determine important operating window parameters for the two-product distillation column in Figure 2.18 with disturbances in the feed flow (4-12 kmole/min) and feed light key (0.3-0.6 mole fraction). The controlled variables, the light key in the overhead and bottoms products, need to maintained at their design values in spite of disturbances in the feed composition and the total feed flow rate. In this example, the reflux and reboiled vapor flow rates are selected as manipulated variables. In this example, we will determine the required range for these manipulated variables for a specified variation in the disturbance variables. The constant relative volatility model for this process is given in Marlin (2000) and summarized in Appendix A of this chapter.

The calculations for this example involve setting the disturbance variables to sample values selected from their allowable ranges; this is Problem Type I. For all cases, the dependent controlled variables are set equal to their set points. For each set of sample disturbance values, the values for the manipulated variables are determined using the model. Since the model is complex, each solution involves an iterative numerical method to solve the non-linear equations describing the tray, reflux drum, and reboiler material balances.

The results of the calculations are shown in Figure 2.19. The original design ranges for the manipulated variables are 3000-12000 mole/min for the reflux flow rate and 5000-19000 mole/min for the reboiled vapor flow rate (i.e., reboiler duty); we conclude that the manipulated variable range is adequate. However, we must consider additional potential equipment limitations, such as the following.

- Condenser duty
- Tray hydraulics
- Product flow rates

Let's say that the condenser and product feed capacities and turndown are adequate. Limitations imposed by distillation tray hydraulics have been discussed in Section 2.3.1. We find that the equipment in this design can experience tray weeping (liquid exiting the trays through the tray openings meant for vapor flow). Weeping will occur at reboiled vapor flow rates less than 7500 mole/min. Therefore, the section of the operating window in the red-shaded box represents unacceptable equipment performance. How can a design range be expanded by changing operating conditions? We will see a method for allowing distillation operation at low feed rates in the next chapter.

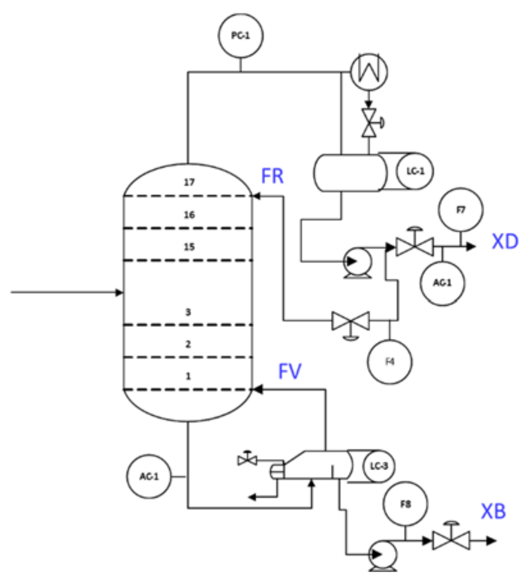


Figure 2.18. Distillation column for Example 2.3.

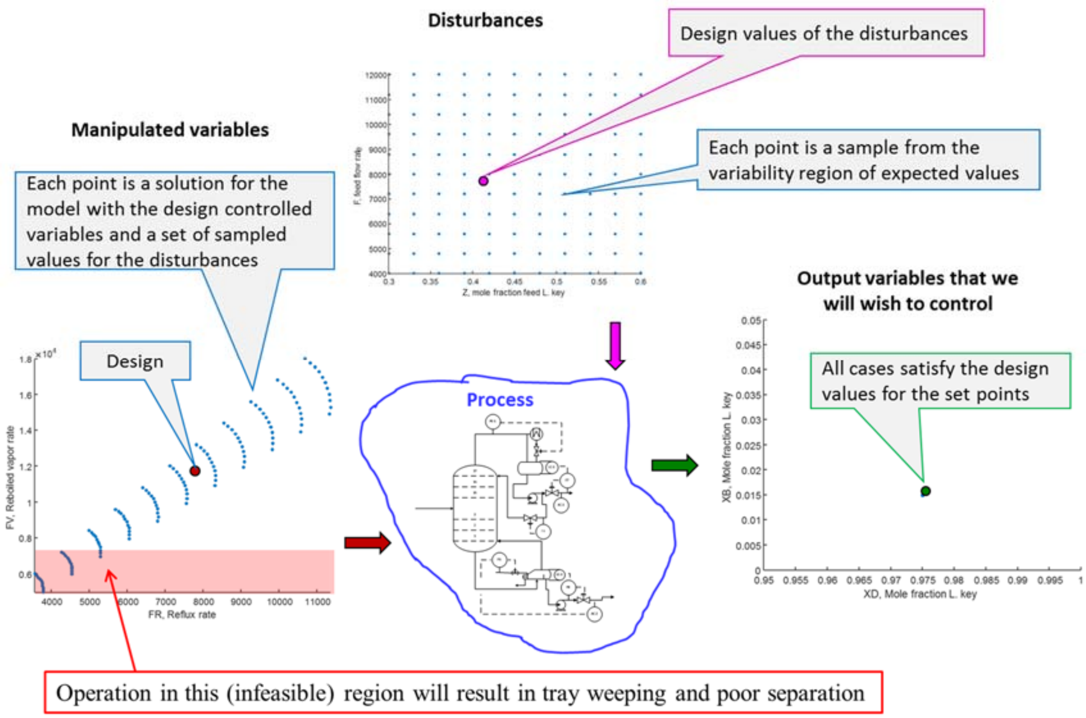
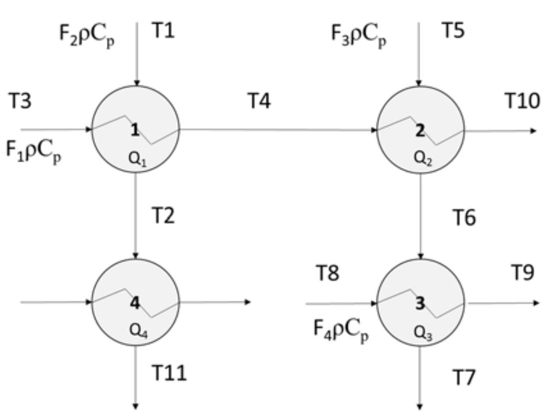


Figure 2.19. Results for Problem Type I for the distillation column in Example 2.3.

Example 2.4. We want to determine important operating window parameters for the heat exchanger network in Figure 2.20. The design base case flow rates and temperatures are given in the figure with values for the input variables. Conditions for the case studies for this heat exchanger network are given in Table 2.4.



$F_1\rho C_p = 2$ kW/K	$T_1 = 620$ K
$F_2\rho C_p = 1.5$ kW/K	$T_3 = 388$ K
$F_3\rho C_p = 1$ kW/K	$T_5 = 583$ K
$F_4\rho C_p = 3$ kW/K	$T_8 = 313$ K

Figure 2.20 Heat exchanger network for Example 2.4 with base case input variable values.

Table 2.4 Definition of heat exchanger network cases for Example 2.4

Case	Output variables	Variability	Adjustable input variables	Bounds on adjustable variables
A	$T_7 <= 323$ K $T_9 = 393$ K $T_{10} = 563$ K $T_{11} = 350$ K	$350 \le T_3 \le 450$ $550 \le T_5 \le 650$	Q_i for i =1,3	$Qi \ge 0$ for i =1,3 $Q_4 = 75$ kW
B	$T_7 <= 323$ K $T_9 = 393$ K $T_{10} = 563$ K $T_{11} = 350$ K	$350 \le T_3 \le 450$ $550 \le T_5 \le 650$	Q_i for i =1,4	$Qi \ge 0$ for i =1,4
C	$T_7 <= 323$ K $T_9 = 393$ K $T_{10} = 563$ K $T_{11} = 350$ K	$350 \le T_3 \le 450$ $550 \le T_5 \le 650$	Q_i for i =1,4	$Qi \ge 0$ for i =1,4 $Q_4 \le 100$ kW
D	$T_7 <= 323$ K $T_9 = 393$ K $T_{10} = 563$ K $T_{11} = 350$ K	$350 \le T_3 \le 450$ $550 \le T_5 \le 650$ $1.2 \le F_2\rho C_p \le 1.55$	Q_i for i =1,4	$Qi \ge 0$ for i =1,4

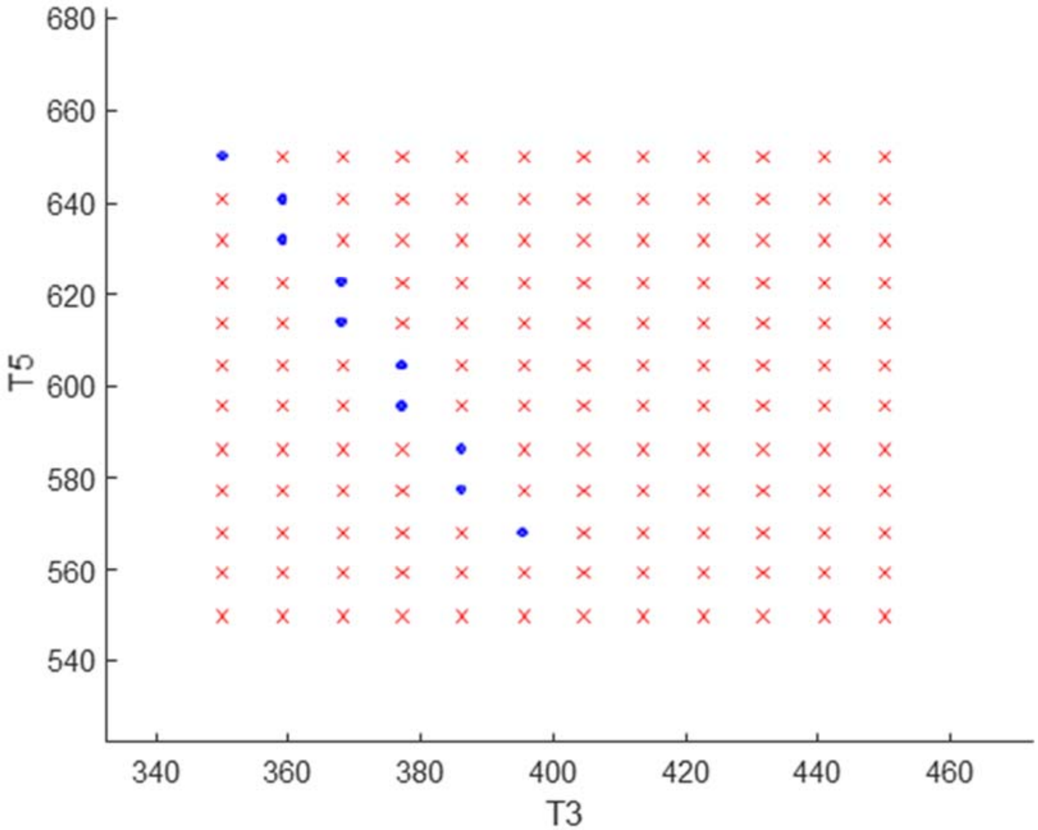
A model for this process is given in Biegler et.al. (1997) and summarized in Appendix A of this chapter. The model consists of energy balances for all streams in each heat exchanger. The problem also must observe practical limitations on the heat transfer, because regardless of how large the heat transfer areas might be, the heat transfer is limited by temperatures of the hot and cold streams becoming equal, that is, by a pinch in the driving forces. We know that heat cannot flow "uphill". Therefore, the following additional limitations exist for this process. (A more realistic definition of these bounds would include an approach temperature that is greater than zero, but we will use these bounds to be consistent with the previously published formulation.)

- $T1 - T4 \ge 0$
- $T2 - T3 \ge 0$
- $T4 - T3 \ge 0$
- $T5 - T10 \ge 0$
- $T6 - T4 \ge 0$
- $T5 - T6 \ge 0$
- $T6 - T9 \ge 0$
- $T7 - T8 \ge 0$
- $T6 - T7 \ge 0$
- $T2 - T11 \ge 0$

The solution for this problem is not as straightforward as the previous examples. The results for several cases will be discussed here, and the model formulation and solution method are given in Appendix A of this chapter.

Case A. Duties in exchangers 1, 2, and 3 can be adjusted as manipulated variables, with the duty in exchanger 4 fixed at 75 kW. A typical reason for the exchanger 4 not being adjusted to satisfy the limits in this example would be the requirement to provide heat transfer at a specified rate to another part of the plant; for example, exchanger 4 could be preheating water to a boiler or preheating feed to a chemical reactor.

We note that the controlled variable space has four dimensions (T10, T9, T11, and T7), which makes results display difficult. The variability for this case will be in two parameters, the

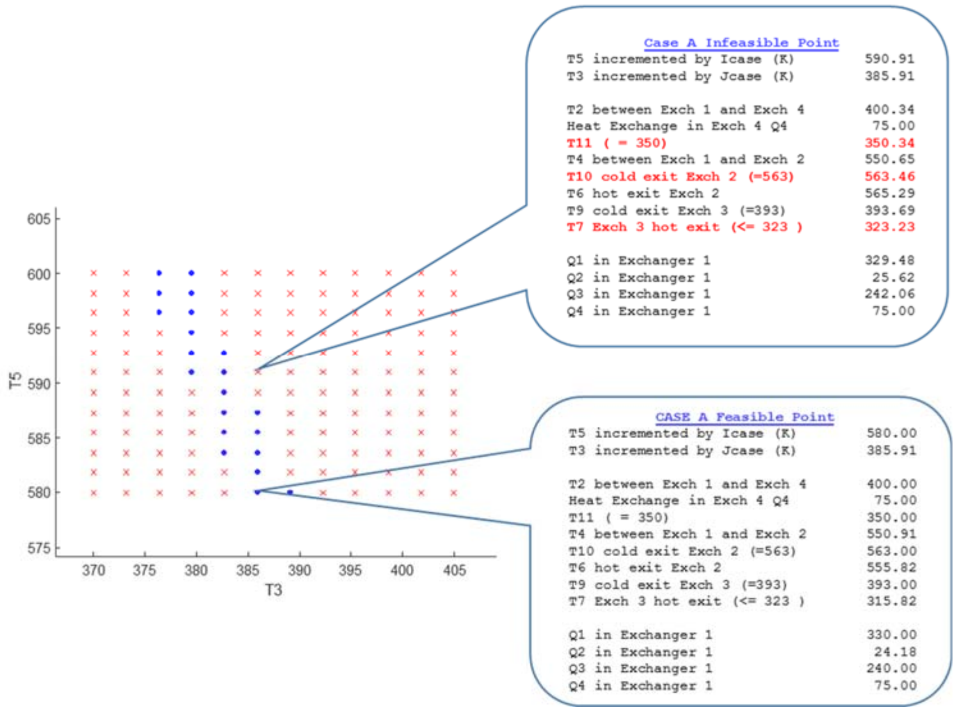


• = feasible point in the operating window
x = infeasible point outside of operating window

Figure 2.21 Example 2.4 Case A showing the feasible operating window and infeasible points in the disturbance space.

temperatures T3 and T5. Therefore, we will plot the results in the disturbance space that has two dimensions. The results are show in Figure 2.21 with the distinction displayed between feasible region, i.e., the operating window, and infeasible region using colored symbols in the scatter plot. We observe that the operating window is quite small; this design would not likely be acceptable.

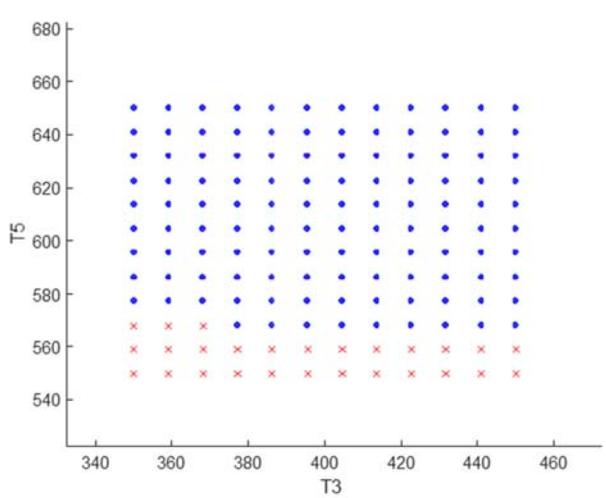
While the results in Figure 2.21 clearly show the operating window, the engineer would like additional insight. Greater resolution can be achieved by additional cases with smaller ranges for the disturbance variables, as shown in Figure 2.22. In addition, values of the key variables can be ascertained for any of the cases, as shown in Figure 2.22. The data from a feasible point shows that all equality and inequality limits are satisfied. In contrast, the data from an infeasible point highlights the variables that fail to satisfy the equality and inequality limits. This information would help the engineer understand the limitations in a proposed design and introduce modifications to alleviate limits and expand the operating window.



• = feasible point in the operating window
x = infeasible point outside of operating window

Figure 2.22 Example 2.4 Case A with higher resolution and smaller range. The engineer can interrogate any point on the plot to observe the results of the model solution.

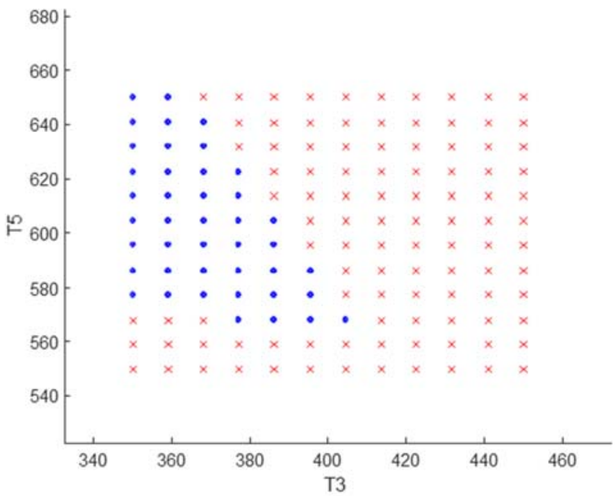
Case B. This case is identical to Case A except the duty in exchanger 4 can be changed to any value consistent with the inequality constraints given above. The duty in exchanger 4 could be free to vary without upper limit (in the design case) if a utility stream, such as cooling water, were the cold stream. The resulting operating window is shown in Figure 2.23, which is much larger than for Case A.

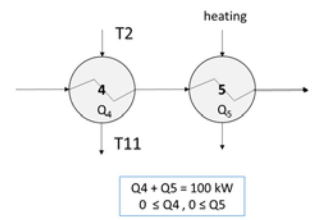


• = feasible point in the operating window
x = infeasible point outside of operating window

Figure 2.23 Operating window for Example 2.4 Case B

Case C. In this case, the duties in all four exchangers can be adjusted, but the maximum duty in exchanger 4 is limited to 100 kW. This case represents the situation in which the cold stream in exchanger 4 requires 100 kW and another heating stream is available to makeup for any heating deficiency due to the adjustment of the exchanger 4 duty. The resulting operating window is shown in Figure 2.24. As expected, the operating window is larger than Case A and smaller than Case B.



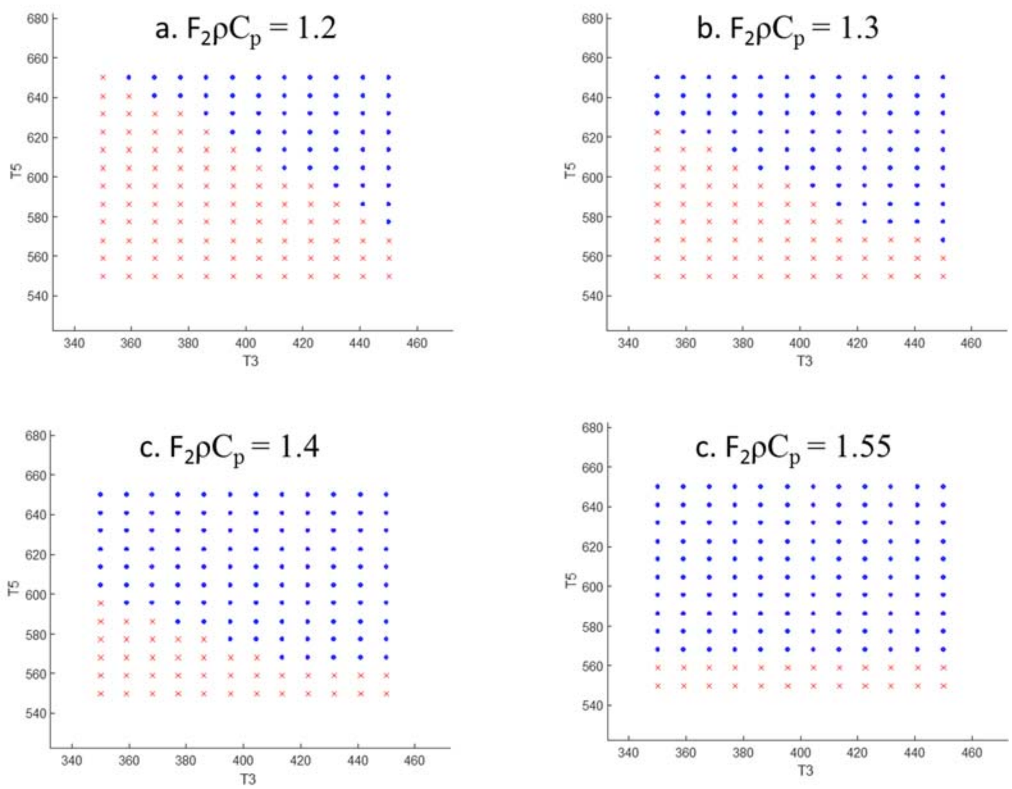


● = feasible point in the operating window
x = infeasible point outside of operating window

Figure 2.24 Operating window for Example 2.4 Case C

Case D. In this case, three parameters will be variable. This will be achieved by repeating Case B with variability in T3 and T5 and additional variability in F2. Since three variable parameters exist in this problem, the results will be presented in a series of two-dimensional figures, with each figure presenting the results for a different value of the flow F2 within its variability range. The results are shown in Figure 2.25. Clearly, as the flow F2 decreases, the size of the operating window decreases because lower F2 values provides less heating.

In the exchanger network Example 2.4, we have investigated several cases to demonstrate the ease with which the method can be modified to analyze various situations. Naturally, only one of these would be relevant to a specific design. How would these results be used in the design of the heat exchange equipment? First, the operating window would have to be acceptable for the expected variability in the process being designed. Second, every point within the operating window corresponds to heat exchangers able to achieve the required heat transfer. A design capable of providing adequate heat transfer can be achieved by calculating the heat transfer area for each point in the operating window and selecting the largest area for each exchanger. The insightful reader might ask, "How can a heat exchanger satisfy all of the cases in the operating window, each of which requires a different duty?" The answer to this question is given in the next chapter that introduces operating flexibility in the equipment design.



• = feasible point in the operating window
x = infeasible point outside of operating window

Figure 2.25 Operating window analysis for three variable parameters.
(Recall that Figure 2.23 shows the operating window for $F_2\rho C_p = 1.5$)

2.5 Summary of the method with limitations

2.5.1 Summary of method

The method for evaluating the operating window described in this chapter is selected to have specific advantages. First, it is easy to define and execute. Second, the method can use existing non-linear models available in commercial flowsheeting software. Third, it provides insight into the causes of limitation through interrogations of the individual simulation results.

This introduction to the operating window and computational methods has limitations as well.

- This method considers only steady-state behavior
- Dynamic behavior is not considered
- Only typical variability is considered; major equipment faults and human failures are not considered. (These major faults are addressed in the chapters on reliability and safety.)
- Parameter uncertainty is considered, but structural uncertainty is not. For instance, structural uncertainty could result from unknown chemical reactions occurring.
- Complex process behavior, like multiple steady states, is not considered
- Solutions at multiple points does not ensure operability between these points

The method relies on the engineer to define a "reasonable" set on manipulated variables that can be adjusted in response to variability to maintain specific variables at set points or within bounds.

We will consider a situation in which "n" adjustable manipulated variables exist and "m" dependent variables must be maintained at set points and/or within specific bounds. There are three situations to consider.

- $n = m$ Given an adequate range of adjustment (and conditions described below) a finite operating window exists. Each point in the window is exactly specified.
- $n < m$ No solution exists for this situation; the operating window has no feasible points (or one point, the design case). This is not an acceptable design; more adjustable variables must be added.
- $n > m$ Given an adequate range of adjustment (and conditions described below) multiple solutions can exist for feasible operating points within the operating window. The calculations for each point should be modified to represent some additional considerations. For example, heat might be provided by two exchangers, one process heat integration and the other steam-heated. For this situation, the simulations (actually, optimizations) would have additional requirements, like minimizing the more costly steam exchanger duty.

;

Naturally, the manipulated variables cannot be selected arbitrarily; what criteria must be satisfied. First, we will consider the case with n = m? Second, there must be independent causal relationships between the manipulated and controlled, dependent variables.

Engineers with some experience with the process being designed generally can select a good set of manipulated variables; engineers new to practice or to the specific process might have some difficulty. There is no direct mathematical manner for determining the independent causal relationships for a set of non-linear, algebraic equations over the entire range of variable values. However, a linear test exists for a solution in the local region of a specific set of values; the set of non-linear equations can be linearized about a specific point to yield the linear set of equations shown in the following.

$$\begin{bmatrix} \boldsymbol{CV}'_1 \\ \dots \\ \boldsymbol{CV}'_{\boldsymbol{n}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{K}_{11} & \boldsymbol{K}_{12} & \boldsymbol{K}_{1\boldsymbol{n}} \\ \boldsymbol{K}_{21} & \boldsymbol{K}_{22} & \boldsymbol{K}_{2\boldsymbol{n}} \\ \boldsymbol{K}_{\boldsymbol{n}1} & \boldsymbol{K}_{\boldsymbol{n}2} & \boldsymbol{K}_{\boldsymbol{nn}} \end{bmatrix} \begin{bmatrix} \boldsymbol{MV}'_1 \\ \dots\dots \\ \boldsymbol{MV}'_{\boldsymbol{n}} \end{bmatrix} \tag{2.3}$$

with
$\boldsymbol{CV}'_i$ = the output variables as deviation from the base case values
$\boldsymbol{MV}'_i$ = the input variables as deviation from the base case values
$\boldsymbol{K}_{ij}$ = the linearized coefficients relating the input to output variables

A solution exists if the gain matrix is non-singular, or equivalently, if the determinant of the gain matrix is not equal to zero. This test establishes the existence of a solution at the point about which the model has been linearized, but it does not guarantee a solution for other values of the variables.

The third criterion is that the manipulated variables must have sufficient range to compensate for disturbances and achieve desired set points changes, if any. Since we are concerned with large changes, analysis of the linearized model is not appropriate. The adequacy of the manipulated variables for the non-linear system can be determined by defining steady-state simulation cases in which includes a range of variability in the disturbances and set points from their base case design values. These simulation case will not converge to a solution if the required independent causality does not exist. (Unfortunately, the simulation might not converge because of numerical issues, so that lack of a solution does not prove that the manipulated variable set is inadequate.) We note that these cases will also establish the steady-state controllability for the non-linear system.

The fourth criterion involves interactions. The manipulated variables should not unduly influence operation of the integrated plant. For example, adjusting steam to a reboiler is acceptable because the boiler and steam system are designed to quickly respond to demands from numerous consumers without disturbing other process production or product quality. A counter example involves adjusting the production rate of one process to provide sufficient heat transfer to another process; this would not be acceptable.

The fifth and final criterion addresses dynamics. Fast feedback correction is desirable, so we select manipulated variables with fast effects on the output variables. This criterion is not addressed in the methods in this chapter, but dynamics is addressed in the next three chapters on reliability, safety, and process control.

2.5.2 Large number of variable parameters – Curse of dimensionality

In the method described in the previous section, each point involves the solution of a steady-state flowsheeting model of the process for sampled values of the variable parameters taken from their distribution. The number of simulation solutions grows rapidly for the grid evaluation method used in the examples, as shown in Table 2.5.

Table 2.5 The number of process simulations required

Number of parameters, n	Number of simulation solutions for number of samples/parameter = 5	Number of simulation solutions for number of samples/parameter = 10
1	5	10
2	25	100
3	125	1000
4	625	10,000
5	3125	100,000

Typically, a solution of a single simulation does not require a great deal of computer time, especially when starting from a good initial condition like the base case design conditions. However, the completion of the four-parameters case with ten samples per parameter using a grid method with a simulator that required two seconds per solution would take nearly six hours of single-CPU computing time. Clearly, some adaptations to the method are required for many variable parameters.

- *Preliminary parameter screening* – The engineer can perform a few initial case studies to evaluate the effect of candidate parameters on the operating window. Parameters that have a weak effect or small variability range can be eliminated from the subsequent calculations.
- *Large initial grid spacing* – An initial grid with few points per parameter would require substantially less computing time. The results can be used to define a smaller range of parameters where the boundary between feasible and infeasible points exists.
- *Worst case analysis* – Generally, the operating window analysis is performed to ensure that the equipment has the required capacity. In some cases, the limiting capacity can be determined by worst case analysis, in which the values of the variable parameters can be selected based on qualitative reasoning. An example is the water-cooled heat exchanger in Figure 2.26. The result of the operating window analysis is the heat transfer area. The engineer asks, "What set of variable parameters requires the largest area to achieve the desired value of the temperature T1?" The answer is straightforward.

  - Highest cooling medium temperature. The cooling water temperature varies a great deal during the year, so the highest temperature is taken. This value is often cited at about 20 °C (68 °F).
  - Highest flow rate of hot fluid.
  - Highest hot fluid inlet temperature
  - Lowest overall heat transfer coefficient. The heat exchanger surface fouls during prolonged operation. When the equipment is clean, during initial startup and immediately after cleaning maintenance (that requires taking the exchanger out of service), the heat transfer coefficient has its largest value. Just before cleaning maintenance when the fouling is at its maximum, the heat transfer coefficient has its lowest value. These two conditions are often referred to as "start of run" and "end-of-run". Fouling film heat transfer values are given for common fluids (H&C, 2012). The heat exchanger area should be adequate to achieve desired value for T1 for the worst case operating conditions and the end-of-run heat transfer coefficient.

When a legitimate worst-case condition can be identified, the operating window analysis can be simplified to eliminate the associated manipulated and controlled variables.

Engineers should always apply their process knowledge to identify worse-case situations and design equipment to function properly in these scenarios.

2.5.3 Safety margins – Built into equipment design

Safety margins that increase the capacity of process equipment occur for two basic reasons. First, equipment is manufacturer in a discrete number of sizes. When an engineer completes a design calculation for an equipment, the result (heat exchanger area, valve size, pump motor power, and so forth) generally does not equal one of the commercially available discrete sizes. The typical response is to select the closest larger

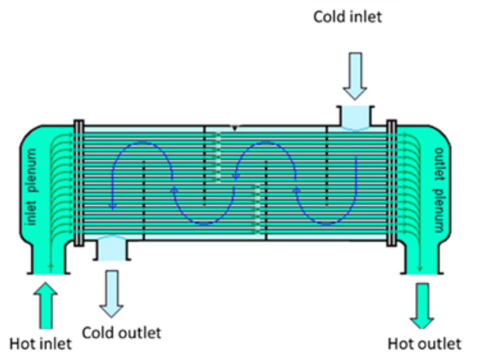


Figure 2.26 Shell and tube heat exchanger (Padleckis, 2006B)

capacity, so that some extra capacity is included in the plant design. This form of safety margin is reasonable. However, the amount of the safety margin is essentially random; it could be a small fraction to nearly the total incremental capacity between the discrete equipment sizes available.

The second source of safety margin is based on guidelines (rules of thumb) for individual equipment. For example, a control valve may be sized to allow the design flow when the valve opening is 70%. This guideline allows for extra flow when required and provides good resolution (change in flow for a 1% change in valve opening) around the base case design conditions. The engineer should not follow these guidelines blindly. Special conditions like startup, shut down, disturbance transients, transitions among product grades, and emergency situations can demand much more capacity.

The method in this chapter is recommended to evaluate the operating window for expected variability. Naturally, the two approaches just described should also be included in equipment design. Recall that the goal of operating window analysis is neither to provide too little nor too much safety margin; it is to provide the right amount of safety margin in the required places in the process. It is worthwhile considering the following quotation from an industrial practitioner and textbook author.

> In fact, students should come away from a design course with disdain for gross overdesign of plants; for example, a 25 percent design (safety) factor can be excessive for some equipment, while being much too small for equipment experiencing large variation.
>
> "For well tested processes, safety factors can approach 0%" (Valle-Riestra, 1993).

2.5.4 Alternative operating window formulations

The method selected for this chapter emphasizes simple calculations using existing software and provides good visual results to support an engineer's decision making. Other formulations give greater information at the cost of more complex formulations and software development.

- *Characterizing the size of the operating window* – This approach determines a shape that fits inside of the operating window, with the largest shape that fits taken as a measure of the size of the operating window (Biegler et.al., 1997)). The area of the shape (or the hyper-volume in higher dimensions) is used to measure the size of the operating window; naturally, the larger the shape, the better the design. This approach requires greater engineering time and mathematical skills to perform. While the volume of the window is important, the importance in various directions is not accounted for.
- *Evaluating the probability of feasibility* – This approach evaluates the conditions for many samples of the variable parameters and determines whether the conditions are within or outside the operating window (Wechsung et.al., 2010)). Advanced sampling methods reduce the number of cases to achieve reasonable computation time, and advanced numerical methods seek to reduce or eliminate simulations that do not converge. Results can be presented graphically, and the design with the highest percentage of points in the operating window is best. With the exception of the advanced numerical method, this approach requires limited engineering time and can be implemented using commercial software.
- *Evaluating the average profitability* – In most processes, capability exists to maintain feasible operation for most variability. For example,
    - If the capacity is below the turndown, some flow can be recycled around a unit to achieve the minimum acceptable.
    - If the maximum capacity of some equipment would be exceeded, the total production rate can be reduced to match the capacity of the equipment.
    - If low production rate in a distillation tower leads to tray weeping weeping, the reflux and reboiler duties can be increased to increase the internal liquid and vapor flows. These actions would increase the operating cost and provide products that are overly pure, but feasibility would be achieved.

  The proper responses could be included in the simulation cases, and the average profit calculated for all feasible points. This approach would require an intermediate (but not insignificant) amount of engineering time and mathematical skills.

2.6 Conclusion: Wrap up and look ahead

The major accomplishment in this chapter is establishing the importance of variability in process design. Many causes for limitations to operating conditions have been introduced. While these examples have been selected to be the more common causes of limitations, the reader should recognize that every process should be investigated for its unique limitations and that this investigation requires a good understanding of the equipment principles.

A computational method has been introduced for evaluating the operating window. The method requires a base case design simulation and defines additional cases based on variable parameters. Typically, the solutions for a large number of cases are required, and flowsheeting software is recommended to facilitate the model formulation and solution. Graphical scatter-plot displays aids the interpretation of results.

Once an appropriate operating window is determined, the equipment to achieve the window can be determined. The equipment must include means for adjusting the variables defined in the operating window calculation, such as heat duty, flow rate, and so forth. The largest capacity and the lowest capacity (highest turndown ratio) determined in the operating window cases can be used in the equipment design.

Designing equipment that can achieve all points in the operating window does not ensure that the process will achieve feasible operation when possible. The following topics salso need to be addressed to achieve an operable design.

- *Flexibility in Chapter 3* - The operating window defined manipulated variables with ranges of adjustment. Therefore, the design must ensure that these manipulated variables can be adjusted in a timely manner. The equipment must be flexible.
- *Reliability in Chapter 4* – The operating window evaluation considered “normal” variation, excluding major faults in equipment. Since a process involve thousands of pieces of equipment, the likelihood of faults occurring is high. Therefore, the engineer needs to include additional equipment so that a process can remain in operation when faults occur.
- *Safety in Chapter 5* – In process design and operation, the highest priority is safety, which must be achieved even when equipment faults and human error occurs. A systematic safety analysis must be performed by engineers. Based on the analysis, the design is enhanced with components of the safety hierarchy.
- *Process Control in Chapter 6* – Designing equipment with the correct flexibility to (1) achieve the operating window, (2) reliably respond to faults, and (3) operate safely does not ensure that the equipment will make the correct adjustments in a timely manner. Automated process control is required to “steer” the process.

Because each is a substantial topic, these future topics are addressed in individual chapters. However, the reader is encouraged to consider Chapters 2 to 6 to contain integrated methods for achieving an operable process design.

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Chapter 2 Appendix A – Process Models

The chapter contains simulation results for several chemical processes. To avoid clutter when concentrating on the operating window method, the model details are given in this appendix.

A.1 Stirred tank chemical reactor

Example 2.2 evaluated the operating window for a continuous stirred tank chemical reaction. The reactor shown in Figure 2A.1 includes cooling heat exchange and has a first-order chemical reaction with Arrhenius temperature dependence. The liquid volume is constant, so that the flows in and out are equal. The reactor is well mixed, shaft work is negligible, and the physical properties are constant. The mathematical model for the component and energy balances are given in the following equations; the steady-state model is achieved by setting the derivatives to zero..

$$V\frac{dC_A}{dt} = F(C_{A0} - C_A) - Vk_0 e^{-E/RT} C_A \tag{A2.1}$$

$$V\rho C_p \frac{dT}{dt} = \rho C_p F(T_0 - T) - \frac{aF_c^{b+1}}{F_c + \dfrac{aF_c^b}{2\rho_c C_{pc}}}(T - T_{cin}) + (-\Delta H_{rxn}) V k_0 e^{-E/RT} C_A \tag{A2.2}$$

Data for the system are from Marlin (2000) Appendix C, Case I and are given in the following.

1. $F = 1\ \text{m}^3/\text{min}$; $V = 1\ \text{m}^3$; $C_{A0} = 2.0\ \text{kmole/m}^3$; $T_0 = 323\ \text{K}$; $C_p = 1\ \text{cal/(g K)}$; $\rho = 10^6\ \text{g/m}^3$; $k_0 = 1.0 \times 10^{10}\ \text{min}^{-1}$; $E/R = 8330.1\ \text{K}$; $-\Delta H_{rxn} = 130 \times 10^6\ \text{cal/(kmole)}$; $T_{cin} = 365\ \text{K}$; $(F_c)_s = 15\ \text{m}^3/\text{min}$; $C_{pc} = 1\ \text{cal/(g K)}$; $\rho_c = 10^6\ \text{g/m}^3$; $a = 1.678 \times 10^6\ \text{(cal/min)/(K)}$; $b = 0.5$.
2. For this data, the steady-state values of the dependent variables are $T_s = 394$ K and $C_{As} = 0.265\ \text{kmole/m}^3$.

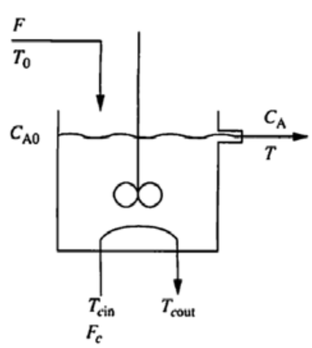


Figure A2.1 Continuous flow stirred tank chemical reactor

A.2 Distillation tower

Example 2.3 evaluated the operating window for a two-product distillation tower. The tower is shown in Figure A2.2 along with base case data. The tower has one feed stream consisting of two components. It has two products, both of which are liquids. Assumptions used in the model are given in the following.

1. Constant relative volatility and equilibrium achieved on all trays
2. Tower pressure is constant
3. The accumulators are well mixed
4. Equal molal overflow

The basic equations for the model are the equilibrium express and the light key component balance on each tray "n", which is given in the following.

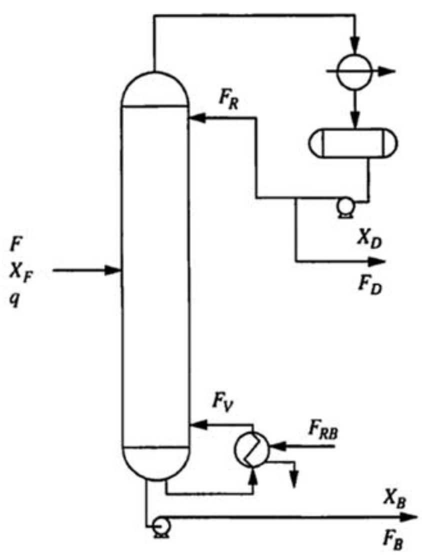
$$y_n = \frac{\alpha x_n}{1 + (\alpha - 1)x_n} \tag{A2.3}$$

$$0 = L_{n+1}x_{n+1} - L_n x_n + V_{n-1}y_{n-1} - V_n y_n + F_n(q)x_{nF} + F_n(1-q)y_{nF} \tag{A2.4}$$

with

L_i = liquid flow from tray i
V_i = vapor flow from trayi
F_i = feed flow to tray i
α = relative volatility

x_i = light key mole fraction in liquid
y_i = light key mole fraction in vapor
q = fraction liquid in feed
x_{iF} = mole fraction light key in liquid feed
y_{iF} = mole fraction light key in vapor feed



Base-Case Data

Feed rate	8.00 kmole/min
Feed composition, XF	0.45 mol fract L.K.
Feed liquid	1.00 fraction
Feed tray	10
Relative vol.	2.20
Trays	21 + reboiler
Distillate, XD	0.975 mol fract L.K.
FD	3.625 kmole/min
FR	7.487 kmole/min
Bottoms, XB	0.015 mol fract L.K.
FB	4.375 kmole/min
FV	11.11 kmole/min
FRB	6.945 kmole/min

Figure A2.2 Binary distillation tower (Marlin, 2000)

A.3 Heat exchanger network

Example 2.4 evaluated the operating window for a simple heat exchanger network. This process was described by Biegler et. al. (1997), who also analyzed the operating window using a different approach from the one proposed in this chapter. The process is shown in Figure 2.20 and all data is given in the body of the chapter. The model of this process accounts for the energy balance and limits to the heat transferred because of outlet temperature pinch. Detailed heat transfer modelling is not included because this operating window evaluation is performed before the exchanger area is determined. When an adequate operating window has been determined, the feasible case with the largest heat transfer area will be used for detailed design of the equipment.

The model is given in the following.

Heat Exchanger 1	**Heat Exchanger 2**	**Heat Exchanger 3**	**Heat Exchanger 4**
T2 = T1 - Q1 / F2	T6 = T5 - Q2 /F3	T7 = T6 - Q3 / F3	F2*(T2 - T11) = Q4
T4 = T3 + Q1 / F1	T10 = T4 + Q2 / F1	T9 = T8 + Q3 / F4	0≤Q4 ≤ Q4max
T1 - T4 ≥ 0	T5 - T10 ≥ 0	T6 - T9 ≥ 0	
T2 - T3 ≥ 0	T6 - T4 ≥ 0	T7 - T8 ≥ 0	

The model can be formulated so that it always has a solution, even if the real process operation is infeasible. This is achieved by replaced strict limits with “soft constraints”, as shown in the following.

T7 - T7viol ≤ T7max
0 ≤ T7viol
T9 – T9slack = 393
T10 –T10slack = 563
T11 – T11slack = 350

The modeling problem is always feasible. When the real process is feasible, T7viol = T9slack = T10slack = T11slack = 0. When one or more of these variables are non-zero, the mathematical problem remains feasible, but the real process is infeasible. The solution to the problem is found using mathematical programming, which minimizes the following objective function.

Objective function = $\text{T7viol}^2 + \text{T9slack}^2 + \text{T10slack}^2 + \text{T11slack}^2$

Therefore, the optimization method seeks to reduce these penalty variables to zero while solving the defining equations; if this is possible, the real process will be feasible, and the solution is in the operating window. If the solution objective is greater than zero, the process is infeasible.