National Program on Technology Enhanced Learning (NPTEL)

Plantwide Control of Integrated Chemical Processes

Indian Institute of Technology Kanpur 208016

Course Coordinator
Dr Nitin Kaistha
Professor
Department of Chemical Engineering
Indian Institute of Technology Kanpur, INDIA

TABLE OF CONTENTS

MODULE II: Control of Common Unit Operations

Chapter 0. Introduction to Course

0.1. Background and Motivation

Chemical processes are designed and operated for manufacturing value added chemicals, the value addition providing the economic incentive for the existence of the process. The fiercely competitive business environment constantly drives research and innovation for significantly improving existing process technologies and for developing new technologies to satisfy man's ever growing needs. On the operation side, the processes are operated to meet key production objectives that include process safety, product specifications (production rate and quality) and environmental regulations. These key production objectives must be satisfied even as the process is subjected to disturbances such as changes in the fresh feed composition, variation in the ambient temperature, equipment fouling, sensor noise / bias etc. In other words, the process operation must ensure proper management of the process variability so that the key production objectives are met even in the presence of the process variability. This naturally leads to the idea of proper management of process variability, the task accomplished by a well designed automatic process control system.

Consider the heat exchanger in Figure 0.1. Steam is used to heat a process stream to a certain temperature. Due to variations in the process stream flow rate and inlet temperature, the stream outlet temperature varies over a large range. From the process operation perspective, this is unacceptable since the large variation in the process stream temperature disturbs the downstream unit (eg. a reactor). The installation of a temperature controller that manipulates the steam flow rate to hold the outlet stream temperature constant mitigates this problem to a very large extent. This is illustrated in the outlet stream temperature and steam flow rate profiles in Figure 0.2. For open loop operation (no temperature control), the temperature varies over a large range while the steam flow rate remains constant. On the other hand, for closed loop operation (with temperature control), the variation in the outlet stream temperature is significantly lower with the steam flow rate showing large variability. The temperature controller thus transforms the variability in the outlet stream temperature to the steam flow rate. This simple example illustrates the action of a control loop as an agent for transformation of process variability.

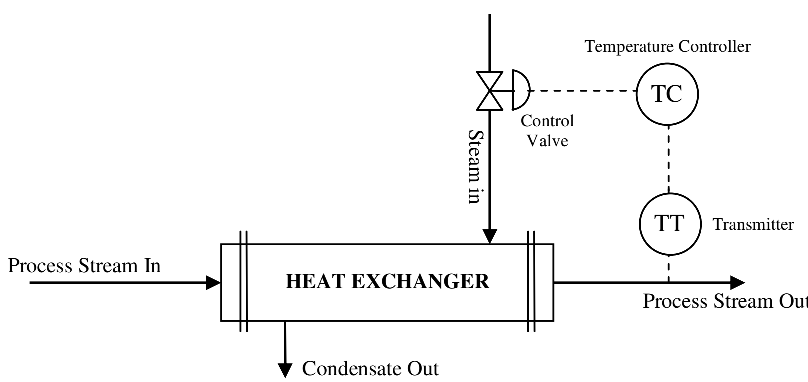


Figure 0.1. Heat exchanger with temperature controller

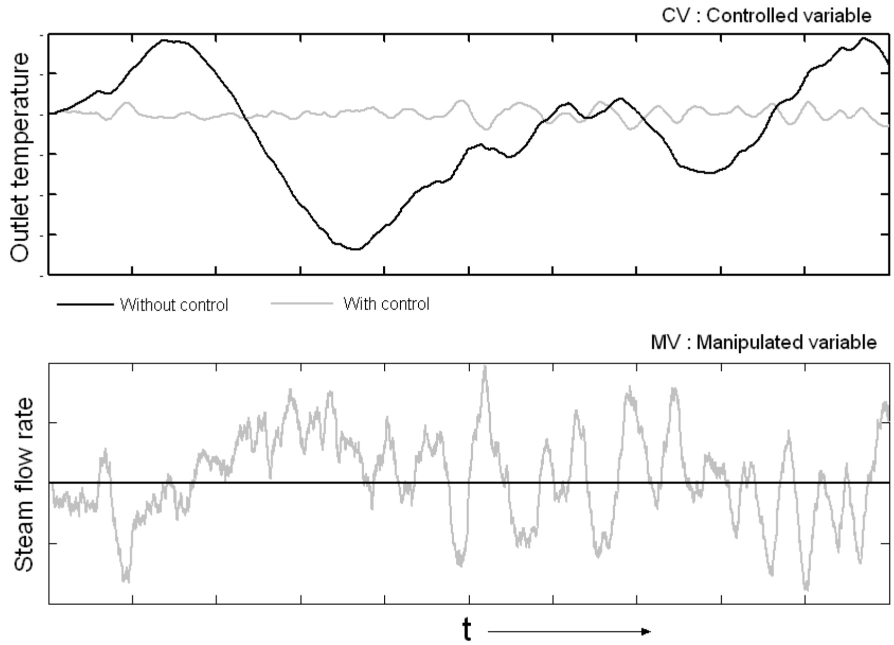


Figure 0.2. The manipulated (steam flow rate) and controlled variable (outlet temperature of process stream) with and without control

A chemical process consists of various interconnected units with material and energy recycle. Controlling a process variable by adjusting the flow rate of a process stream necessarily disturbs the downstream / upstream process due to the interconnection. Material and energy recycle can cause the variability to be propagated through the entire plant. Considering the plant-wide propagation / transformation of process variability, the choice of the variables that are controlled (held at / close to their set-points), the corresponding variables that are manipulated and the degree of tightness of control (loose / tight control) are then key determinants of safe and stable process operation. The choice of the controlled and manipulated variables is also sometimes referred to as the control structure. Modern control text books provide very little guidance to the practicing engineer on the key issue of control structure selection for individual unit operations and the complete process, choosing instead to focus on the control algorithms and their properties with typical mathematical elegance. How does one go about choosing the most appropriate plant-wide control structure for a given set of production objectives? This work attempts to provide an engineering common sense approach to the practicing engineer for answering this key question.

Given a control system that ensures safe and stable process operation in the face of ever present disturbances, crucial economic variables must be maintained to ensure economically efficient or optimum process operation. Depending on the prevailing economic circumstances, optimality may require process operation at the maximum achievable throughput or lower throughputs. At the optimum steady state, multiple process constraints are usually active such as reactor operation at maximum cooling duty/level/temperature/pressure or column operation at its flooding level etc. How close can the process operate to these constraint limits is intimately tied with the basic plant-wide control strategy implemented. The converse problem is that of designing the regulatory plantwide control system such that the back-off from the constraint limits is the least possible. In this work, we also develop a systematic procedure for designing such an economic plantwide control system.

In summary, this book is targeted at the practicing engineer to help him design effective plant-wide control systems through an appreciation of the major issues the control system must address. It is hoped that the targeted audience finds the work of practical utility. The author invites suggestions, comments and criticisms for improving upon the work.

0.2. Organization of the Course

The course is organized into four modules, excluding this Introduction. In Module 1, the reader is introduced to the essentials of process control. Only the most practical aspects of process control theory are presented. Mathematical rigor is deliberately done away with in favour of a more colloquial style to keep the discussion focused on the most essential and practical aspects of process control theory. Module 2 is devoted to the control of common unit operations found in the process industry. The control of distillation columns is exhaustively dealt with and includes simple, heat integrated and complex column configurations. The control of industrially common reactor configurations and heat exchangers is covered next. Finally common control configurations for miscellaneous systems such as furnaces, heat refrigeration systems and compressors are discussed. Module 3 elaborates upon the key issues in the design of a plant-wide control system. The need for balancing the reactant inventory and the interaction between the reaction and separation section of a plant are described. We then go about developing a systematic procedure for economic plantwide control system design. Three elaborate case studies on realistic chemical processes are then presented to demonstrate the application of the methodology. Comparisons with conventional plantwide control structures show that an economic plantwide control structure can significantly improve (2-20%) the achievable profit (or maximum throughput) for a given process. Proper design of the plantwide control system is thus shown to be crucial to achieving economically optimal process operation.

MODULE I

ESSENTIAL PROCESS CONTROL BASICS

In this module, we cover essential aspects of process control theory, necessary for proper control system design. A hands-on approach to covering process dynamics, PID control algorithm, identification, tuning, advanced control structures and multivariable decentralized control is used, in contrast to the mathematically elegant but abstruse treatment in most controls texts. Only the most essential and relevant aspects are covered. In the interest of brevity, since this is a course on plantwide control and not control theory, we do not provide many detailed solved examples to back the theory and refer the reader to standard text-books for the same.

Chapter 1. Process Dynamics

Process dynamics refers to the time trajectory of a variable in response to a change in an input to the process. All of us have an inherent appreciation of process dynamics in the sense that the effect of a cause takes time to manifest itself. It thus takes 20 minutes for a pot of rice to cook over a flame, 5-10 minutes for the water in the geyser to heat up sufficiently, years and years of dedicated practice to become an adept musician (or a good engineer, for that matter!) and so on so forth. In each of these examples, a change in the causal variable (flame, electric heating or dedicated practice) results in a change over time in the effected variable (degree of "cookedness" of rice, geyser water temperature or a musician's virtuosity). Process dynamics deals with the systematic characterization of the time response of the effected variable to a change in the causal variable. In process control parlance, the causal variable is referred to as an input variable and the effected variable is referred to as an output variable.

In order to fix ideas in the context of chemical processes, Figure 1.1 shows the schematic of a simple distillation column. An equimolar ABC feed is separated to recover nearly pure A as the distillate with the bottoms being a BC mixture with trace amounts of A. The fresh feed, reflux and reboil constitute the inputs to the column while the distillate and bottoms flow / composition and the tray composition / temperature profiles constitute the outputs.

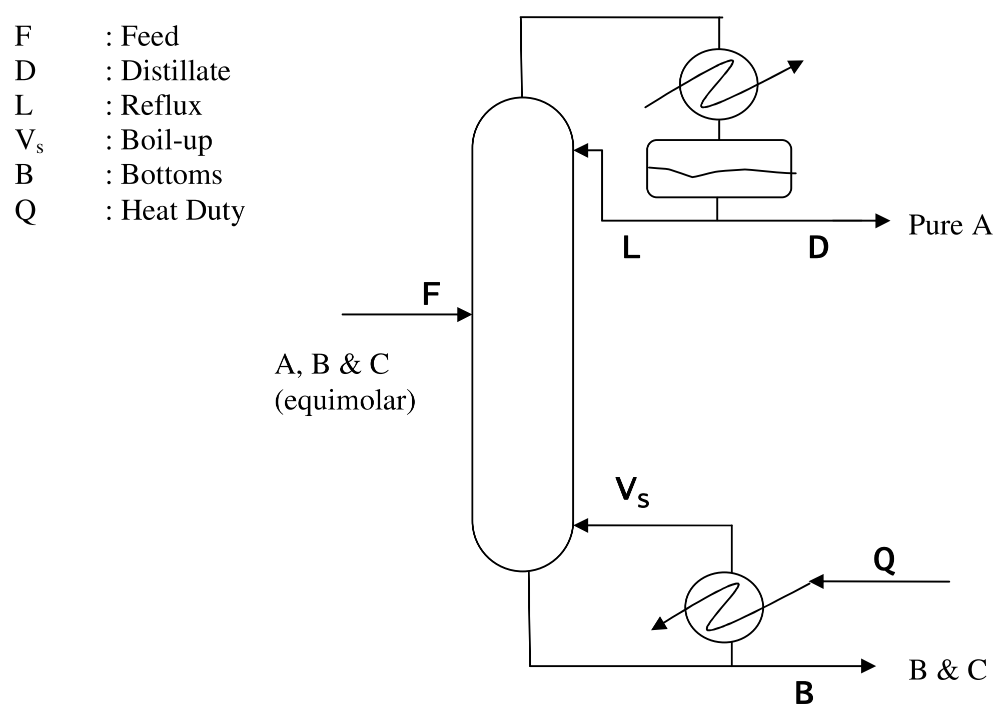


Figure 1.1. Schematic of a distillation column

1.1. Standard Input Changes

To systematically characterize the transient response of an output to a change in the input, the input change is usually standardized to a step change, a pulse change or an impulse change. These standard input changes are depicted in Figure 1.2. A step change in the input, the simplest input change pattern, is used in this work to characterize the process dynamics.

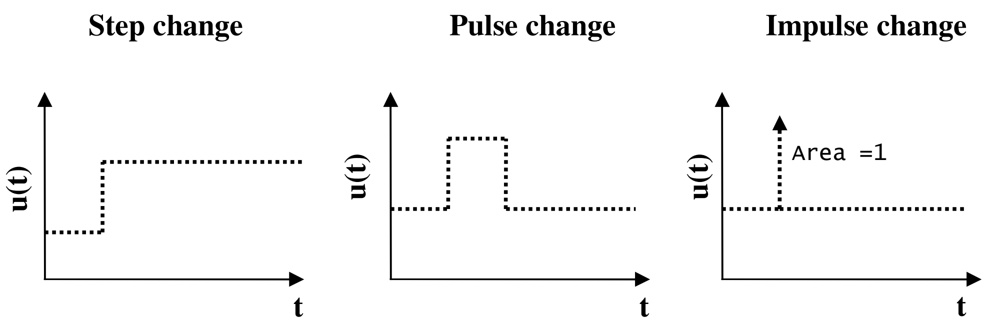


Figure 1.2. Standard input changes

1.2. Basic Response Types

The dynamics of every process are. Even so, the variety of transient responses can be characterized as an appropriate combination of one or more basic response types. These transient responses correspond to the solution of linear ordinary differential equations (ODEs). Linear ODEs can be compactly represented using Laplace transforms. For example consider a second order differential equation

$$\tau^2 \frac{d^2 y(t)}{dt^2} + 2\zeta\tau \frac{dy(t)}{dt} + y(t) = K_P u(t)$$

where y(t) and u(t) are the process output and input respectively. The Laplace transform representation in the *s* domain is obtained by replacing the n^{th} order derivative operator by s^n so that for the second order ODE above

$$\tau^2 . s^2 y(s) + 2\zeta\tau . s . y(s) + y(s) = K_P u(s)$$

Rearranging, the input-output transfer function becomes

$$G_P = \frac{y(s)}{u(s)} = \frac{K_P}{\tau^2 s^2 + 2\zeta\tau s + 1}$$

The ODEs and corresponding Laplace transform representation is noted in Table 1.1.

1.2.1. First Order Lag

The first order lag is the simplest transient response where the output immediately responds to a step change in the input (see Figure 1.3(a)). The ratio of the change in the output to the change in the input is referred to as the process gain, K_p. The time it takes for the output to reach 63.2% of its final value corresponds to the first order time constant τ_p. The output reaches ~95% of its final value in 3 time constants.

Table 1.1. Various differential equations and their Laplace transform

Terminology	Differential equation	Laplace Transform $\frac{y(s)}{u(s)}$
Gain	$y(t) = K.u(t)$	K
Derivative	$y(t) = \frac{du(t)}{dt}$	s
Integrator	$y(t) = \int_0^t u(t).dt$	$\frac{1}{s}$
First order lag	$\tau \frac{dy(t)}{dt} + y(t) = u(t)$	$\frac{1}{\tau s+1}$
First-order lead	$\tau \frac{du(t)}{dt} + u(t) = y(t)$	$\tau s+1$
Second Order Lag		
Underdamped $\zeta < 1$	$\tau^2 \frac{d^2 y(t)}{dt^2} + 2\zeta\tau \frac{dy(t)}{dt} + y(t) = K_p u(t)$	$\frac{K_p}{\tau^2 s^2 + 2\zeta\tau s + 1}$
Critically damped $\zeta = 1$	$\tau^2 \frac{d^2 y(t)}{dt^2} + 2\tau \frac{dy(t)}{dt} + y(t) = K_p u(t)$	$\frac{K_p}{(\tau s+1)^2}$
Overdamped $\zeta > 1$	$\tau_1\tau_2 \frac{d^2 y(t)}{dt^2} + \zeta(\tau_1+\tau_2) \frac{dy(t)}{dt} + y(t) = K_p u(t)$	$\frac{K_p}{(\tau_1 s+1)(\tau_2 s+1)}$
Deadtime	$y(t) = u(t-\theta)$	$e^{-\theta s}$
Lead-lag	$\tau_2 \frac{dy(t)}{dt} + y(t) = \tau_1 \frac{du(t)}{dt} + u(t)$	$\frac{\tau_1 s+1}{\tau_2 s+1}$

1.2.2. Higher Order Lags

If the output from a first order lag is input to another first order lag, the latter's output behaves as a second order lag with respect to the input to the first lag. The overall transient response is S shaped with the output not responding immediately to a change in the input. When the time constant of the two lags are different, the response is called an over-damped second order response. The response for the special case where the two time constants are equal is called the critically damped second order response. Higher order systems result as more first order lags are connected in series with the transient response becoming increasingly sluggish.

1.2.3. Second Order Response

Sometimes, a step change in the input causes the output to oscillate before settling at the final steady state. The simplest such response corresponds to a second order underdamped system. The damping coefficient, ζ, can be used to characterize all second order responses – overdamped ($\zeta > 1$), critcally damped ($\zeta = 1$) and underdamped ($\zeta < 1$). The second order response is shown in Figure 1.3(b).

To gain an appreciation of the impact of damping coefficient on the transient response, Table 1.2 reports the ratio of the second overshoot to the first overshoot for different values of ζ. A quarter decay ratio is observed for a damping coefficient of 0.218. Sustained oscillations (decay ratio = 1) are observed for a damping coefficient of 0. As ζ increases to 1, the overshoot in the output disappears.

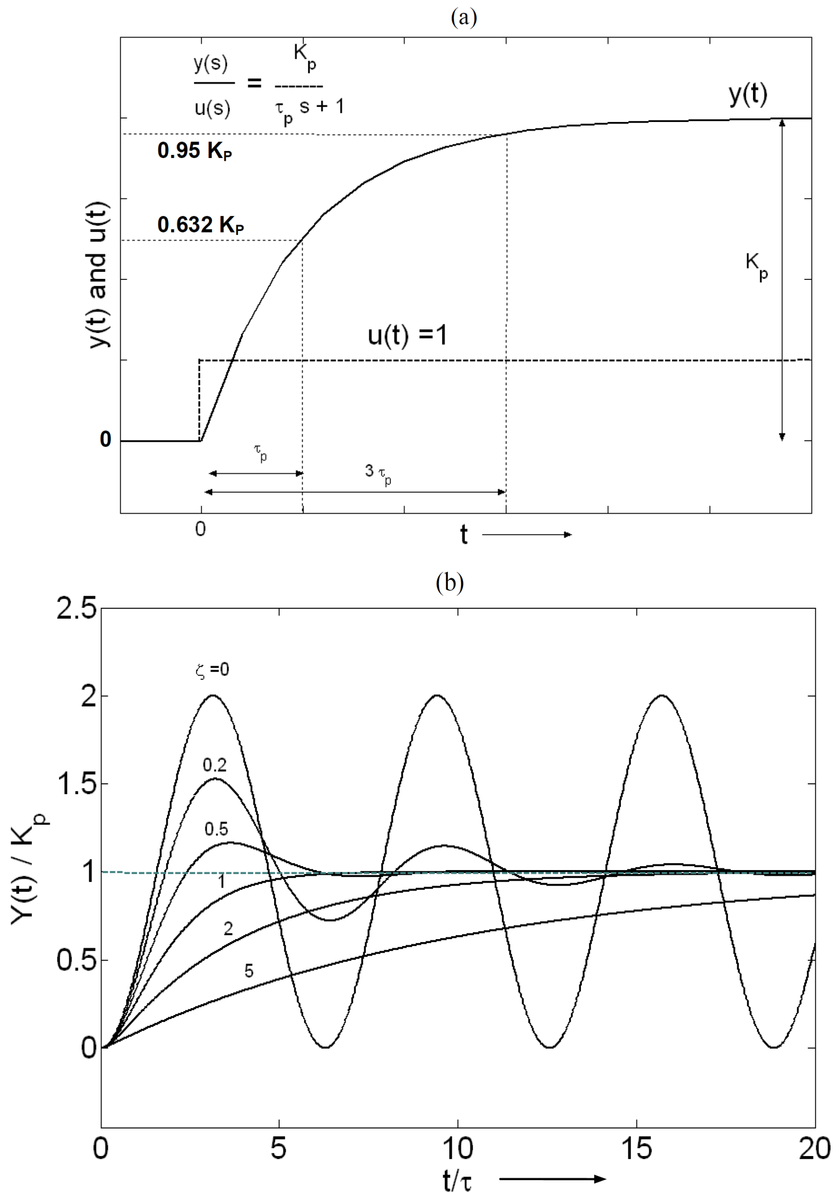


Figure 1.3. Output response for unit step change to (a) First order & (b) Second order process.

Table 1.2. Decay ratio for various different damping coefficients

Damping Coefficient, ζ	0	0.05	0.1	0.2	0.218	0.4	0.6	1
Decay ratio	1.000	0.730	0.532	0.277	0.250	0.064	0.009	0.000

1.2.4. Other Common Response Types

Other types of responses include the pure integrator, the pure dead-time, and the inverse response. The transient response to a unit step change can be seen in Figure 1.4 and are self explanatory.

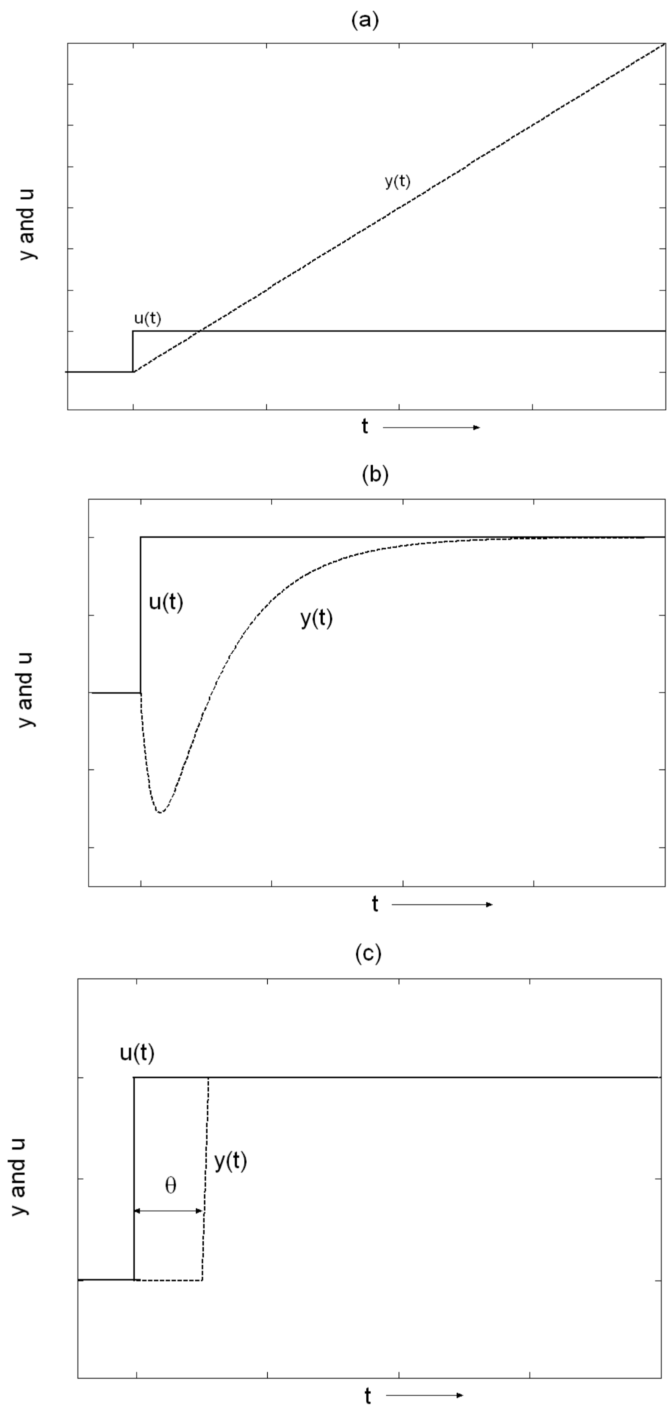


Figure 1.4. The output response for a unit step change for (a) pure integrator, (b) inverse response and (c) pure dead time process.

The most common example of a pure integrator is the response of the tank level to change in the inlet / outlet feed rate. Unless the inlet and outlet flows are perfectly equal, the tank level is either rising or falling in direct proportion to the mismatch in the flows. The level in a tank is thus non-self regulating with respect to the connected flows. A controller must be used to stabilize all such non-self regulating process variables. Dead time is very common in chemical processing systems and is due to transportation delay. A very common example of the inverse response is the response of the liquid level in a boiler to a change in the heating duty. As the heating duty is increased, the vapour volume entrapped in the liquid increases causing the liquid interface level to rise initially. Over longer duration, the level of course reduces since more liquid is being vaporized. As will be seen later, dead time and inverse response can create control difficulties.

1.2.5. Unstable Systems

Some systems may be inherently unstable. Unstable transient responses are shown in Figure 1.5. The unstable response may be non-oscillatory or oscillatory as in the Figure. Reactor temperature runaway is an example of an unstable process. A control system must be used to stabilize an inherently unstable system.

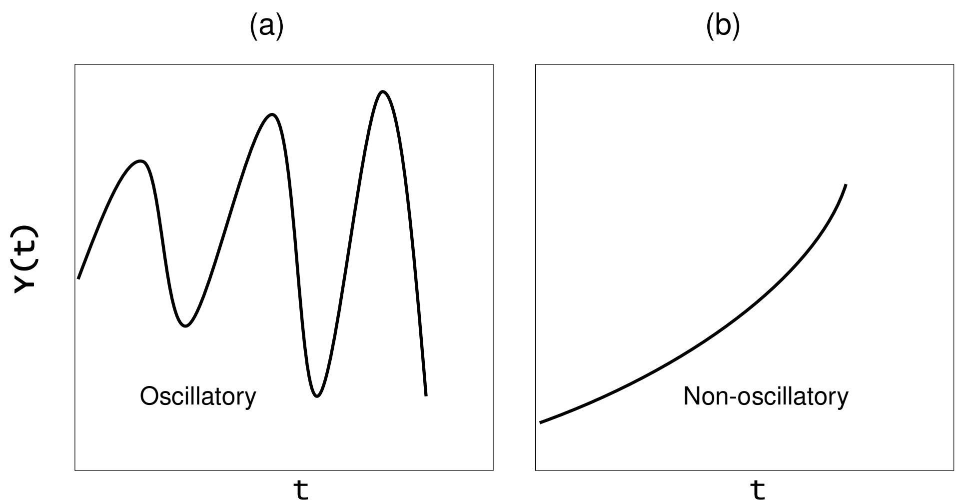


Figure 1.5. The output response for unstable process. (a) Oscillatory and (b) non-oscillatory

1.3. Combination of Basic Responses

Any transient response can be reasonably represented as a combination of the above basic response types. One such combination is the first order lag plus dead time that has been found to represent the transient response of many chemical processing systems very well. The response is illustrated in Figure 1.6(a). Another example of such a combination is the inverse response which can be represented by the parallel combination of two first order lags. One of the lags has a small gain and a small time constant (ie a fast response) while the other lag has a gain of larger magnitude and opposite sign with a much larger time constant (i.e. a slow response in the opposite direction). Figure 1.6(b) illustrates this concept.

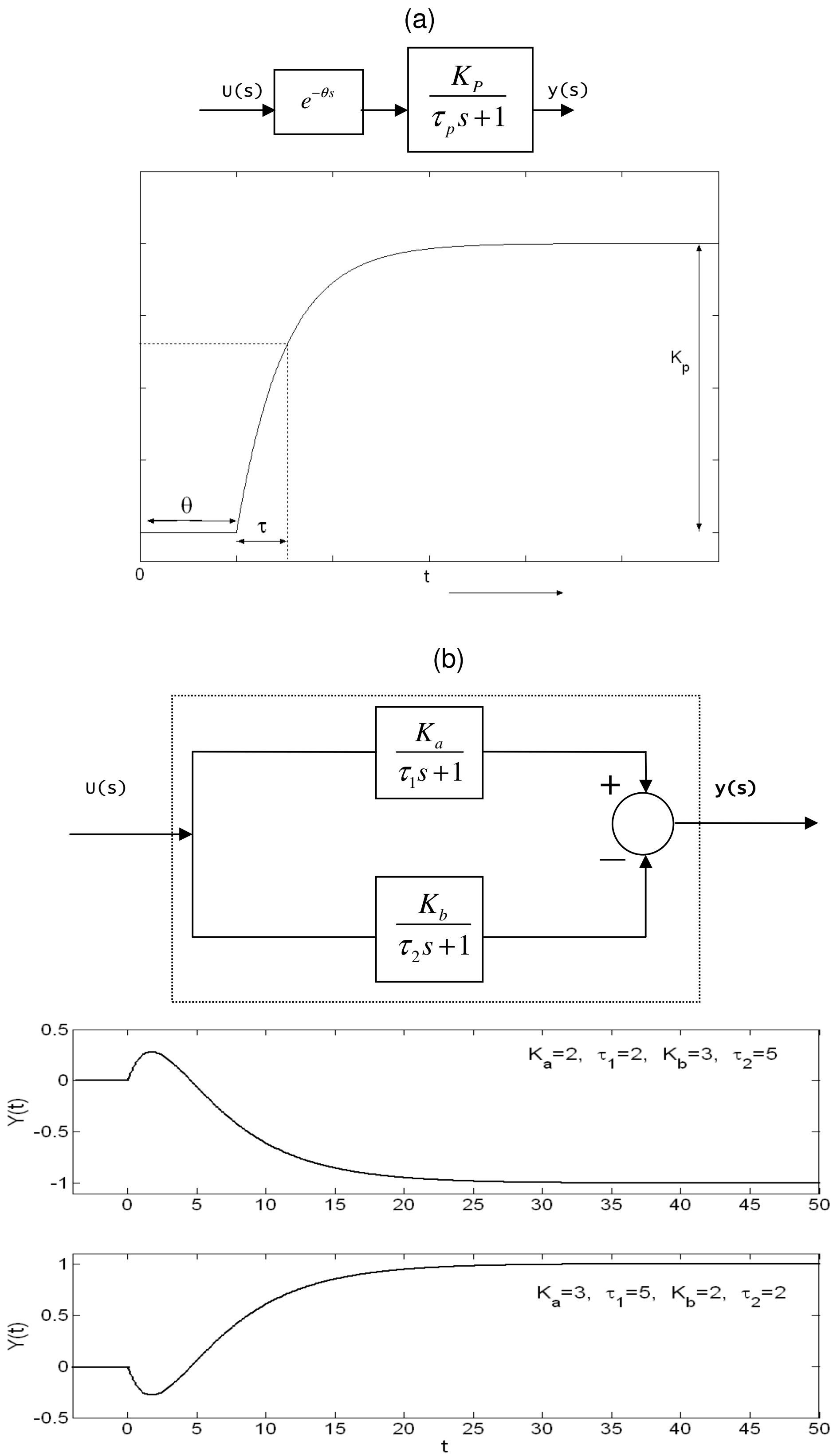


Figure 1.6. Unit step responses (a) first order plus dead time process (FOPDT) and (b) Inverse response

Chapter 2. Feedback Control

The safe and stable operation of a process requires that key variables be maintained at or close to their design values in the face of disturbances entering the process. For example, it may be necessary to hold a process stream flow rate nearly constant even as the upstream / downstream pressure fluctuates. Similarly the temperature at the inlet to a packed bed reactor must be maintained at its design value to prevent reactor run-away and also ensure the desired conversion to products(s) for varying flow rates of the process stream. Maintaining a process variable at or near a certain value requires a manipulation handle that can be appropriately adjusted. For example, the valve opening can be adjusted to maintain the flow rate through the pipe. Similarly the heating duty of the furnace can be used to heat the process to maintain the reactor inlet stream temperature. This leads to the idea of feedback control where the deviation in the variable to be maintained at / near its design value is used to make appropriate adjustments in the manipulation handle. The variable to be maintained at its design value is referred to as the controlled variable and the adjustment handle is called the manipulated variable. The algorithm / procedure used to quantitatively translate the deviation in the controlled variable to the adjustment in the manipulated variable is known as the control algorithm.

2.1. The Feedback Loop and its Components

A feedback control loop is schematically illustrated in Figure 2.1. Its primary components are the sensor, transducer, transmitter, controller, I/P converter and the final control element. The sensor is the sensing element used to measure the controlled variable (and other important process variables that may not be controlled). Flow, temperature and pressure sensors are routinely used in the process industry. Composition analyzers are used less frequently to measure only key compositions such as the product purity. Most sensors translate a change in the state of the variable to be measured into an equivalent mechanical signal such as the stretching / bending of a Bourdon tube. The mechanical signal needs to be converted into an electrical signal for onward transmission to the control room (or stand-alone controller). This is accomplished by the transducer. For standardization across different manufacturers, the range of the input and output signal from a controller is 4-20 mA. The range corresponds to the sensor / final control element span. The transmitter converts the electrical signal from the transducer to the 4-20 mA range. The transmitter signal is input to the controller. The desired value for the controlled variable, referred to as the set-point, is also input to the controller. The controller output signal is again between 4-20 mA. In the process industry, this electrical signal is converted to an equivalent 3-15 psig pneumatic pressure signal using an I/P converter. The pressure signal (or rather change in the pressure signal) is used to move the final control element to bring about a change in the manipulated variable. In the process industry, almost all final control elements are control valves that adjust the flow rate of a material stream.

The controller subtracts the current value of the controlled variable from its set-point to obtain the error signal as

$$e_t = y^{SP} - y_t$$

where y is the controlled variable. The subscript t refers to the current time. The error signal is input to the control algorithm to determine the change in the manipulated variable (control input) to be implemented. This is schematically illustrated in Figure 2.2. The most popular control algorithm, namely the PID algorithm is discussed next.

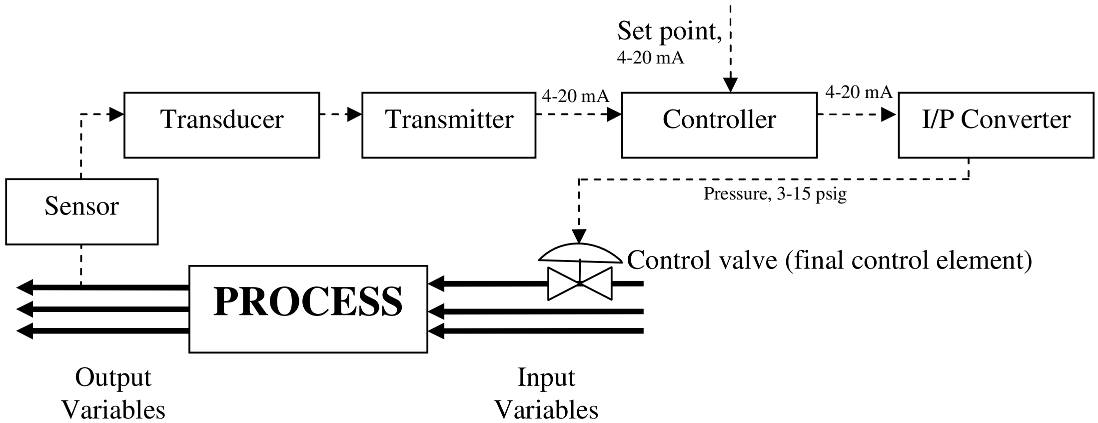


Figure 2.1. Schematic of a process with feed back control scheme

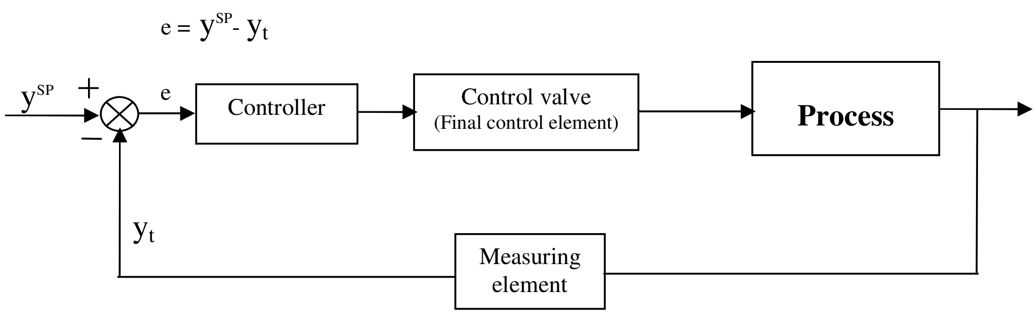


Figure 2.2. Block diagram of a feed back control

2.2. PID Control

2.2.1. The Control Algorithm

Almost all controllers in the process industry use the Proportional Integral Derivative (PID) control algorithm. Even as instrumentation and computation technologies have witnessed a transition from the analog era to the digital revolution, the good old PID control algorithm remains the most widely used algorithm, not withstanding the onslaught of advanced model predictive control algorithms. The positional form of the algorithm states that

$$u_t = K_C\left(e_t + \frac{1}{\tau_I}\int_0^t e(t)dt + \tau_D \frac{de_t}{dt}\right) + bias$$

where u is the controller output (input to the process), e is the error in the controlled variable, and K_C, τ_I and τ_D are controller tuning parameters. The tuning parameters are referred to respectively as the controller gain, reset (or integral time) and derivative time. The bias term in the expression is provided to make the LHS equal the RHS at time $t = 0$ for proper initialisation. The three terms in the algorithm correspond to Proportional, Integral and Derivative action, hence the acronym PID.

The velocity form of the algorithm is more amenable to understanding the effect of each of the P, I and D actions. Differentiating the above equation, we get

$$\frac{du_t}{dt} = K_C \left(\frac{de_t}{dt} + \frac{1}{\tau_I} e_t + \tau_D \frac{d^2 e_t}{dt^2} \right)$$

The controller gain or proportional gain, K_C, determines the fastness of response with larger values resulting in a fast response to deviations from set-point. This can be verified from the first term in the velocity form equation where the rate of change of the control input is directly proportional to the rate of change in the error, K_C being the proportionality constant. The larger the K_C, the larger the change in the control input, the faster the return to set-point.

The integral action is provided to ensure zero offset in the controlled variable. If the controlled variable deviates from its set-point, the controller acts to settle the system at a new steady state. At this new steady state all time derivatives are zero (by definition) implying the LHS in the equation above is zero. The RHS also therefore must be zero which requires that the error term, e_t, must be zero at the final steady state ($t \rightarrow \infty$). The error term in the velocity form above is due to the integral mode so that integral action moves the control input until the error in the controlled variable is driven to zero i.e. ensures a zero offset. P and D action do not guarantee zero offset as at the final steady state, the LHS and RHS terms corresponding to P and D action are zero. For a P or PD controller with no integral action, the velocity form of the algorithm imposes no restriction on the output error at the final steady state. A non-zero offset thus can and does result sans integral action.

The derivative action causes the controller to "think ahead" and is usually introduced to suppress oscillations from the "seeking behaviour" caused by integral action. In effect, the derivative action puts brakes on the control action as the controlled variable approaches the set-point thus avoiding large oscillations around the set-point. Most controllers in the industry are P or PI controllers and the D action is set to zero. This is because the D action amplifies noise so that the controller input signal must be pre-filtered appropriately to reap the benefit of D action. It is easier to simply turn the D action off and properly tune the controller gain and reset time for the desired control performance.

2.2.2. Controller Tuning

Empirical rules have been developed for tuning PID controllers. These tuning rules are based on the idea of ultimate gain and ultimate period. Figure 2.3 plots the closed loop response for a unit step change in the set-point of a first order plus dead time process for a P only controller as the controller gain is increased. Notice that as the controller gain is increased, the steady state offset reduces. Also, the response becomes faster. For larger gains the closed loop response is oscillatory. As the gain is increased further, sustained oscillations result. Any further increase in the controller gain results in an unstable system with the oscillations increasing in magnitude with time. The controller gain for which the closed loop response exhibits sustained oscillations corresponds to the transition from a stable to an unstable closed loop response. This controller gain at which the closed loop system borders on instability is referred to as the ultimate gain, K_U. The period of the sustained oscillations is known as the ultimate period, P_U. The empirical tuning rules recommend the controller gain to be a fraction of the ultimate gain and the reset time and derivative time as fractions (multiples) of P_U. Two popular tuning rules are the Zeigler-Nichols and Tyreus-Luyben tuning rules are tabulated in Table 2.1. For a given ultimate gain and ultimate period, the controller gain is the least for a PI controller. This is due to the "seeking behaviour" caused by integral action for zero offset. The closed loop system thus goes unstable for a lower controller gain implying that it should be lower. The controller gain is the maximum for a

PID controller due to the stabilizing effect of D action. As discussed before, D action is however used rarely in practice due to noise amplification. The PI algorithm is most commonly used in the industry. The tuning rules show that Zeigler-Nichols tuning is more aggressive than the Tyreus-Luyben tuning. Application of the ZN tuning rule can cause process upsets such as a distillation column flooding due to a sudden large increase in the vapour boil-up caused by a controller. The more conservative TL tuning rule is preferred in the process industry for a smooth and bumpless handling of transients avoiding large and sudden changes in the control input.

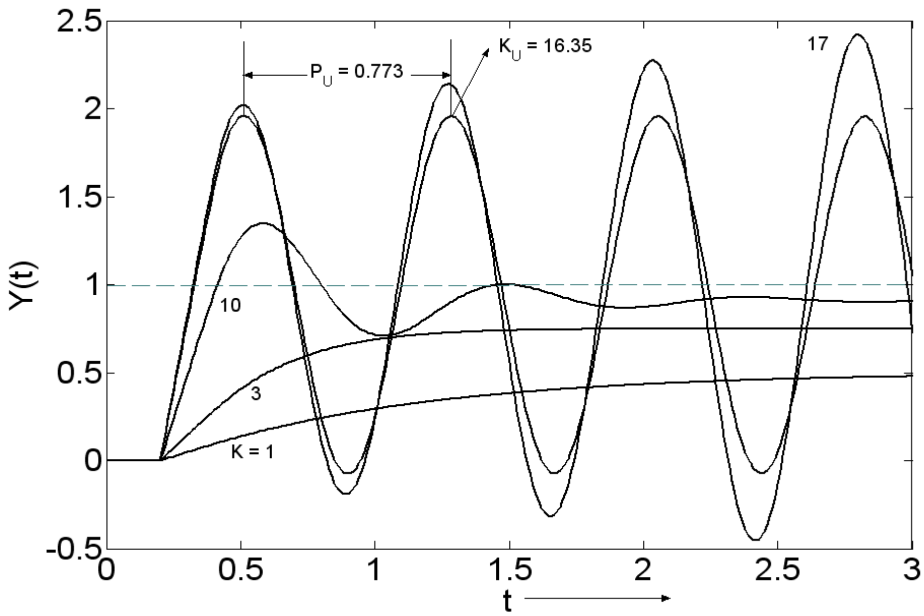


Figure 2.3. Closed loop response of a first order plus dead time process using P controller with different controller gains (K).

Table 2.1

	P	PI	PID
	Ziegler-Nichols		
K_C	$K_U/2$	$K_U/2.2$	$K_U/1.7$
τ_I	--	$P_U/1.2$	$P_U/2$
τ_D	--	--	$P_U/8$
	Tyreus -Luyben		
K_C	--	$K_U/3.2$	$K_U/2.2$
τ_I		$2.2P_U$	$2.2P_U$
τ_D	--	--	$P_U/6.3$

It is appropriate to highlight that a controller is required to handle two types of changes namely, a change in the output set-point and a change in the measured / unmeasured disturbance into the process. The closed loop response for these is respectively referred to as the servo and the regulator response. A disturbance into a process is also sometimes referred to as a load change. Control systems in the process industry are typically designed for effective load rejection. In contrast, set-point tracking is the primary objective in the design of control systems for aerospace systems such as aeroplanes, rockets and missiles.

Figure 2.4 plots the regulator response for a unit step in the load variable with a P, PI and PID controller tuned using the ZN and TL tuning rules for the first order plus dead time process considered earlier. Notice that P only control results in an offset at the final steady state. This offset is larger for TL tuning due to the lower controller gain. The PI and PID regulator responses show no offset at the final steady state due to integral action. Also notice that the aggressive ZN tuning results in a quicker but oscillatory return to the set-point for the PI controller. These oscillations are suppressed by the D action in a PID controller. PID control leads to a faster and smoother return to set-point due to the stabilizing effect of D action. It is also highlighted that the TL tuning leads to a comparatively sluggish but non-oscillatory response due to the more conservative tuning parameters. Large and sudden changes in the control input are not desirable in the process industry to avoid hitting operating constraints (e.g. flooding / weeping in sieve tray towers) during transients. Also, the process equipment changes its dynamic characteristics due to equipment fouling, change in process through-put, wear and tear over time etc so that the need for retuning a control loop is mitigated using conservative controller settings. The TL settings thus represent a good compromise between control performance and robustness.

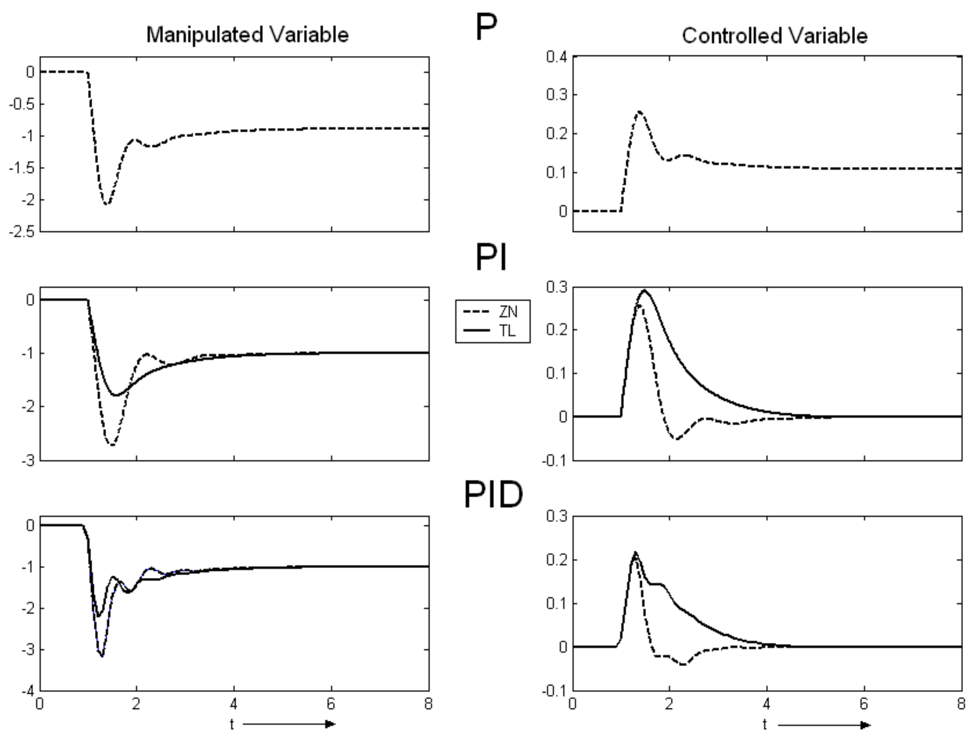


Figure 2.4. Dynamics of manipulated and controlled variables using P, PI and PID controllers with ZN and TL controller parameters for a unit step change in load. (Regulatory response).

2.3. Process Identification

Obtaining the ultimate gain and period of a control loop by increasing the controller gain causes the process to be driven towards instability. Considering the hazardous nature of chemicals processed in any chemical plant, such a methodology for tuning loops must be avoided. Alternative methods are needed that can be used for proper tuning. Two practical methodologies namely, the process reaction curve and auto-tune variation are presented next.

2.3.1. Process Reaction Curve Fitting

The process reaction curve is the open-loop response of the output variable to a step change in the manipulated variable which usually corresponds to a step change in a valve position. Most of the transient responses can be well represented by a first order plus dead time model. The model parameters are obtained as illustrated in Figure 2.5. The model parameters can be obtained by two methods as illustrated in Figure 2.5. In both methods, the ratio of the change in the controlled variable (output) from the initial to the final steady state to the magnitude of the step change gives the process gain K_P. For the controller, both input and output are 4-20 mA signals corresponding to the sensor and final control element span. In most commercial DCS systems, this range is represented as an equivalent 0-100% range. The units of K_P are then % change in controlled variable per % change in manipulated variable.

The two methods differ in the manner in which the dead time, θ, and the first order time constant, τ_P, are obtained. In Method 1, a tangent at the inflection point in the process reaction curve is drawn. Its intersection with the time axis gives the dead time θ. Its intersection with the horizontal line $Y = Y_{SS}$' where Y_{ss} is the final steady state equals $\theta + \tau_P$, from where τ_P is obtained. Equivalently, τ_P is obtained as

$$\tau_P = \frac{K_P}{S}$$

where S is the slope of the tangent drawn at the inflection point.

In Method 2, the time it takes for the response to reach 28.3% and 63.2% of the final steady state are noted. Denote these two times with $t_{28.3\%}$ and $t_{63.2\%}$ respectively. Noting that for a first order lag, 28.3% and 63.2% response completion occurs in $\tau_P/3$ and τ_P time units respectively, we have

$$\theta + \tau_P/3 = t_{28.3\%}$$

$$\theta + \tau_P = t_{63.2\%}$$

Subtracting the two equations to eliminate θ, we have

$$\tau_P = 1.5(t_{63.2\%} - t_{28.3\%})$$

and finally $\theta = 1.5\, t_{28.3\%} - 0.5\, t_{63.2\%}$

The response of the fitted model using the two methods in shown in Figure 2.11. Method 2 is clearly simpler and fits the actual process reaction curve better.

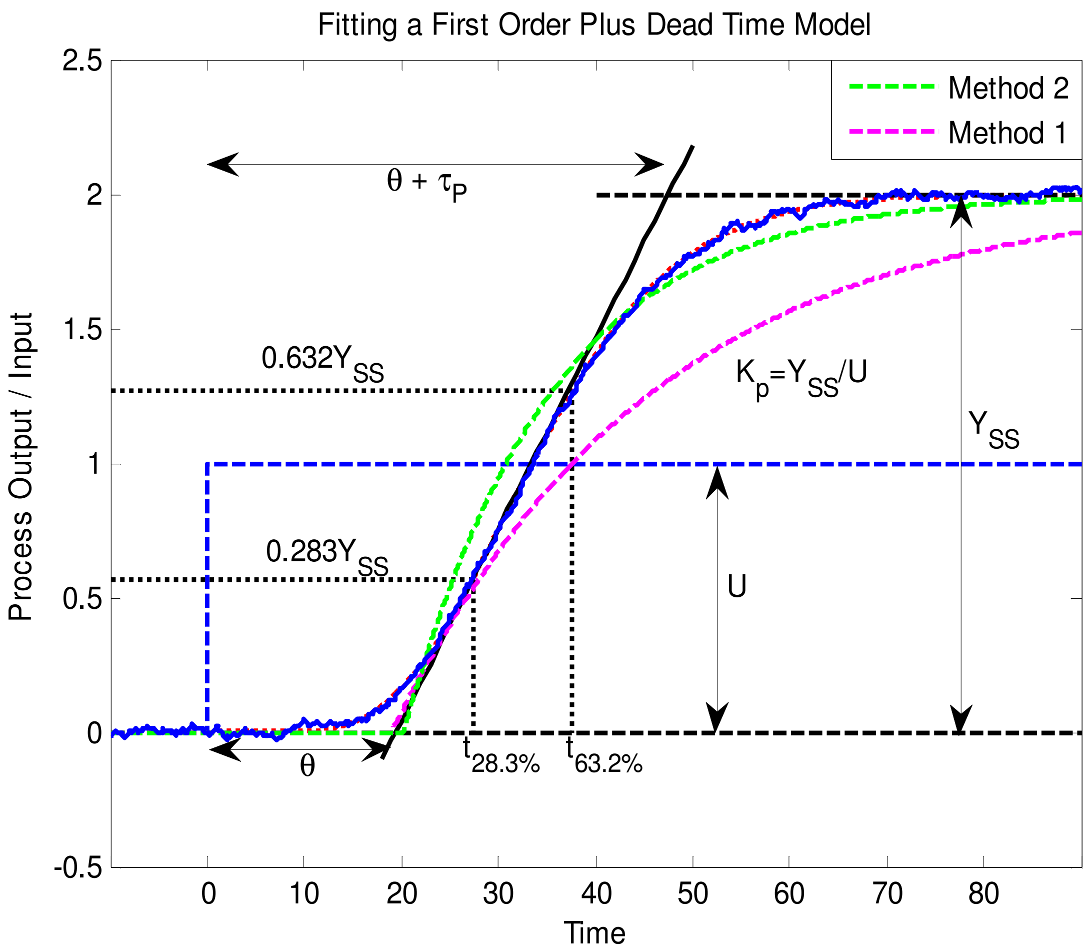


Figure 2.5. Fitting a first order plus dead time model to the process reaction curve

With the fitted model, K_U and P_U can be obtained either by simulation or complex variable analysis. The ZN or TL tunings can then be calculated as in Table 2.1.

2.3.2. Autotuning

Astrom and Hagglund (1984) proposed a powerful auto-tune variation (ATV) method for obtaining the ultimate gain and ultimate period. The method consists of putting a relay at the error signal that toggles the process input by $\pm h\%$ on detecting a zero crossing. This is schematically illustrated in Figure 2.6(a). The action of the relay causes the process input to toggle around the steady state by $\pm h\%$ for every zero crossing in the error signal corresponding to the output crossing the set-point. Sustained oscillations result and the system ends up in a limit cycle as depicted in Figure 2.6(b). The period of oscillations is the ultimate period P_U. The amplitude a of the output oscillations gives the ultimate gain K_U as

$$K_U = \frac{4h}{a\pi}$$

The ATV method has advantages over open loop step methods. The method automatically finds the critical frequency (or period) of the process. Also, large deviations away from the steady state are avoided as this is a closed loop test. Finally, the amplitude at the critical frequency (ultimate period) is obtained so that the identification procedure is more accurate than step / pulse tests.

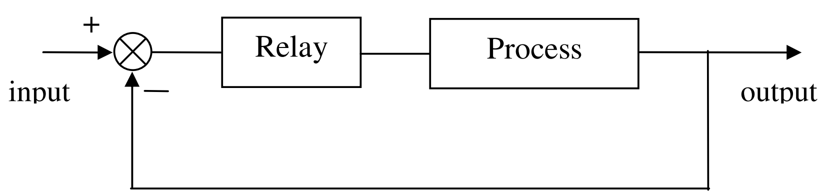


Figure 2.6(a). Block diagram of relay feedback approach

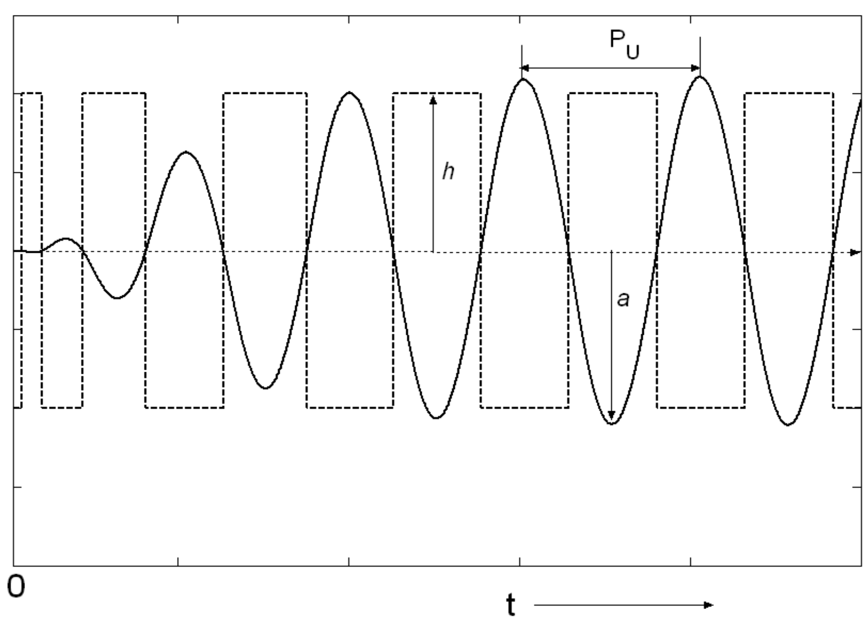


Figure 2.6(b). Relay feed back experiment a process with positive steady state gain

2.4. Controller Modes and Action

In all DCS systems, the controller can be in the indicator, manual, automatic or cascade mode. In the indicator mode, the controller is off and the process variable (controlled variable) is displayed. The control valve position cannot be adjusted by the operator. In the manual mode, the controller is off. The process variable reading is displayed and the operator can manually input the control valve position. Open loop step / pulse tests are performed in the manual mode with the operator giving a step change to the control valve position. In the automatic mode, the controller is on so that the control valve position is now set by the controller. The operator inputs the set-point for the controlled variable. In the cascade mode, the controller receives the set-point for the controlled variable from a master controller (and not the operator).

Depending on the sign of the process gain, the controller action must be specified to be “direct” or “reverse”. Usually a “direct” acting controller increases the controller output as the controlled variable increases above the set-point. A reverse acting controller, on the other hand, decreases the controller output as the controlled variable increases above set-point. For a negative process gain, the controller is “direct” acting while for a positive process gain the controller is “reverse” acting. The definition of “direct” or “reverse” action can vary from one vendor to the other and it is always best to confirm the definition. Another consideration in correctly specifying the controller action is whether the control valve fails open (air-to-close) or fails closed (air-to-open). Process safety considerations dictate if a control valve fails open or fails closed. For example the cooling water valve for removing heat from a reactor would fail open while the steam valve into a reboiler would fail close. If the controller action for a fail open valve is “direct”, the action would be “reverse” for a fail close valve in the same control loop.

In control parlance, the controller gain is many-a-times reported as proportional band. The proportional band is defined as

$$PB = \frac{100}{K_C}\ \%$$

The higher the proportional band, the lower the controller gain and vice versa.

2.5. Rules of Thumb for Controller Tuning

Almost all control loops in the process industry are one of the following

- Flow control loop
- Pressure control loop
- Level control loop
- Temperature control loop
- Product quality control loop

Some heuristics are discussed for tuning these loops that reflect common industrial practice. Depending on the application, exceptions to these heuristics are always possible.

2.5.1. Flow Loops

Flow is usually controlled using a PI controller. The signal from the flow sensor is noisy due to turbulent flow so that a large proportional band (about 150%) is used. A small reset time (10-20s) is used for good set-point tracking.

2.5.2. Level Loops

Most liquid levels provide surge capacity for filtering out flow disturbances. For example, the reflux drum in a distillation column allows for the reflux into the column to be held constant even as the vapour condensation rate and distillate rate vary. If the drum is not provided, the reflux into the column would fluctuate unnecessarily disturbing the column. The reflux drum thus acts as a surge capacity. In order to filter out flow disturbances, the level should be controlled loosely. The control objective is to maintain the liquid level within acceptable limits. Accordingly, a P controller is used for level control. A proportional band of 50% is commonly used so that the valve fully closes / opens for a 25% change in the level assuming the valve is initially 50% open. Note the use of PI controllers for level control of surge capacities is not recommended as a change in the inlet (outlet) flow would require that the outlet (inlet) flow increase above (decrease below) the inlet flow before becoming equal to the inlet flow in order to bring the level back to its set-point (zero offset). The flow disturbance thus gets magnified downstream (upstream). This magnification would only worsen for a series of interconnected units defeating the very purpose of providing surge capacity for attenuating flow disturbances. There are, of course, exceptions where tight level control is desired. For example, the level in a CSTR should be controlled tightly to maintain the residence time.

2.5.3. Pressure Loops

The dynamics of pressure in a can be very fast (flow like) or slow (level like) depending on the process system. For example, the pressure dynamics are extremely fast for a valve throttling the vapour outlet line from a tank. On the other hand, the dynamics are slow for the cooling water flow adjusting the pressure in a condenser due to the heat transfer and water flow lag. PI controllers are usually used for pressure loops with a small proportional band (10-20%) and integral time (0.2-2 mins) for tight pressure control. Tight pressure control is usually desired in most processing situations. For example, in distillation columns, the pressure must be controlled tightly as large pressure deviations would require compensation of the temperature controller set-points that ensure inferential product quality control. Similarly, most gas phase reactors are designed for near maximum pressure operation for maximum reaction rates so that large pressure deviations are not acceptable.

2.5.4. Temperature Loops

Temperature loops are moderately slow due to sensor lags and heat transfer lags. PI and PID controllers are often used. In most processing situations, tight temperature control is desired so that the proportional band is low (2-20%). The integral time is usually set to about the same value as the process time constant. In situations where derivative action is used for faster closed loop response, the derivative time constant is set to about one-fourth the process time constant or less depending on the transmitter signal noise.

2.5.5. Quality Loops

Composition control loops are usually applied for maintaining the product quality. In terms of relative importance, these loops are probably the most crucial for process profitability. If the product quality shows large variability, the process must be operated at a mean product quality that is significantly better than the quality specification to ensure the production of on-spec or better quality product all the time. This results in a quality giveaway adversely affecting the process profitability. The quality giveaway can be reduced by ensuring tight product quality control. The concept of quality give-away is illustrated in Figure 2.7.

Typical composition measurements involve large dead-times or lags. For example the dead-time introduced by a gas-chromatograph can vary from a few minutes to an hour. Some compositions may be measured once a shift or once a day through laborious analytical measurements. Of all the measurements, analytical composition measurements are the most expensive and unreliable. The product specifications increasingly require the measurement of ppm / ppb levels of trace impurities so that a logarithmic scale is more appropriate in many situations. Product quality measurements are typically used to make small / incremental adjustments in the set-point of a loop. The frequency of the changes may vary from once a day to once every hour etc. Whenever PID controllers are applicable, a large proportional band is used (100-2000%). A large reset time (0.1 – 2 hrs) must be used due to the lag introduced by the composition measurement as well as the usually slow process dynamics.

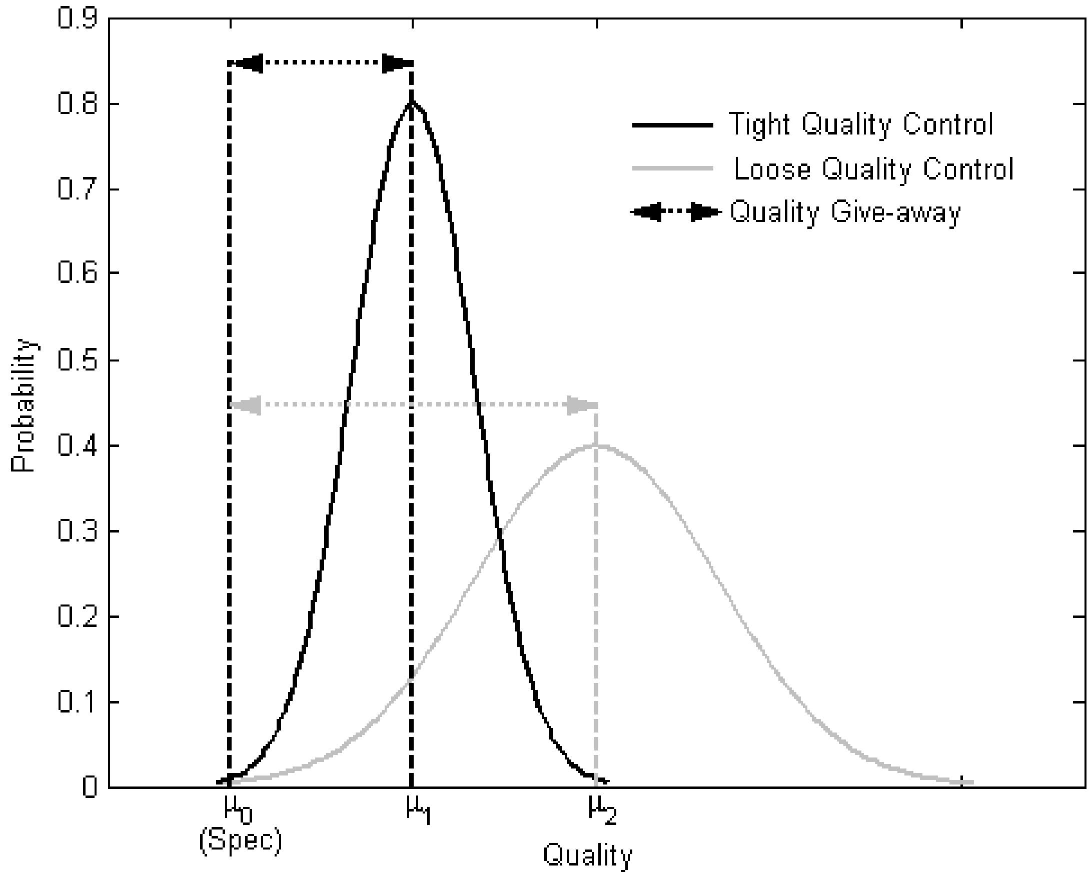


Figure 2.7. The concept of quality give-away

Chapter 3. Advanced Control Structures

The feedback control loop, discussed at length, forms the backbone of control systems applied in the process industry. Some typical feedback control loops are schematically illustrated in Figure 3.1. Over the years, enhancements to the basic feedback control structure that lead to significant improvement in control performance, have been developed. These advanced control structures include ratio control, cascade control, feed-forward control, over-ride control and valve positioning control and are briefly described in the following.

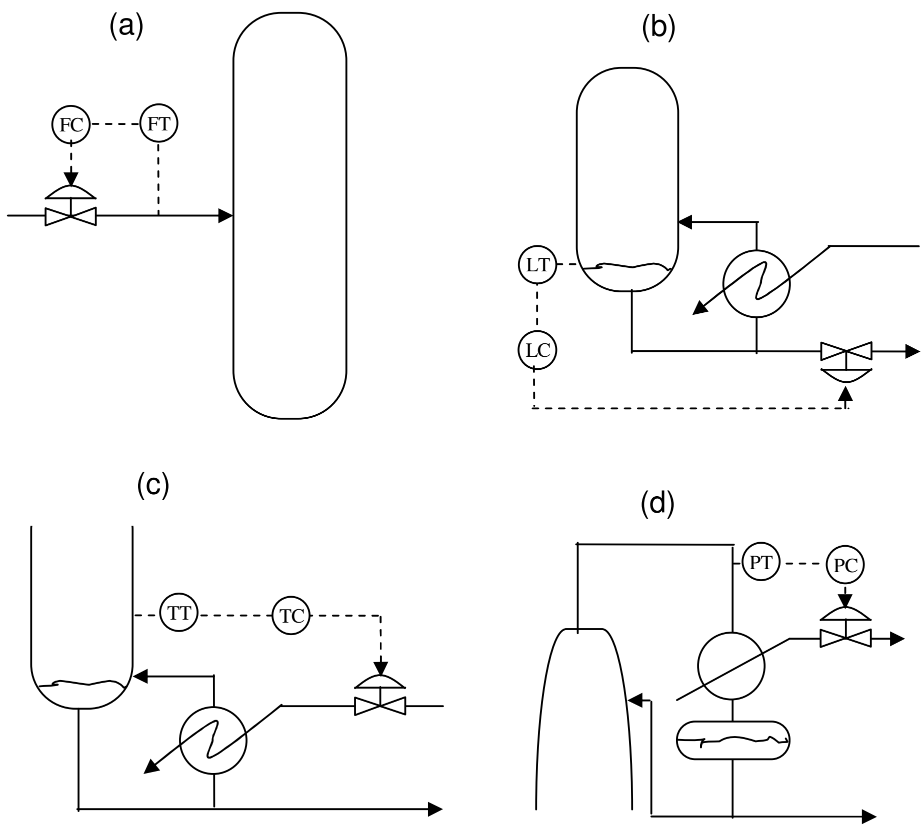


Figure. 3.1. Typical feed back control schemes commonly employed in distillation columns. (a) Feed flow control, (b) Level control in reboiler drum using bottoms flow, (c) Tray temperature control using reboiler duty and (d) Column pressure control using condenser duty.

3.1. Ratio Control

Ratio control, as the name suggests, is used for maintaining the ratio between two streams. The independent stream is referred to as the wild stream. The ratio controller adjusts the flow of the other stream to keep it in ratio to the wild stream. The implementation of ratio control is illustrated in Figure 3.2. The wild stream flow measurement is multiplied by the ratio set-point to obtain the flow set-point for the manipulated stream. The calculated flow set-point is input to the flow controller on the manipulated stream. Ratio control is implemented as a feed-forward strategy (to be discussed later) where two flows are increased in tandem so that the change in the wild stream is compensated for before it affects the process output. For example, if the feed flow rate into a distillation column increases by 10%, the reboiler duty necessary to maintain the same separation should also increase by about 10%. It therefore makes sense to ratio the reboiler duty to the fresh feed rate so that the necessary change in the reboiler duty is implemented apriori. This leads to tighter product purity control with the change in the feed rate causing only small deviations in the product purity.

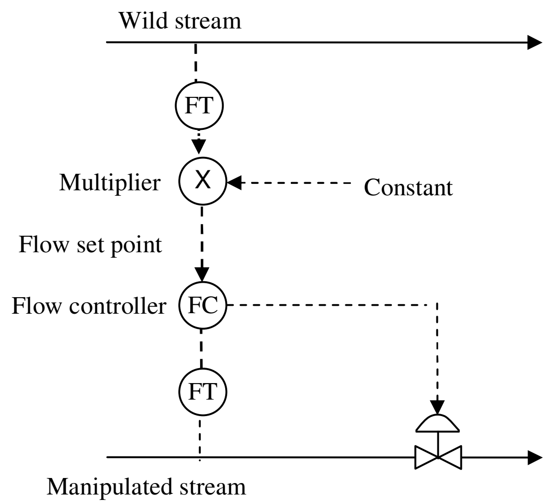


Figure. 3.2. Implementation of ratio control.

3.2. Cascade Control

Cascade control is arguably one of the most useful concepts in chemical process control. The cascade control scheme consists of two control loops, namely the master loop and the slave loop, with the master loop setting the set-point for the slave loop. The concept is best illustrated by an example. Consider a jacketed CSTR where cooling water is recirculated in the jacket to remove the exothermic reaction heat. The typical feedback reactor temperature control scheme and the cascade reactor temperature control scheme is shown in Figure 3.3. In the feedback arrangement, the reactor temperature controller directly adjusts the cooling water valve to maintain the reactor temperature at set-point. In the cascade arrangement, a slave loop is introduced that controls the jacket temperature by manipulating the cooling water valve. The master reactor temperature loop adjusts the jacket temperature set-point.

At first glance, the advantage of cascade arrangement over simple feedback control is not very obvious. To appreciate the same, consider an increase in the coolant temperature as an input disturbance. In the simple feedback scheme, the reactor temperature must rise before the controller opens the cooling water valve to bring the reactor temperature back to set-point. In the cascade control scheme, the jacket temperature controller senses the increase in the cooling water temperature and adjusts the cooling water valve to maintain the jacket temperature. The reactor temperature would thus show comparatively much smaller / negligible deviations from set-point. The slave controller acts to remove local disturbances into the process and prevents its effect on the primary controlled variable. Another subtle advantage is that the slave controller compensates for the non-linearity in the slave loop so that the master controller ‘sees’ a more linear system. In the current example, the non-linear characteristics of the cooling water valve are compensated for by the slave controller. Since the slave loop has much faster dynamics than the master loop (else the cascade arrangement is infeasible), the master loop does not have to compensate for the valve non-linearity. It therefore sees a less non-linear system compared to simple feedback control resulting in improved control performance. The improvement is however at the expense of installing, tuning and maintaining an additional slave controller.

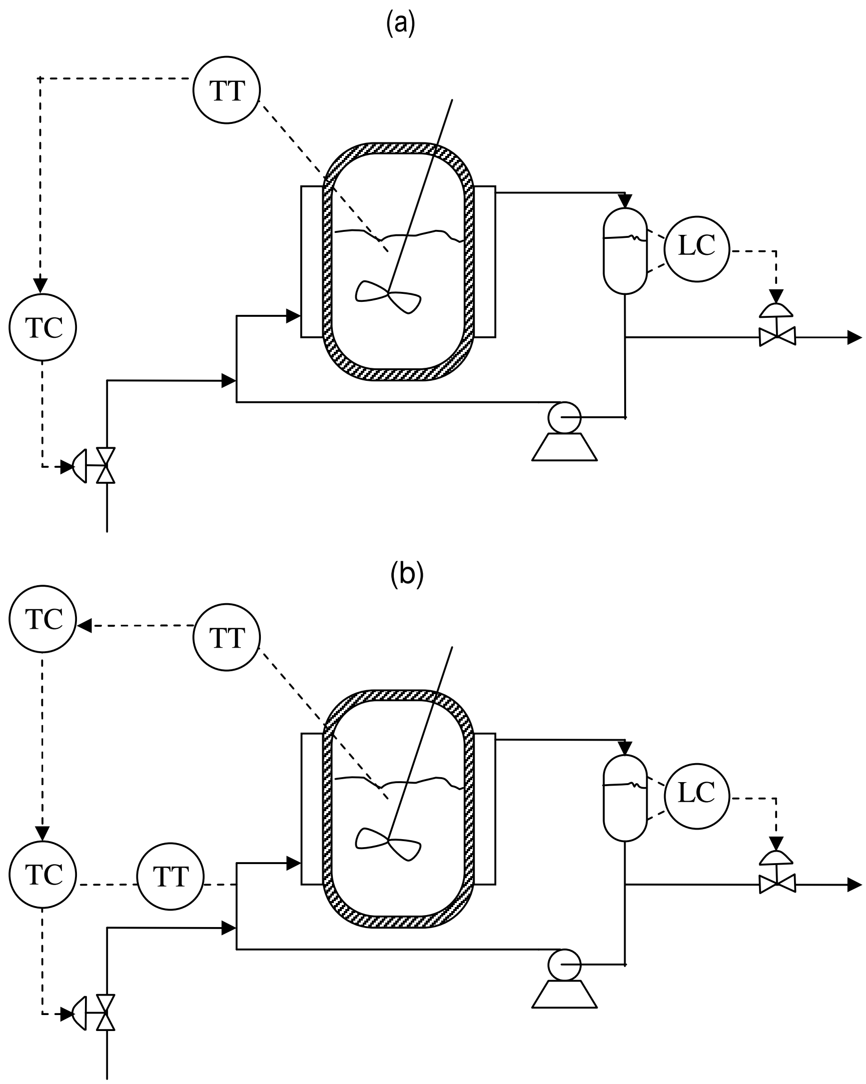


Figure 3.3. Temperature control of an exothermic CSTR. (a) the typical feedback reactor temperature control scheme and (b) the cascade reactor temperature control scheme.

To tune a cascade control structure, the slave loop is first tuned with the master loop in manual. P only controllers with a small proportional band (large controller gain) are commonly used in the slave loop for a fast response to a set-point change from the master controller. Integral action is usually not applied in the slave loop as an offset in the secondary measurement is acceptable. The tuned slave loop is then put on automatic and the master loop is tuned. Note that for the cascade control system to be stable, the dynamics of the slave loop should be much faster than the master loop allowing the slave loop to keep-up with the set-point changes received from the master loop. A typical rule of thumb is that the time constant for the master loop should be more than thrice that of the slave loop.

Cascade control loops are quite common in the process industry. Some common configurations are shown in Figure 3.4. The interpretation of these configurations is left as an exercise to the reader.

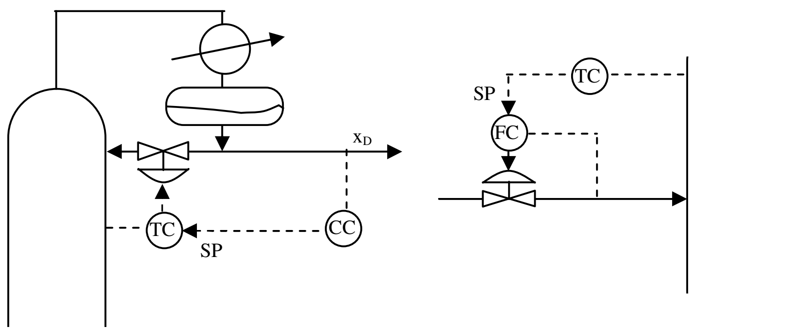


Figure 3.4. Some typical cascade arrangements

3.3. Feed-forward Control

The concept of feed-forward control has already been alluded to earlier. If a measured disturbance enters a process, the control input can be adjusted to compensate for effect of the disturbance on the output. Perfect compensation would cause the controlled output to show no deviations from its set-point even as a disturbance has entered the process. This apriori compensation to mitigate the transient effect of a measured disturbance on the controlled output is referred to as feed-forward control. A very simple example of feed-forward control is driving a car. Adjusting the hot and cold water knobs for the right temperature water from the shower is an example of feedback control. As discussed previously, ratio control compensates for disturbances in a feed-forward manner.

The design of a feed-forward compensator is illustrated using block diagrams in Figure 3.5. G_d represents the disturbance to output transfer function while G_p represents the control input to output transfer function. The control input u must be varied such that

$$G_p.u + G_d.d = 0$$

The control input is adjusted by the feed-forward compensator with the transfer function G_{ff} so that

$$u = G_{ff}.d.$$

Substituting into the previous equation and solving for G_{ff} gives the feed-forward compensator design as

$$G_{ff} = -G_d/G_p$$

Assuming that G_d and G_p are first order plus dead time transfer function, the feed-forward compensator is then a lead-lag plus dead time transfer function. Modern DCS allow lead-lag plus dead time blocks to be configured into the control system.

For a better appreciation of the improvement in control performance using feed-forward compensation, consider a very simple example where

$$G_d = 1/(s+1)$$

and $$G_p = 1/(5s+1)$$

Then $$G_{ff} = -(5s+1)/(s+1)$$

Figure 3.6. plots the simulated transient output response for a unit step change in the measured disturbance with and without feed-forward compensation.
Since there is no plant-model mismatch, perfect feed-forward compensation is observed with the output showing no deviations from set-point. In a real-life scenario, the presence of a plant-model mismatch may cause small transient deviations. The feed-back controller compensates for these small deviations resulting in an overall tighter closed loop response.

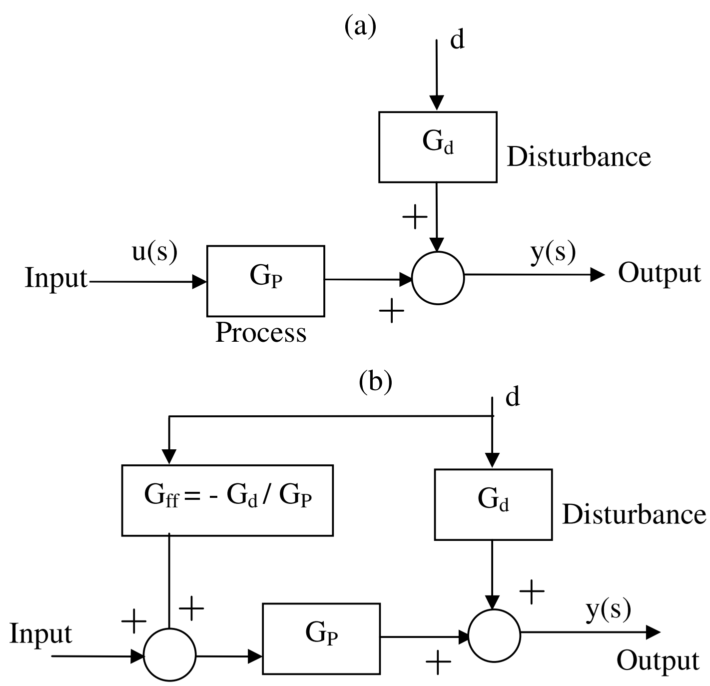


Figure 3.5. Design of feed forward compensator. (a) Process and (b) process with feed forward compensator.

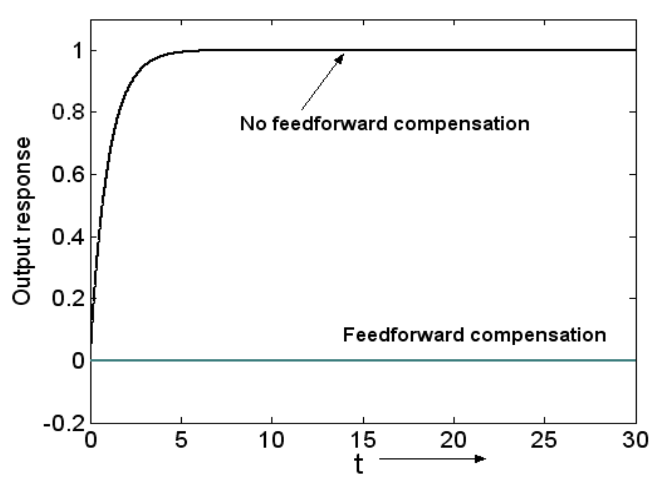


Figure.3.6. Deviation in the output with and without feed forward action

3.4. Override Control

Over-ride control is employed to ensure that an unsafe condition does not arise during process operation. As the name suggests, an over-ride controller over-rides the output of another controller as an unsafe condition develops and acts to move the process away from the unsafe condition. This is an example of multivariable control where the same manipulated variable can be adjusted at any time by one of many controlled variables. An example best illustrates the concept of over-ride or selective control. Consider the bottom section of a distillation column. The bottom sump level is controlled by the bottoms flow rate. During normal operation, the steam rate into the reboiler is manipulated to control a tray temperature. During severe transients, a situation may arise where the bottoms level is low and continues to fall even as the bottoms flow rate is zero. An unsafe situation can arise with the reboiler tubes getting exposed to vapour and fouling. Also, the bottoms pump may lose suction as the reboiler dries up. A sensible operator would put the temperature loop on manual and cut back on the steam rate to ensure the reboiler tubes remain submerged. In effect, the temperature controller output, the signal to the steam valve, gets over-ridden to maintain the liquid level. The over-ride controller automates this action as shown in Figure 3.7. The base level signal is input to a multiplier. A multiplier value of 5 is used so that if the level is above 20%, the multiplier output is above 100%. As the level decreases below 20%, the multiplier output decreases below 100%. If the level continues to decrease, the multiplier output would eventually decrease below the temperature controller output. The low select would then pass on the multiplier signal to the steam valve over-riding the temperature controller. The steam rate would thus decrease. Once the level begins to rise, the multiplier output would increase above the temperature controller output so that the low select would pass the manipulation of the steam valve back to the temperature controller. In addition to the level over-ride controller, the low select may also receive signals from a pressure over-ride controller or a

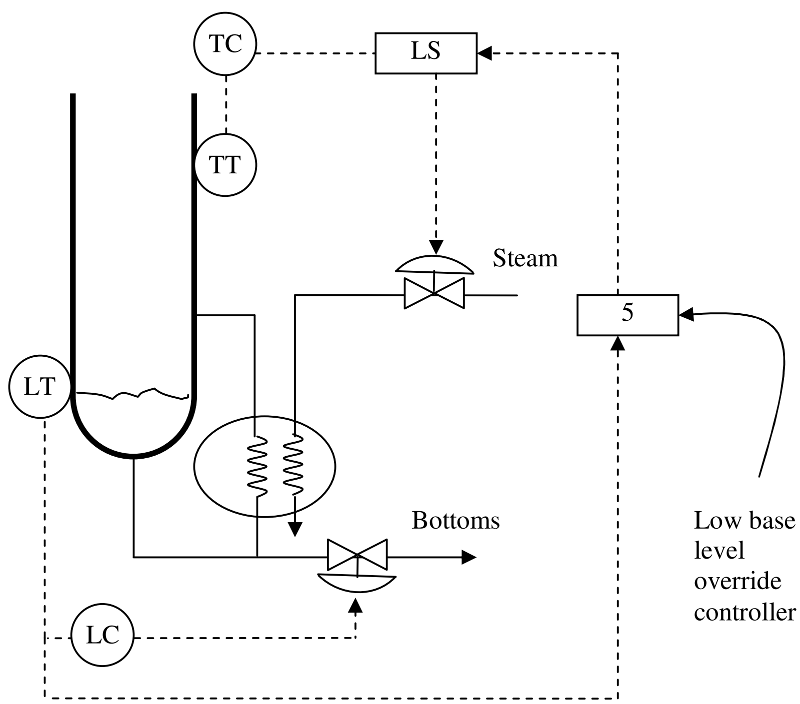


Fig. 3.7. Override control scheme

temperature over-ride controller to reduce the steam flow rate. Pressure over-ride would be needed if the column pressure goes too high. Similarly temperature over-ride may be necessary if the base temperature goes too high.

In temperature or pressure over-rides, a PI controller is needed unlike the P only controller for a level over-ride. This is because a pressure / temperature over-ride is needed only for a very small range of the total transmitter span. A very large proportional gain would then be necessary which can destabilize the closed loop system. Therefore a PI controller with lower gain and fast reset action is used to achieve the tightest control possible.

3.5. Valve Positioning (Optimizing) Control

Valve positioning control was originally proposed by Shinskey as an effective way of minimizing the energy consumption in distillation columns. The pressure in a distillation column is set by the condenser cooling duty. For a given separation, as the column pressure increases, more stages are needed as the x-y VLE plot moves towards the 45 degree line as shown in Figure 3.8. Translated to process operation, the same separation can be achieved at lower reboil as the column operating pressure is reduced. To minimize energy consumption, the column should be operated at lowest possible pressure corresponding to the maximum condenser duty. This can be accomplished by the valve positioning control scheme as illustrated Figure 3.9. The column pressure is typically controlled by adjusting the condenser cooling water valve. The VPC controller takes in the pressure controller output signal and adjusts the pressure set-point. If the valve is not nearly open, the controller reduces the column pressure set-point so that the pressure controller increases the cooling duty to reduce the column pressure. The VPC controller thus ensures that any underutilized cooling capacity is exploited to reduce the column operating pressure. The column pressure thus floats with the condenser duty being near maximum. The VPC controller is tuned to be slow with the fast pressure controller rejecting any pressure disturbances.

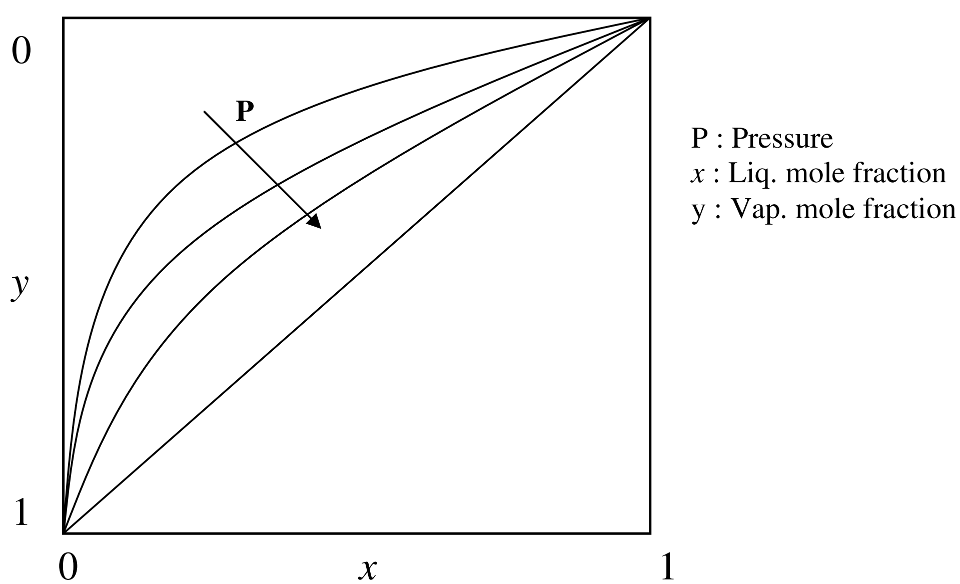


Figure 3.8. Typical x-y diagram with varying Pressures

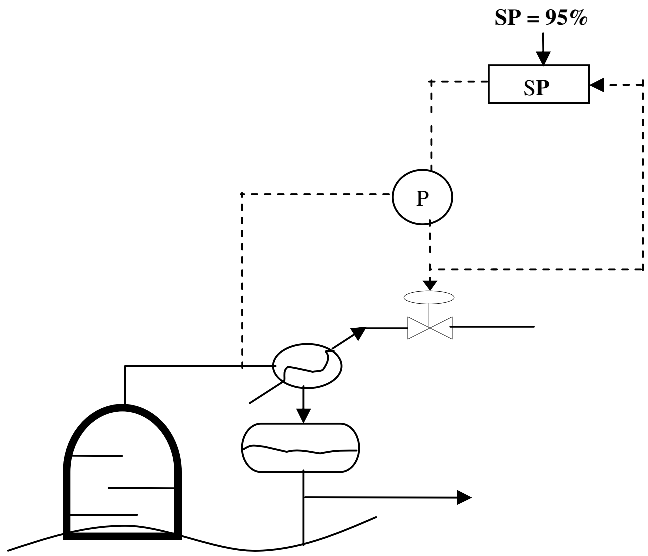


Figure 3.9.Valve positioning control

Another simple VPC application is shown in Figure 3.10. Let us say a high capacity variable speed pump is providing feed to N parallel trains of processes. We would like to minimize the pump electricity consumption while ensuring the desired flow setpoints for each of the parallel trains is achieved. The electricity consumption gets minimized by running the pump at as low an rpm as possible. This gets achieved by ensuring that the most open process feed valve is nearly fully open. The high select passes the position of the most open valve. A valve position below the nearly fully open VPC setpoint (say 80%) indicates unnecessary valve throttling. The VPC then reduces the pump rpm. In response, the flow controllers would open the valves to maintain the flow. The VPC reduces the pump rpm till the most open valve position reaches the VPC setpoint (80%) ensuring the pump operates at as low an rpm as possible while maintaining the desired flow to each of the parallel trains.

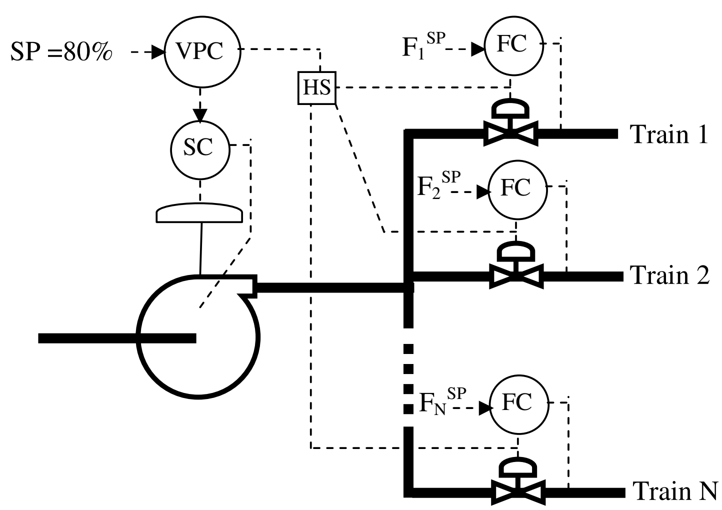


Figure. 3.10. VPC for minimizing variable speed pump electricity

Chapter 4. Multivariable Systems

Single input single output (SISO) systems have been treated till now. Most practical control system design problems are multivariable in nature with multiple inputs multiple outputs (MIMO). A 2 X 2 multivariable system is shown in Figure 4.1. There are two inputs, u_1 and u_2 and two outputs y_1 and y_2. In the most general case, a step change in an input causes a transient response in both the outputs. The input output relationship may be compactly represented in matrix notation as

$$\begin{bmatrix} y_1(s) \\ y_2(s) \end{bmatrix} = \begin{bmatrix} G_{11}(s) & G_{12}(s) \\ G_{21}(s) & G_{22}(s) \end{bmatrix} \begin{bmatrix} u_1(s) \\ u_2(s) \end{bmatrix}$$

and the corresponding block diagram is shown in Figure 4.1.

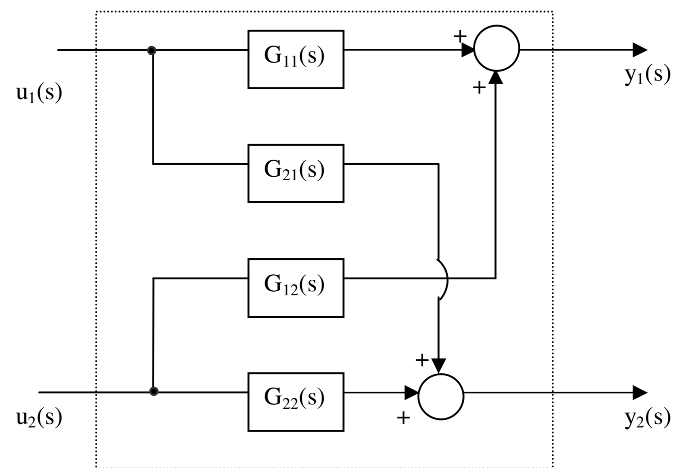


Figure 4.1. A block diagram of a 2 X 2 multi variable system

In general, G_{ij} denotes the transfer function between the j^{th} input and the i^{th} output. The non-diagonal terms with $i \neq j$ are the interaction terms. The simplest way of controlling a multivariable process is to control each of the outputs by manipulating an input using a PID controller. This is referred to as multivariable decentralized control and is illustrated in Figure 4.2. for the example 2x2 system. Controller 1 manipulates u_1 to maintain y_1 and controller 2 adjusts u_2 to maintain y_2.

In the design of a multivariable decentralized control system, choice exists as to which manipulated variable is used to control an output. For the 2x2 example, there are a total of two control structures with y_1 being controlled by u_1 or u_2. The number of such possibilities grows exponentially as the number of inputs / outputs increase. In the most general sense, the design of a plant-wide decentralized control system for a complex chemical process is a multivariable problem of high order. The high order problem is naturally broken down into smaller process unit specific controller design problems and controller design for managing plant-wide issues such as inventory balancing. A high order unit specific controller design problem can also be further broken down into a smaller subset of fast loops and slow loops based on the process dynamics. An example is the simplification of the 5x5 controller design problem for a simple distillation column into a 2x2 problem. In a distillation column, the pressure, reflux drum and bottom levels and two temperatures (or compositions) may be controlled. Since the tray temperature dynamics are significantly slower than the pressure /

level dynamics, SISO controllers are applied for the latter reducing the 5x5 problem into a 2x2 design problem for the two temperature controllers. Any complex high order control system design problem can thus be simplified into subsets of simple SISO, 2x2 or in the worst case 3x3 decentralized control system design problems. A systematic unit specific and plant-wide control system design methodology for complete chemical plants will be developed in the subsequent chapters.

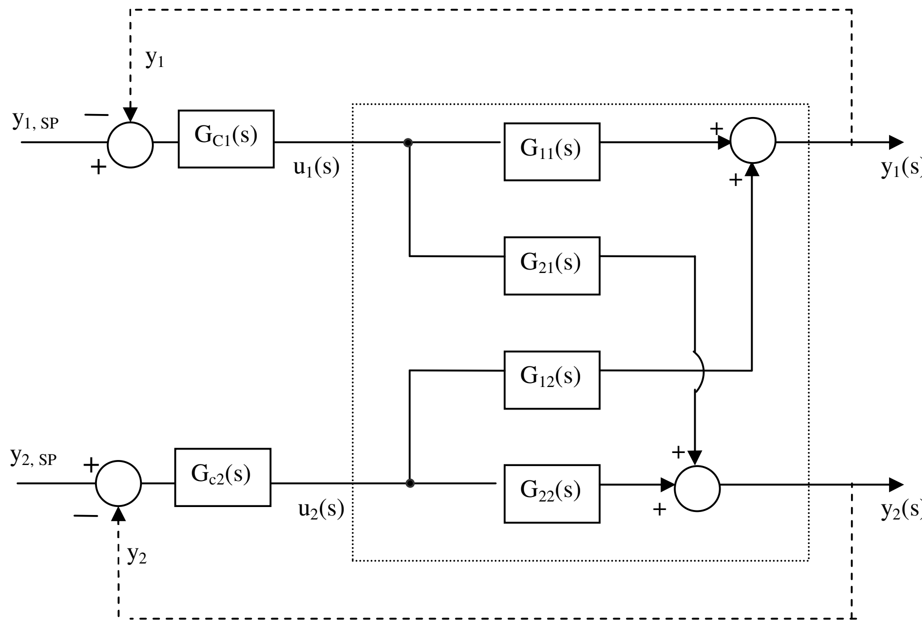


Figure 4.2. Block diagram of a multivariable decentralized control for a 2X2 system

4.1. Interaction Metrics

The selection of the input-output pairing in a decentralized control system is usually made based on engineering considerations which shall be covered in greater detail in subsequent chapters. The individual controllers in a decentralized control system may need to be detuned in order to maintain process stability. This is because the interaction between the loops during closed loop operation can lead to instability. The magnitude of interaction depends on the aggressiveness of the individual controller tunings employed. Detuning or less aggressive tuning mitigates the interaction to ensure closed loop stability. The Niederlinski Index and Relative Gain Array are two commonly used quantitative measures of interaction between control loops. Both are based on the open-loop steady state gain matrix $\mathbf{K_P}$, where

$$\mathbf{y} = \mathbf{K_P}\,\mathbf{u}$$

4.1.1. Niederlinski Index

The Niederlinski Index for a control structure where the i^{th} input is used to control the i^{th} output is then defined as

$$NI = \frac{|K_P|}{\prod_i K_{ii}}$$

The NI for any control structure can thus be obtained through appropriate relabeling of the outputs and inputs so that the i^{th} input controls the i^{th} output. If the Niederlinski Index is negative, the closed loop system is guaranteed to be integral closed loop unstable. If the NI is positive, the closed loop system may or may not be stable. In other words, the criteria NI>0 is a necessary but not sufficient condition for closed loop stability. Input-output pairings with small positive or large positive (>>1) NI values indicate ill-conditioning problems and should be avoided. Control structures with NI close to 1 indicate favourable interaction. For example, an NI value of 1 for a 2X2 system indicates that either K_{12} or K_{21} or both are zero implying one-way or no steady state interaction between the loops. The primary use Niederlinski Index is for rejecting unworkable control structures.

4.1.2. Relative Gain Array

The relative gain is another popular metric that measures the interaction of a control loop with other loops as the ratio of the steady state process gain the controller sees with all other loops off to the process gain with all other loops on (all other outputs at their set-points). Mathematically, if the i^{th} output is controlled by the j^{th} input, its relative gain is defined as

$$\lambda_{ij} = \frac{\left(\frac{\partial y_i}{\partial u_j}\right)_{u_k = constant, k \neq j}}{\left(\frac{\partial y_i}{\partial u_j}\right)_{y_k = constant, k \neq i}}$$

If the relative gain is negative, the i^{th} output should not be paired with the j^{th} input as the process gain sign would change depending on whether the other loops are on automatic or manual mode. Input-output pairings with relative gain close to 1 may be preferred as the process gain the controller sees is independent of the state of the other loops. The relative gain array is obtained as i and j are varied for respectively all outputs and inputs.

The relative gain array is an effective tool for input-output pairing when the primary control objective is set-point tracking. For set-point tracking, lower interaction between the loops increases the degree of independence of the different control loops so that each can be separately tuned for tight set-point tracking. Interaction is thus undesirable for set-point tracking. For load disturbance rejection, interaction is not necessarily undesirable and may actually favour disturbance rejection. This was demonstrated in an early article by Niederlinski (1971). Since the primary objective in chemical process control is load rejection, the application of RGA for control structure selection makes little sense. Candidate control structures should be proposed based on engineering considerations and unworkable structures further eliminated using the Niederlinski Index. The same arguments can be applied to recommend the use of dynamic decouplers only when the primary control objective is set-point tracking. Dynamic decoupling is not covered here as load rejection is the primary control objective in chemical process control systems.

4.2. Multivariable Decentralized Control

Consider the 2x2 multivariable open loop system in Figure 4.1. We would like to hold both the outputs at their respective setpoints. The simplest way to do it is to implement individual PI controllers for y_1 and y_2. Without loss of generality, let us assume that y_1 is paired with u_1 and y_2 is paired with u_2. The multivariable control system is shown in Figure 4.2. Notice that even as u_1 and u_2 affect both y_1 and y_2 through the interaction transfer functions G_{12} and G_{21}, the adjustment made to u_1 is based purely on e_1 and the adjustment made to u_2 is based purely on e_2. In other words, the y_1 controller moves are based purely on y_1 and does not consider the effect of the control moves made by the y_2 controller. Similarly, the y_2 controller moves are based purely on y_2 and does not consider the effect of control moves made by the y_1 controller. Thus even as the actual system is multivariable, the individual controllers do not take the interaction into consideration. This is referred to as decentralized control.

For the decentralized control system, notice that the interaction terms introduce an additional feedback path as shown in blue in Figure 4.3. This additional feedback tends to further destabilize the closed multivariable control system. If each controller is tuned individually with the other controller on manual (other loop is open) and the Zeigler Nichols tunings applied, then when both the loops are closed, the system response is likely to be highly oscillatory and may even be unstable due to the additional feedback path. In the individual tuning of the controllers, since the other loop is open, this additional feedback path is inactive and therefore not accounted for in the determination of the tuning parameters. Clearly the individual ZN tuning parameters need to be detuned due to the additional feedback path to ensure the overall closed loop response is sufficiently away from instability.

4.2.1. Detuning Multivariable Decentralized Controllers

The obvious next question is that how does one tune a decentralized multivariable controller. Typically, in practical settings, tight control of one of the outputs is much more important than the other. A sequential tuning procedure can then be applied, where the more important output controller is tuned individually so that we get the tightest possible controller tuning. The less important output controller is then tuned with the other loop on automatic. Since the other loop is on, the additional feedback path is active and the necessary detuning due to the same gets accounted for in the tuning parameters of this less important loop. This sequential tuning procedure thus gives the tightest possible control of the more important output at the expense of a highly detuned controller for the less important output. The sequential procedure can be easily extended to more than 2 outputs when the prioritization of the controlled outputs is clear.

There are however situations where the need for tight control of each of the outputs is comparable. The detuning due to multivariable interaction then needs to be taken in all the loops. How does one systematically go about the detuning. For the 2x2 multivariable system, we have for the open loop system

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

or more simply

$$\boldsymbol{y} = \boldsymbol{G_P}\, \boldsymbol{u}$$

where G_P is the open loop process transfer function matrix. For a decentralized controller, we have

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} G_{C1} & 0 \\ 0 & G_{C2} \end{bmatrix} \begin{bmatrix} y_1^{SP} - y_1 \\ y_2^{SP} - y_2 \end{bmatrix}$$

or in matrix notation

$$\boldsymbol{u = G_C (y^{SP} - y)}$$

where the controller matrix, G_C, is diagonal for decentralized control. Combining the above two matrix equations, we get

$$\boldsymbol{y = G_P G_C (y^{SP} - y)}$$

or $$\boldsymbol{(I + G_P G_C) y = G_P G_C y^{SP}}$$

or $$\boldsymbol{y = (I + G_P G_C)^{-1} G_P G_C y^{SP}}$$

This is the multivariable closed loop servo response equation and its analogy with SISO systems is self evident. Each element of the $\boldsymbol{(I + G_P G_C)^{-1}}$ matrix would have $\det(\boldsymbol{I + G_P G_C})$ as its denominator. The closed loop multivariable characteristic equation is then

$$\det(\boldsymbol{I + G_P G_C}) = 0$$

Similar to SISO systems, if any of the roots of the multivariable characteristic equation is in the right half plane, the closed loop multivariable system is unstable.

To systematically detune the controllers, an empirical analogy with the Nyquist stability criterion for SISO systems is used. For a SISO system, the closed loop servo response equation is

$$y = [G_P G_C/(1 + G_P G_C)]\, y^{SP}$$

where G_P is the open loop transfer function and G_C is the controller transfer function. The Nyquist stability criterion then guarantees stability for the closed loops system if the polar plot of the open loop transfer function between y^{SP} and y, ie G_PG_C, does not encircle (-1, 0). Gain margin and phase margin are criteria that are commonly used to quantify the distance from (-1, 0) at a particular frequency. To ensure that the distance from (-1, 0) is sufficient at all frequencies, the 2 dB closed loop maximum log modulus criterion is often used, where the closed loop log modulus is defined as

$$L_{CL}(\omega) = 20 \log|G_PG_C / (1+G_PG_C)|_{s=j\omega}$$

L_{CL} is calculated by putting $s = j\omega$ in the transfer functions, G_P and G_C, and is therefore a function of ω. The SISO PI tuning parameters (K_C and τ_I) are chosen such that the maximum closed loop log modulus (with respect to ω) is 2dB. This ensures that the closed loop servo response is fast and not-too-oscillatory.

To develop a closed loop maximum log modulus criterion for multivariable systems, we note that the SISO closed loop characteristic equation is

$$1 + G_PG_C = 0$$

and the transfer function whose polar plot is used to see encirclements of (-1,0) is then

$$-1 + (1+G_PG_C)$$

ie -1 + closed loop characteristic equation

For a multivariable system, we then define by analogy

$$W = -1 + \det(\boldsymbol{I + G_P G_C})$$

where W is -1 + closed loop characteristic equation. The multivariable closed loop log modulus (L_{MVCL}) is then defined as

$$L_{MVCL} = 20 \log|W/(1+W)|.$$

The tuning parameters for the individual controllers should be chosen such that

$$L_{MVCL}^{MAX} = 2\, N_C$$

where N_C is the number of loops.

A simple algorithm for systematic detuning of the individual controller for the 2x2 decentralized control system is then:

1. Obtain individual ZN tuning parameters, $(K_{C1}^{ZN}, \tau_{I1}^{ZN})$ and $(K_{C2}^{ZN}, \tau_{I2}^{ZN})$, for each loop.
2. Detune the individual tuning parameters by a factor f ($f > 1$) to get the revised tuning parameters as $(K_{C1}^{ZN}/f, f.\tau_{I1}^{ZN})$ and $(K_{C2}^{ZN}/f, f.\tau_{I2}^{ZN})$
3. Adjust f such that $L_{MVCL}^{MAX} = 4$ dB.

The above procedure can be easily extended to an NxN (N > 2) decentralized control system.

As a parting thought, we re-emphasize that in chemical processes, the dominant time constants of different loops can differ by up to two orders of magnitudes. Thus for example, the residence time of a surge drum may be ~5 minutes while it may take 2-5 hrs for transients caused by a change in its setpoint to reach back after passing through the different downstream units, the material recycle and the upstream units. Similarly, on a distillation column, while the column pressure time constant with respect to condenser duty is ~1 min and the reflux drum / bottom sump level residence times are ~ 5 mins, the tray temperature response times to changes in reflux / boilup rates are much slower (~15-20 mins). Thus even as the dual-ended distillation column control problem is 5x5 (2 levels, 1 pressure and 2 temperatures), the separation in time constants allows the level and pressure controllers to be tuned first followed by the two temperature controllers. The 5x5 problem thus reduces to a 2x2 problem due to the separation in time constants. In industrial practice, most high order multivariable problems reduce to 2x2 or at most 3x3 problems, which are mathematically tractable.

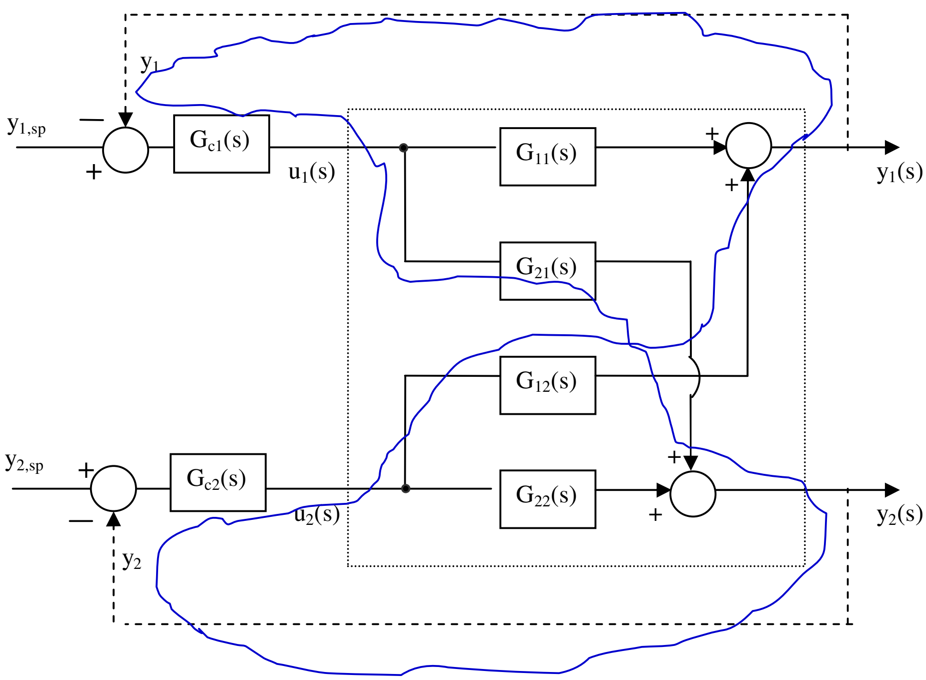


Figure 4.3. Additional feedback path due to multivariable interaction

Illustrative Example:
Consider a 2x2 openloop multivariable system

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} \dfrac{-18.9e^{-3s}}{21s+1} & \dfrac{12.8e^{-s}}{16.7s+1} \\ \dfrac{-19.4e^{-3s}}{14.4s+1} & \dfrac{6.6e^{-7s}}{10.9s+1} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

(a) Calculate its RGA. Based on the RGA, what input-output pairing would you recommend.
(b) Calculate the Niederlinski Index for the recommended pairing. What can you say about closed loop integral stability of the recommended pairing.
(c) Calculate the Niederlinki Index for the other alternative pairing (the one that is not recommended). What can you say about the closed loop integral stability of this other pairing.
(d) For the recommended pairing, design a feedforward dynamic decoupler showing its complete block diagram and also the physically realizable feedforward compensator transfer functions.

Solution:
(a) The steady state input-output relationship is

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} -18.9 & 12.8 \\ -19.4 & 6.6 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

so that the steady state gain matrix is

$$\boldsymbol{K} = \begin{bmatrix} -18.9 & 12.8 \\ -19.4 & 6.6 \end{bmatrix}$$

Inverting the matrix, we get

$$\boldsymbol{K}^{-1} = \begin{bmatrix} 0.0534 & -0.1036 \\ 0.1570 & -0.1529 \end{bmatrix}$$

The RGA is then obtained as

$$\boldsymbol{RGA} = \boldsymbol{K}.*(\boldsymbol{K}^{-1})^T$$

where the '.*' operator denotes element-by-element multiplication. Performing the necessary operations, we get

$$\boldsymbol{RGA} = \begin{bmatrix} -1.0094 & 2.0094 \\ 2.0094 & -1.0094 \end{bmatrix}$$

Notice that the row/column sum of the RGA is 1. This is a property of the RGA (can you prove it?).
Rejecting the IO pairings corresponding to the negative RGA elements, the recommended pairing based on the RGA is y_1-u_2 and y_2-u_1.

(b) The steady state IO relation for the recommended pairing is

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 12.8 & -18.9 \\ 6.6 & -19.4 \end{bmatrix} \begin{bmatrix} u_2 \\ u_1 \end{bmatrix}$$

The Niederlinski Index is then

$$NI = \frac{12.8 \times (-19.4) - 6.6 \times (-18.9)}{12.8 \times (-19.4)} = 0.4977$$

Since NI > 0 for the recommended pairing, the multivariable decentralized control system may be integrally stable.

(c) The other possible pairing is y_1-u_1 and y_2-u_2. For this pairing, the IO relation is

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} -18.9 & 12.8 \\ -19.4 & 6.6 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

The Niederlinski Index is then

$$NI = \frac{6.6 \times (-18.9) - 12.8 \times (-19.4)}{(-18.9) \times 6.6} = -0.99$$

Since the NI for this pairing is < 0, the multivariable decentralized control system is guaranteed to be integrally unstable. This pairing should therefore not be implemented.

(d) If we look at the open loop 2x2 system with the recommended pairing (y_1-u_2 and y_2-u_1), a change in u_2 affects both y_1 (its controlled variable, CV) and y_2 (other CV). Similarly, a change in u_1 affects both y_2 (its CV) and y_1 (other CV). When both the control loops are on, the adjustment made by a loop ends up disturbing the other loop. A dynamic decoupler uses feedforward compensation ideas to make appropriate adjustments in the "other" process input so that a change in a process input only affects its CV and not the other CV. The dynamic decoupler block diagram for the recommended pairing is shown in Figure 4.4. We are looking for the feedforward compensator G_I^{ff} (G_{II}^{ff}) so that a change in u_2^* (u_1^*) only affects its CV, y_1 (y_2) with no effect on the other CV y_2 (y_1).

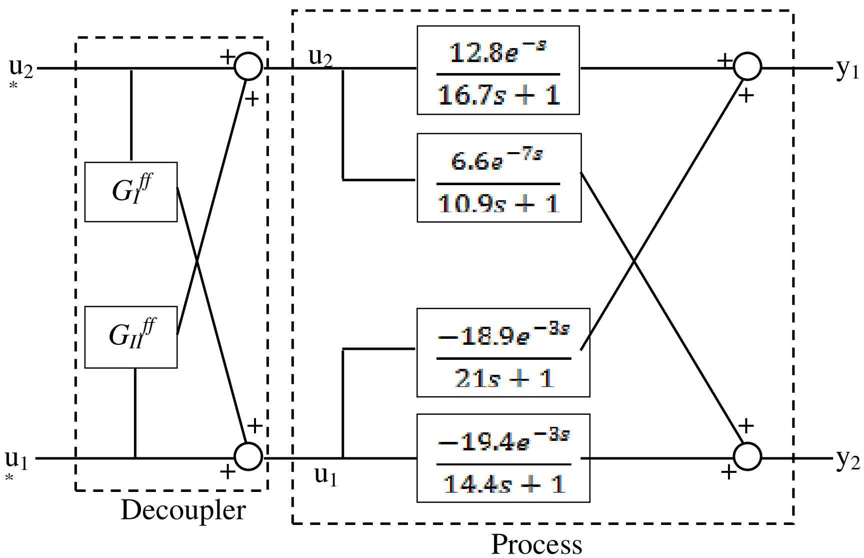


Figure 4.4. 2x2 process example with dynamic decoupler

From the block diagram, the ideal compensator G_I^{ff} would be such that

$$y_2 = G_{22}u_2^* + G_{21}G_I^{ff}u_2^* = 0$$

so that $G_I^{ff} = -G_{22}/G_{21}$

Similarly, we have $G_{II}^{ff} = -G_{11}/G_{12}$

Putting in the appropriate transfer functions, we get

$$G_I^{ff} = -\frac{\frac{6.6e^{-7s}}{10.9s+1}}{\frac{-19.4e^{-3s}}{14.4s+1}} = 0.3402\frac{14.4s+1}{10.9s+1}e^{-4s}$$

$$G_{II}^{ff} = -\frac{\frac{-18.9e^{-3s}}{21s+1}}{\frac{12.8e^{-s}}{16.7s+1}} = 1.4766\frac{16.7s+1}{21s+1}e^{-2s}$$

The feedforward compensators consist of a gain, a lead-lag and a deadtime. In some cases, it is possible that we get an exponential term of form e^{+Ds} ($D > 0$) implying a negative deadtime. This means that a change in the causal variable leads to a change in the effected variable in the past, which is impossible. The term e^{+Ds} is then physically unrealizable and dropped from the compensator.

MODULE II

CONTROL OF COMMON UNIT OPERATIONS

Having covered the essential aspects of control theory, in this module we consider control systems as applied to common unit operations in the process industry. We thus treat simple and complex distillation configurations (including heat integrated sequences), reactors, heat exchangers and miscellaneous systems such as furnaces, compressors, refrigeration cycles and boiler houses. Several of the examples shown here can be found in "Plantwide Process Control" by Luyben, Tyreus and Luyben (McGraw Hill, 1998) and "Process Control Systems" by Shinskey (McGraw Hill, 1996). We have attempted to present these examples afresh in the hope that readers readily assimilate the concepts.

Chapter 5. Control of Distillation Systems

5.1. Distillation Basics

Distillation is unarguably the most preferred unit operation used for separating mixtures. In the design of chemical processes, other separation techniques are considered only if distillation is found to be economically unviable. It is thus not surprising that the final product stream from a plant is typically a product steam from a distillation column. This Chapter provides guidelines for designing effective control systems for distillation columns.

5.1.1. The Simple Distillation Column

A proper understanding of the basic physics of a distillation column (or any other process for that matter) is a pre-requisite for designing an effective control system. Figure 5.1 shows the schematic of a simple distillation column along with the control valves. It consists of a tray section, a condenser, a reflux drum and a reboiler. The feed mixture is fed on a feed tray. The trays above the feed tray constitute the rectifying / enriching section and those below constitute the stripping section. The overhead distillate and the bottoms are the two product streams from a simple distillation column. Steam is typically used to provide vapour reboil into the stripping section. The liquid reflux into the enriching section is provided by the condenser. Cooling water is commonly used as the coolant in the condenser. The condenser may be a total condenser, where all the vapour is condensed, or a partial condenser where only a part of the vapour is condensed. The overhead distillate is a liquid stream for a total condenser. A partial condenser column may be operated at total reflux where all the liquid is refluxed back into the column and the distillate stream is a vapour stream. Alternatively (and more commonly) both a vapour and a liquid distillate stream are drawn. The reflux drum provides surge capacity to adjust the reflux and distillate rate during transients. The bottom sump provides the surge capacity for adjusting the bottoms and steam rate.

The vapour generated when a volatile liquid feed mixture is boiled is richer in the more volatile component. The remaining liquid is then richer in the heavier components. Chemical engineers refer to this as flashing a mixture. If the flashed vapour is condensed and partially vaporized again, the vapour from the second flash would be further enriched in the volatiles (light boilers). Similarly, if the liquid from the first flash is further vaporized, the heavies composition of the liquid from the second flash would increase. Theoretically speaking, a sufficiently large number of flash operations on the vapour can result in a final vapour stream that is almost 100% pure lightest component. Similarly a series of flash operations on the liquid can result in a final liquid product that is 100% heaviest component. The array of trays in a distillation column accomplishes this series of flash operations. The temperature difference between the liquid and vapour streams entering a tray causes condensation / vaporization so that as one moves up the column, the composition of the lightest component increases monotonically. Alternatively, as one moves down the column, the composition of the heaviest component keeps on increasing. Since heavier components boil at higher temperatures, the tray temperature increases as one moves down the column with the condenser being the coolest and the reboiler being the hottest. The reboiler and the condenser are the source of vaporization and condensation respectively for the series of vaporization / condensation.

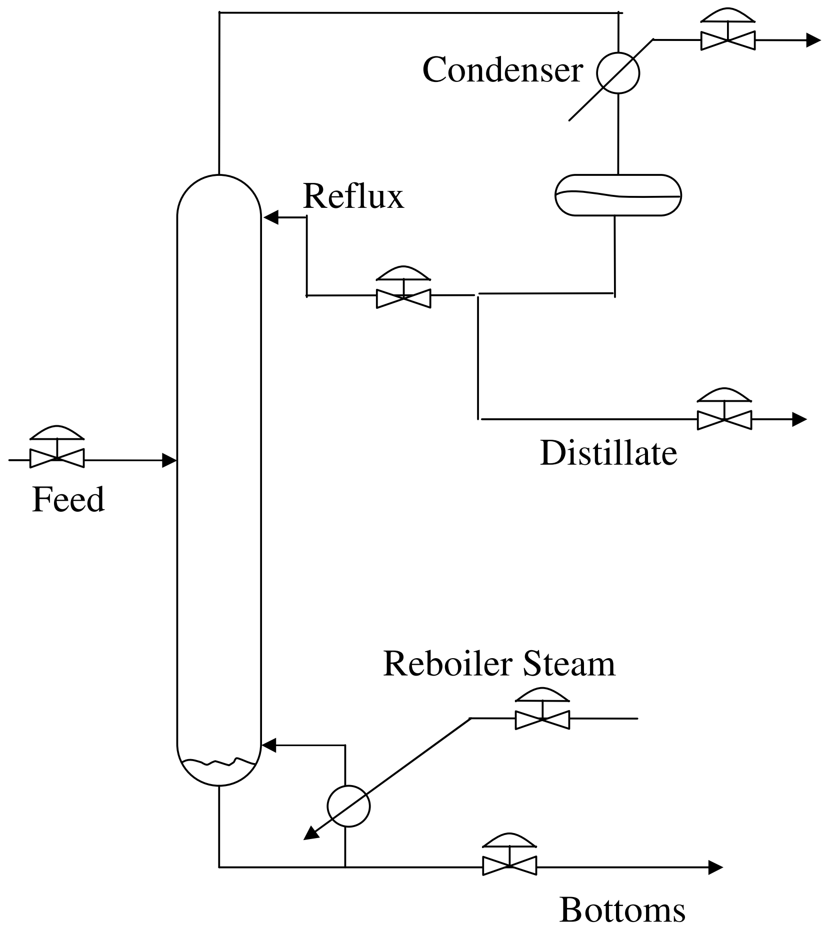


Figure 5.1 Schematic of a simple distillation column along with the control valves.

5.1.2. Splits in a Simple Distillation Column

Consider a five component equimolar ABCDE mixture feed into a simple distillation column. The components are in decreasing order of volatility so that A is the lightest and E is the heaviest. The feed rate is 100 kmol/h. The steady state distillate to bottoms product split is primarily determined by the choice of the distillate (or bottoms) rate. Assuming a sufficiently large number of trays, adequate reboil and reflux, for a distillate rate of 40 kmol / hr, which is equal to the component A and component B flow rate in the feed, essentially all of the A and B would leave up the top so that the distillate would contain traces C, D and E impurities in decreasing order of composition. The bottoms would be a CDE mixture with traces of B and A, in decreasing order of composition. The column thus accomplishes a split between components B and C with the liquid preventing C from escaping up the top and the vapour reboil preventing B from escaping down the bottoms. Components B and C, are referred to as the light key (LK) and heavy key (HK) respectively. The LK is the dominant impurity in the bottoms stream and the HK is the dominant impurity in the distillate stream. The component split is referred to as an AB/CDE split. The component that is the next lighter component than the LK is called the lighter than light key (LLK). The heavier than heavy key (HHK) can be defined in a complementary manner. Components A and E are respectively the lightest and heaviest and therefore referred to as the lightest key and the heaviest key.

For the ABCDE mixture, there are four possible splits – A/BCDE, AB/CDE, ABC/DE and ABCD/E. The first one, where the light key is also the lightest key is referred to as the direct split. The last one, where the heavy key is also the heaviest key is referred to as an indirect split. The remaining splits where the key components are intermediate boilers are referred to as intermediate splits. It is helpful to categorize the column split into these basic types.

5.2. Basic Control Structures

A simple distillation column with a total condenser has a total of six valves as in Figure 5.1. Of these six valves, the feed valve is usually set by an upstream unit in the process. Also two valves must be used to control the reflux drum level and the reboiler level as liquid levels are non-self regulating. Another valve must be used to regulate the column pressure which represents the vapour inventory in the column. Typically, the cooling duty valve in the condenser is used for pressure control. After implementing the three inventory loops, the position of the remaining two control valves can be set by an operator or a controller to regulate the separation. This gives a operation degree of freedom of two for a simple distillation column. The operation degree of freedom is more for complex column configurations that are considered later.

Four control structure types result for a distillation column corresponding to the choice of valve used for reflux drum and reboiler level control. These are the LQ, DQ, LB and DB structures and are illustrated in Figure 5.2. The nomenclature corresponds to the two control degrees of freedom (valves) that remain to regulate the separation. The LQ control structure corresponds to the distillate (D) controlling the reflux drum level and the bottoms (B) controlling the reboiler level. This leaves the reflux (L) and reboiler duty (Q) as the two valves for regulating the separation achieved, hence the label LQ. In the DQ structure, the condenser level is controlled using the reflux while in the LB structure, the bottoms level is controlled using the reboiler duty. Lastly in the DB control structure, the reboiler duty and reflux are used for controlling the reboiler and condenser levels respectively.

5.2.1. The Energy Balance (LQ) Structure

The LQ control structure is the most natural control structure for a simple distillation column. This is because the separation in a distillation column occurs due to successive condensation and vaporization of the counter-current vapour and liquid streams flowing through the column. Adjusting the cold reflux, the source of condensation, and the reboiler duty, the source of vaporization, is then a natural choice for regulating the separation achieved in the column. The LQ control structure is thus the most commonly applied distillation control structure. It is also sometimes referred to as an energy balance structure as changing L (cold reflux) or Q alters the energy balance across the column to affect the distillate to bottoms product split.

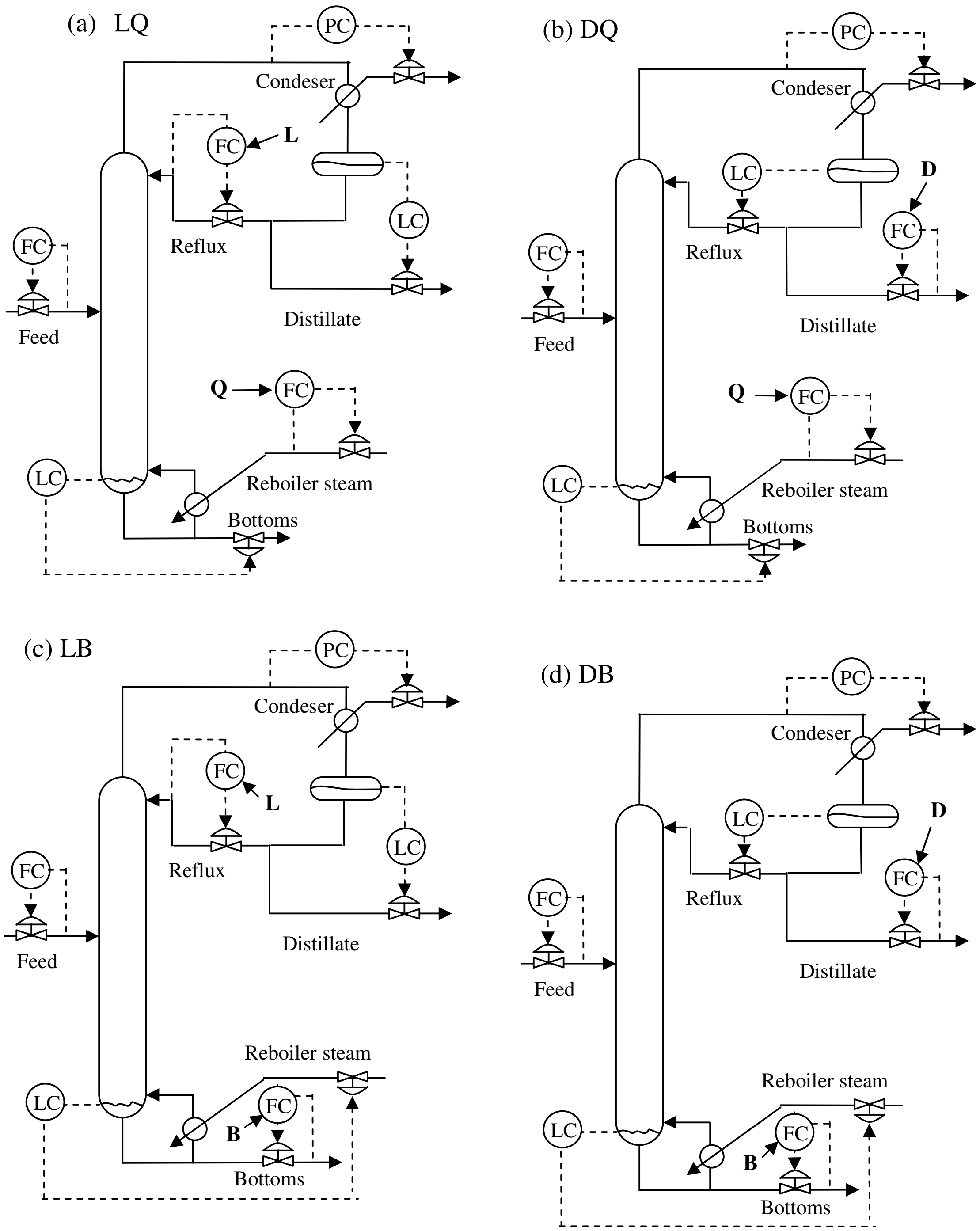


Figure 5.2. Schematics of LQ, DQ, LB and DB control structures

5.2.2. Material Balance Structures

The other control structures are referred to as material balance structures as the product split is directly adjusted by changing the distillate or bottoms stream flow rate. The material balance structures are applied when a level loop for the LQ structure would be ineffective due to a very small product stream (D or B) flow rate. The DQ structure is thus appropriate for columns with very large reflux ratio (L/D > 4). The distillate stream flow is then a fraction of the reflux stream so that the reflux drum level cannot be maintained using the distillate. The level must then be controlled using the reflux. The LB structure is appropriate for columns with a small bottoms flow rate compared to the boil-up. The bottoms stream is then not appropriate for level control and the reboiler duty must be used instead. The DB control structure is used very rarely as both D and B cannot be set independently due to the steady state overall material balance constraint. In dynamics however, the control structure may be used when the reflux and reboil are much larger than the distillate and bottoms respectively. This occurs in super fractionators which will be discussed later in this Chapter.

5.2.3. Other Control Structure Variants

Other variants of the basic control structure types include the L/D-Q, L/D-B and D-Q/B. In the first two structures the reflux ratio is adjusted for regulating the separation. In the last structure the reboil ratio is adjusted. These control structures are illustrated in Figure 5.3. Note that when the reflux is adjusted in ratio with the distillate, the distillate stream can be used to control the reflux drum level even as it may be a trickle compared to the reflux rate. Similarly, when the reboil rate is adjusted in ratio with the bottoms, a small bottoms stream can provide effective level control.

Maintaining the reflux ratio is quite common in distillation control as it provides feedforward compensation in the reflux for a change in the distillate rate. Such a feedforward compensation can significantly improve quality control as the column dynamics are slow with respect to a change in the reflux rate due to the slow liquid hydraulics with every tray having a time constant of 15-30 s. Pure feedback adjustment of the reflux can thus result in large purity deviations. Maintaining the reboil ratio is not very popular. This is because all the tray compositions / tray temperatures respond almost immediately to a change in the reboil due to the fast vapour dynamics. Adjustment of the reboiler duty in a feedback arrangement is thus usually sufficient for effective regulation.

5.3. Temperature Based Inferential Control

The distillation column performs a separation between the light key and the heavy key so that heavy key and light key impurity levels respectively in the distillate and bottoms are below design specifications. The primary control objective then is to ensure these impurity levels remain below specifications for load changes. A change in the flow rate and composition of the feed into the column are the two major load disturbances that must be rejected by the control system. Feedback control based on the impurity levels in the product streams is usually not acceptable due to the large delays / lags introduced by composition measurements. Also, control action would only be taken after the product purity deviates in a feedback system. Considering that the column consists of an array of trays, the trays would respond to a load disturbance much before the effect of the disturbance reaches the product streams. It therefore makes sense to control an appropriate tray process variable so that the disturbance is compensated for before the product purities are affected. This would lead to tighter product purity control.

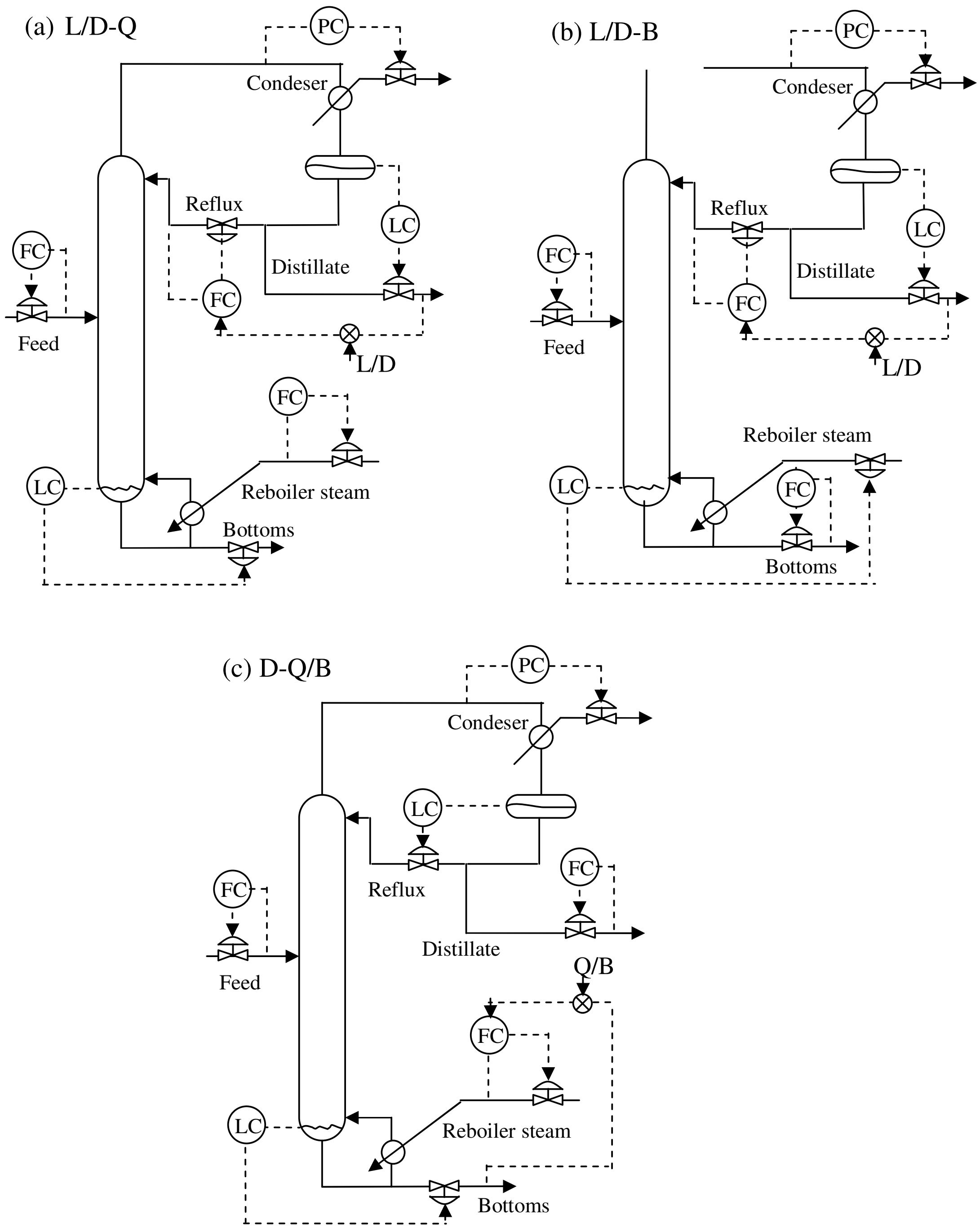


Figure 5.3. Schematics of L/D-Q, L/D-B, and D-Q/B control structures.

The tray temperature is almost always used as an inferential variable for the tray composition. The boiling point of a mixture depends on the pressure and the mixture composition. At a constant pressure, the boiling point increases as the concentration of heavies increases and vice versa. A change in the tray composition can thus be inferred from a change in the tray temperature. The relationship is exact for a binary mixture and is approximate for a multi-component mixture.

5.3.1. Single-Ended Temperature Control

Controlling a single tray temperature in a column is usually referred to as single-ended temperature control. Either of the two operation degrees of freedom can be used as the manipulation handle. For example, in the LQ control structure, the reflux rate or the reboiler duty can be manipulated for maintaining a tray temperature. This is shown in Figure 5.4(a). Manipulation of Q is usually preferred due to the fast response of all the tray temperatures to a change in Q. The dynamics with respect to reflux rate are slower due to the associated tray liquid hydraulic lags. The reflux rate can also be used for maintaining a tray temperature if the control tray location is not too far below the reflux (say about 10 trays). The single ended variants for the DQ and LB control structures are shown in Figure 5.4(b) and (c) respectively. In the DQ structure, if the distillate rate is used to control a tray temperature, the temperature controller is nested with the reflux drum level controller. This means that the temperature controller would work only if the reflux drum level controller is working. Similarly, in the LB structure, if the bottoms flow rate controls a tray temperature, the temperature controller is nested with the reboiler level controller. In both these cases, the level controller must be a tightly tuned PI controller, else the temperature control would be extremely sluggish. Note that the reflux and the reboil are the only two causal variables that affect the tray temperature so that any control scheme must directly / indirectly effect a change in these causal variables.

5.3.2. Dual-Ended Temperature Control

Theoretically speaking, since the column degree of freedom is two, two tray temperatures can be controlled in a column. This is referred to as dual-ended temperature control. For example, in the LQ control structure, the reflux rate can be used for controlling a rectifying tray temperature and the reboiler duty can be used to control a stripping tray temperature as in Figure 5.5. Industrial practice is to control a single tray temperature as controlling two tray temperatures usually requires detuning of the temperature controllers due to interaction between the temperature loops. More importantly, the two controlled tray temperatures may not be sufficiently independent so that, in the worst case, the control system may seek infeasible temperature set-points. Dual temperature control is possible for long towers so that two tray temperatures that are far apart are sufficiently independent.

5.4. Temperature Sensor Location Selection

Various criteria have evolved for the selection of the most appropriate tray location(s) for temperature control. Prominent among these are selection of tray with the maximum slope in the temperature profile, sensitivity analysis and SVD analysis.

5.4.1. Maximum Slope Criterion

The maximum slope criterion is the simplest to use and requires only the steady state temperature profile. From the temperature profile, the tray location where the temperature changes the most from one tray to the other is chosen as the control tray. The temperature profile usually also shows a large change / break at the feed tray location. The feed tray should however not be chosen for control as the changes in temperature would be due to changes in the feed composition / temperature and not due to a change in the separation. A large change in the temperature from one tray to the other reflects large separation between the key components so that disturbances in the separation would affect this separation zone much more than other locations. It therefore makes sense to place the temperature sensor at that location.

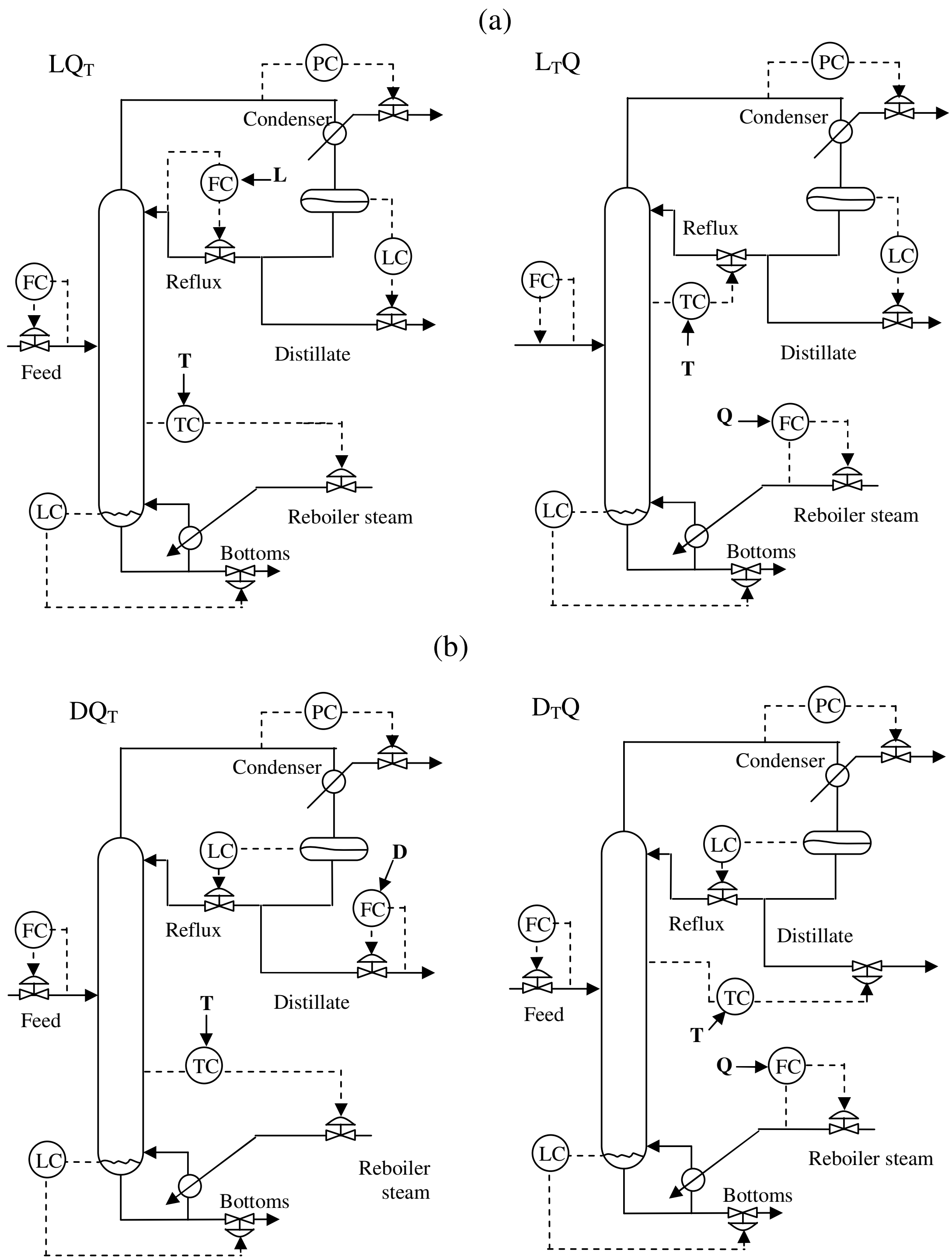
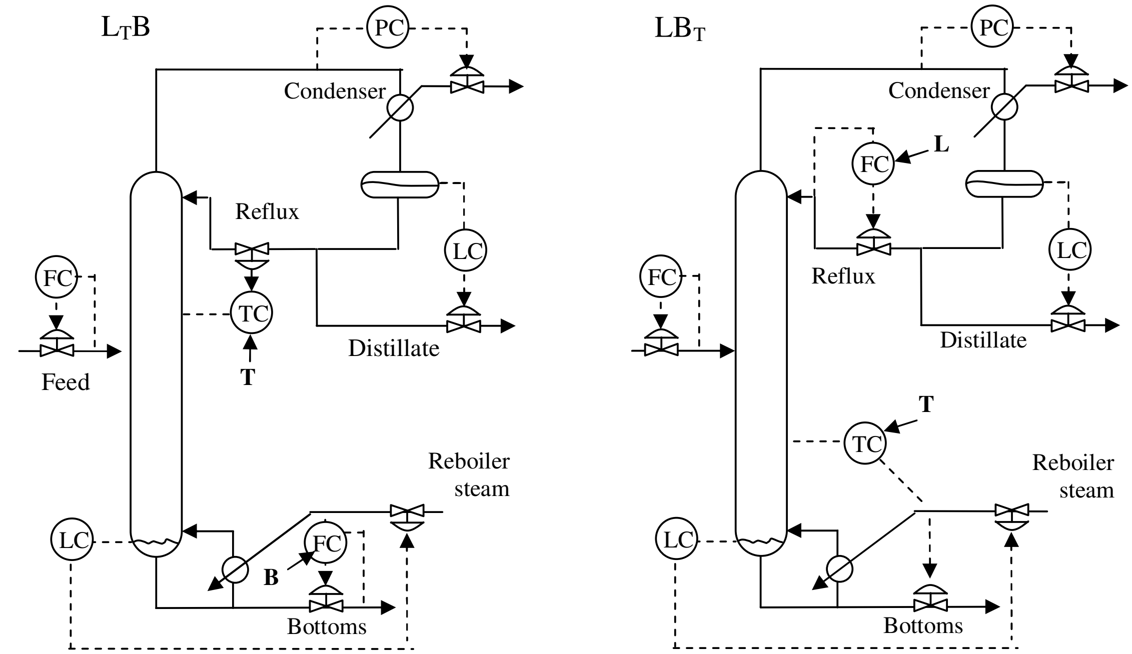


Figure 5.4 Single ended temperature control structures using LQ and DQ scheme

(c)



(d)

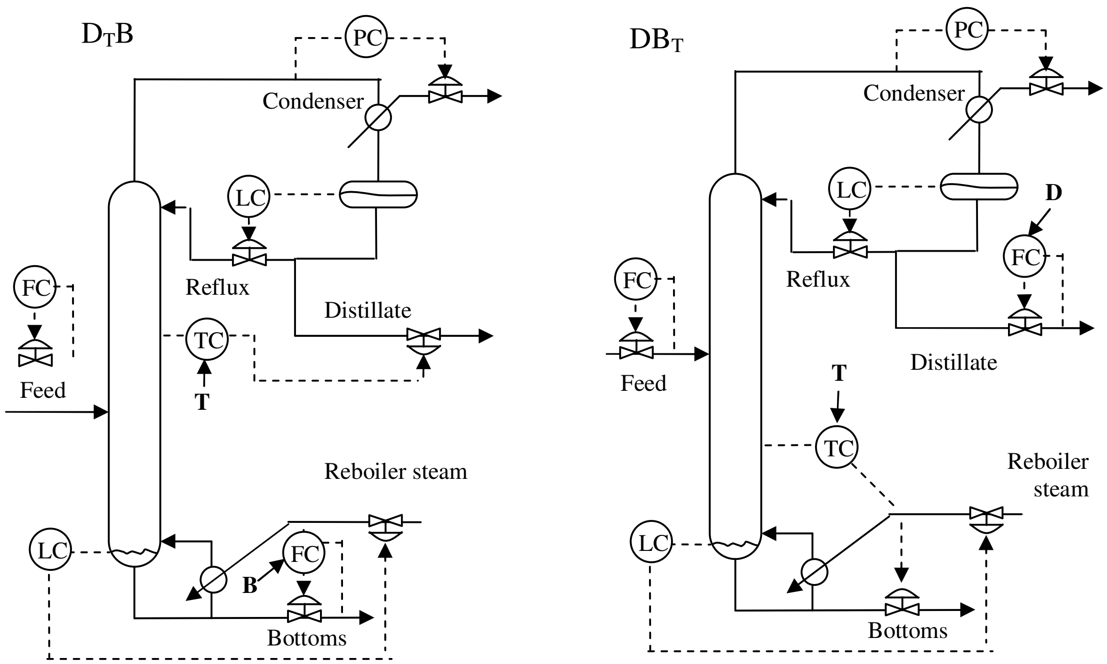


Figure 5.4 Single ended temperature control structures using LB and DB scheme

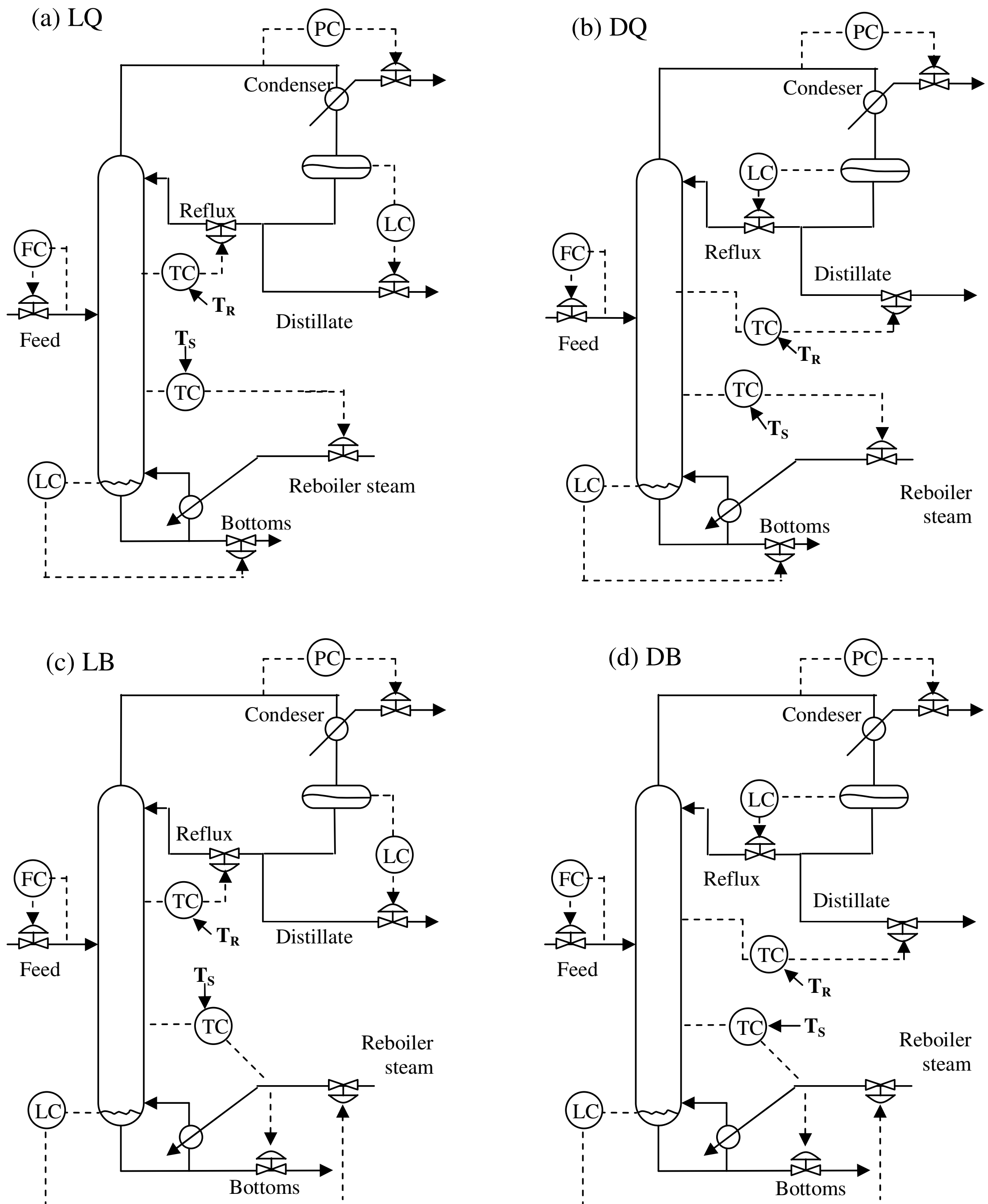


Figure 5.5. Dual ended temperature control structures using LQ, DQ, LB and DB schemes.

5.4.2. Maximum Sensitivity Criterion

Sensitivity analysis recommends controlling the tray with maximum sensitivity to the control input. The causal variables that effect a change in the tray temperature are the reflux rate (or ratio) and the reboiler duty. The sensitivity of the i^{th} tray temperature to the reflux rate (L) and reboiler duty (Q) is defined as

$$S_{iL} = \frac{\partial T_i}{\partial L}$$

and

$$S_{iQ} = \frac{\partial T_i}{\partial Q}$$

respectively. Controlling the most sensitive tray location provides muscle to the controller as a smaller change in the manipulated variable is needed to bring the deviating temperature back to its set-point. The open loop steady state gain is large so that a low controller gain suffices. The low controller gain mitigates sensor noise amplification. Also, a small bias in the temperature sensor can be tolerated. Plotting the sensitivity of all the trays with respect to Q and L would reveal the most sensitive tray location. In case two distinct regions of high sensitivity are observed, dual temperature control should be possible. If not, dual temperature control is likely to result in the two temperature controllers fighting each other.

5.4.3. SVD Criterion

The SVD analysis is another useful technique for selecting the tray temperature locations. The sensitivity matrix

$$\mathbf{S} = [\mathbf{S}_L\ \mathbf{S}_Q]$$

where $\mathbf{S}_L$ and $\mathbf{S}_Q$ are column vectors of tray sensitivities, is decomposed using the singular value decomposition (SVD) as

$$\mathbf{S} = \mathbf{U\Sigma V}^T.$$

In the above **U** and **V** are orthogonal matrices with the columns constituting the left singular and right singular vectors, respectively. The $\mathbf{\Sigma}$ matrix is a diagonal matrix. A plot of the first two left singular vectors (first two columns of **U**) shows the two most independent locations in the column. The index of the element of the first left singular with the maximum magnitude corresponds to the tray location that should be controlled in a single-ended scheme. If dual temperature control is to be implemented, the corresponding index for the second left singular vector gives the tray location for the second temperature sensor. The feasibility of dual ended temperature control is reflected in the ratio of the two diagonal elements, σ_1 and σ_2, of $\mathbf{\Sigma}$. The diagonal elements in $\mathbf{\Sigma}$ are always in decreasing order of magnitude. If the two singular values are comparable, ie the ratio σ_1/σ_2 is not too large (say < 10), dual temperature control should be possible.

Of the above three criteria, the maximum slope criteria is the simplest to use. Sensitivity analysis and SVD analysis requires the availability of a rating program to calculate the tray temperature sensitivities to the manipulated variables. The SVD technique further requires a module to obtain the SVD decomposition of the sensitivity matrix **S**. In most distillation column studies, the three techniques would agree on sensor location. However, for columns with highly non-ideal columns, the use of the SVD technique is recommended for selecting the tray location.

5.5. Considerations in Temperature Inferential Control

5.5.1. Effect of LLK / HHK

The temperature composition relationship is not exact for multi-component mixtures. If the feed LLK composition increases, the LLK must leave up the top of the column. For the same LK/HK split, the tray temperatures in the enriching section should be lower as the LLK composition must increase due to the increase in its feed composition. This dip in the temperature would be more as one moves up the enriching section since the LLK accumulates at the top. If a tray temperature near the top is controlled using the reboiler duty and the tray temperature set-point is not reduced on increase of feed LLK, more of the HK would be pushed up the top of the column by the action of the controller. Controlling a tray temperature near the feed tray would mitigate this effect. Another option is to measure the HK composition in distillate and use it to compensate the control tray temperature set-point. Note that the volatilities dictate that any LLK entering the column must exit up the top. In case LLK in the distillate is not acceptable, action must be taken upstream to ensure LLKs do not enter the column. Troubleshooting the process would typically reveal an upstream column not doing its job.

Similar to LLK, if a stripper tray temperature low down the column is being controlled using boilup, an increase in feed HHK would cause more LK to leak down the bottoms, unless the tray temperature setpoint is appropriately increased.

5.5.2. Flat Temperature Profiles

When the key components in a mixture are close boiling, the column temperature profile is flat with only a small change in adjacent tray temperatures. This is typical of superfractionators that use a large number of trays and a high reflux ratio as the separation is inherently difficult. Controlling a tray temperature is then not desirable as variations in the tray pressure with changes in column internal flow rates would swamp any subtle variations in the tray temperature due to composition changes. Controlling the difference in two tray temperatures that are located close by mitigates the effect of pressure variation as the change in the local pressure for the two trays would be about the same. The differential temperature measurement then reflects the change in the HK (or LK) composition between the trays. Care must be exercised in the use of a differential temperature measurement as the variation in ΔT with the bottoms composition depends on the location of the separation zone inside the column. If the measurement trays are below the separation zone, ΔT increases as the steam rate is decreases. Once the separation zone passes below the ΔT trays, a decrease in the steam would cause the ΔT to decrease. The gain thus changes sign depending on the location of the separation zone inside the column.

5.5.3. Easy Separations

The other extreme to a flat temperature profile is an extremely sharp temperature profile. This occurs when the separation is very easy so that the separation zone shows a large change in temperature over a few trays ie a sharp temperature profile. During transients, this sharp separation zone may move up or down the column leading to temperature transmitter saturation. Once the separation zone moves up and continues to move up, the error signal that the controller sees does not change so that the burden of bringing the profile back falls on the integral action. The problem is compounded by the low controller gain due to the extreme sensitivity of the tray temperature to a change in the manipulated variable. The problem is solved by controlling the average temperature of the trays over which the profile moves.

5.6. Control of Complex Column Configurations

5.6.1. Side-draw Columns

Side product streams are sometimes withdrawn from a column when the product purity specifications are not very tight and there is small amount of impurity in the feed that must be purged. Two common configurations are a liquid side-draw from a tray above the feed tray or a vapour side draw below the feed tray. Consider an ABC ternary mixture. If the component flow rate of A in the fresh feed is small, the liquid side stream withdrawal above the feed tray allows most of the B to be removed in the side stream. The side-draw must be liquid as A being the LLK would be present in smaller amounts in the liquid phase. The vapour side draw below the feed tray is used when there is a small amount of C (compared to A and B) in the fresh feed. The C HHK would separate into the liquid phase so that a vapour side stream that is mostly B with small amounts of C can be withdrawn below the feed tray. The side stream (liquid or vapour) provides an additional opearation degree of freedom and its flow rate may be adjusted to maintain the B purity in the side draw. The control schemes are illustrated in Figure 5.6.

Alternative simpler control schemes are possible when the light A or heavy B impurities occur in very small amounts in the fresh feed. The purge rate is flow controlled with a set-point corresponding to the maximum expected impurity component flow in the feed. When the impurity is below this maximum, small amount of LK or HK would be lost with purge. However, the loss is acceptable due to the very small purge rate. The alternative simpler control schemes for the two common side draw configurations are shown in Figure 5.7.

5.6.2. Side Rectifier / Side Stripper Columns

The side rectifier and side stripper columns are an extension of the side-draw column discussed above. As with side-stream columns, these are used when there is a small amount of light or heavy impurity in the feed that is removed as a small purge stream. However the purity specs on the main products are tight. The vapour or liquid side stream respectively, must then be further rectified or stripped to ensure that the impurity is pushed back into the main column and does not escape with side-product stream to ensure high purity. The side stripper and side rectifier column arrangements are shown in Figure 5.8(a) and (b). An additional operation degree of freedom is introduced in the form of the reflux rate or the reboiler duty. The side draw rate and the reflux rate or reboiler duty can then be adjusted to maintain the two impurities in the side-product. The corresponding control schemes are shown in Figure 5.8(a). Along with the two composition loops in the main column, these schemes represent a highly coupled 4X4 multivariable system. Simpler control schemes with only one temperature (or composition) being controlled in each of the main column and the side-column are much more practical.

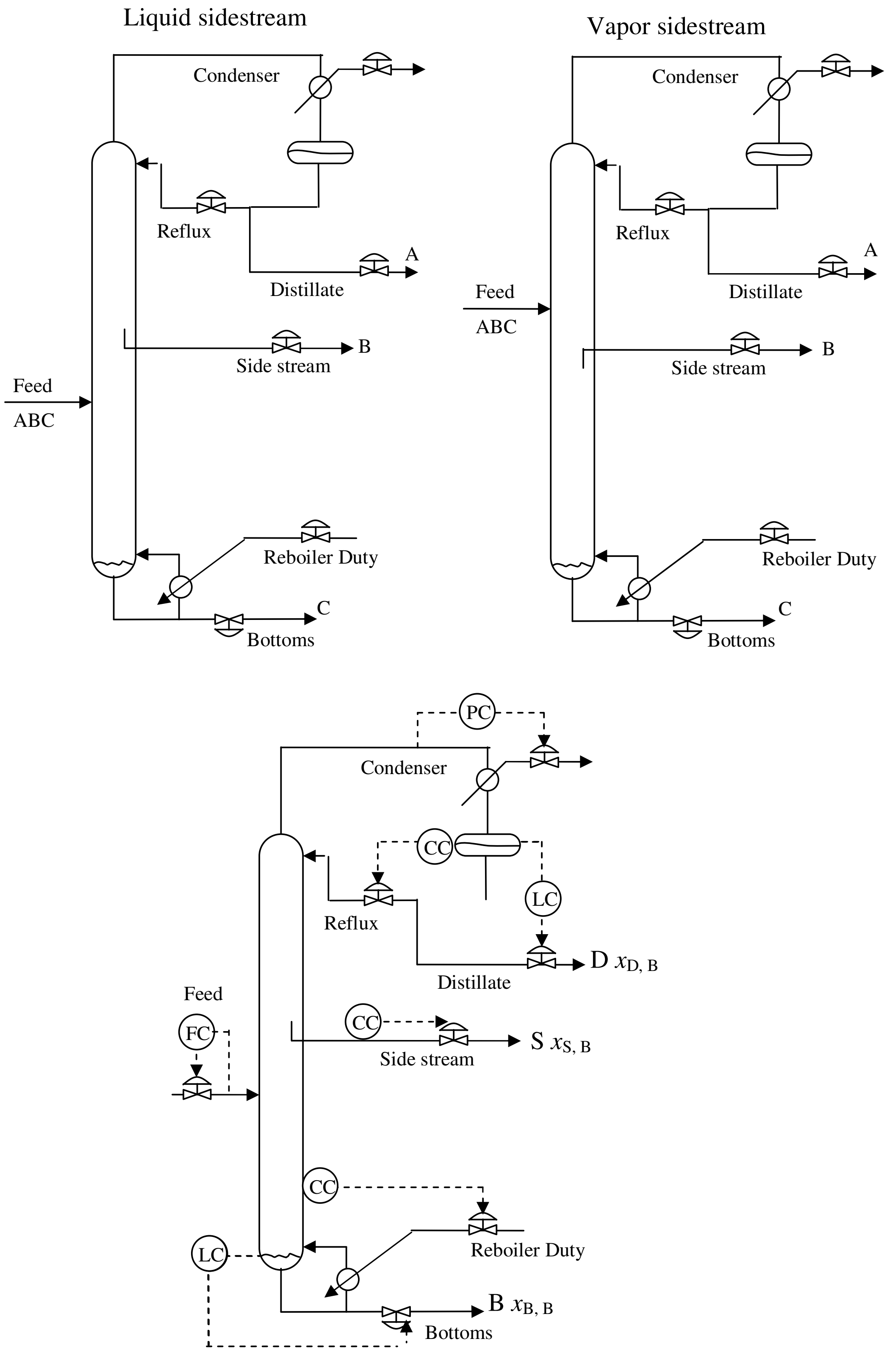
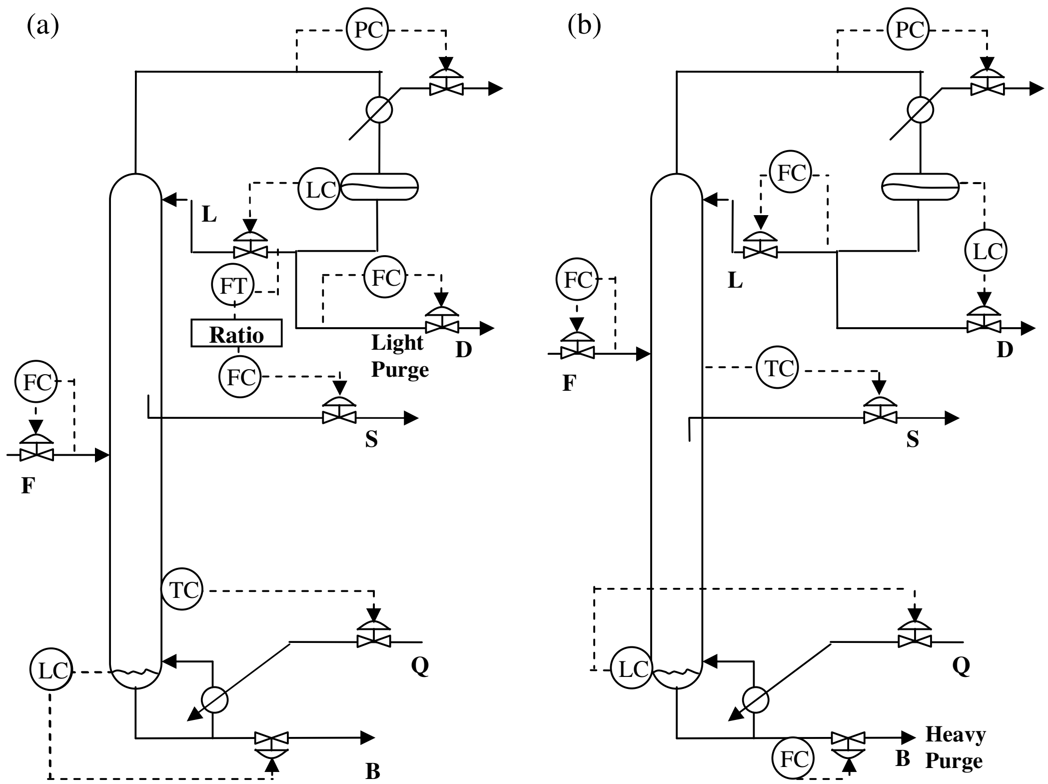


Figure 5.6. Control of side stream column



F	Feed
B	Bottoms
D	Distillate
Q	Reboiler Duty
L	Reflux

Figure 5.7. Control of purge columns of (a) Liquid side draw and (b)Vapor side draw

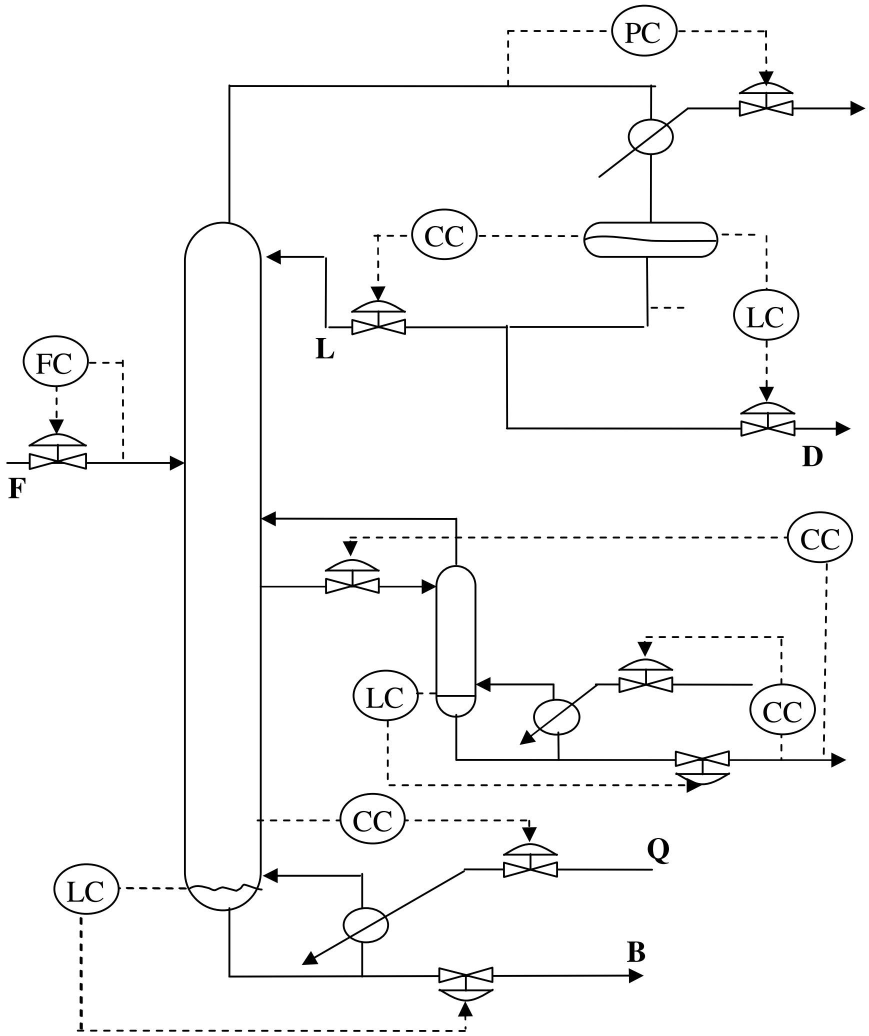


Figure. 5.8(a). Side stream column with stripper

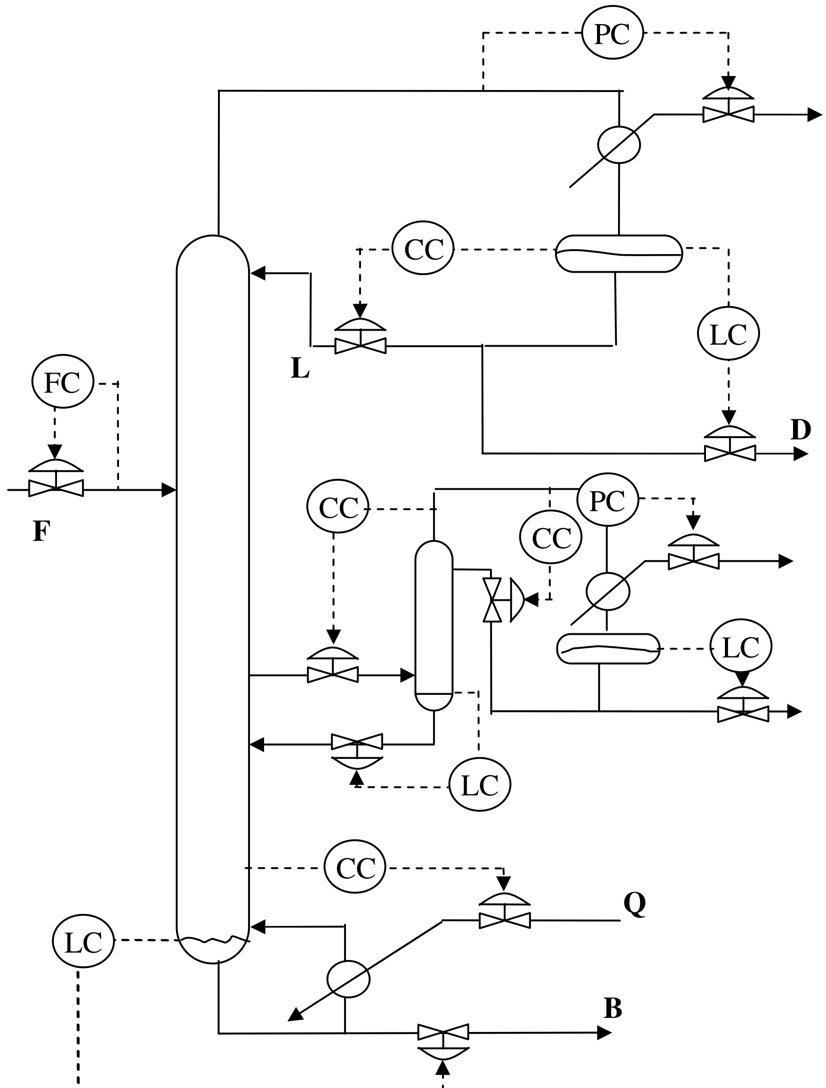


Figure 5.8(b). Side stream column with rectifier

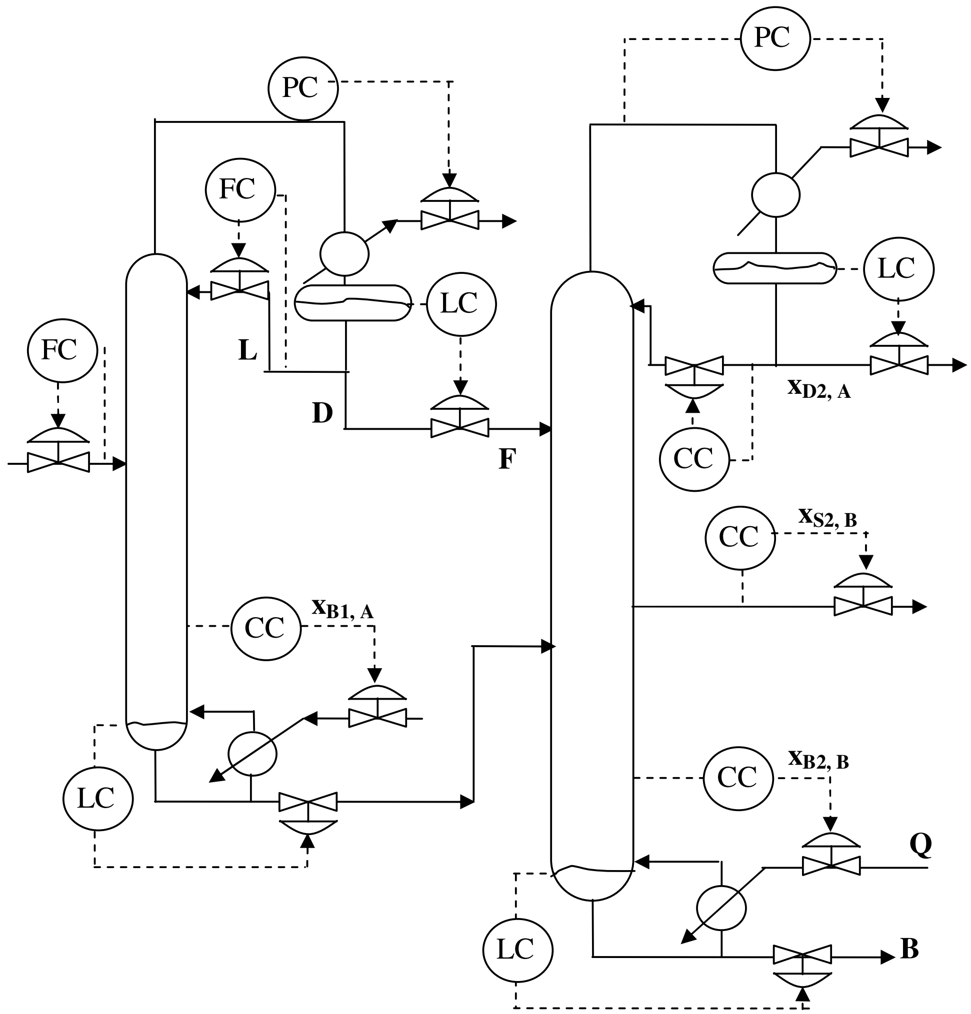
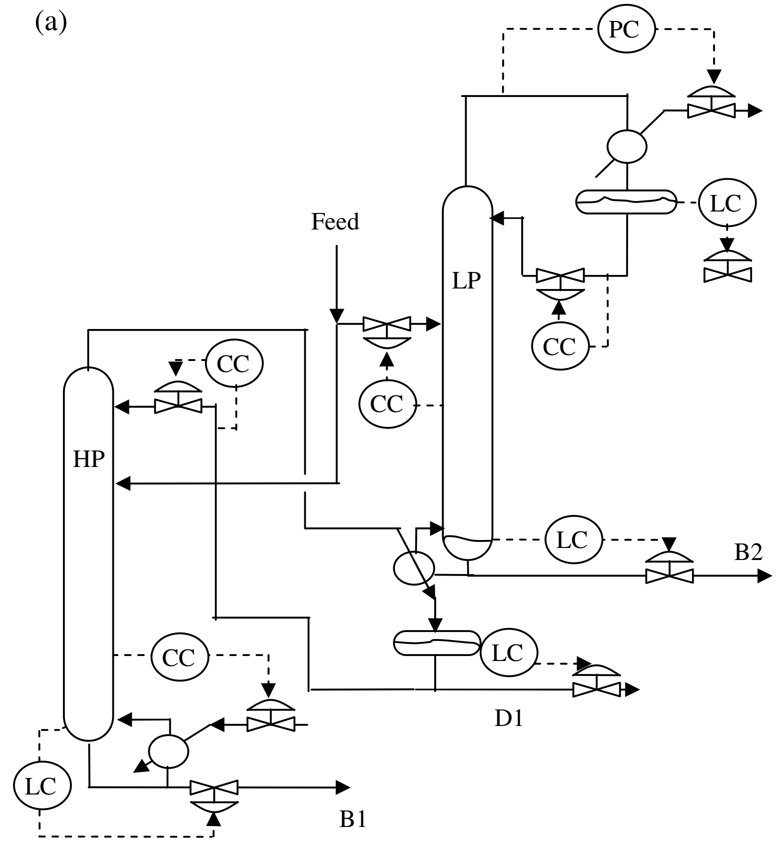


Figure 5.9. Side stream column with prefractionator

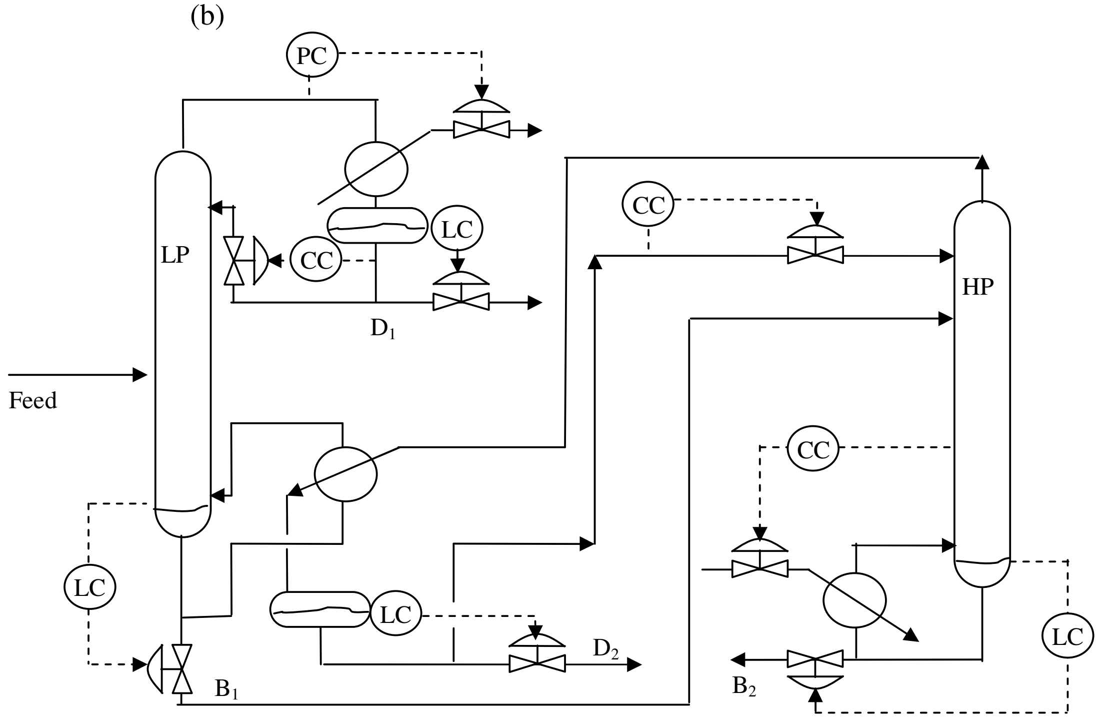
5.7. Control of Heat Integrated Columns

Heat integration arrangements in columns consist of the hot vapour from high pressure column providing the energy for reboil in a low pressure. The reboiler for the low pressure column then also acts as the condenser for the high pressure column. Three possible heat integration schemes are shown in Figure 5.10. In the feed split scheme (Figure 5.10(a)), a binary fresh feed is split and fed to two columns. One of the columns is operated at high pressure and the other at low pressure. The pressure difference is chosen so that the hot vapour is 10-15 C hotter than the low pressure column reboiler temperature. The temperature difference provides the driving force for reboiling the liquid in the low pressure column. In the control structure shown, note that the feed to the low pressure column is adjusted so that the bottoms composition is maintained. This is because the reboiler duty in the low pressure column cannot be manipulated. Heat integration thus leads to the loss of a control degree of freedom. Also note that this heat integration scheme is used for a binary separation as the presence of LLK / HHK components can affect the column temperature profiles sufficiently so that the temperature driving force necessary for heat transfer in the low pressure column reboiler disappears.

(a)


PC
LC
Feed
LP
CC
CC
CC
HP
LC
B2
LC
CC
D1
LC
B1

(b)


PC
LP
CC
LC
D_1
Feed
CC
HP
CC
LC
LC
D_2
B_1
B_2
LC

(c)

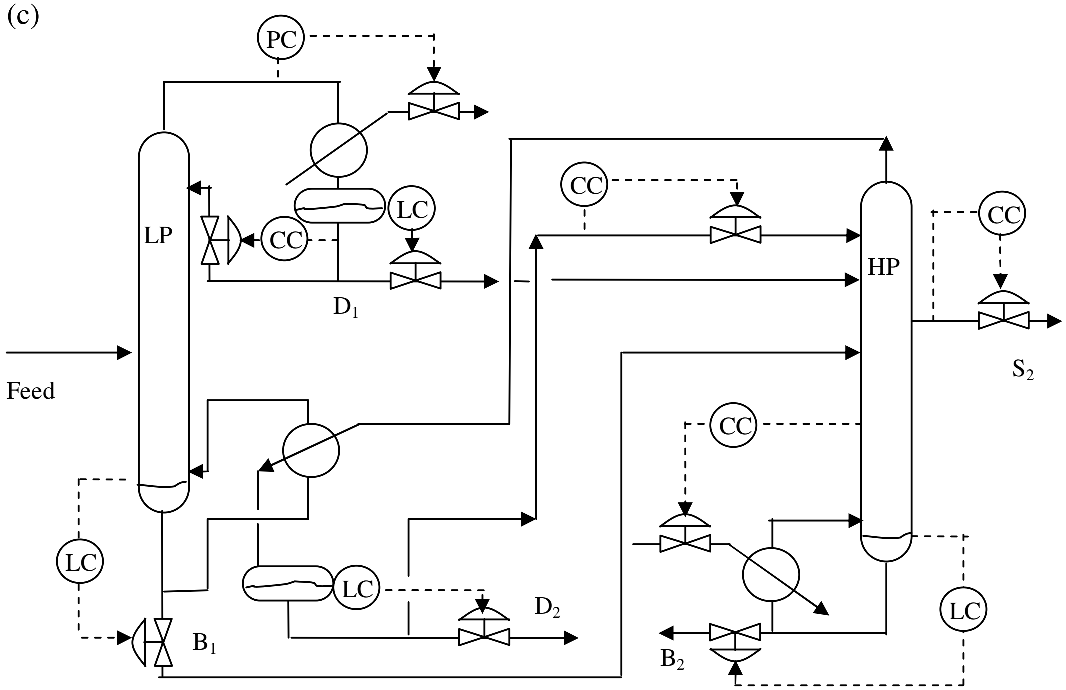


Figure. 5.10. Heat integrated columns (a) Split of feed (binary); (b) Light split reverse (binary); (c) Prefractionator reverse (ternary)

Figure 5.10(b) shows the reverse light split heat integration scheme. Approximately, half the light component is removed as the distillate from the first low pressure column. The bottoms is fed to the high pressure column to remove the light and heavy components as the distillate and bottoms respectively. The hot vapour from the top of this column is condensed to provide vapour reboil into the low pressure column. The direction of heat integration is reverse to that of the process flow. Hence the name, reverse light split. The forward light split configuration is also possible. The control structure for this heat integration scheme is self-explanatory.

Figure 5.10(c) shows another heat integration scheme that can be used for ternary mixtures. The scheme is the same as prefractionator side-draw complex column discussed previously (Figure 5.9) except for reboiler in the pre-fractionator (low pressure column) acting as the condenser for the main column (high pressure) through heat integration. The control structure for this configuration is again self explanatory.

5.8. Control of Homogenous Extractive Distillation System

Homogenous extractive distillation is used to separate a binary AB mixture that cannot be separated due to relative volatility approaching one or the presence of a binary azeotrope. As shown in Figure 5.11, A heavy solvent S is added near the top of the first column, the extractive column, to soak in one of the components (say B). The distillate from the first column is then near pure A. The bottoms, a mixture of S and B, are fed to the solvent recovery column that recovers the heavy S in the bottoms and recycles it back to the extractive distillation column. The distillate from the solvent recovery column is pure B. The control scheme depicted in the Figure manipulates the reboiler duty in the two columns to keep respectively A and B from falling down the bottoms in the two columns. The solvent into the extractive column is ratioed to ensure fresh feed rate to ensure enough solvent for extracting component B. Note that the bottom sump level is not controlled and the sump must provide enough surge capacity for handling the expected variation in the fresh feed flow rate. Any loss of the solvent over long time is made up by a make-up solvent stream (not shown).

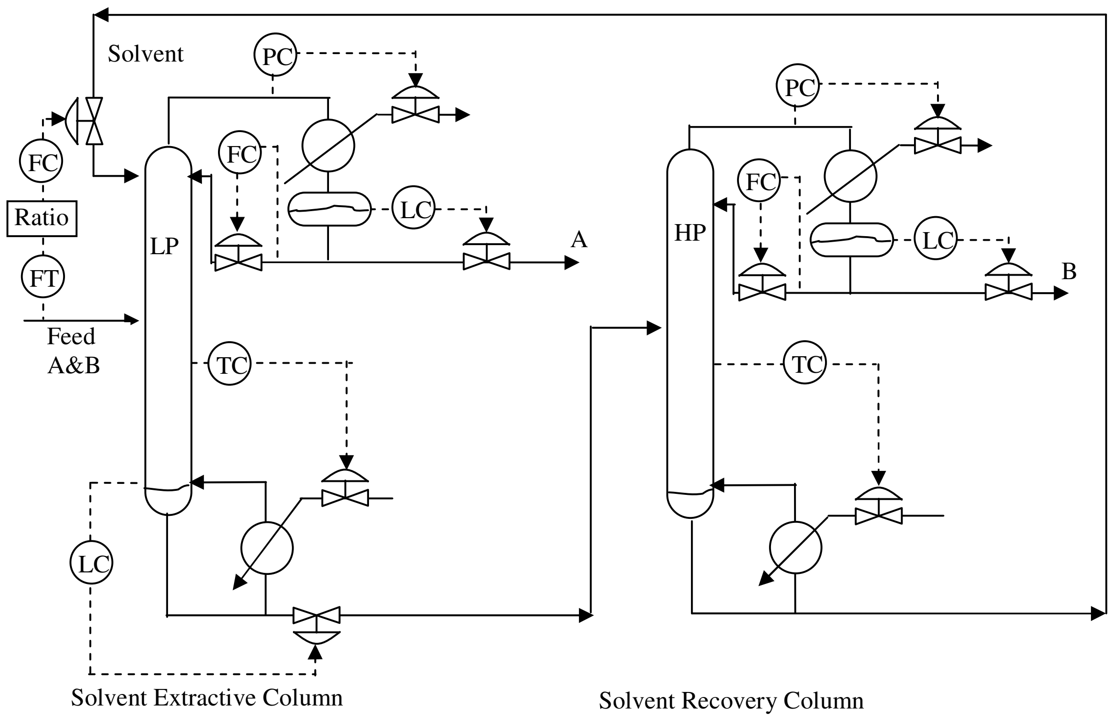


Figure 5.11. Control of Extractive distillation column

5.9. Plant-wide Considerations

In the plant-wide context, the distillate and / or bottoms would feed into a downstream unit such as another distillation column. The variation in the distillate / bottoms flow rate then acts as a disturbance into the downstream unit. The LQ control structure is particularly preferable as the reflux drum and reboiler levels are controlled using the P only controller which results in a smooth flow change into the downstream unit. If however, the DQ (or LB) control structure is used in a high reflux ratio (reboil ratio) column and a tray temperature is controlled using D, the reflux drum level controller manipulates L and must be tightly tuned for a fast dynamics of the of closed loop temperature controller. The D would then show large changes disturbing the downstream unit. Feedforward control action can and should be used to mitigate the propagation of variability to downstream units. For example, the distillate rate may be ratioed to the feed rate with the composition / temperature controller setting the ratio set-point. Alternatively, the distillate may be moved in ratio with reflux with the composition controller setting the reflux ratio set-point. The reflux level controller is then tuned as a P only controller for smooth changes in the reflux and hence the distillate. The variability in the distillate rate can thus be greatly reduced improving the overall plant-wide control performance.

The vapour distillate from a partial condenser can be manipulated to control the tower pressure. This is however not a good idea if the vapour stream feeds directly into a downstream unit and not a surge tank. In such a scenario, the column pressure should be controlled using the condenser cooling duty, the reflux drum level controlled using the reflux rate and the vent rate moved in ratio with the reflux. This arrangement mitigates the propagation of variability downsteam.

The control of energy integrated distillation columns can also be problematic as a disturbance on the hot vapour side necessarily affects the boil-up in the reboiler using the hot vapour as the heat source (instead of steam). To maintain the control tray temperature in the heat integrated column, an auxiliary reboiler (or condenser, as appropriate) is provided. The heat integrated reboiler and the auxiliary reboiler may be arranged in a parallel or a series arrangement. The series arrangement is preferred as the temperature variations in the hot vapour are attenuated due to variation in the temperature driving force in the auxiliary reboiler as shown in Figure 5.12(a). In the parallel arrangement, the auxiliary reboiler must adjust for the variability on the hot vapour side after it has entered the column. One way to prevent this is to use a total heat input controller as shown in Figure 5.13.

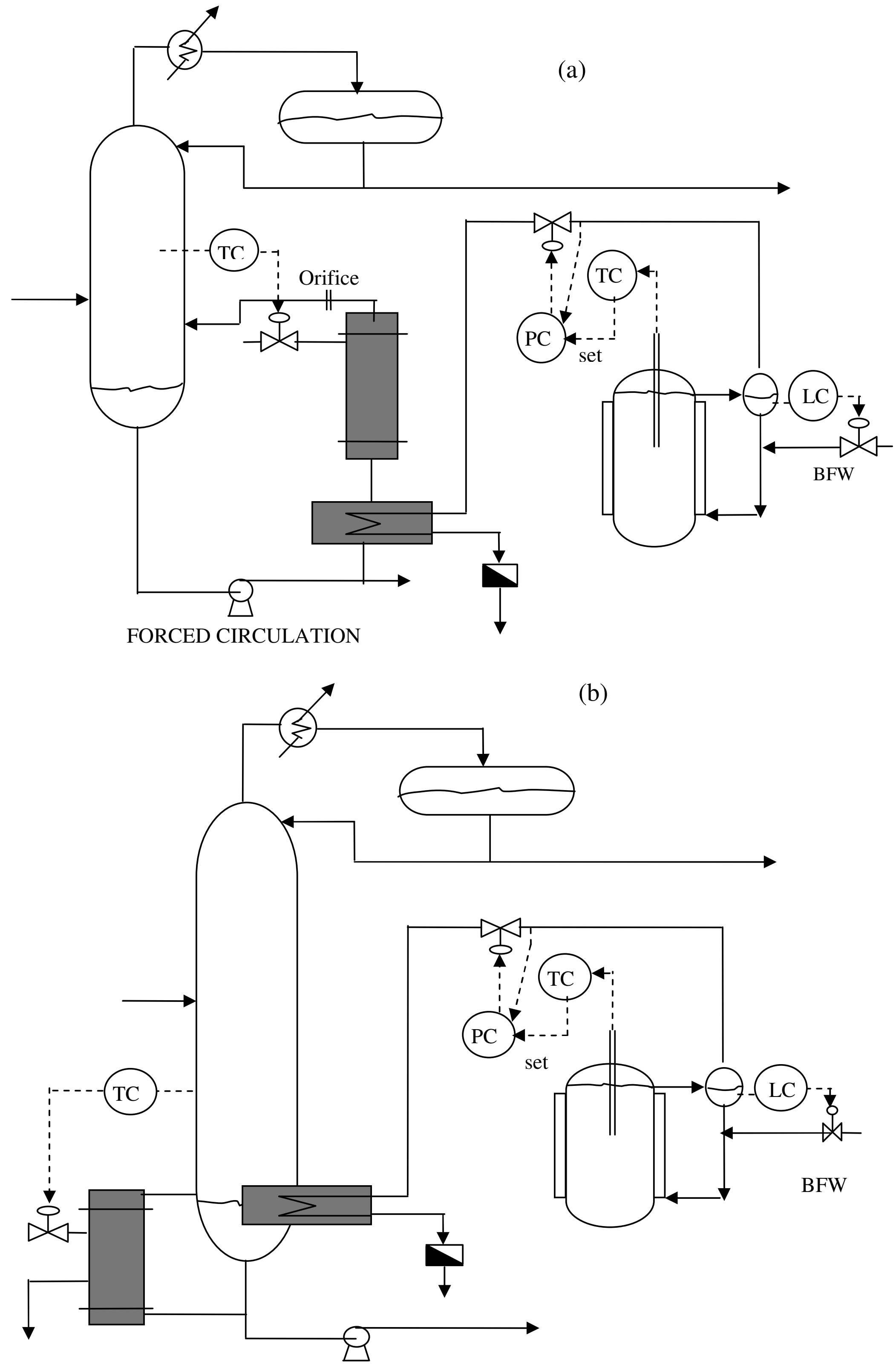


Figure 5.12. Reactor/column heat integration with auxiliary reboiler in (a) series (b) parallel

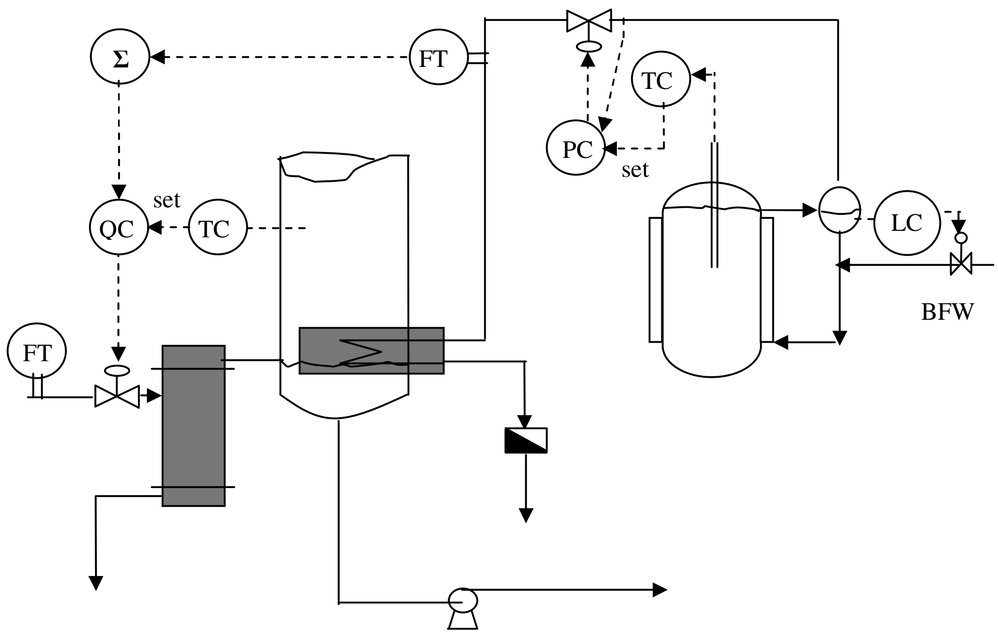


Figure 5.13 Reactor/column heat integration with auxiliary reboiler in parallel and Q controller

Chapter 6. Control of Reactors

A reactor is the heart of a chemical process where the reactants undergo the desired chemical transformation to the products. The transformation is usually incomplete and is also accompanied by undesirable transformation to by-products through side reactions. The reactor operating conditions of temperature, concentration and flow rates determine the production rate of the main product and the side-products. The downstream separation load for separating the unreacted reactants from the products and recycling them back to the reactor is also determined by the reactor. Proper operation and control of the reactor is then crucial to determining the overall process operating profit. The reactor conversion (or yield) and selectivity are the two most commonly used reactor performance metrics that are directly related to the economics of the process. The conversion is defined as the fraction (or %age) of reactant in the feed that reacts to form product(s). The yield is the conversion of a key reactant, usually the limiting reactant. The selectivity is defined as the desired product generation rate relative to the total product generation rate (including all undesired side products). The yield and selectivity represent two key economic objectives of any process. A lower conversion would result in greater energy consumption to separate the unreacted reactants from the products and recycle them back to the reactor. The energy cost per kg product would then go up. A low selectivity represents an economic loss as more of the costly reactant gets converted to the undesired product with lower (or worse, a negative) profit margin. Typically, as the conversion increases, the selectivity decreases so that the usual philosophy is to operate the reactor near the maximum conversion for which the selectivity is acceptable (say >95%).

Even as proper reactor operation is the key to profitability, controlling a reactor offers unique challenges as most reactions are accompanied by the generation or consumption of heat. The reaction heat generation / consumption alters the temperature of the reaction mixture which in turn affects the reaction rate and hence the rate of heat generation / consumption. The coupling of the thermal and reaction effects leads to a highly coupled non-linear system. The reaction rate, r (kmol.s^{-1}.m^{-3} or kmol.s^{-1}.kg^{-1} catalyst), for an irreversible reaction A + B → C would generally vary as

$$r = k.c_A^{\alpha}.c_B^{\beta}.$$

In the above expression, c_A and c_B are the concentrations (kmol.m^{-3}) of A and B respectively, k is the reaction rate constant, and α and β are the reaction order (typically > 0) with respect to A and B respectively. The units of the reaction rate constant depend on the reaction order and it follows the Arrhenious temperature dependence as

$$k = k_0.e^{(-E/RT)}$$

where E is the activation energy and k_0 is the Arrhenius frequency factor.

The form of the kinetic expressions above shows that the reactant concentration and the reaction temperature are the two basic manipulation handles for adjusting rate of product generation in a reactor. The reaction rate doubling for every 10 deg C increase in the temperature is an oft quoted rule of thumb. The reactor temperature is thus a dominant variable that significantly affects the reaction rate. When the reactant concentration is adjusted for changing the production rate, altering a key reactant concentration affects the reaction rate more than changing the concentration of other reactants. This is because most reactors must be operated such that one of the reactants is limiting, i.e. in excess of other reactants. The non-stoichiometric environment is necessary to suppress side reactions. For example, consider the main irreversible reaction A + B → C. The product C can further react irreversibly with B to form an undesired product D as C + B → D. For this reaction scheme, the reactor must be operated in an excess A environment so that the limited availability of B for further participation in the side-reaction suppresses by-product generation. Clearly, changing the limiting reactant B concentration would affect the reaction rate more than changing the excess reactant A concentration. In many industrial reactors, the reactor temperature and the limiting reactant concentration are the two dominant variables that are directly / indirectly adjusted for changing the product generation rate.

In exothermic reactions, the use of a selective catalyst lowers the activation energy for the main reaction. The activation energy for the side reactions is thus more than for the main reaction. In case the temperature is increased for increasing the production rate, the Arrhenius temperature dependence of the rate constant causes a larger relative change in the side-reaction rate. Thus if the main reaction rate increases by say 5%, the side reaction rate would increase by more than 5% (say ~10%). The reaction selectivity thus goes down. The adjustment of the reactor temperature for increasing the production rate thus must consider the detrimental effect on selectivity. In many industrial reactors, the reactor temperature is usually adjusted to compensate for catalyst poisoning / deactivation so that the overall reaction rates do not decrease over time.

6.1. Basic Reactor Types

The continuous stirred tank reactor, the plug flow reactor and the packed reactor are the most common reactor types used in the continuous process industry. These basic reactor types are shown in Figure 6.1. The PFR and PBR are similar except that the latter holds a catalyst bed to facilitate the reaction. The CSTR and the PFR (or PBR) differ fundamentally in terms of back mixing. In the PFR (and PBR), the fluid travels along a pipe as a plug so that every atom entering the reactor spends the same amount of time inside the reactor before exiting. This time is also referred to as the reactor residence time. Plug flow, by definition, implies no back mixing. The exact opposite of plug flow is perfect back mixing as in the CSTR. The back mixing is accomplished using agitators, spargers and fluidization.

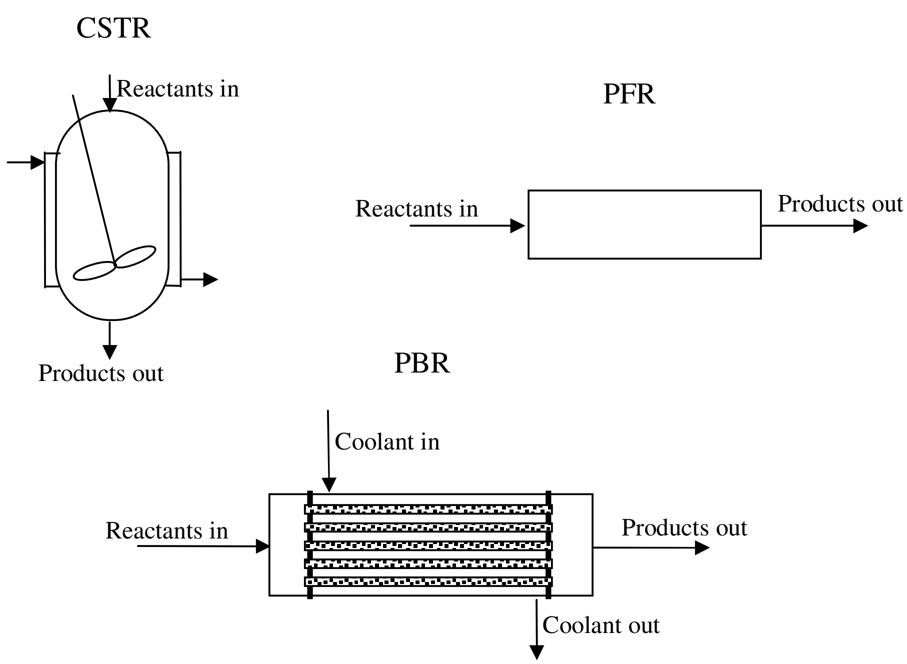


Figure 6.1. Basic reactor types

6.2. Plug Flow Reactor

6.2.1. PFR Basics

To understand the behaviour of a PFR (or PBR), imagine a plug of fluid flowing through the reactor. As it moves through, the concentration of the reactants goes down as they undergo reaction. Assuming adiabatic operation and an exothermic reaction, the heat released due to reaction would heat up the plug. The increase in the plug temperature causes the reaction rate to increase further so that the temperature in the initial part of the reactor increases exponentially. At a sufficient length down the reactor, the reaction rate begins to decrease due to the limited availability of reactants. For a large enough reactor length, the reaction rate would go to zero as the limiting reactant gets exhausted. The temperature profile for an adiabatic PFR thus resembles a sigmoid as shown in Figure 6.2. The difference in the inlet and outlet temperature is referred to as the adiabatic temperature rise. If the reaction is highly exothermic, the adiabatic temperature rise is large, which is usually unacceptable due to reasons such as promotion of side reactions at the higher temperatures, possibility of catalyst sintering in a PBR, increase in the material of construction cost etc. The cooled PFR / PBR is then used

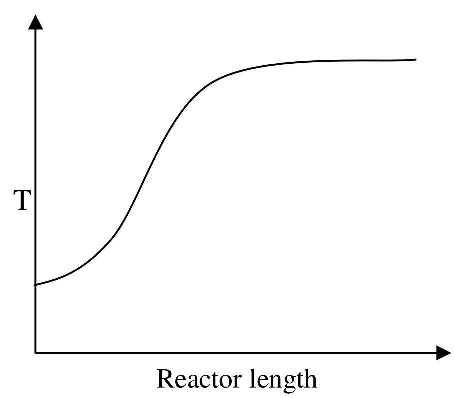


Figure 6.2. Temperature profile for an adiabatic PFR

.

The most common cooled PBR arrangement is shown in Figure 6.3. Catalyst is loaded in the tubes of a shell and tube heat exchanger. Pressurized water is re-circulated on the shell side. The water carries the reaction heat to form steam in the steam drum. The high recirculation rate ensures a near constant temperature on the shell side. Unlike adiabatic operation, the temperature profile initially increases as the rate of heat generation is more than the cooling rate and later decreases with the reaction rate decreasing due to reactant depletion and the cooling rate increasing due to the higher temperature driving force. The temperature profile thus exhibits a maximum, also referred to as the hot spot. For highly exothermic systems, the reactor temperature profile can be extremely sensitive to the operating conditions, in particular the reactor inlet temperature and the shell side temperature.

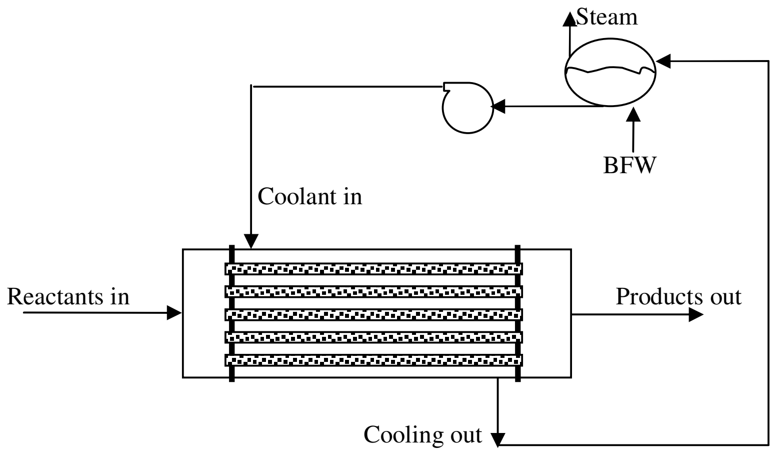


Figure 6.3. Cooled Packed bed reactor

If the reactant inlet temperature (or coolant temperature) is too low, reaction may not kick in leading to the quenched state. If the reactant inlet temperature is too high, the reaction can proceed so fast that only a small fraction of the heat released gets removed resulting in a temperature run-away. The quenched, hot-spot and run-away reactor temperature profiles are illustrated in Figure 6.4.

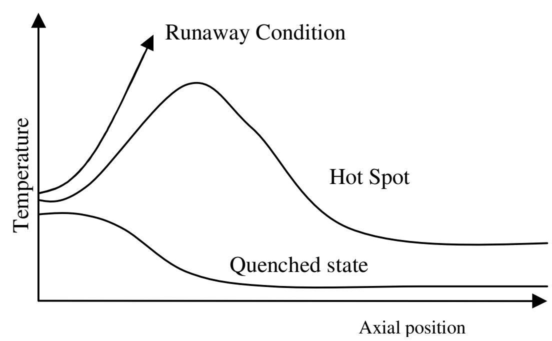


Figure 6.4 Cooled plug flow reactor temperature profiles

The adiabatic or cooled tubular reactor is commonly used in the process industry for gas phase reactions. The reactor is usually operated at the maximum equipment pressure so that the reactant partial pressures are as high as possible for maximum reaction rate. This also reduces the design volume of the reactor for a given conversion. The control of PFRs is considered next.

6.2.2. Control of PFRs

6.2.2.1. Adiabatic PFR

The adiabatic PFR is the simplest reactor configuration and is used when the adiabatic temperature rise is acceptable. The reactants (fresh + recycled) are heated to the reaction temperature using a furnace. The furnace heat duty holds the reactor inlet temperature constant. This is shown in Figure 6.5(a). The adiabatic temperature rise sets the reactor outlet temperature. Sometimes the outlet temperature is also controlled to maintain the reactor conversion and selectivity. The limiting reactant fresh feed rate may be used as the manipulation handle as illustrated in Figure 6.5(b).

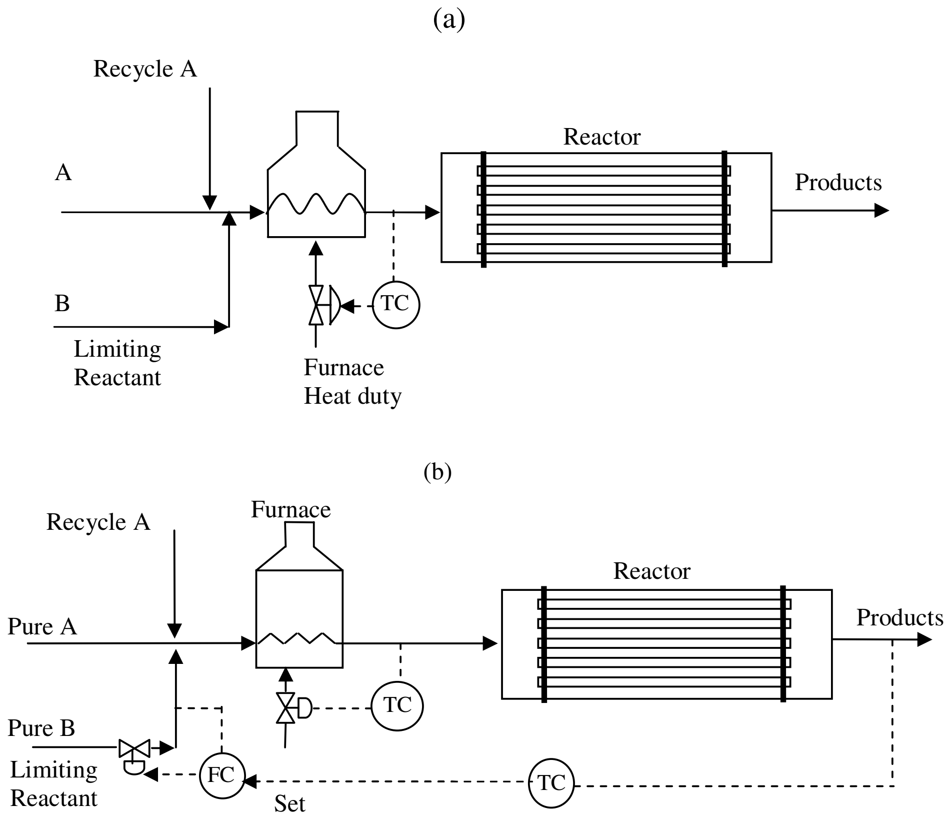


Figure 6.5. Simple adiabatic PFR structures

6.2.2.2. Cooled Tubular Reactors

Cooled tubular reactors are more challenging from the control perspective. The hot spot temperature must be tightly controlled to prevent a runaway. This is accomplished using auctioneering temperature control as illustrated in Figure 6.6. The measurements from an array of thermocouples (or RTDs) placed along the length of the reactor are input to a high selector that passes the maximum temperature to the hot spot temperature controller. This controller typically manipulates the reactor cooling duty. The control structure for the most common cooled PBR arrangement is shown in Figure 6.6. The temperature controller sets the steam drum pressure set-point. A change in the drum pressure alters pressurized water boiling point which in turn changes the temperature driving force for heat removal from reactor.

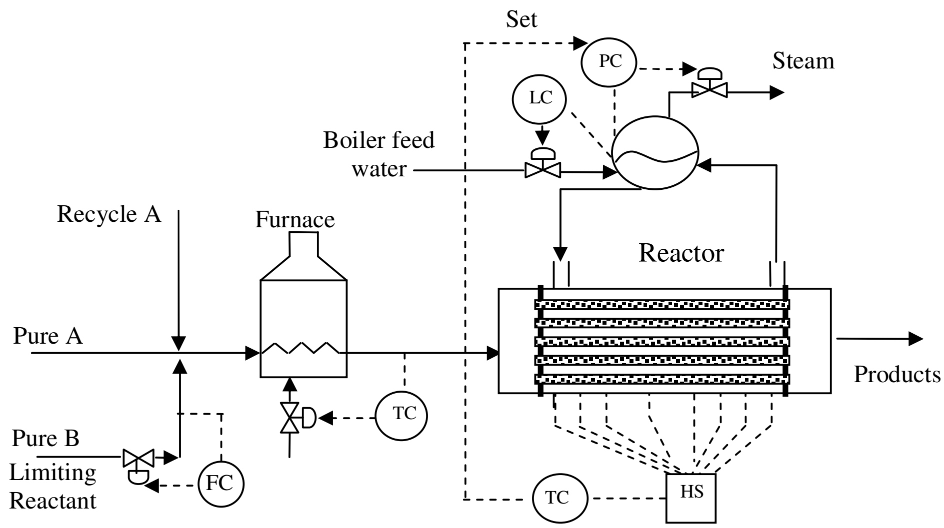
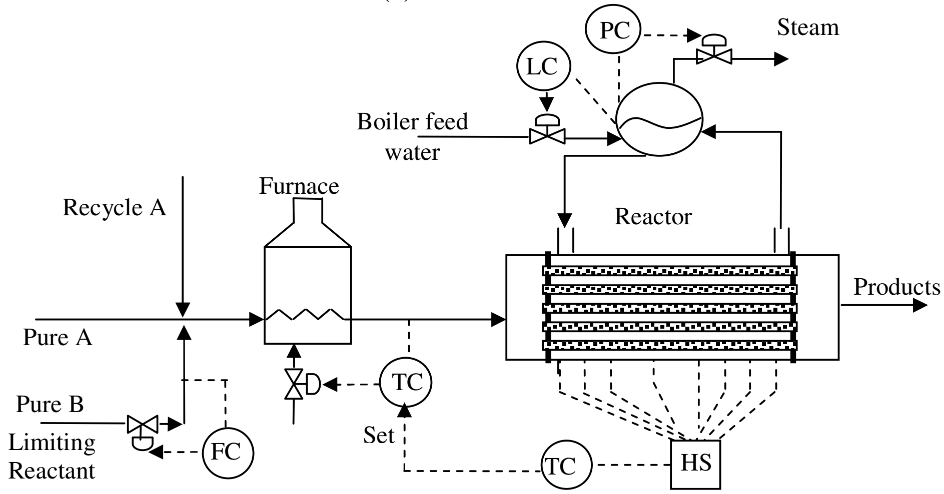


Figure 6.6. Auctioneering temperature control structure

In addition to the reactor cooling duty, there are two other possible manipulation handles for reactor heat management, namely the reactor inlet temperature set-point and the limiting reactant flow rate into the reactor. The schemes are shown in Figure 6.7. Both the schemes work by changing the heat generation due to reaction. The non-linearity between the controlled and manipulated variable is severe in all the three schemes. This may be understood using the analogy of a fire. It is very easy to make a fire whereas extinguishing one requires much effort. Similarly, it requires much more control effort to adjust for an increase in the hot-spot temperature than for the same decrease. The controller thus must be aggressive for deviations in one direction and not too aggressive in the other. Gain scheduling is sometimes used with the magnitude of the controller gain depending on the magnitude and sign of the error signal (or a more sophisticated schedule). The possibility of temperature run-away also requires that large overshoots above the set-point be avoided even as the controller is aggressive. The derivative action is often employed to suppress closed loop oscillations.

(a)



(b)

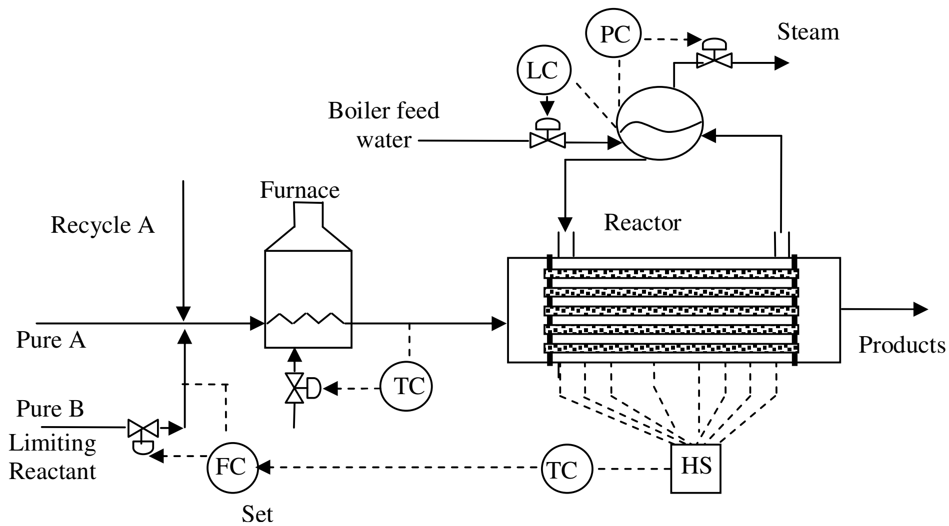
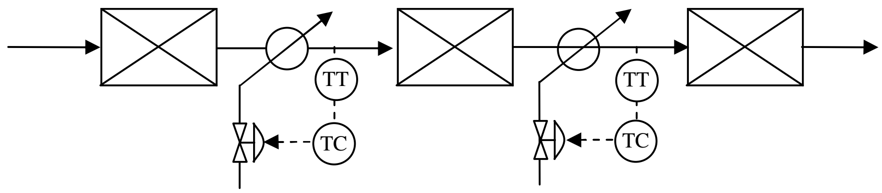


Figure 6.7. Two other possible manipulation handles for reactor heat management

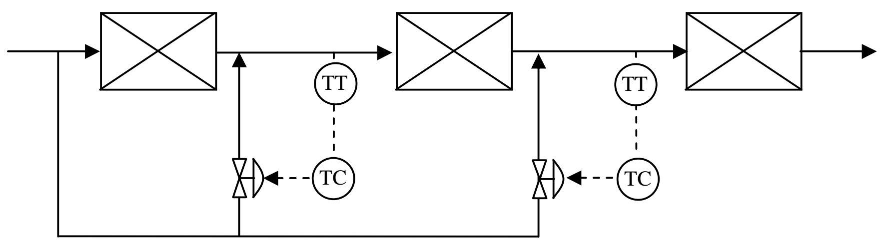
It is noted that controlling the reactor outlet temperature may sometimes provide adequate regulation of the hot spot temperature. The applicability of this much simpler scheme depends on how close the outlet is to the reactor hot spot at the base design condition. When the hot spot is close to the reactor outlet, a change in the outlet temperature correlates well with the change in the hot spot temperature so that controlling the outlet temperature provides adequate regulation of the hot spot temperature.

6.2.3. Intermediate Cooling and Cold–Shot Cooled Reactors

Two other commonly used heat removal configurations, namely, intermediate cooling and cold shot cooling, are shown in Figure 6.8 along with the control structure. Explicit intermediate coolers are provided in equilibrium limited exothermic reactions to increase the overall equilibrium conversion. Cold shot cooling is frequently employed in polymerization reactors where it is extremely important to hold the temperature profile in the reactor to maintain the molecular weight and polydispersity of the product polymer.



(a)



(b)

Figure 6.8. (a) Intermediate cooling in sequence reactors
(b) Cold shot cooling

Modern chemical plants frequently recover the reaction heat using heat integration. A common heat integration scheme employs the feed effluent heat exchanger to preheat the cold reactor feed using the hot reactor effluent gases as in Figure 6.9. The heat integration results in energy recycle loop which can lead to instability. Consider the extreme case of a FEHE that heats the reactants to the reaction temperature so that there is no furnace. If the temperature of the cold reactants rises, the reactor inlet temperature will increase. This would cause more reaction accompanied by heat release resulting in an increase in the hot reactor effluent gas. The hotter effluent would cause a further increase in the reactor inlet temperature resulting in a temperature runaway or instability. This instability can be prevented if the reactor inlet temperature (or outlet temperature) is controlled. The furnace performs this function by breaking the positive thermal feedback loop. An alternative to the FEHE is to recover the reaction heat as steam in a waste heat boiler and feed it to the steam utility network. This removes the thermal feedback while ensuring almost 100% heat recovery.

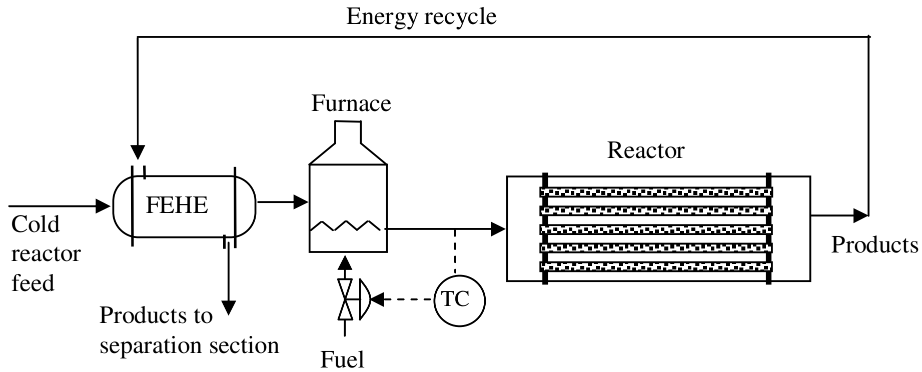


Figure 6.9. Heat integration scheme

Catalytic packed bed reactors differ from simple plug flow reactors in that that the catalyst bed constitutes a significant thermal capacitance. The heat capacity of the packed bed can sometimes lead to the outlet temperature exhibiting an inverse response with respect to the inlet temperature. This effect is due to the difference in the propagation rate of the gas and the bed thermal effect through the reactor. If the reactor inlet temperature decreases, the bed temperature does not decrease immediately. The cooler gas plug thus comes in contact with the hot packing and heats up. The reaction now kicks off leading to the outlet temperature increasing. Once the catalyst bed cools down, the outlet temperature of course decreases. This inverse response or "wrong" way behaviour destabilizes the control loop so that a PID controller must be detuned. In cases where the closed loop performance is not satisfactory, the application of advanced control techniques such as the Smith predictor is recommended.

6.3. Continuous Stirred Tank Reactor

Perfect back-mixing occurs in ideal continuous stirred tank reactors. Due to the mixing, the composition at the reactor is the same as the composition inside the reactor. The reaction thus occurs at the reactor outlet concentration. The reactant, upon entering the reactor, thus gets diluted instantaneously to the lower reactor composition. Since the reaction occurs at the exit conditions, the steady state conversion now depends on both the inlet and outlet conditions. This creates higher non-linearity so that the existence of multiple steady states is a distinct possibility. This is in direct contrast to PFRs where the outlet conditions are uniquely determined by the inlet conditions. Back-mixing thus causes material feedback with the possibility of multiple solutions.

Consider a jacketed CSTR as in Figure 6.10. Assume that the coolant flow rate is high so that the jacket temperature is nearly constant. The heat removal rate varies linearly with the jacket-reactor temperature difference. The heat generation due to reaction is an S-shaped sigmoid with respect to the reactor temperature. At steady state the heat removal rate and the heat generation rate must balance each other. The reactor can exhibit a unique steady state or multiple steady states. These scenarios are depicted in Figure 6.11. For multiple steady states, there are three steady states corresponding to a high, intermediate and low temperature. The high and low temperature steady states are stable while the intermediate temperature steady state is unstable. This is because around the intermediate steady state, if the temperature increases slightly, the rate of heat generation increases more rapidly than the rate of heat removal so that the temperature would continue to rise and not return back to the intermediate steady state ie an open loop unstable system. In contrast, at the high / low temperature steady state, the slope of the heat removal curve is more than the heat generation curve in the vicinity of the steady state implying stable open loop behaviour. Typically, reactor operation at the intermediate steady state is desired as the high temperature steady state may lead to catalyst sintering and undesirable side reactions while the reaction rate is small at the low temperature steady state. For such open loop unstable reactors, a temperature controlled must be used to stabilize the reactor. The closed loop system becomes stable for a controller gain above a critical value. At lower gains, the feedback action is not enough to stabilize the unstable system. For extremely large controller gains, the closed loop system becomes unstable due to too much feedback, similar to open loop stable processes. The closed loop system is thus stable only for a range of controller gain. Conventional tuning rules such as the ZN / TLC procedure should therefore not be applied. Multiple steady states are avoided when a large heat transfer area is provided. Unique solution CSTRs are much easier to control and the heat transfer system for CSTRs should be properly designed to avoid multiplicity.

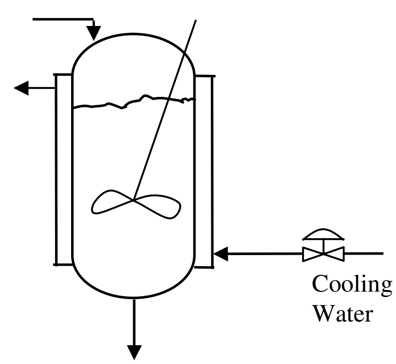


Figure 6.10. High flow rate cooling water temperature control

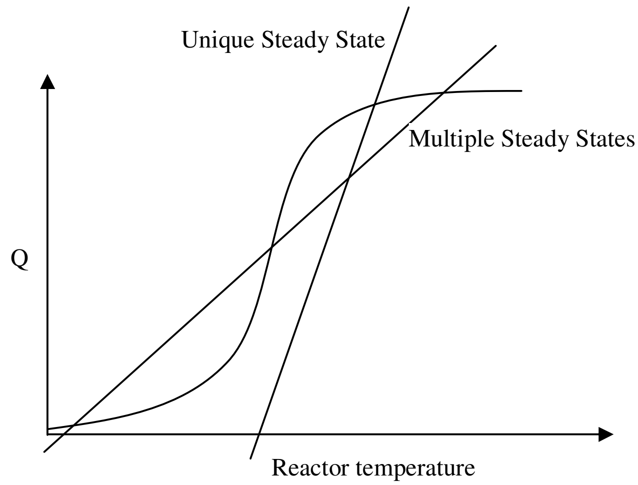


Figure 6.11. Steady states in CSTR

6.3.1. Jacket Cooled CSTR

Evidently, proper regulation of the reaction heat removal is one of the main control tasks. The simplest heat transfer arrangement is that of a jacketed CSTR with cooling water flowing along the jacket. Its flow rate is adjusted to maintain the reactor temperature as shown in Figure 6.12. This approach suffers from drawbacks such as a non-linear process gain due to variation in the heat transfer coefficient with cooling water flow and local reactor hot spots due to the jacket temperature profile. These problems can be mitigated by using a recirculation loop as shown in Figure 6.13(a). The recirculation allows for a constant coolant flow rate so that the jacket temperature is constant. The reactor temperature is maintained by adjusting the fresh coolant flow rate into the recirculation. The recirculation loop introduces and additional thermal lag into the heat transfer loop resulting in a slow closed loop response. The use of a cascade control scheme as in Figure 6.13(b), where the jacket temperature is tightly controlled by adjusting the coolant flow (slave loop) and the reactor temperature loop adjusts this set-point, significantly improves the closed loop reactor temperature control.

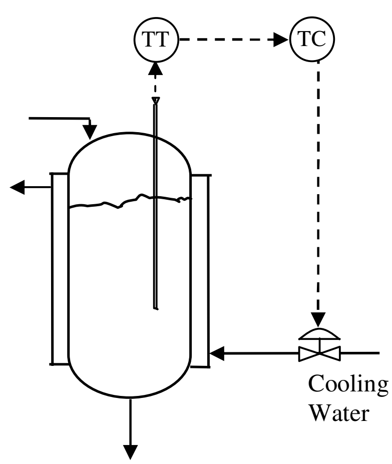
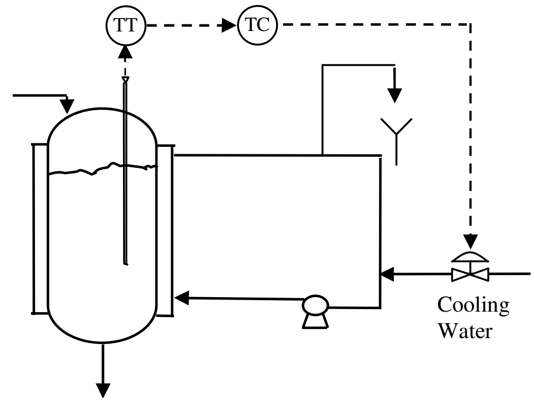
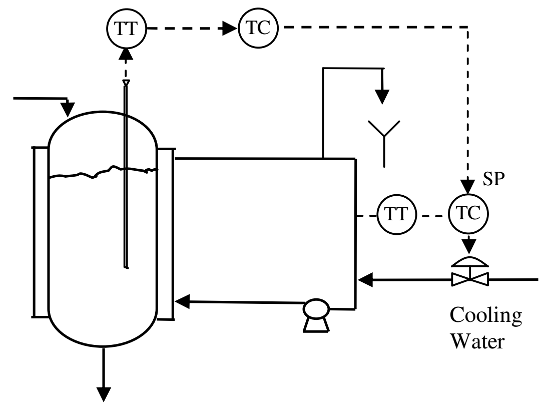


Figure 6.12. Simplest CSTR Control Structure



(a)



(b)

Figure 6.13 (a) Circulating cooling water temperature control
(b) Cascade control

6.3.2. Reaction Heat Removal as Steam

A common arrangement for recovering the reaction heat is to generate steam from the hot pressurized water recirculating in the jacket recirculation loop. The heat removal scheme and the control structure are shown in Figure 6.14. The level in the steam drum would exhibit the inverse response so that the boiler feed water flow into the drum is ratioed to the steam flow with the level controlled adjusting its set-point. This arrangement allows for the feed water to move in the correct direction for load changes.

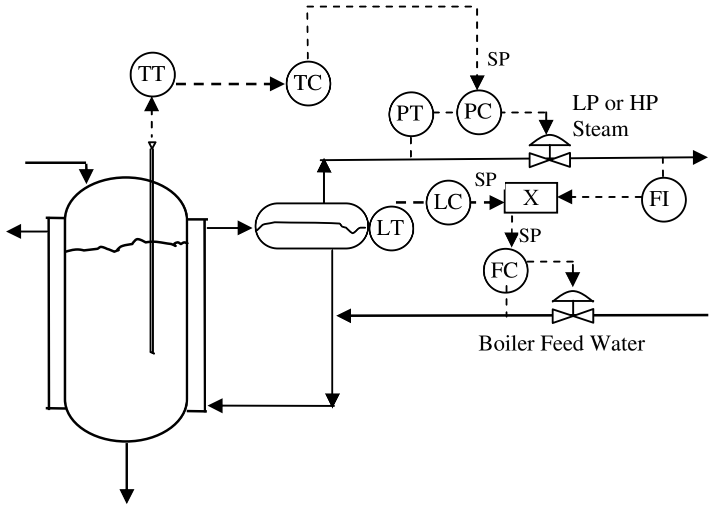


Figure 6.14. Temperature control through steam generation

6.3.3. External Heat Exchanger

In high temperature applications, the generation of steam is not possible so that expensive proprietary coolant oils must be used. An external heat exchanger is then provided as in Figure 6.15 for a closed circuit coolant loop. Cooling water is used as the coolant in the external heat exchanger to remove the reaction heat carried by the hot oil. The control structure shown in the Figure is self explanatory.

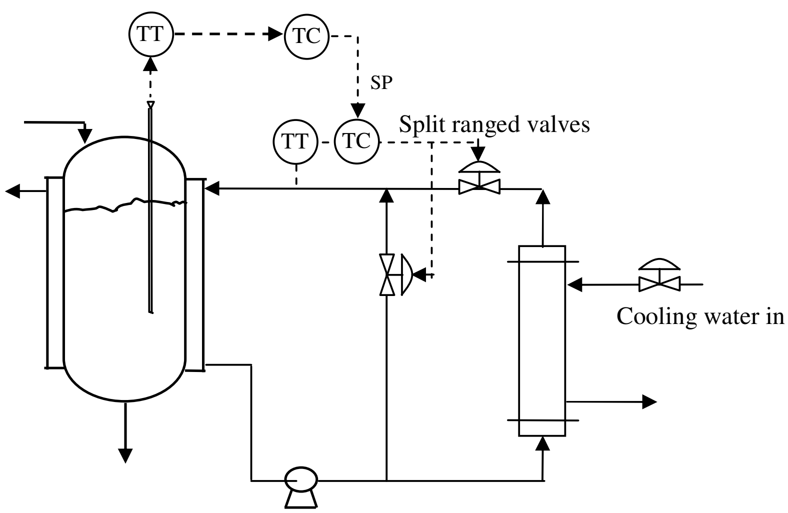


Figure 6.15. Use of external Heat exchanger for temperature control

6.3.4. Cooling Coils

In the jacketed CSTR, the heat transfer area is determined by the reactor volume and may not be sufficient. Cooling coils, as in Figure 6.16, are used for higher heat transfer area per unit volume. The control scheme adjusts the coolant flow rate for maintaining the jacket temperature.

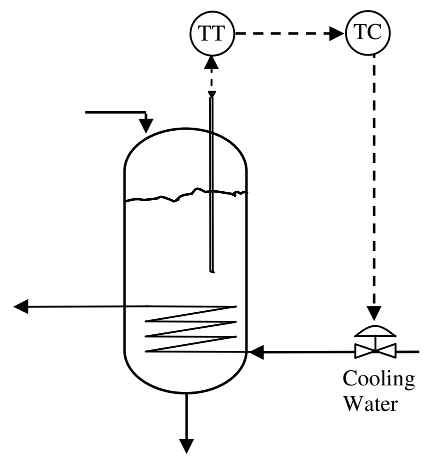


Figure 6.16. Extended heat transfer area through use of cooling coils

6.3.5. External Cooling by Content Recirculation

Another alternative for removing the reaction heat when the jacket heat transfer area is insufficient is to circulate the reaction mixture through an external heat exchanger and feed it back into the reactor. This scheme is shown in Figure 6.17. The reactor temperature is maintained by manipulating the temperature of the cooled reaction mixture from the external heat exchanger. The cooling water flow rate into the heat exchanger is adjusted to maintain the cooled reaction mixture temperature. In this control scheme, the external heat exchanger introduces a significant thermal lag into the slave loop. The dynamics of the slave loop can be significantly improved by a slight design modification providing for bypassing a small fraction of the reaction mixture stream around the external heat exchanger. This is illustrated in Figure 6.18. The thermal lag is thus replaced by the negligible mixing lag as the dominant time constant of the slave loop resulting in significantly improved reactor temperature control.

6.3.6. Boiling CSTR with External Condenser

When the reaction mixture boils, excellent reactor temperature control can be achieved using an external condenser that condenses the vapour and refluxes the cold condensate back into the reactor. The arrangement is shown in Figure 6.19. Note that the condensate flows back into the reactor by gravity so that the condenser should be at a sufficient elevation above the reactor. The U-leg seal is provided to force the vapour to enter the condenser from the correct entry port. Note that the reactor temperature in this case is self-regulatory..

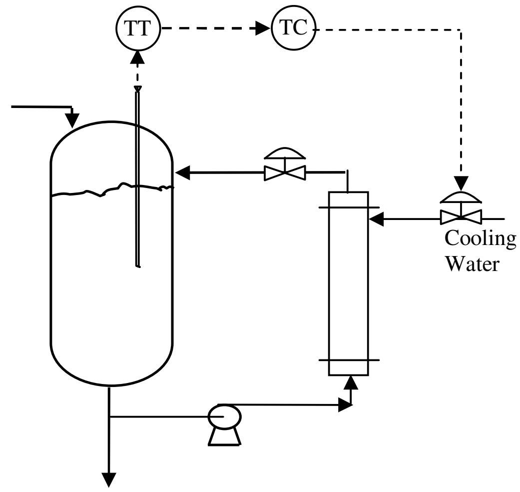


Figure 6.17. Circulation of reactor contents through external heat exchanger

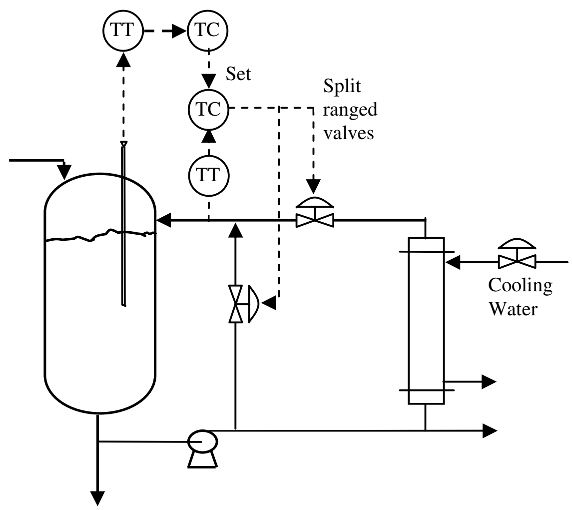


Figure 6.18. Bypass of circulating reactor content around external Heat exchanger

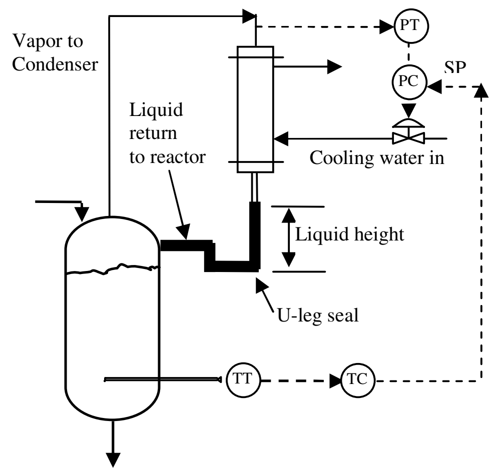


Figure 6.19. Cooling through vaporization of reactor content

6.3.7. Reactor Heat Removal Capacity Constraint

A possibility for controlling the reactor temperature when the heat transfer area is limiting is to adjust the reactant feed rate so that the heat generation due to reaction changes appropriately. The cooling water valve is fully open. The scheme is shown in Figure 6.20. While, appealing in its own right, this control strategy should not be implemented in practice (or used with due caution) as the open loop dynamics of the temperature loop is slow due to the composition lag introduced by the reaction mixture volume. As the feed rate changes, the composition of the reaction mixture changes slowly due to the large reactor hold up. The reaction heat generation thus changes slowly. In case the reactor temperature goes down, the temperature controller would add more feed. The unreacted reactant amount in the reactor thus goes up. Once the reactor temperature begins to increase, reaction would "kick-in" due to the large amount of unreacted reactant inside the reactor. The possibility of a reactor run-away is thus always lurking in the back-drop, especially for highly exothermic reactions. The scheme may be workable for mildly exothermic reactions.

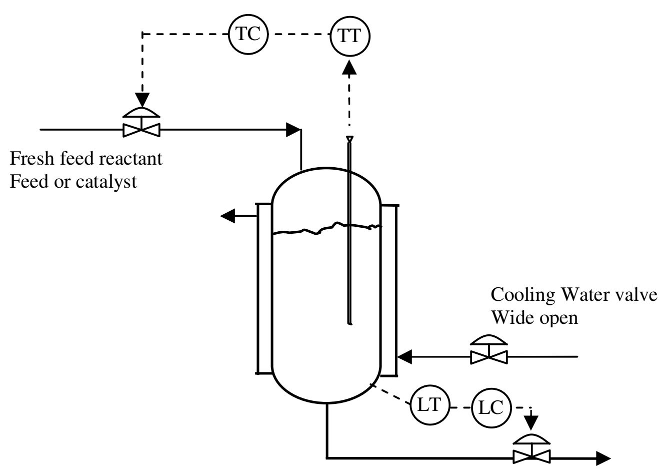


Figure 6.20. Temperature control by manipulating the fresh feed rate

The problem of reactor runaway can be circumvented by the use of a valve positioning scheme as illustrated in Figure 6.21. The reactor temperature is controlled by adjusting the reactor cooling duty. The valve positioning controller measures the cooling duty valve position and slowly adjusts the feed rate so that eventually the cooling duty valve is near fully open and the reactor operates at maximum through-put. In this scheme, the temperature control loop effectively rejects short term disturbances as its dynamics are much faster compared to controlling the reactor temperature directly using the fresh feed rate. Over the long term, the VPC ensures the reactor is operating at near maximum cooling duty, ie maximum through-put. Note that the feed rate can be directly manipualted in a PFR since the material flows through as a plug and there is no back-mixing implying little / no build-up of unreacted reactants inside the reactor.

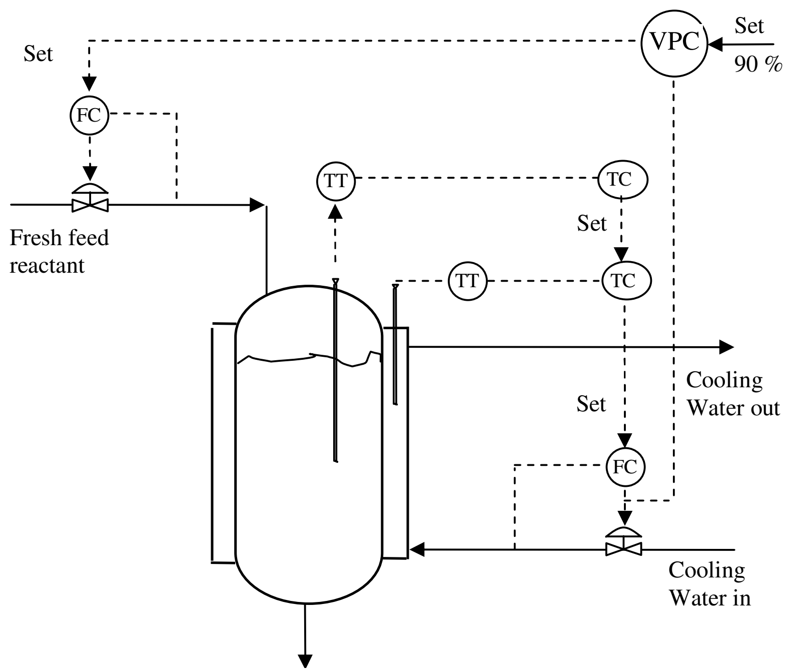


Figure 6.21. Valve positioning control for throughput maximization

Chapter 7. Heat Exchanger Control

Heat exchangers are widely used for heating / cooling process streams to the desired temperature or to change the phase of a stream. The heat exchanger is thus for removing / adding sensible or latent heat. Figure 7.1 shows the schematic of a counter-current shell and tube heat exchanger. The hot stream flows through the tubes and loses its heat to the cold stram flowing through the shell. The heat exchange is driven by the temperature difference between the shell side and the tube side. For a given inlet temperature of the hot and cold streams, the temperature driving force is more for the counter-current flow arrangement. Most exchangers are thus operated with counter-current flow.

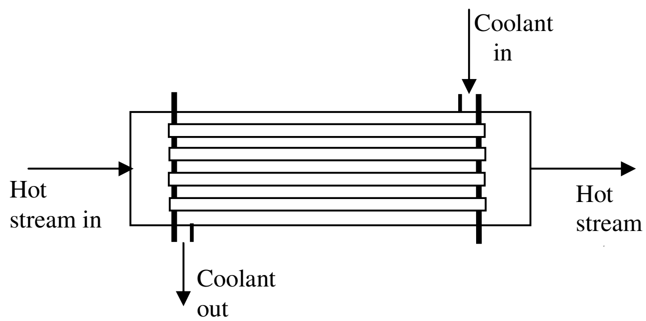


Figure 7.1. Counter current Shell and Tube heat exchanger

The heat exchangers in a process can be usefully classified into utility heat exchangers or process-to-process heat exchangers. Utility heat exchangers typically use steam or cooling water to respectively add or remove heat from a process stream. In process-to-process heat exchangers, both the hold and cold streams are process streams.

7.1. Control of Utility Heat Exchangers

The purpose of a utility heat exchanger is to provide (remove) as much heat as is necessary to maintain the process stream temperature. A simple temperature controller that adjusts the utility flow rate to maintain the process stream temperature accomplishes this function. Figure 7.2(a) shows a cooler that uses cooling water for heat removal. Figure 7.2(b) shows a heater using steam as the utility fluid. The control loops are self-explanatory.

Sometimes the heat transfer is controlled without adjusting the utility flow. For example in a partial condenser that vents the non-condensables as a vent stream, the cooling water valve is fully open and the vent rate is adjusted to control the condenser pressure. The pressure sets the dew point temperature of the condensables in the vapour stream fixing the temperature driving force across the tubes. The control scheme is illustrated in Figure 7.3.

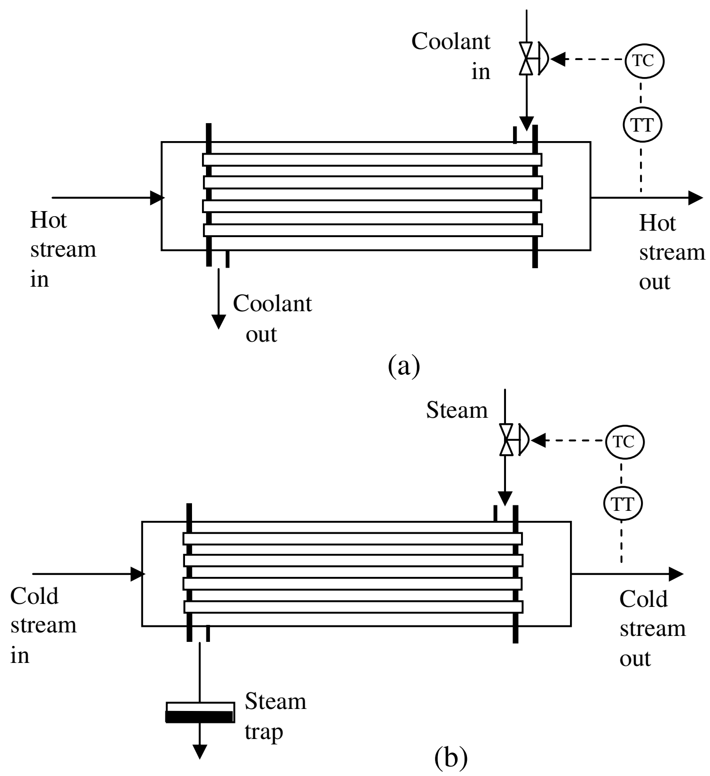


Figure 7.2. Control of utility exchangers

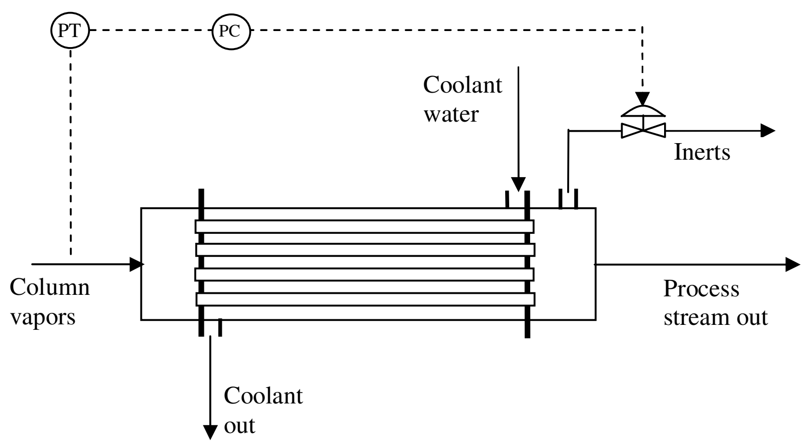


Figure 7.3. Indirect control of Heat exchanger using partial pressure of non-condensable

The flooded condenser is another common arrangement where the level of the condensate determines the number of tubes that are submerged. Heat is thus transferred only across the tubes exposed to the vapour. The cooling rate thus gets adjusted to maintain the pressure by manipulating the condensate draw which affects the level. The liquid hold up inside the condenser represents a significant lag (~2-5 minutes) so that the pressure cannot be controlled very tightly. Flooded condenser arrangement is shown in figure 7.4.

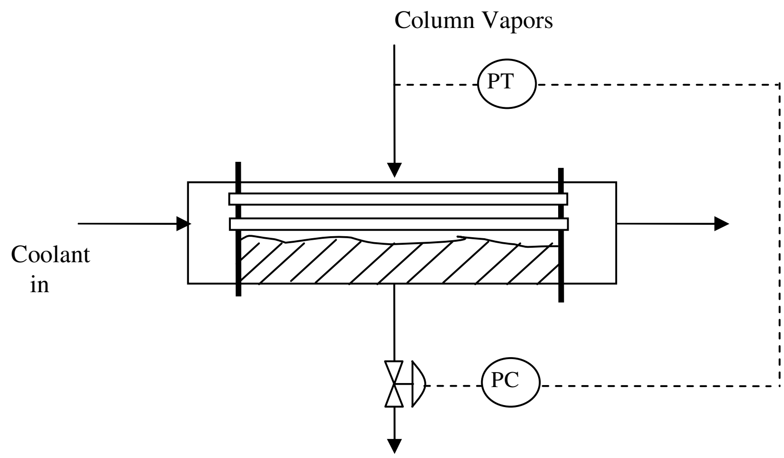
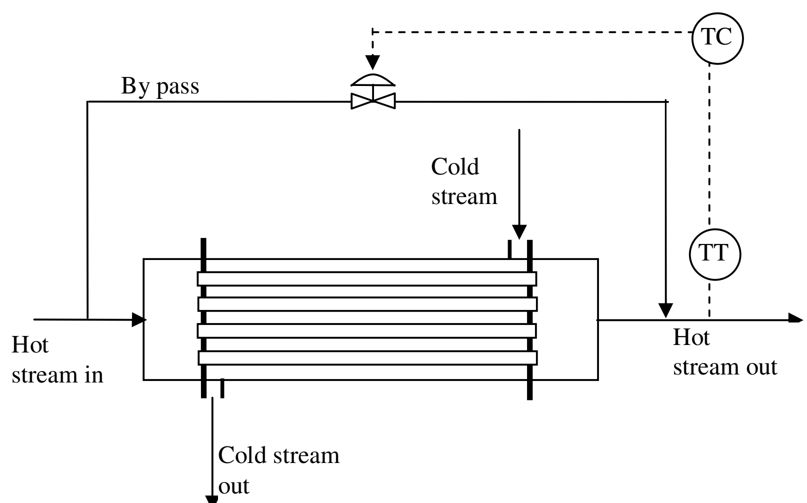


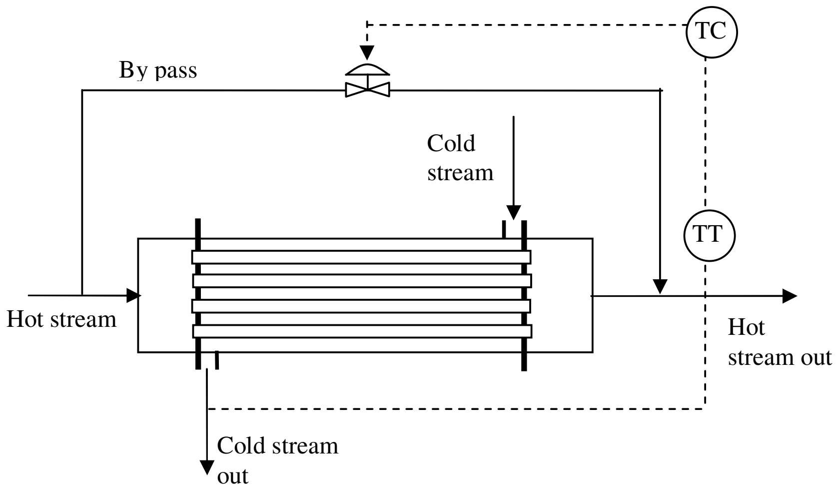
Figure 7.4. Heat transfer control by variable heat transfer area in flooded condenser

7.2. Control of Process-to-Process Heat Exchangers

Process to process heat exchangers transfer heat between two process streams. The flow of these process streams is usually set elsewhere in the plant so that adjusting the flow rate of one of the process streams to regulate the amount of heat transferred is not possible. To provide a control degree-of-freedom for regulating the heat transferred, a small by-pass (~5-10%) of one of the process streams around the heat exchanger is provided. The outlet temperature of this process stream or the other process stream can be controlled by manipulating the by-pass rate. These two schemes are illustrated in Figure 7.5. In the former, tight temperature control is possible as the amount of heat transferred is governed by the bypass. In the latter, a thermal lag of the order of 0.5 to 2 minutes exists between the manipulated and controlled variable.



(a)



(b)

Figure 7.5. By-pass control of process to process heat exchangers
(a) Controlling and bypassing hot stream
(b)Controlling cold stream and bypassing hot stream

Process-to-process heat exchangers are increasingly used for heat integration to minimize the energy consumed per kg product. Given that the flow of the two process streams into the heat exchangers is set elsewhere, an auxiliary utility heat exchanger is often provided to control the temperature of the more important process stream. The size of the auxiliary utility heat exchanger should be large enough for effective disturbance rejection.

In the plant-wide context, heat integration using process-to-process heat exchangers causes interaction between the interconnected units. In particular, it is necessary to ensure that in the quest for maximum energy recovery, energy recycle circuits do not lead to instability. Sufficient control degrees-of-freedom should be provided in the form of auxiliary utility exchangers so that the variability is transferred to the plant utility system.

Chapter 8. Control of Miscellaneous Systems

In this chapter, the control of other common units in the industry such as furnaces, compressors, refrigeration systems and plant utility systems is briefly described.

8.1. Furnace Controls

A furnace heats a process stream to high temperature using combustion of a fuel as the heat source. It consists of a fire box or combustion zone with tube bundles carrying the process stream to be heated. Fuel is burnt with air in the combustion zone to heat the tubes to very high temperatures. Typically a convective heat transfer zone is also provided in furnaces to recover heat from the hot flue gases. The furnace is essentially a reactor combusting fuel with air. The control objective is to satisfy the 'on-demand' heat load. The control system shown in Figure 8.1 is typically used. The fuel-to-air ratio must be nearly stoichiometric for complete combustion of the fuel. Excess air is not fed in as that would increase the flue gas discharge rate. Less than stoichiometric air would lead to partial combustion or worse, unburnt fuel remaining in furnace. The flue gas oxygen concentration is a good indicator of the quality of combustion and adjusts the fuel-to-air ratio set-point. The air is fed in ratio to the fuel. The forced draft fan speed is varied to change the air feed rate. An induced draft fan is provided at the outlet to suck the flue gases out of the furnace. Its speed is controlled to maintain the pressure inside the combustion chamber.

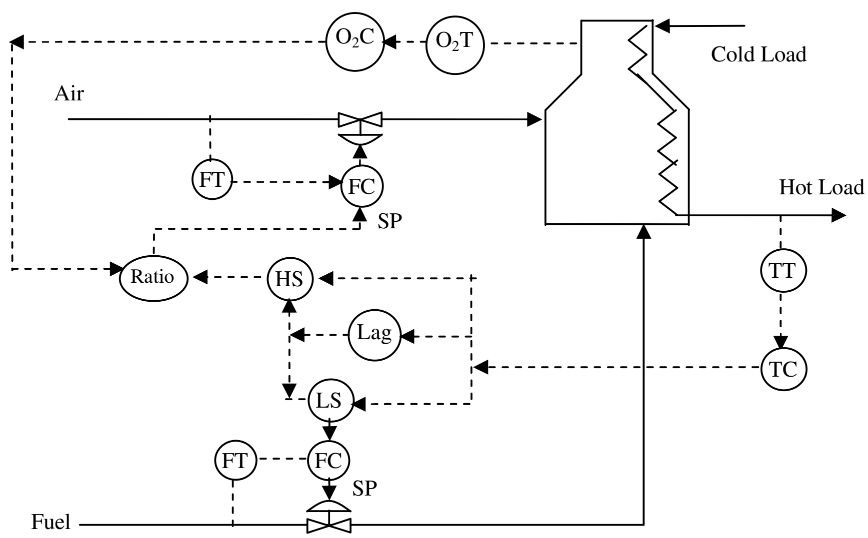


Figure 8.1. Furnace firing controls

A critical safety requirement is to operate the furnace such that the air is fed in excess during transients (load changes). This is necessary to ensure that all the fuel fed into the furnace is burnt and no unreacted fuel remains inside, lest it combust later to damage the furnace. Thus if the heat load increases, the air rate must be increased before the fuel valve is opened. On the other hand, if the heat load decreases, the fuel valve must be closed before the air flow is reduced. This control action is accomplished by lagging the heat load signal as shown in Figure 8.1. The lagged and the unlagged signals are then input to a high selector and a low selector. The output of the high selector sets the air flow controller set-point. The output of the low selector sets the fuel flow controller set-point. If the heat load increases, the high selector sends the unlagged signal to the air flow controller causing an instantaneous increase in the air flow. The low selector sends the lagged signal to the fuel flow controller. The fuel flow thus lags behind the air flow for an increase in the heat demand. For a decrease in the heat load, the high selector sends the lagged heat load to the air flow controller while the low selector sends the unlagged heat load to the fuel flow controller. The air thus lags behind the fuel for a heat load decrease. Furnace operation in excess air is thus ensured during transients.

8.2. Compressor Controls

Compressors are used to increase the pressure of gas stream. A cooler with a knock-out pot is typically provided at the compressor outlet to cool the hot pressurized gas and remove any condensables that liquefy due to the higher pressure and cooling. There are three important types of compressors used in plants, namely, centrifugal, axial and reciprocating. In reciprocating compressors, the through-put is adjusted by manipulating the strokes per minute or the length of a stroke. A recycle is always provided around the outlet of the compressor for the safety of the compressor.

Centrifugal compressors are similar to centrifugal pumps in that a rotating motor is used to impart energy to the fluid. To control the through-put, three configurations are typically used, namely, exit recycle, suction throttling and motor speed manipulation. These three schemes are illustrated in Figure 8.2. In the exit recycle scheme, a recycle around the compressor back to the inlet is provided which is adjusted to manipulate the through-put. Note that the total (recycle + fresh) flow rate through the compressor remains the same so that compressor operates at a single point on its characteristic curve. This is the most energy inefficient method of compressor operation. Also, note from the figure that the recycle is provided after the cooler so that energy recycle is prevented. In suction throttling, a valve is provided at the compressor suction and the through-put is manipulated by adjusting the suction pressure. At lower through-puts lesser energy is consumed as the amount of material flowing through the compressor is less. The most energy efficient method of throughput manipulation is to vary the rpm of a variable speed drive. High pressure steam, as in a turbine, is used many a times to provide the motive force for rotation. A cascade speed controller that adjusts the steam flow rate set-point maintains the drive speed. The drive speed set-point is input remotely by the through-put controller.

Another important consideration in compressor control is the prevention of surge at low flow rates. The compressor characteristic curve shows a maximum and the compression ratio dips a low flow rates due to compressibility. So much so, that if the flow rate goes low enough, the flow through the compressor can reverse direction. This causes the suction pressure to build and the flow almost immediately reverses direction again (i.e. flows out the compressor). This flow reversal cycle repeats in less than a second. To prevent the compressor surge phenomenon, the compressor discharge is recycled to the compressor suction. An anti-surge controller, as in Figure 8.3 adjusts the recycle rate to prevent the flow through the compressor from dropping below a minimum. Note that this minimum must be sufficiently above the surge flow rate for the particular compressor rpm (or maximum rpm for variable speed drives).

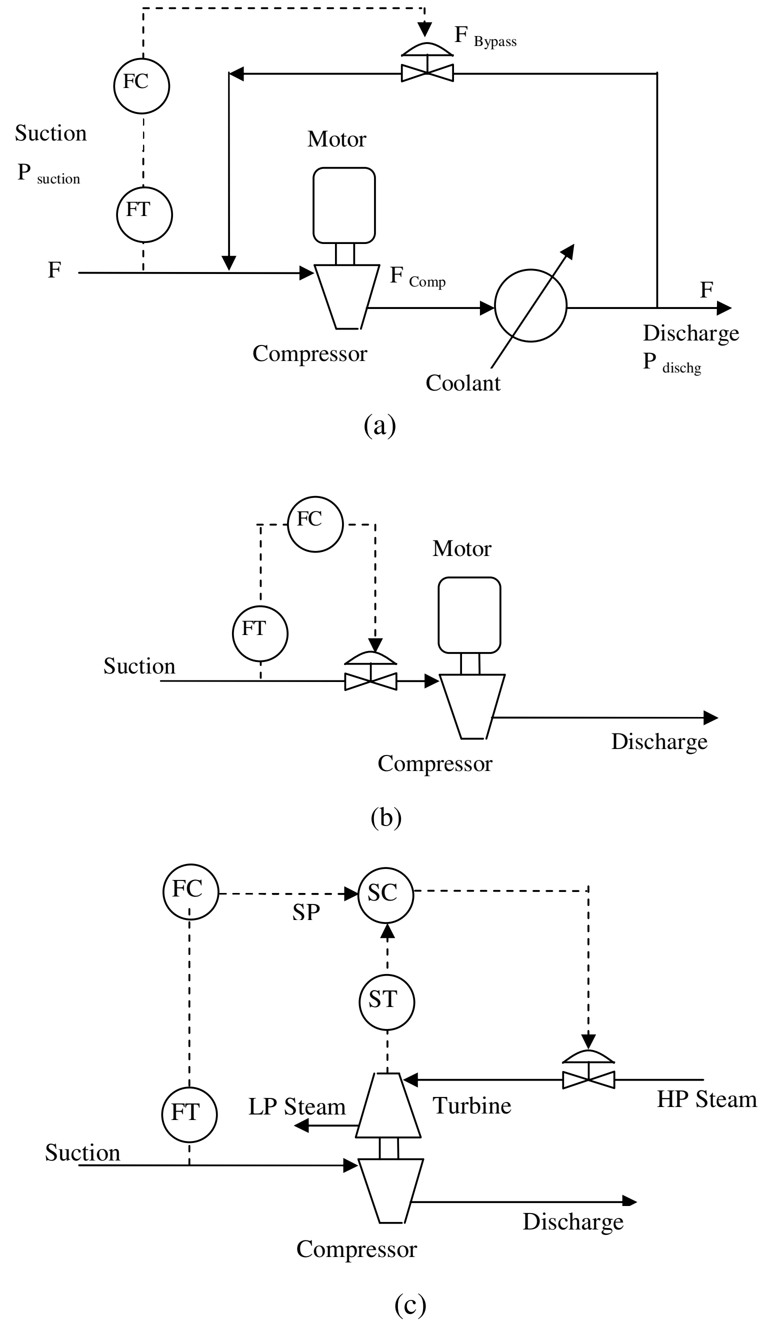


Figure 8.2. Compressor controls
(a) Exit recycle
(b) Suction throttling
(c) Motor speed manipulation

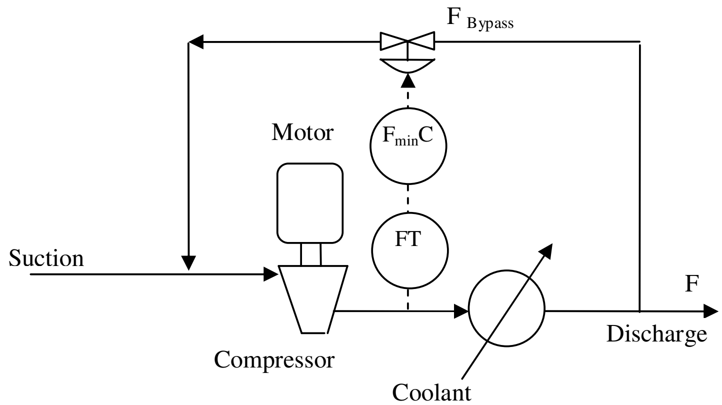


Figure 8.3. Compressor antisurge controller

8.3. Decanter Control

Decanters separate a heterogenous liquid-liquid mixture into its constituent liquid phases by utilizing the density difference between the liquid phases. The heterogenous mixture phase separates into a heavy and light liquid phase. Typically, the heavy liquid phase is aqueous while the light liquid phase is organic. Appropriately located withdrawal ports are provided in a decanter for removing aqueous and organic streams. To prevent the aqueous liquid from entering the organic liquid withdrawal port, the level of the liquid-liquid interface must be controlled. Also the organic phase level must be controlled. The simplest scheme, shown in Figure 8.4(a) manipulates the organic and aqueous stream flow rates to adjust the respective levels. The organic level controller must however interacts with the aqueous level controller. A simple and effective strategy for removing the interaction is to adjust the total flow out from the decanter to control the organic phase level. Figure 8.4(b) shows the corresponding control scheme. The organic stream flow is manipulated to maintain total flow (organic + aqueous) out of the decanter. The organic level controller sets the total flow set-point.

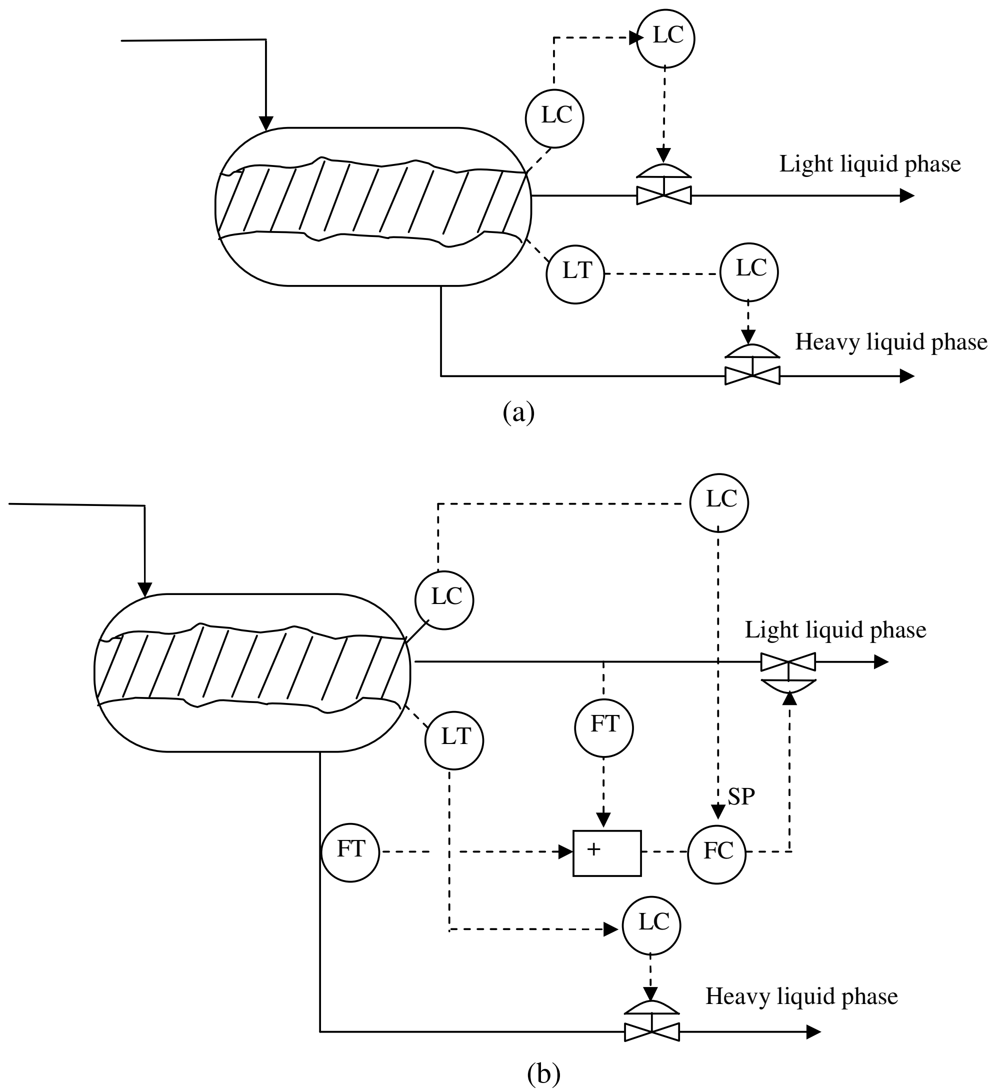


Figure 8.4. Decanter Controls
(a) Conventional level control
(b) Buckley control structure to eliminate interaction

8.4. Control of Refrigeration Systems

We study control schemes for the commonly used vapor compression and vapour absorption refrigeration cycle.

8.4.1. Vapor Compression Cycle

The refrigeration cycle typically employs compression. The cold refrigerant absorbs heat from the process stream and vaporizes in the evaporator. The vapour is compressed so that at the higher pressure, cooling water can be used to condense the refrigerant. The condensed refrigerant is collected in a surge drum and fed to evaporator. Figure 8.5 shows control schemes for the compression refrigeration cycle. The chilled process stream temperature controller sets the evaporator pressure set-point. The evaporator pressure is controlled by adjusting the compressor suction valve. The level in the evaporator is controlled by adjusting the liquid refrigerant inlet valve. In case a variable speed drive compressor is used, the pressure controller is done away with and the temperature controller directly sets the drive speed set-point. The pressure controller is necessitated in the compressor suction throttling scheme to compensate for the throttling valve non-linearity. In the variable drive speed compressor, the variation in the suction pressure (evaporator pressure) with respect to the drive speed is relatively linear so the drive speed can be directly adjusted by the temperature controller. The level in the refrigerant surge drum is not controlled as the refrigerant forms a closed circuit. Notice that the heat transfer rate changes as the temperature driving force across the condenser changes due to the dependence of refrigerant boiling temperature on the evaporator pressure.

8.4.2. Vapor Absorption Cycle

In addition to compression systems, refrigerant absorption systems are also applied industrially. The absorption based refrigeration cycle and its control scheme is shown in Figure 8.6. Ammonia (refrigerant) rich strong liquor is distilled at high pressure to recover liquid ammonia as the distillate and ammonia lean weak liquor as the bottoms. The liquid ammonia is fed to the evaporator where it absorbs heat from the process stream to be chilled and evaporates. Vapor ammonia is absorbed by the 'weak liquor' water stream. The 'strong liquor' so formed is fed to the distillation column to completed the closed circuit refrigerant loop. The temperature of the chilled process stream is controlled by adjusting the level set-point of the evaporator. The heat transfer rate is thus varied by changing the area across which heat transfer occurs. The evaporator level controller adjusts the distillate liquid ammonia flow. An increase in the level of the evaporator implies an increase in the ammonia evaporation rate so that the weak liquor rate is increased in ratio to absorb the ammonia vapours. The strong liquor is cooled and collected in a surge drum. The level of the surge drum is not controlled. Liquid from the surge drum is pumped back to the distillation column through a process-to-process heater that recovers heat from the hot 'weak liquor' bottoms from the distillation column. The flow rate of the strong liquor to the column is adjusted to maintain the column bottoms level. Also, the steam to the reboiler is manipulated to maintain a tray temperature.

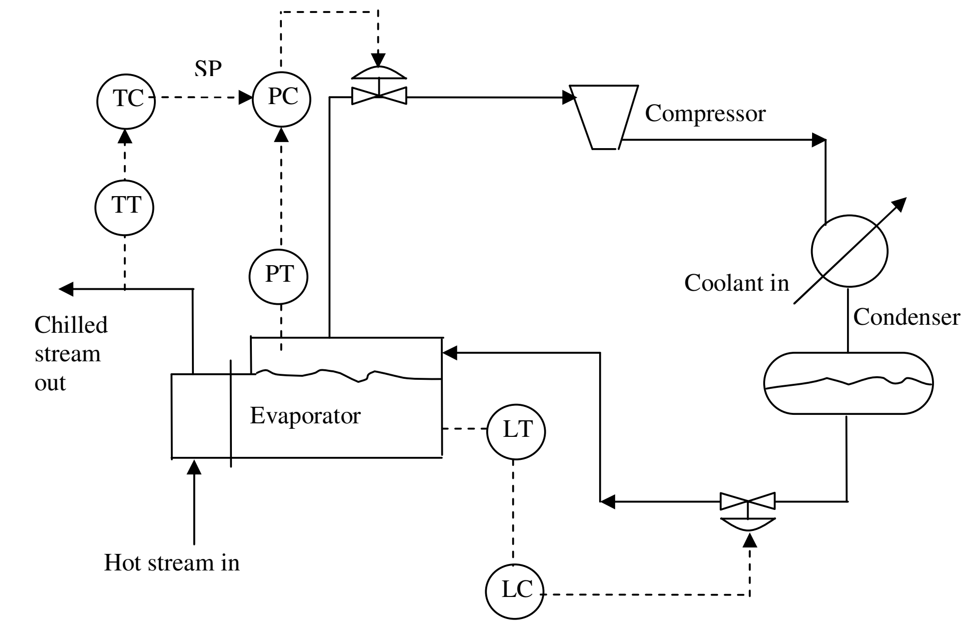


Figure 8.5. Compression refrigeration controls

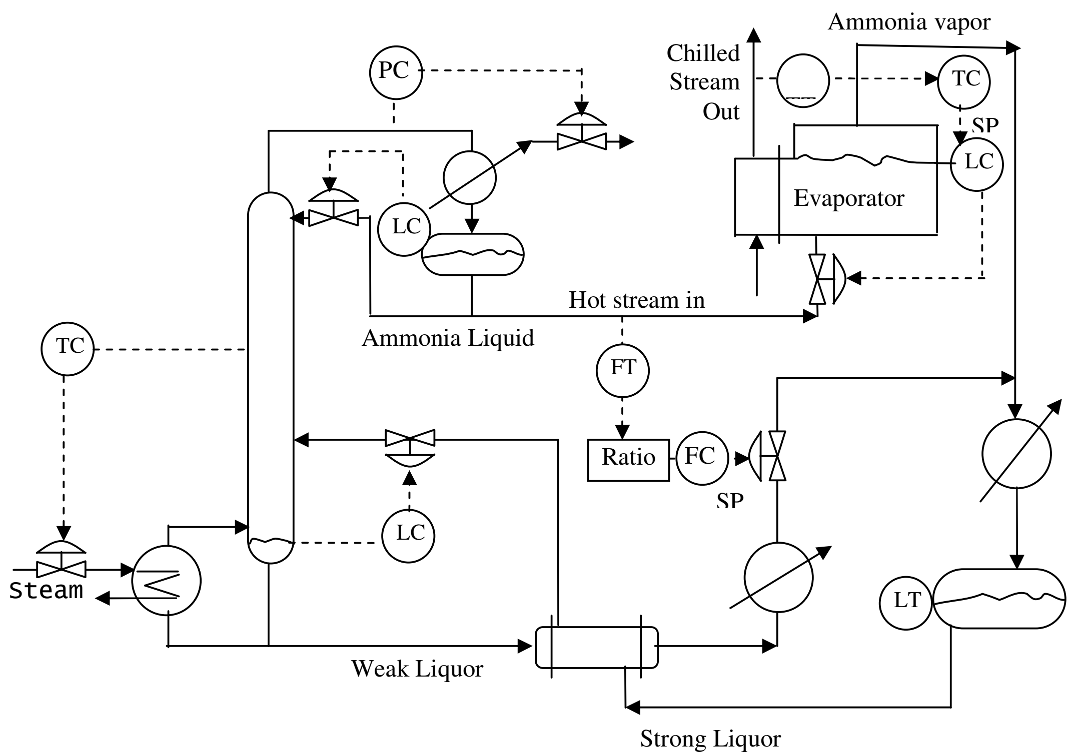


Figure 8.6. Absorption refrigeration controls

8.5. Control of Steam Utility System

Figure 8.7 schematically shows a plant power and utility system. Boiler feed water is heated in a furnace to produce saturated steam. The saturated steam is passed through the furnace to produce superheated steam at 1000 psia pressure. The superheated LP steam drives a turbine to produce electricity. Steam at different pressures is extracted form the turbine for process steam utility requirements. Typically, steam at 300 psia (high pressure steam), 150 psia (medium pressure steam) and 50 psia (low pressure steam) is made available as a heat source at different temperature levels for process use. The pressure of the superheated steam from the furnace is maintained by adjusting the furnace duty. The steam drum level is controlled by adjusting the boiler feed water rate. The pressure of the 300 psia header is maintained in a split range arrangement as shown in the Figure. Steam from the higher pressure header is let in for a decrease in the header pressure while steam is dumped to the lower pressure header for an increase in the header pressure.

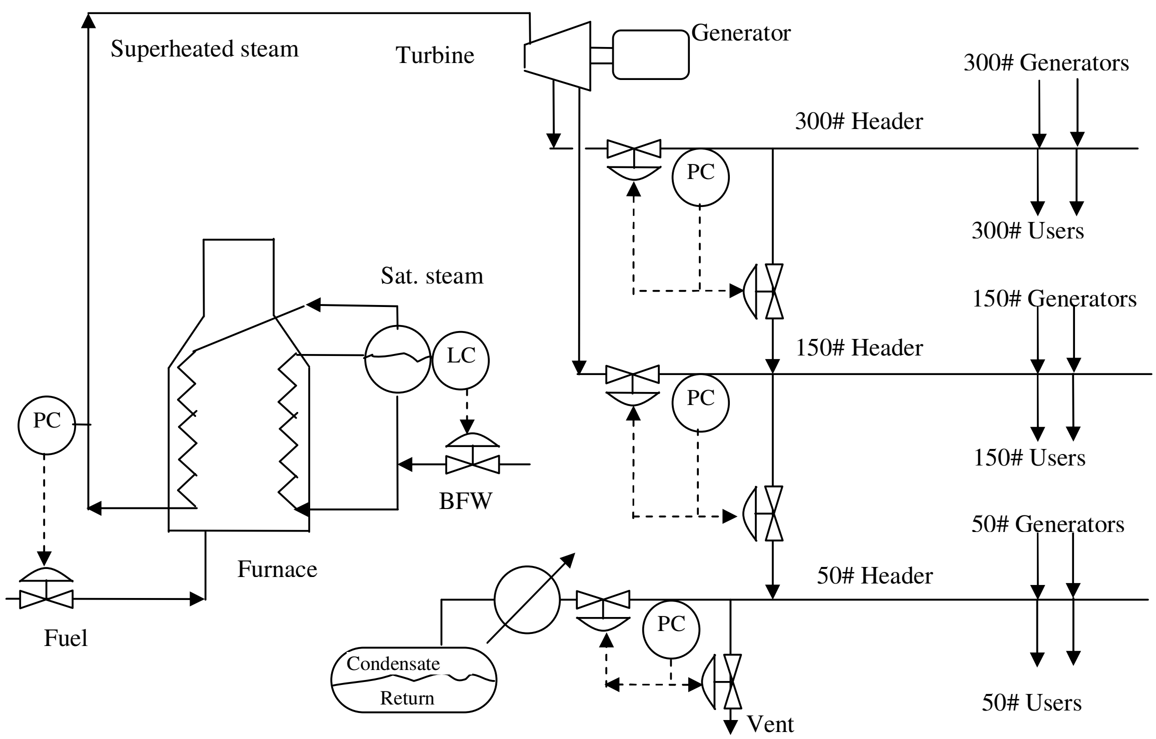


Figure 8.7. Power plant utility system controls

MODULE III

ISSUES IN PLANTWIDE CONTROL SYSTEM DESIGN

The control structures for common unit operations as presented in the previous section may give the impression that developing effective control systems for a complete plant should be a piece of cake in that we simply put in the control structures for each of the individual unit-operations. As we will see in this module, there are unique challenges presented by material / energy recycle that make the plantwide control structure design problem much more challenging than simply putting in structures for each of the individual unit operations. In fact, there are many-many reasonable structures that will work to provide safe and stable operation on a given process. The economic performance of these different structures can however be significantly different. Industrial examples with prudent altering of the control structure resulting in the maximum achievable throughput for the same plant increasing by as high as 20-30% are part of industry folklore. What are the specific plantwide issues that must be considered and addressed in the design of such effective (including economics) plantwide control systems is the focus of this module.

For a firm grip on the plantwide control problem, we start from scratch covering degrees of freedom (control and steady state) and the tremendous flexibility that exists in the choice of the controlled variables (CVs) corresponding to these dofs as well the combinatorial complexity in the manipulated variables (MVs) used to regulate these CVs. We also discuss the snowball effect due to non-linearity caused by material recycle and the integrating nature of the component inventories in a recycle loop. We then discuss the design of the plantwide regulatory control system using the conventional CV-MV pairing approach and the more recent, Luyben pairing approach, along with an illustration on two toy-problems. Finally we bring in economic considerations and show how these considerations may require operating the plant at or close to equipment capacity constraints. We also discuss different ways of handling these constraints and their pros and cons in the plantwide context including illustrations on the two toy examples.

Chapter 9: Control and Steady State Degrees of Freedom

9.1. Control Degrees of Freedom

The plantwide control system design problem can be considered as devising the "best" strategy for managing the available degrees of freedom (dof) in a process. From the operations perspective, a degree of freedom may quite simply be interpreted as having the freedom to make an adjustment, usually to a process / utility flow (a control valve opening). With no control system on a process, the operator is free to adjust the opening of the available independent control valves. These are referred to as the control degrees of freedom. By independent control valves, we imply respecting hydraulic fluid flow laws so that eg on a fluid flow pipe, only a

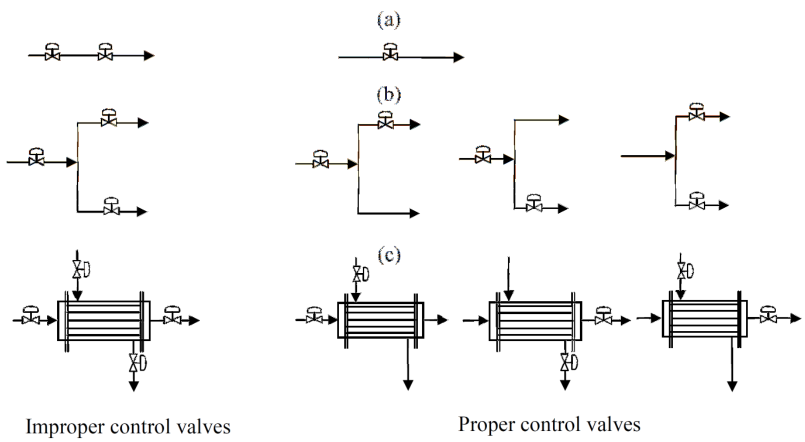


Figure 9.1. Examples of properly and improperly installed control valves
(a) Flow through a pipe
(b) Flow splitter
(c) Process to process heat exchanger

single control valve is adjusted. Figure 9.1 provides illustrative examples of proper and improper installation of independent control valves.

How should adjustments be made to the independent control degrees of freedom (control valves). First and foremost, these adjustments must ensure safe and stable process operation. This requires using a control system for stabilization of potential instabilities and avoiding undesirable drifts in process variables. Reactor thermal runaway is an example potential instability. Process inventories such as liquid levels or gas pressure are examples of process variables that drift in the absence of proper regulation leading to potentially unsafe situations such as a tank running dry / overflowing or a rupture disc breaking open to release pressure. The control system for safe and stable process operation is referred to as the basic regulatory plantwide control system.

Given basic regulatory control that ensures safety, stability and acceptably small drifts, further adjustments may be made to any remaining valves or to the setpoints in the regulatory control system for ensuring the process is operated in the most profitable manner. This may correspond to operating condition adjustments (valve positions or regulatory loop setpoints) to e.g. minimize steam consumption per kg product, maximize yield to the desired product, on-aim product quality with no product give-away, proper effluent discharge management etc.

9.2. Steady State Degrees of Freedom

For continuous chemical processes, it is the steady state at (around) which the process is being operated that determines the operating profit. Of all the control degrees of freedom, not all affect the steady state. This is illustrated for a very simple 'three-tanks-in-series' process in Figure 9.2. There are four control valves. Since liquid level in a tank is non-self regulatory (i.e. unless the inflow and outflow are exactly balanced, the level is either rising or receding), all three tank levels must be controlled to avoid large drifts in the levels. This would take away three control valves leaving one valve free. Let us say this free valve is at the process feed. We may then flow control the feed stream using this valve to set the fresh feed flow at the desired value. The level controllers then adjust the respective tank outlet valves as shown in Figure 9.2. The operator can adjust 4 setpoints (one fresh feed flow setpoint and three level setpoints). Of these the final steady state is determined only by the fresh feed flow setpoint and not by the choice of the level setpoints, which only has a dynamic effect. We therefore distinguish between the steady state operating degrees of freedom and the control degrees of freedom. The steady state operating degrees of freedom is the number of independent adjustments (to valve positions or regulatory setpoints) that affect the process steady state. For the simple example process, the

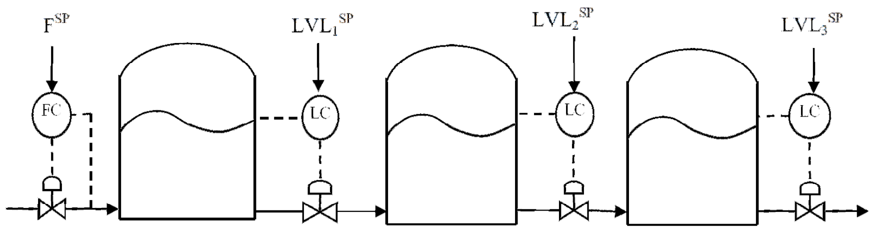


Figure 9.2. Three-tank-in-series process

steady state operating dof is 1, corresponding to the steady flow through the process, while the control dof is 4 corresponding to the number of independent control valves. Notice that the number of setpoints that the operator must input to the control system is 4, the same as the number of independent valves. Of these, the level setpoints have no steady state effect. Only the feed flow setpoint affects the steady state.

This then leads to a very simple procedure for calculating the steady state degrees of freedom for a process. We count the number of independent control valves and subtract the number of non-reactive surge levels as they have no effect on the steady state solution. If the inventory however is reactive, eg level in a liquid phase CSTR, it must not be subtracted (discounted) as the inventory (reactor holdup) affects the reaction extent (conversion) and hence the steady state solution. We also subtract any other variables (e.g. column pressures) that must be kept fixed at a given value for operational reasons to obtain the steady state operating degrees of freedom.

As an illustration, consider a simple distillation column. It has six valves (including feed). Two valves will get used for reflux drum and bottom sump level control. One valve would get used to control the column pressure. Usually the column pressure must be maintained at the design value so that temperature inferential control can be applied. Also the column feed is not in our hands and is specified by an upstream process. Thus for a given feed and column pressure, the steady state operating dof of a simple distillation column is 6 - 2 levels - 1 column pressure - 1 column feed = 2. The operator is free to make 2 independent adjustments. These 2 independent adjustments may be made for maintaining 2 variables such the light key impurity in the bottoms and the heavy key impurity in the distillate.

In Figure 9.3, we show typical steady state dofs for simple unit operations with the implicit assumption that the feed to the unit is given (eg set by an upstream process). Figure 9.4 shows the steady state dof calculation for two example chemical processes. Notice the ease with which dofs can be calculated without having to worry about number of independent variables and number of independent constraints, counting which can befuddle even experienced engineers.

9.3. Degrees of Freedom, Controller Variables (CVs) and Control Structures

The steady state operating dofs are the number of independent adjustments an operator can make to a process that would affect the steady state solution of the process. Consider a simple distillation column. Given the column pressure and feed rate, the operator may choose to keep two appropriately chosen variables constant, corresponding to the two steady state dofs. The simplest option is to fix the reflux rate(L) and the boilup(V). This is equivalent to choosing L and V as the two column specifications. For changes in the feed rate / composition, the light key and heavy key impurity in respectively, the bottoms and the distillate, would show unacceptably large variation. To prevent excessive heavy key leakage down the bottoms, the operator may choose to adjust the boilup to maintain a sensitive stripping tray temperature (T_S). To ensure that the light key leakage up the top is regulated, at least for changes in the feed flow, the operator may choose to maintain L in ratio with the column feed F. This is equivalent to T_S and L/F as the two column dof specifications. We may similarly have the operator maintaining T_S and T_R, a sensitive rectifying tray temperature, or alternatively the distillate heavy key mol fraction (x_{hk}^D) and the bottoms light key mol fraction (x_{lk}^B). Many other choices can be made for the 2 specification variables for simple distillation column. This example shows that there are several options for choosing the specification variable corresponding to steady state dofs.

From the discussion above, it is apparent that holding a particular variable constant implicitly assumes a control loop that manipulates an appropriate valve (or setpoint) in order to maintain the variable. Figure 9.5 shows example control structures corresponding to L-V, L/F-T_S, T_R-T_S and x_{hk}^D-x_{lk}^B as the specification (controlled) variables on a simple distillation column. In these structures a basic regulatory control structure is assumed where feed flow is controlled by the feed valve, column pressure is controlled by the condenser duty and the reflux drum and bottoms levels are controlled using respectively the distillate and bottoms.

Implicit in the pairings implemented in the structures shown in the Figure are some common sense principles. For fast level and pressure control, the manipulated variables are chosen 'local' to the concerned unit. Similarly, reflux is used to control a variable related to the rectifying section (T_R or x_{hk}^D) and boilup is used to control a variable related to the stripping section (T_S or x_{lk}^B). This pairing philosophy reflects the heuristic:

"Choose close by manipulated variables for controlling a process variable for a fast dynamic pairing".

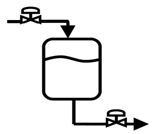
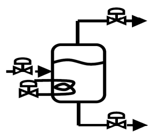
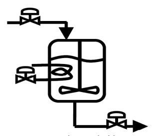
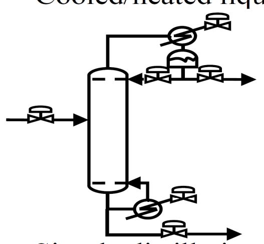
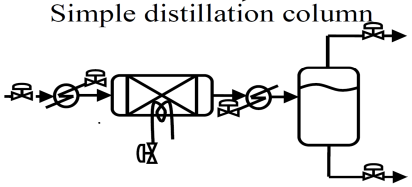
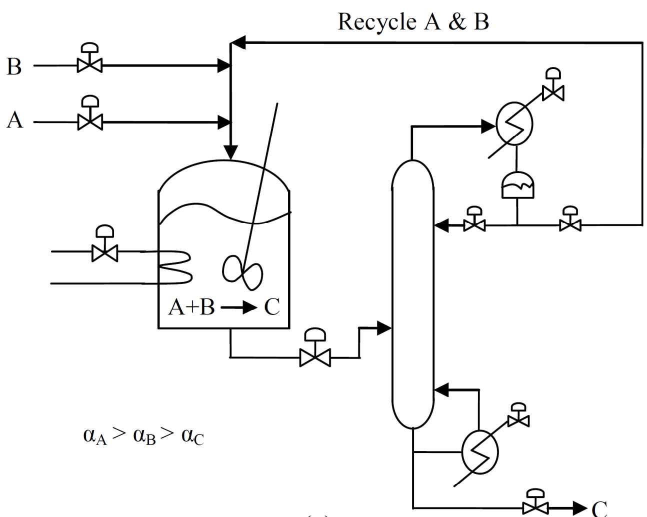
	Unit Operation	Independent control valves (Control dof)	Non-reactive surge levels	Other specification	Steady state dof	Typical steady state dof specification
(1)	 Liquid surge drum	**2**	**1**	**1** (Throughput)	**0**	---
(2)	 Flash drum	**4**	**1**	**2** (Throughput, Drum pressure)	**1**	Drum temperature
(3)	 Cooled/heated liquid CSTR	**3**	**0**	**1**	**2**	Reactor temperature Reactor hold up
(4)	 Simple distillation column	**6**	**2**	**2** (Throughput, Column pressure)	**2**	Reflux & boil up or distillate heavy key impurity & bottoms light key impurity
(5)	 Gas phase packed bed reaction section	**6**	**1**	**2** (Throughput, Flash drum pressure)	**3**	PBR inlet temperature, PBR hot spot/outlet temperature, Cooler outlet temperature

Figure 9.3. Illustration of control and steady state dofs for some typical unit operation

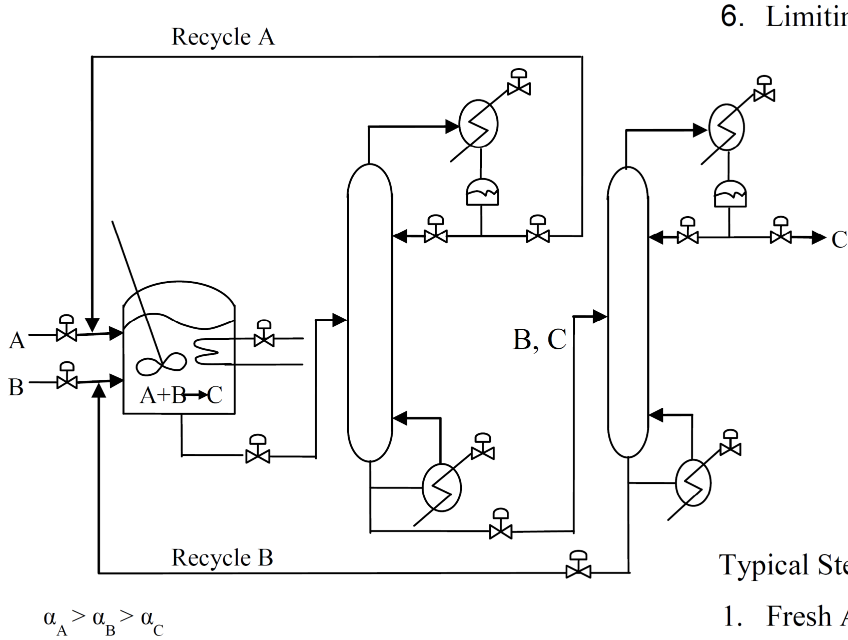


(a)

Control dofs:	9
Non-reactive surge levels:	2
Given column pressure:	1
Steady state dofs:	6

Typical Steady State Specifications

1. Fresh A feed rate (throughput)
2. Reactor temperature
3. Reactor level
4. C impurity in recycle stream
5. B impurity in product C
6. Limiting reactant conc. in reactor



(b)

Control dofs:	14
Non-reactive surge levels:	4
Given column pressures:	2
Steady state dofs:	6

Typical Steady State Specifications

1. Fresh A (or B) feed rate
2. Reactor temperature
3. Reactor level
4. C impurity in recycle A
5. A impurity in column 1 bottom
6. B impurity in product C
7. C impurity in recycle B
8. Total (recycle + fresh) B (or A)

Figure 9.4. Illustration of dof analysis for complete chemical plants

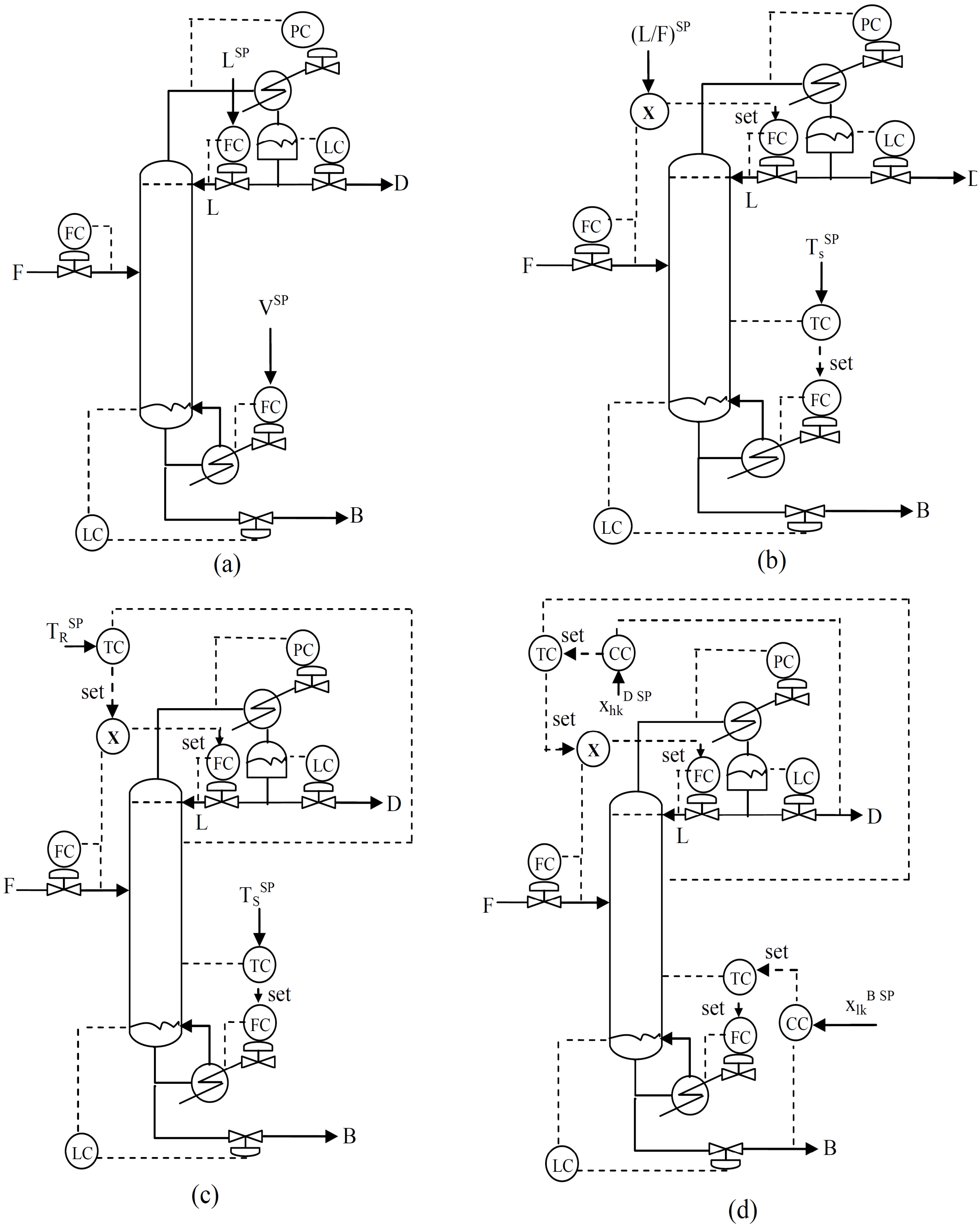


Figure 9.5. Alternative CV_s corresponding to steady state dof_s on a simple distillation column.
(a) L-V (b) L/F-T_S (c) T_R-T_S (d) $x_{hk}^D - x_{lk}^B$

If we let go of the "close-by" pairing philosophy, for the same set of CVs, several alternative pairings can be proposed. Giving up close-by pairing on a unit would usually be due to plantwide control considerations that require tighter control of a particular plant subsection. For example, let us say the distillate from the column feeds the reaction section of a plant, where a highly exothermic reaction occurs. We would like to hold the flow to the reactor section constant to prevent propagation of transients to this section as it is hard to stabilize and variability in the reaction section upsets the downstream product separation section. So now, the distillate must be flow controlled to eliminate flow transients to the reaction section. This flow setpoint then sets the flow through the column, instead of the column feed. Since distillate is fixed, reflux drum level gets controlled using the reflux. The bottoms level is controlled as before using the bottoms. Since it is important to have tight impurity control in the distillate (which feeds a reactor), we use boil-up to control a rectifying tray temperature, as a change in boilup has an almost immediate effect on tray temperature, unlike reflux which has a slower effect particularly if the control tray is further down from the top. This pairing would give tighter distillate impurity regulation. The stripping tray temperature then gets controlled using the column feed. Figure 9.6 shows four alternative pairings for T_R-T_S as the CVs on a column. These structures differ particularly in the location where the flow through the column, also referred to as the throughput, is set. Which structure should get implemented would depend on the specific plantwide context. Even as we have not said much about plantwide control considerations, the point of the whole exercise is to show that even for a simple distillation column with 2 steady state dofs, there exists tremendous flexibility in the control structure that can be implemented on it due to the choice of the specification variable corresponding to the steady state dofs as well as the pairings for the CVs (including regulatory level and pressure loops).

How do we go about systematically choosing the CVs and the corresponding pairings is like piecing a puzzle together. In what follows, we look at different ways of piecing together this puzzle. The first step, as evident in what has already been discussed previously, is to count the number of control and steady state degrees of freedom. The next step is to tabulate the different control objectives and appropriate controlled variables (CVs) for those objectives. All control objectives regulate some process inventory, inventory being interpreted in its most general sense to include total material, phase, component and energy contained in a process unit and the overall process. The regulatory control system is required to ensure (In – Out + Generation) of the inventories in a unit and the overall process is zero so that accumulation is forced to zero to ensure unit specific / plantwide drifts are avoided / mitigated.

The number of CVs are the same as the number of control degrees of freedom and would encompass all inventory regulation objectives. Of these, pure surge capacities have no steady state impact and are therefore economically not relevant. The level of component inventories in recycle loops and product / purge streams on the other hand usually impact the steady state plant economics significantly. The reactor operating conditions (temperature and composition) also are usually important as the single-pass conversion and selectivity determine the cost for recycling unreacted reactants and side-product processing cost.

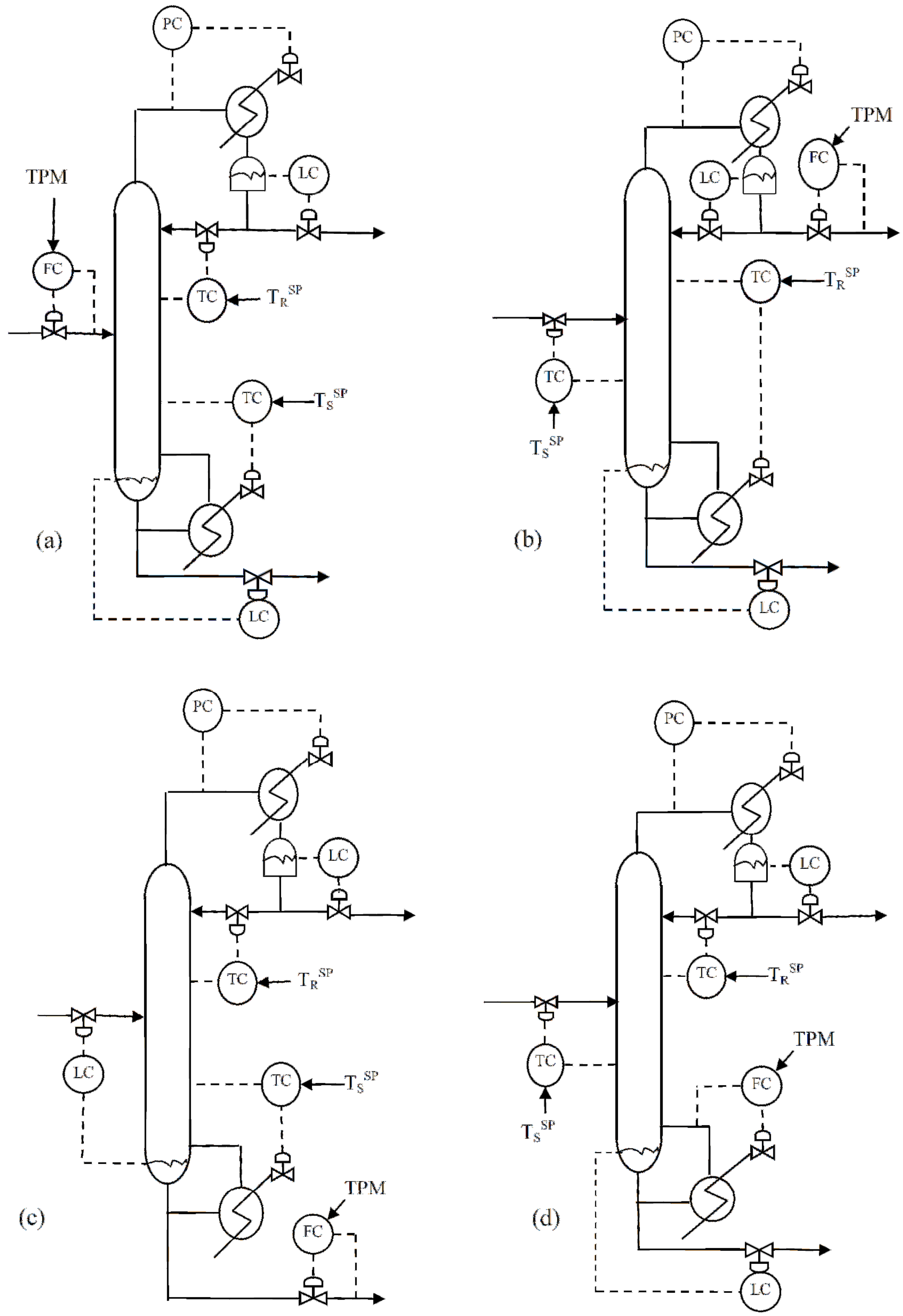


Figure 9.6. Alternative pairings (structure) for holding T_R-T_S as the two steady state dof CV_S as a simple distillation column

9.4. Control Objectives and Choice of CVs

Given a set of control objectives and corresponding CVs plus the prioritization of the CVs, it is relatively straightforward to devise the control loop pairings. How does one go about systematically determining the control objectives and corresponding CVs. To the experienced engineer, control objectives and corresponding CVs for a process are usually evident. To the novice however, this is usually not very clear. In the following we attempt to provide a basic framework to help figure out the control objectives and appropriate CVs.

The control system on a continuous chemical process with material and energy integration may be viewed as an automatic mechanism for ensuring that all process inventories are regulated at safe / optimal levels and not allowed to drift, regardless of process disturbances such as changes in the process throughput, ambient conditions, equipment characteristics etc. All the CVs directly/indirectly reflect process inventories; e.g. level reflects liquid inventory, pressure reflects gas/vapor inventory, temperature reflects energy inventory and composition reflects component inventory (inferential measurements such as column tray temperature or a recycle flow or an appropriate separator level also indirectly reflect component inventory). Since inventories are prone to large drifts (accumulation/depletion) unless regulated, the plantwide control system attempts to maintain them at desired values for economic reasons or at the very least, within an acceptable band (e.g. surge drum levels) to avoid unsafe operating conditions. From the economic standpoint, typically component inventory levels in recycle and product/discharge streams have a large impact on the steady state operating profit so that these should be controlled tightly. On the other hand, surge drum levels that are part of the material balance control system have no effect on the process steady state.

As a starting point, let us take a liquid tank with a liquid stream in and a liquid stream out as a very simple example. If both the inlet and outlet control valves are flow controlled as shown in Figure 9.7(a), the control structure is fundamentally flawed as it violates the overall material balance constraint. Two flows are being independently set and any mismatch in the setpoints would necessarily imply the liquid inventory in the tank (indicated by a level sensor) either builds up (*inflow* > *outflow*) or depletes (*inflow* < *outflow*). The tank is then guaranteed to run dry or over flow. In other words the implemented control system is guaranteed to fail.

The novice may argue that to satisfy the material balance constraint, both the setpoints can be set equal. That still does not solve the basic problem as a mismatch in the two tank flows would any way occur since sensors are never 100% accurate, the slightest of biases implying a slow build-up / depletion in the tank level. The basic issue is that the liquid inventory in the tank is non-self regulatory and must therefore be regulated. We need to measure (or estimate) the liquid inventory and adjust one of the flows to ensure that the inventory is maintained within an acceptable band. The other flow is set independently by the operator or an upstream / downstream process. A direct measure of the liquid inventory inside the tank is its level. Figure 9.7(b-c) shows two workable control configurations that respect the material balance constraint by controlling the tank level.

Even as the above is a very trivial example, treating a complex process with several units and recycles as a tank and questioning if the implemented control system ensures all process inventories (material, phase, component or energy) on each of the individual units as well as the overall process are regulated and do not drift would reveal if the control system is workable or not. We note that routine level, pressure, temperature and flow measurements that indicate appropriate inventory levels are usually self evident.

The control structures on individual unit operations that have already been discussed in previous chapters may be interpreted as regulating inventories. For example, in dual ended temperature inferential LV control structure of a simple distillation column, the condenser duty regulates the column pressure (total vapor inventory), the distillate flow regulates the reflux drum level (reflux drum liquid inventory), the bottoms flow regulates the sump level (sump liquid inventory), the reflux rate is adjusted to maintain a sensitive rectification section temperature to regulate the heavy key leakage in the distillate (component inventory) and the boilup is adjusted to maintain a sensitive stripping tray temperature to regulate the light key leakage down the bottoms (component inventory). Each control loop on the column fixes (regulates) a process inventory. Of these, while the two levels have no economic significance, the light key and heavy impurity leakage levels significantly affect the column energy consumption and are therefore economically important. The interpretation can be easily extended to control structures on other unit operations studied earlier.

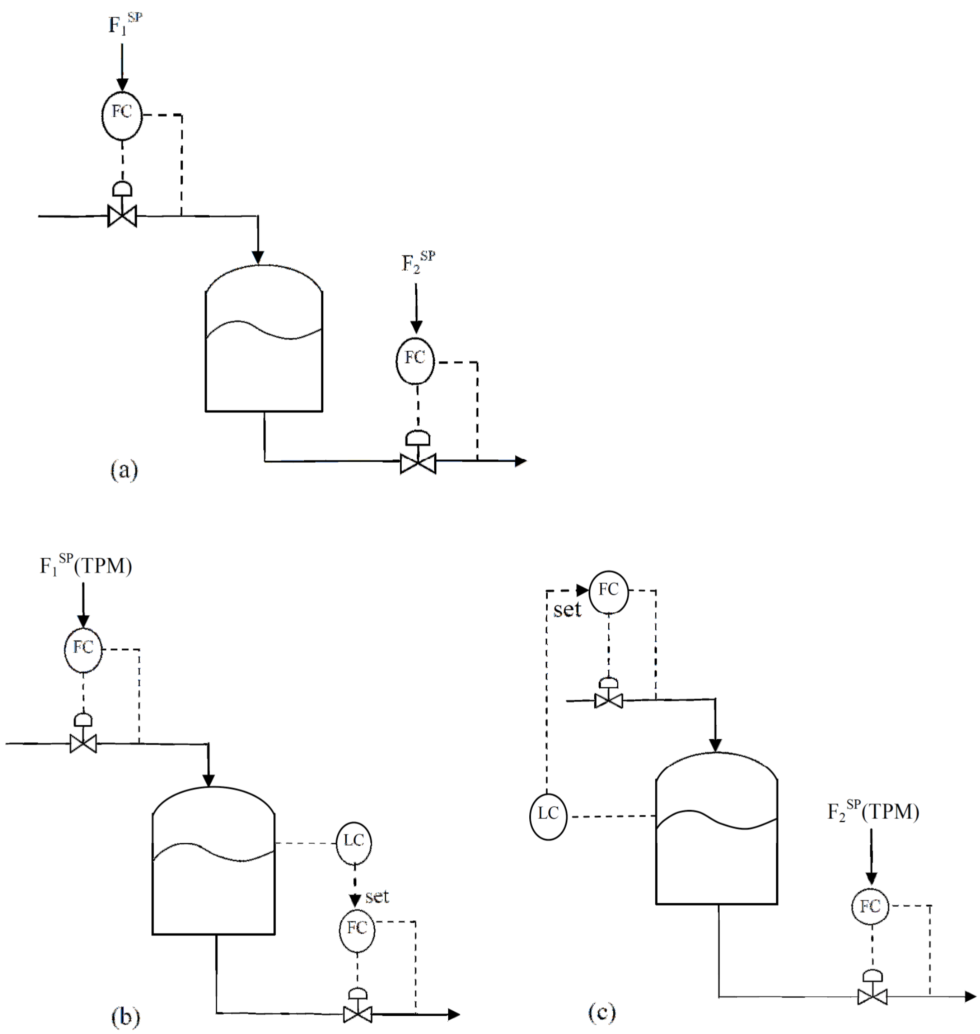


Figure 9.7. Material balance control on a liquid surge drum
(a) Unacceptable control structure
(b) & (c) Acceptable control structure

9.5. Illustration of Control Objectives and CVs for Example Processes

We are now ready to illustrate control objectives and corresponding CVs for a complete plant. Let us consider the process flowsheet in Figure 9.4(a). It has 9 control dofs and these valves can be used for regulating 9 objectives. On the reactor, the total material hold-up and energy hold-up must be regulated. The reactor level and temperature are appropriate CVs for the same (1^{st} – 2^{nd} CVs). On the distillation column, the liquid holdup in the reflux drum and bottom sump must be regulated. Also, the vapor hold-up in the column must be regulated. The reflux drum and sump levels along with the column pressure are appropriate CVs for these inventories (3^{rd}-5^{th} CVs). We also need to regulate the product C leakage up the top and the B impurity leakage down the bottoms. A sensitive stripping tray temperature is a good inferential measure of the latter (6^{th} CV). Holding the reflux in ratio with the column feed would provide loose but adequate regulation of the C leakage in the recycle stream (7^{th} CV).

The remaining 2 control objectives are more subtle. By the design of the process, the recycle stream would contain significant amounts of both the reactants, A and B, with small amounts of C. If we look at the overall material balance across the entire plant, 1 mol A would react with exactly 1 mol of B. The slightest excess of fresh A (or fresh B) is not allowed to leak in the product stream due to a stringent product purity constraint and must necessarily accumulate in the recycle loop. Unless the fresh feeds are balanced exactly as dictated by the reaction stoichiometry, the recycle loop would slowly but surely get filled up with the excess reactant (A or B). The recycle rate and its excess reactant composition would then increase. This slow drift of component inventories inside the recycle loop is referred to as the snowball effect. We need to regulate the component inventory of both the reactants in the recycle loop to ensure stoichiometric feed balancing. This would ensure the recycle rate and its composition does not drift. Since the reactor is inside the recycle loop, one may hold composition of a reactant (usually the limiting reactant) to regulate its inventory (8^{th} CV) and the total flow to the reactor to regulate the inventory of the other component (9^{th} CV). Note that the reactor temperature and composition indirectly sets the production rate inside the reactor through the kinetics. We may change either of these to bring about a change in process production rate.

As another illustration of control objectives, consider the process in Figure 9.4(b). The process control dof is 14. The reactor material and energy inventories are reflected by reactor level and temperature (1^{st} – 2^{nd} CVs). On the first column, the liquid and vapor inventories are reflected by the reflux drum and sump levels and column pressure (3^{rd} - 5^{th} CVs). The column prevents C (heavy key) leakage up the top and A (light key) leakage down the bottoms. Any A that leaks down the bottoms would necessarily end up in the product C stream. It must therefore be tightly regulated and a sensitive stripping section tray temperature is a good inferential measure of the same (6^{th} CV). Since the first column distillate is a recycle stream, loose regulation of the C impurity in it is acceptable. Holding the column reflux to feed ratio (L_1/F_1) constant should suffice (7^{th} CV). On the second column, we again have the reflux drum / bottom sump levels and pressure as measures of liquid and vapor inventories (8^{th} – 10^{th} CVs). The column prevents B (heavy key) leakage up the top and C (light key) leakage down the bottoms. Tight regulation of the B impurity in the product stream (component inventory) is desirable and a sensitive rectifying tray temperature is a good inferential measure of the same (11^{th} CV). Since the bottoms is a recycle stream, loose regulation of the C impurity in it is acceptable. Assuming that boilup is paired for tight control of rectifying tray temperature for tight product quality control, we may hold the reflux-to-feed ratio (L_2/B_1) to indirectly achieve the same (12^{th} CV).

We now consider the stoichiometric balancing of the two fresh feeds to the process. By the design of the process, if an excess of fresh A (fresh B) is being fed, it would accumulate in the A (B) recycle stream. The total (fresh + recycle) A (B) rate would then increase. This total rate to the reactor then indirectly reflects the A (B) inventory in the process. We may then choose the total (recycle + fresh) A to the reactor and total (recycle + fresh) B to the reactor as very convenient measures of the component inventories in the recycle loops (13^{th} – 14^{th} CVs). As in the previous example, the total rate of either reactant to the reactor or the reactor temperature may be adjusted to bring about a change in the process production rate.

Table 9.1 summarizes the regulatory control objectives and corresponding CVs for the two example processes. The relationship of the control objectives with ensuring unit specific and plantwide material and energy balances are evident in the objectives. Comments are also provided to highlight their economic / regulatory significance.

9.6. Snowball Effect

From the discussion above, it is evident that while the inventories that require regulation on a specific unit are quite self-evident, figuring out recycle component inventories that require regulation is subtler and requires some thought with respect to guaranteeing that the overall material balance around the plant for all the components is satisfied. Material recycle introduces high non-linearity into the process with the recycle rates being highly sensitive to small changes in the fresh feed flow(s). This is referred to as the snowball effect.

If we consider the example process in Figure 9.4(a), its steady state dof is 6. The reactor level and temperature and the light key / heavy key leakage in the bottoms / distillate of the column specify four of these dofs. Let us say that we arbitrarily choose the two fresh feed rates as specifications for the remaining 2 steady state dofs. If we try and converge the flowsheet using a commercial simulator, we will find that if the two fresh feeds are specified to be even slightly different, the recycle tear does not converge and keeps on blowing up. This is because the reaction stoichiometry and nearly pure product constraint implies the reactant fed in slight excess has no way out of the process and therefore must necessarily build up in the recycle loop. The sensitivity of the recycle to even the slightest of mismatch between the two fresh feeds is then infinity. If we purge a very small fraction of the recycle stream, the sensitivity of the recycle stream rate to small changes in the fresh feed rates would still be very high, though not infinity. This is the snowball effect.

The choice of the specification variables for the two dofs is not appropriate as the two flows are related by overall process material balance. For robust convergence, a better specification is specifying the total flow rate to the reactor and its A (or B) mol fraction. Both the fresh feeds then get calculated to satisfy these two specifications.

From the operations perspective, if the fresh feed(s) are specified (ie flow controlled), the high sensitivity of the recycle rates to the fresh feeds would cause large swings in the recycle streams and all the equipment in the recycle loop would be subjected to large plantwide transients for small changes in the fresh feed(s). To avoid these large swings, it is better to hold appropriate component inventories in the recycle loop by manipulating the fresh feed(s). The fresh feed(s) are then fed as make-up streams and only as much is fed as gets consumed. Since the reactor is always inside the material recycle loop, a common industrial practice is to hold the total reactant component feed (fresh + recycle) to the reactor constant by adjusting the corresponding fresh feed. In cases where the recycle stream is nearly pure reactant, the corresponding fresh feed may be adjusted to hold the total (recycle + fresh) flow constant. In cases where the recycle stream is a mixture of reactants, appropriate composition(s) inside the reactor and total flow to the reactor are held constant by manipulating the fresh feeds.

The basic idea of feeding fresh feeds to hold appropriate reactor conditions constant achieves two objectives. It ensures the component inventories in the recycle loops are properly managed. Also, by maintaining the reactor operating conditions (flow and composition) constant, robust stabilization of the most non-linear unit operation in the process is achieved mitigating the transients propagated to the downstream separation section.

Table 9.1. Regulatory objectives and CVs for the two example processes

SNo	*Regulatory objective*	*CV*	*Significance*
	Single column recycle process		
1	Reactor liquid inventory	Reactor level	Closes reactor MB[*]. Affects conversion and separation load.
2	Reactor energy inventory	Reactor temperature	Closes reactor EB[**]. Affects conversion and separation load.
3	Column reflux drum liquid inventory	Reflux drum level	Closes reflux drum MB.
4	Column sump liquid inventory	Sump level	Closes sump MB.
5	Column vapor inventory	Column pressure	Closes column EB.
6	Distillate hk[&] (C) leakage	Reflux to feed ratio	Closes the lk/hk balance on the column. Affects column steam consumption. Bottoms B leakage fixed by min product quality. Too much distillate C leakage dilutes reactor reducing conversion.
7	Bottoms lk[%] (B) leakage	Stripping tray temp	
8	Component B circulating in recycle	Reactor B mol fraction	Fixes recycle stream conditions and hence affects column steam consumption.
9	Component A circulating in recycle	Total feed to reactor	
	Two-column recycle process		
1-2	Reactor liquid and energy inventory	Reactor level and temperature	Closes reactor MB and EB. Affects conversion and downstream separation load.
3-6	Reflux drum/sump liquid inventories	Column reflux drum and sump levels	Closes reflux drum/sump MBs
7-8	Vapor inventory in columns	Column pressures	Closes column EBs
9	Column 1 distillate C (hk) leakage	Reflux to col feed ratio	Closes the lk/hk balance on the columns. Affects reboiler steam consumption. Too much C leakage in recycle streams dilute reactor reducing conversion. Col1 bottoms A leakage and Col2 distillate B leakage set by max product impurity specification
10	Column 2 bottoms C (lk) leakage	Reflux to col feed ratio	
11	Column 1 bottoms A (hk) leakage	Stripping tray temp	
12	Column 2 distillate B (hk) leakage	Rectifying tray temp	
13	Component A circulating in plant	Total[#] A to reactor	Fixes recycle stream conditions and hence affects column steam consumption.
14	Component B circulating in plant	Total[#] B to reactor	

*: material balance; **: energy balance; &: heavy key; %: light key; #: recycle plus fresh feed

Chapter 10. The Pairing Issue: Selection of MVs for CVs

Given a set of inventory regulation control objectives and corresponding CVs, the next step is to select the manipulated variable (MV) pairing for each of the CVs. To select pairings for the CVs, they must be prioritized with the pairing for the highest priority CV being selected first followed by the pairing for next one and so on so forth. Different prioritizations would lead to different pairings and hence different control structures.

10.1. Conventional Pairing Approach

The conventional approach to designing the loop pairings is to first choose the process variable that is adjusted for setting the throughput. The setpoint corresponding to that process variable control loop is referred to as the throughput manipulator (TPM). Conventionally, the throughput manipulator is chosen at a fresh feed to the process. Other TPM locations are possible and include the product stream flow for on-demand process operation, where the demand from a customer must be immediately met; an intermediate process stream flow for mitigating transients to the connected unit; directly setting reactor temperature or limiting reactant concentration in a process with a reactor etc.

With the TPM in place, local inventory loops on each of the units are then put in place to establish total material balance / energy balance control. By local, we mean that the MV for controlling the inventory is local to the unit containing the inventory. This is illustrated in Figure 10.1 for the 'three tanks in series process', where the throughput may be set at any of the four process streams. The tank level controllers upstream of the TPM (set flow) are then naturally oriented opposite to the process flow while the level controllers downstream of the TPM are oriented in the direction of process flow. The upstream level controllers act to supply the set flow while the downstream level controlled act to process the set flow. The total material balance control structure thus radiates outwards from the TPM. Local loops for energy balance control would usually include temperature control of an exothermic reactor using reactor cooling duty stabilizing the most non-linear unit in the plant.

With the basic material balance / energy balance control pairings in place, the pairings for the remaining CVs are chosen from the remaining valves. These involve loops for regulating component inventories and are usually economically important. In cases where the open loop response of the CV is sluggish, an appropriate cascade arrangement is implemented with a slave controller holding a faster secondary variable and the master controller holding the primary variable by adjusting the slave loop's setpoint.

10.2. Luyben's Pairing Approach

In the first significant departure from the conventional pairing approach, Luyben et al.[14] insightfully noted that since non-reactive surge inventories have no steady state economic impact, material balance control loops should have lower prioritization so that the best pairings get implemented for the tightest control of economically important CVs. Their prioritization hierarchy thus first fixes the TPM and energy balance control, then establishes loops for economically important objectives (quality, safety, effluent discharge etc) and finally pairs loops for material balance (material inventory) control.

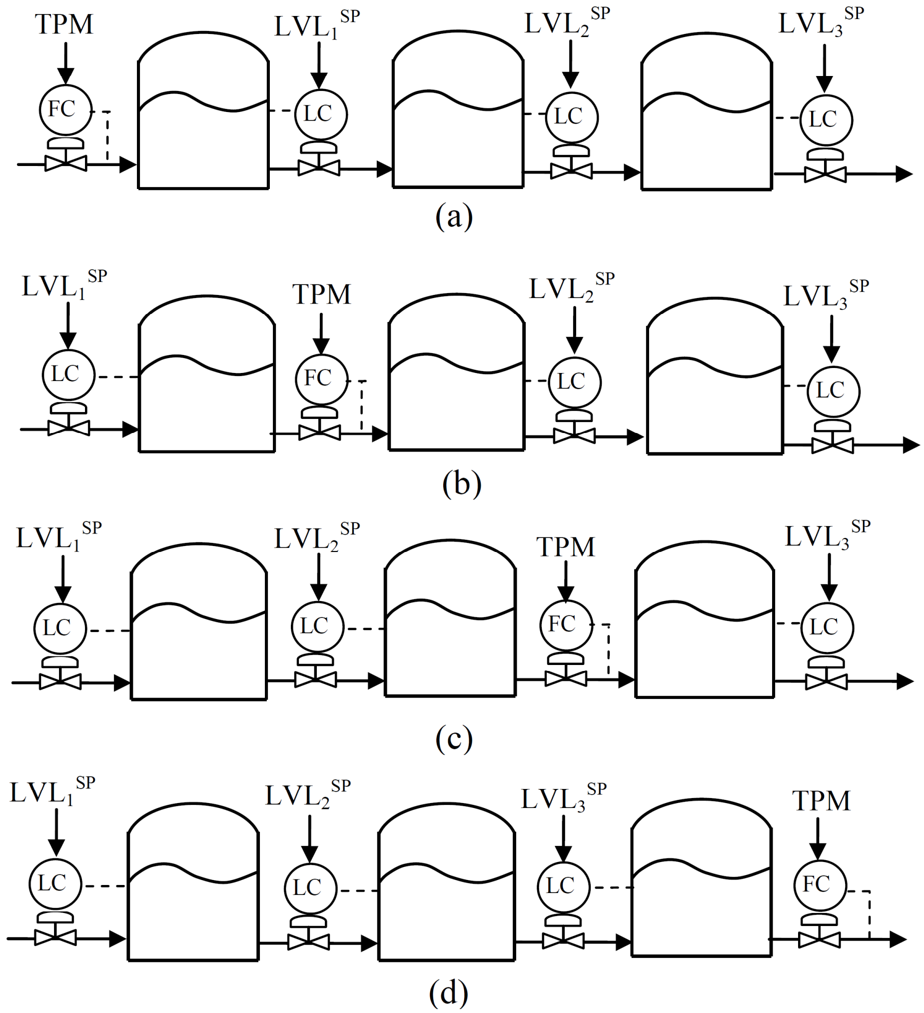


Figure 10.1. Alternative TPM locations and material balance control in three tanks-in-series process

10.3. Regulatory Plantwide Control Structure Synthesis Examples: Conventional vs Luyben's Approach

We are now ready to synthesize and contrast plantwide control structures using the conventional approach and Luyben's approach. For continuity, we consider the two example processes in Figure 9.4.

10.3.1. Single Column Recycle Process

In the conventional approach, the TPM is chosen at a process fresh feed. Let us say the fresh B feed (F_B) is the TPM (1st loop). The reactor temperature (T_{rxr}) is then controlled using its cooling duty (Q_{rxr}), which would provide tight temperature control to regulate the reactor energy balance (2nd loop). Its level (LVL_{rxr}) is controlled using the total flow out of the reactor (F_1) to the column (3rd loop). On the column, the pressure (P_{col}) is controlled using the condenser duty (Q_{cnd}), the reflux drum level (LVL_{RD}) is controlled using the distillate (D_1) and the sump level is controlled using the bottoms (B_1) (4th – 6th loops). The impurity B mol fraction in the product stream (x_B^{B1}) is regulated in a cascade arrangement by adjusting the setpoint of a sensitive stripping tray temperature (T^S_{col}) which manipulates the column boilup (V_1) (7th loop). The C impurity in the distillate (x_C^{D1}) is loosely regulated by holding the reflux in ratio with the column feed (L_1/F_1) (8th loop). Lastly, the B mol fraction in the reactor (x_B^{rxr}) is maintained by adjusting the fresh A to fresh B ratio setpoint (9th loop). Maintaining fresh A in ratio with fresh B ensures the two fresh feeds move together in (near) stoichiometric ratio and large imbalances in the reactant feeds are avoided. The conventional control structure is shown in Figure 10.2(a). Note

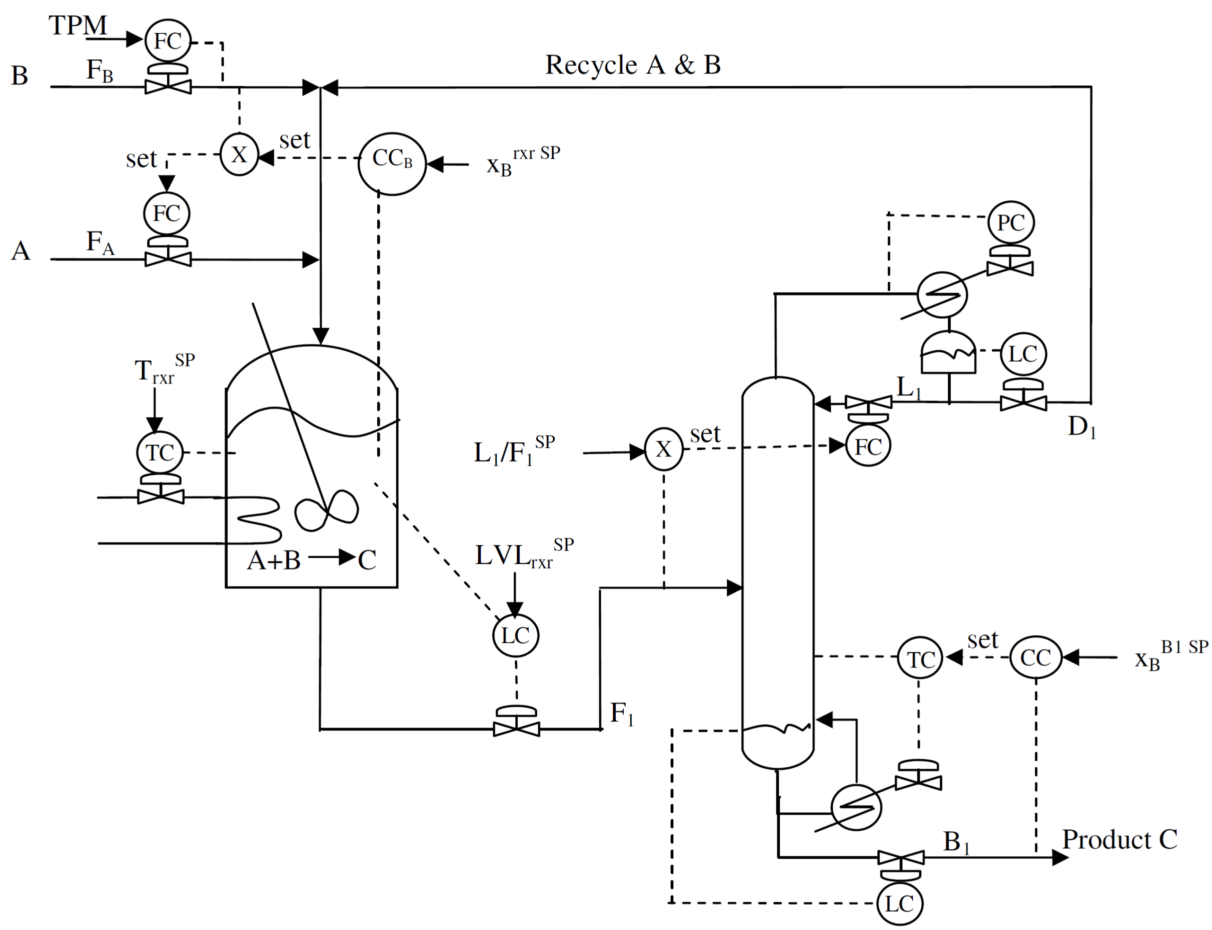


Figure 10.2(a). Conventional control structure with TPM at fresh B

that since F_A is flow controlled, large transient swings in the recycle rate due to the snowball effect are likely with the recycle rate floating to the appropriate value.

In Luyben's approach for plantwide control structure design, the exothermic reactor energy balance regulation loop is first implemented so that a potential instability is first stabilized. The conventional T_{rxr}-Q_{htr} pairing is implemented for tight energy balance regulation (1st loop). We assume the TPM can be placed anywhere in the process and there is no operational constraint such as on-demand operation or a process feed set by an upstream process. Where to locate the TPM is then left as a decision to be taken later. The next loop to be implemented then is the product purity control loop. For tight regulation of x_B^{B1}, a cascade arrangement is implemented with the x_B^{B1} adjusting the setpoint of the T^S_{col} controller which manipulates the column boilup (V_1) (2nd loop). In the absence of any other information, the next loops to be implemented are ones for feeding the fresh feeds as make-up streams. The total flow to the reactor (F_{rxr}) is maintained by adjusting F_B (3rd loop). F_A is maintained in ratio with F_B and its setpoint is adjusted to maintain x_B^{rxr} (4th loop). With these two loops, the recycle rate and composition are not allowed to float or float only within a very narrow band. Snowballing is thus mitigated. We are now ready to put in the material balance control system. The pairings LVL_{rxr}-F_{col}, LVL_{RD}-D_1, LVL_{bot}-B_1 and P_{col}-Q_{cnd} are chosen for regulating the liquid and vapor inventories in the process (5th – 8th loops). Lastly, the L_1/F_1 ratio loop is chosen for managing the column reflux (9th loop). The control structure obtained is shown in Figure 10.2(b). Even as it 'looks' very similar to the conventional structure (Figure 10.2a), the design philosophy including how fresh feeds are managed and the prioritization of the control objectives is very different. To manipulate the throughput, we may adjust either of the T_{rxr}, x_B^{rxr} or F_{rxr} setpoints. Usually T_{rxr} is not adjusted as the catalyst has a very narrow operating temperature range for which the manufacturer guarantees catalyst life. Also, usually the reactor must be operated with one of the reactants being limiting which would fix x_B^{rxr}. F_{rxr}^{SP} is then the only option for the TPM.

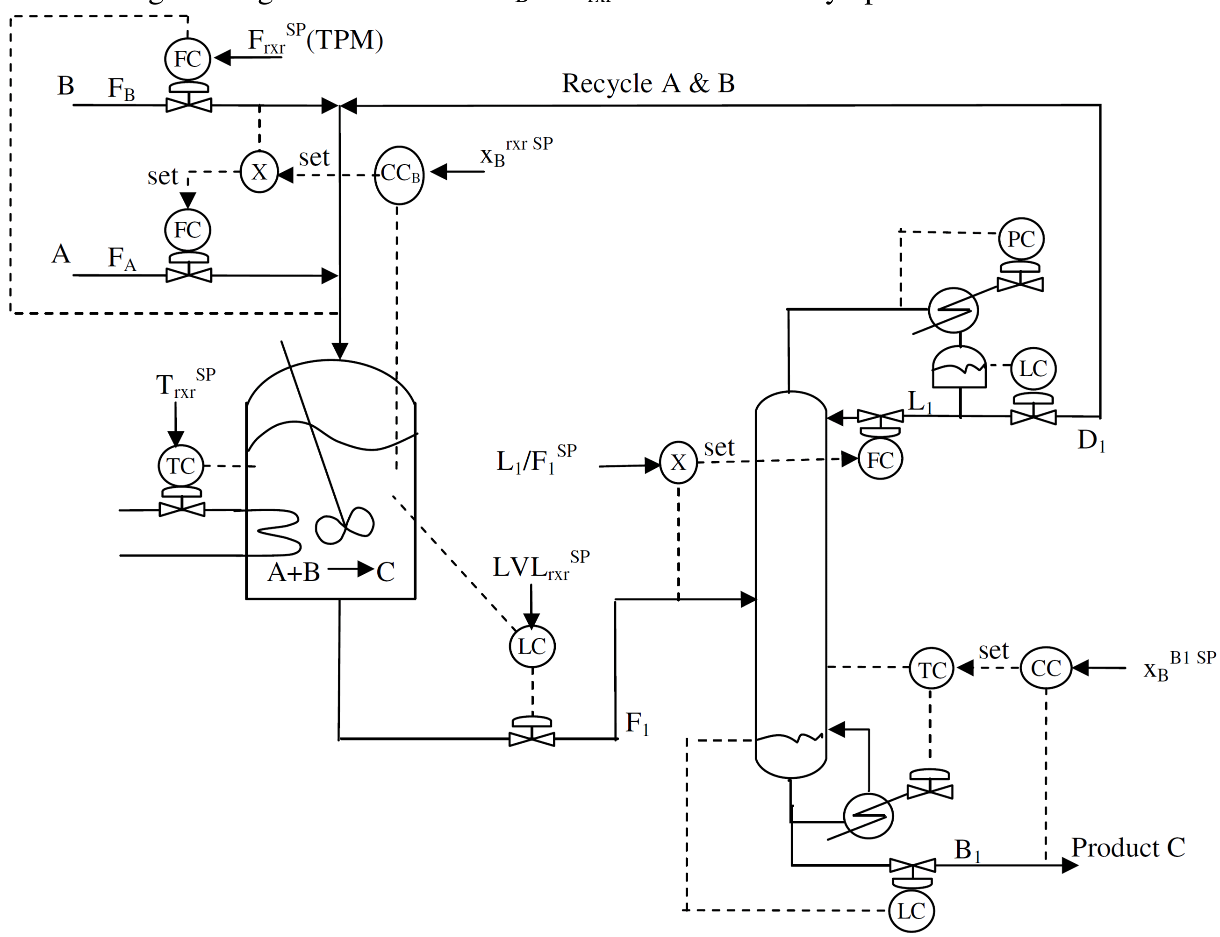


Figure 10.2(b). Luyben's control structure with TPM at reactor inlet

10.3.2. Two Column Recycle Process

The conventional plantwide control structure for the two column recycle process (Figure 9.4b) is synthesized as follows. Let us say the fresh B (F_B) is the TPM (1^{st} loop). The reactor temperature (T_{rxr}) is controlled using the reactor cooling duty (Q_{rxr}) for tight energy balance regulation on the most non-linear process unit (2^{nd} loop). Material balance control consists of controlling reactor level (LVL_{rxr}) using reactor outlet flow (F_{col1}), the two reflux drum levels (LVL_{RD1} and LVL_{RD2}) using the respective distillate flows (D_1 and D_2), the two column sump levels (LVL_{bot1} and LVL_{bot2}) using the respective bottoms flows (B_1 and B_2) and the two column pressures (P_{col1} and P_{col2}) using the respective condenser duty valves (Q_{cnd1} and Q_{cnd2}) (3^{rd} to 9^{th} loops). We now implement component inventory control loops. On the first column, the reflux is maintained in ratio with the feed to provide loose regulation of the C impurity in the A recycle stream (10^{th} loop). A sensitive stripping tray temperature (T^S_{col1}) is maintained by adjusting the boilup (V_1). The temperature setpoint is adjusted by an A impurity in product (x_A^{D2}) controller in a cascade arrangement (11^{th} loop). On the second column, the reflux is maintained in ratio with the feed and the L_2/B_1 ratio setpoint is adjusted by a B impurity in product (x_B^{D2}) controller (12^{th} loop). The column boilup (V_2) is manipulated to hold a sensitive stripping tray temperature (T^S_{col2}) constant to regulate the C leakage down the bottoms (13^{th} loop). The last loop must ensure that F_A exactly balances F_B (TPM) to satisfy the overall plant material balance through the reaction stoichiometry. The total (fresh + recycle) A rate (F_{TotA}) to the reactor is maintained by adjusting F_A (14^{th} loop). The control structure is shown in Figure 10.3(a). Note that in this control scheme, the B recycle can show large swings due to the snowball effect.

We now synthesize the regulatory plantwide control structure using Luyben's pairing approach. The T_{rxr}-Q_{rxr} pairing is first selected for robust stabilization of the reactor energy balance (1^{st} loop). As in the previous example, we assume that the TPM can be chosen anywhere in the plant and leave the decision for later. The next loops to be implemented are for tight product impurity control. The two impurities in the product are A leaking down the first column and B leaking up the second column. For tight regulation of the former, the T^S_{col1}-V_1 pairing is selected with the temperature setpoint cascaded by a x_A^{D2} controller (2^{nd} loop). For tight regulation of x_B^{D2}, a sensitive rectifying tray temperature in the second column (T^R_{col2}) is maintained by manipulating V_2 with its setpoint cascaded by the x_B^{D2} controller (3^{rd} loop). Tray temperature control using boilup achieves the tightest temperature control on a column. Here, this dynamic advantage of the pairing is leveraged for achieving tighter B impurity control than the conventional pairing with reflux rate (or ratio). With the product impurity loops in place, we implement loops for feeding the fresh feeds as make-up streams. The total (fresh + recycle) B (F_{TotB}) to the reactor is maintained constant by manipulating F_B (4^{th} loop). The total (fresh + recycle) A (F_{TotA}) to the reactor is maintained by adjusting F_B and its setpoint is maintained in ratio with F_{TotB} (5^{th} loop). Maintaining F_{TotA} and F_{TotB} using the fresh feeds ensures the unreacted A and B component inventories in the recycle loops are tightly regulated to mitigate snowballing. Maintaining F_{TotA} in ratio with F_{TotB} mitigates the transient variability in the reactor composition. The pairings LVL_{rxr}-F_1, LVL_{RD1}-D_1, LVL_{RD2}-D_2, LVL_{bot1}-B_1, LVL_{bot2}-B_2, P_{col1}-Q_{cnd1} and P_{col2}-Q_{cnd2} are implemented to control the process liquid and vapor inventories (6^{th} – 12^{th} loops). The last two loops to be implemented are holding the two column reflux rates in ratio with the column feeds (L_1/F_1 and L_2/B_1) (13^{th} – 14^{th} loops). In conjunction with the temperature loops on the two columns, these two loops ensure the impurity leakage in the two recycle streams is loosely regulated. The control structure is shown in Figure 10.3(b). To manipulate the throughput, T_{rxr}, F_{TotA} or F_{TotB} may be adjusted. Usually, one is not free to adjust T_{rxr}. Also, the reactor must be operated with a minimum excess of one of the reactants (say A). The total limiting reactant (B) flow to the reactor (F_{TotB}) would then be an appropriate TPM. We again highlight that even as the structures in Figure 10.3(a-b) ‘look’ similar, their synthesis philosophies are very different.

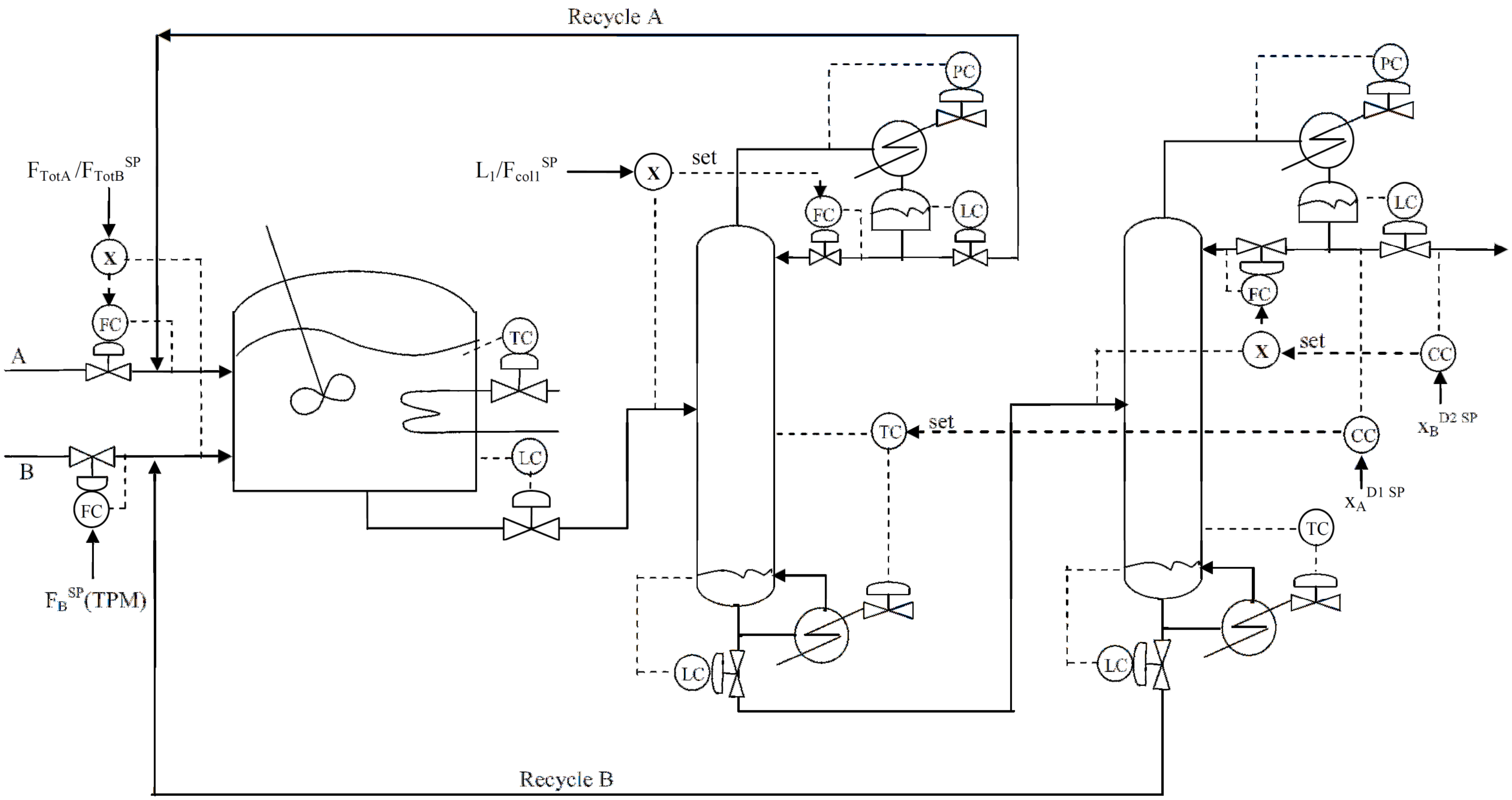


Figure 10.3(a). Conventional control structure for two column recycle process

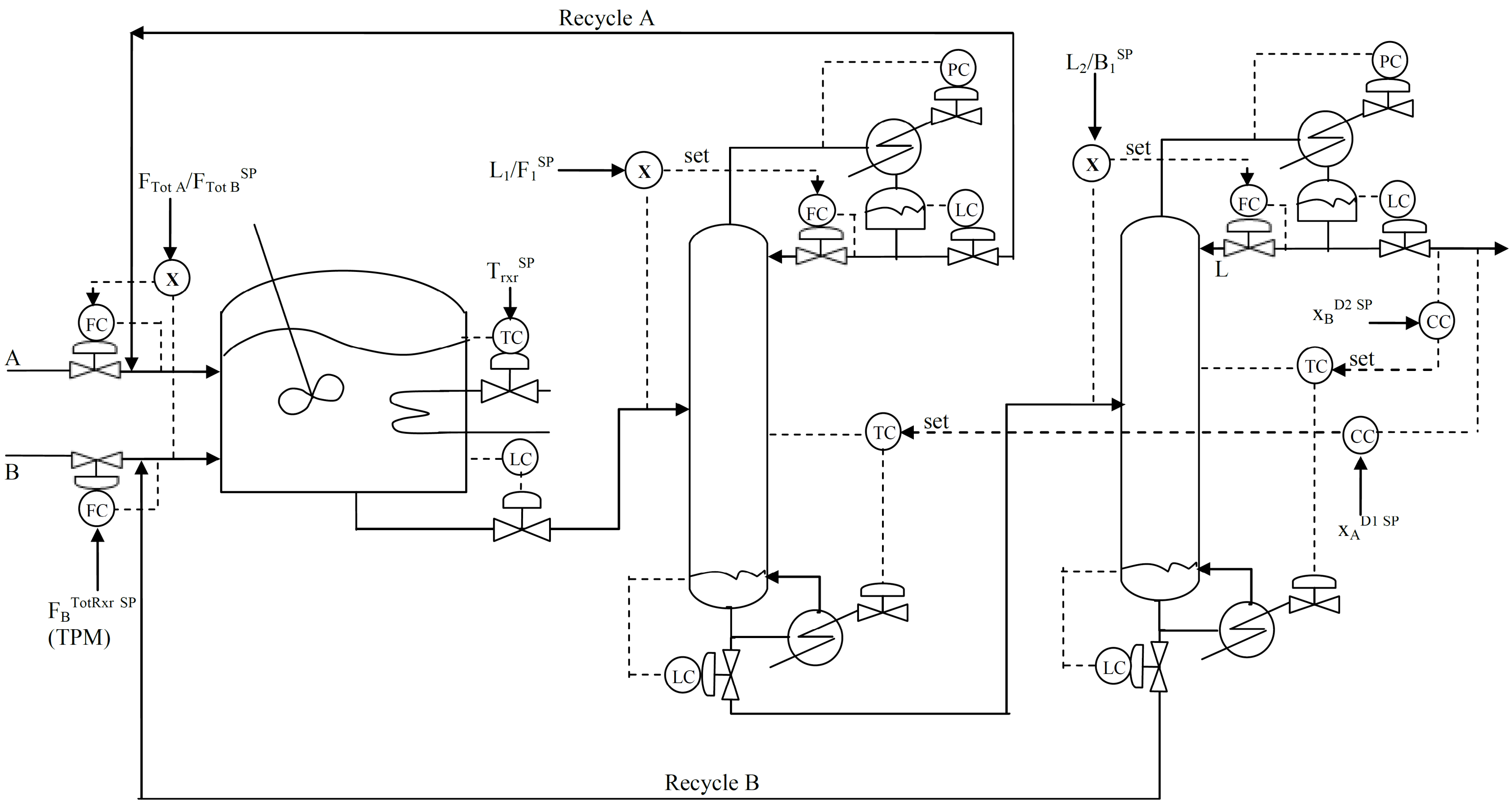


Figure 10.3(b). Luyebn's control structure for two column recycle process

Chapter 11: Economic Considerations in Plantwide Control

Given a regulatory plantwide control structure that ensures the unit specific and overall material and energy balances are satisfied so that the process inventories do not drift or drift within an acceptably small band, we are ready to bring in economic considerations. The key question is, "What are the process inventories that significantly affect steady operating profit and their optimal levels (values)?" Engineering common sense applied to a process would usually reveal the economically important inventories and we discuss some of the considerations below.

11.1. Economic Process Operation Considerations

From the economic point standpoint, on-aim product purity is always desired. The product then contains maximum allowed impurity for zero product give-away or alternatively, for selling maximum allowable cheap impurities for the price of the product (legal adulteration!). Because process raw materials (reactants) are usually quite expensive (much much more than energy), their loss in non-product streams (eg a purge stream or a waste-product stream) discharged from the process must be regulated tightly at an acceptably small value. This includes minimizing the loss of expensive reactants as undesired by-products that are discharged from the plant, since the waste product consumes expensive reactants with no sales revenue.

In reactors, there usually exists a single-pass conversion versus selectivity (yield to desired product) trade-off. Side reactions always occur in any reactor and these are often suppressed by designing the reactor to operate in large excess of a reactant. One would like to maximize the single-pass reactor conversion to reduce the amount of unreacted reactants to be recycled and hence the associated recycle cost. For irreversible reactions, this would correspond to operating the reactor at the maximum allowed temperature. However, because the activation energy of the side reaction(s) is higher than the main reaction with the catalyst significantly reducing the activation barrier for the main reaction, the %age increase in reaction rate per unit temperature increase is higher for the side reaction. Thus for irreversible catalytic reactions, any increase in conversion via an increase in temperature comes at the expense of reduced yield to desired product. The reactor temperature is then likely to have an optimum conversion-yield trade-off with higher single pass conversion reducing the recycle cost (lower unreacted reactants to be recycled) at the expense of lower yield to desired product. If the process is such that the by-product is simply discharged from the process, the loss in yield dominates since energy is significantly cheaper than raw materials and the reactor operating conditions must be chosen to maximize yield. This would usually correspond to maximizing the excess reactant composition in the reactor, usually limited by a recycle equipment capacity constraint, along with an optimal temperature for high yield (say >95%) and not-too-low a conversion. In cases where the by-product is further processed back to the desired product, there is an associated processing cost which goes up as the by-product formation rate goes up (with increase in temperature). The reactor temperature would then still have an optimum; however since both reactant recycle cost and side-product processing cost primarily correspond to energy consumption (which is cheap), it would usually be optimal to have lower than maximum achievable excess reactant in the reactor and a higher operating temperature (as no by-product is discharged).

Unlike the reactor temperature, the reactor hold-up (level for liquid phase reactors and pressure for gas phase reactors) affects all the reaction rates equally with a eg 10% increase in hold-up causing a 10% increase in all reaction rates. For kinetically limited reactors (ie all irreversible reactions and reversible reactions where the reactor is not large enough for equilibrium to be attained), it is then always optimal to operate at maximum reactor hold up (maximum level for liquid phase CSTRs and maximum pressure for gas phase reactors) as we get an increase in conversion with no yield penalty.

For optimal operation, the total energy consumption per kg product should generally be as small as possible. Heuristics for energy efficient operation of common unit operations are well-known and should be liberally applied. This includes preventing over-refluxing in distillation columns by dual-ended control, efficient operation of furnaces by adjusting the fuel to air ratio to maintain stack-gas composition, floating pressure control of a superfractionator, using valve position control on a variable speed pump feeding parallel process trains etc. These heuristics have been discussed earlier.

11.2. Process Operation Modes

Continuous chemical processes are usually operated in 2 modes. In Mode I, the process throughput (production rate) is specified based on market demand-supply considerations and economic operation is equivalent to maximizing process efficiency (eg minimum steam consumption per kg product or maximum yield to desired product etc). In Mode II, the market conditions are such that it is optimal to operate the process at maximum (economic) throughput. Plants immediately after commissioning are often operated at maximum throughput to maximize revenue and pay-off debts. First-to-patent product / process monopolies may also be operated at maximum throughput given sufficient product demand.

11.3. Process Constraints and Economic Operation

The discussion on economic considerations hints at economic process operation requiring operation at or close to constraints. The constraints may be soft, where short duration constraint violations are acceptable, or hard, where constraint violations are unacceptable or not possible. Process operation at the maximum allowed product impurity constraint for no product give-away is an example of a soft constraint. Hard constraints usually correspond to equipment capacity constraints. Examples include operating a gas recycle compressor at maximum duty to maximize gas recycle rate and hence minimize fresh gas consumption, operating a distillation column at its flooding limit (maximum boilup) to maximize the recycle of the excess reactant for suppressing a side reaction etc.

At the design throughput, hard equipment capacity constraints are usually not active (due to equipment overdesign). However, as throughput is increased, equipment successively hit capacity constraints. For example, the boilup in a distillation column is commonly manipulated for stripping tray temperature control. As throughput is increased sufficiently, the boilup would increase to a point where the column approaches its flooding limit with the high boilup not allowing liquid to drop down the trays. Upon hitting the flooding limit (maximum boilup, V^{MAX}), tray temperature control would be lost. The loss in tray temperature control would imply loss in regulation of the light key dropping down the column. Let us say the column bottoms stream is a product stream. Product light key impurity control is then lost, which is unacceptable. If the bottoms is a recycle stream, the light key inventory in the recycle stream is unregulated and can build-up (snowballing) unless the throughput is cut. The point is that as constraints go active, regulation of crucial control tasks may be lost.

11.4. Approaches for Handling Equipment Capacity Constraints

11.4.1. Backed-off Operation

How does one handle equipment capacity constraints going active? Consider the simple distillation column with conventional single ended temperature control using boilup and maximum boilup (V^{MAX}) representing a capacity constraint. The simplest thing to do would be to back-off the column feed sufficiently so that V^{MAX} does not go active for the worst expected disturbance. This is illustrated in Figure 11.1(a). The maximum achievable steady throughput would then be lower, representing an economic loss.

11.4.2. Use of Valve Positioning (Optimizing) Controller

To automate the back-off in throughput, one may implement a valve positioning controller that maintains the boilup at a specified value by manipulating the feed rate. This is shown in Figure 11.1(b). Since an adjustment in feed by the VPC would affect the boilup reasonably quickly through the action of the temperature controller, the back-off would be lower than what was necessary using the strategy in Figure 11.1(a). Even so, some back-off would be necessary representing a loss in maximum throughput ie an economic loss.

In the control system in Figure 11.1(b), the VPC setpoint sets the feed to the column and thus indirectly acts as the TPM. A simple and effective control scheme for handling the V^{MAX} constraint is to directly use the boil-up flow setpoint as the TPM and control tray temperature using the column feed, as shown in Figure 11.1(c). Increasing the boilup would cause the tray temperature to increase and the temperature controller would increase the cold fresh feed to bring the increasing temperature back to setpoint. The temperature control would be reasonably tight as long as the control tray is not too far below the feed tray. Notice that due to tight control of the boilup using reboiler duty, little/no back-off from the V^{MAX} limit would be necessary so that the process can be operated at V^{MAX} with no (or negligible) loss in maximum achievable throughput.

11.4.3. Altering Material Balance Control Structure Using Overrides

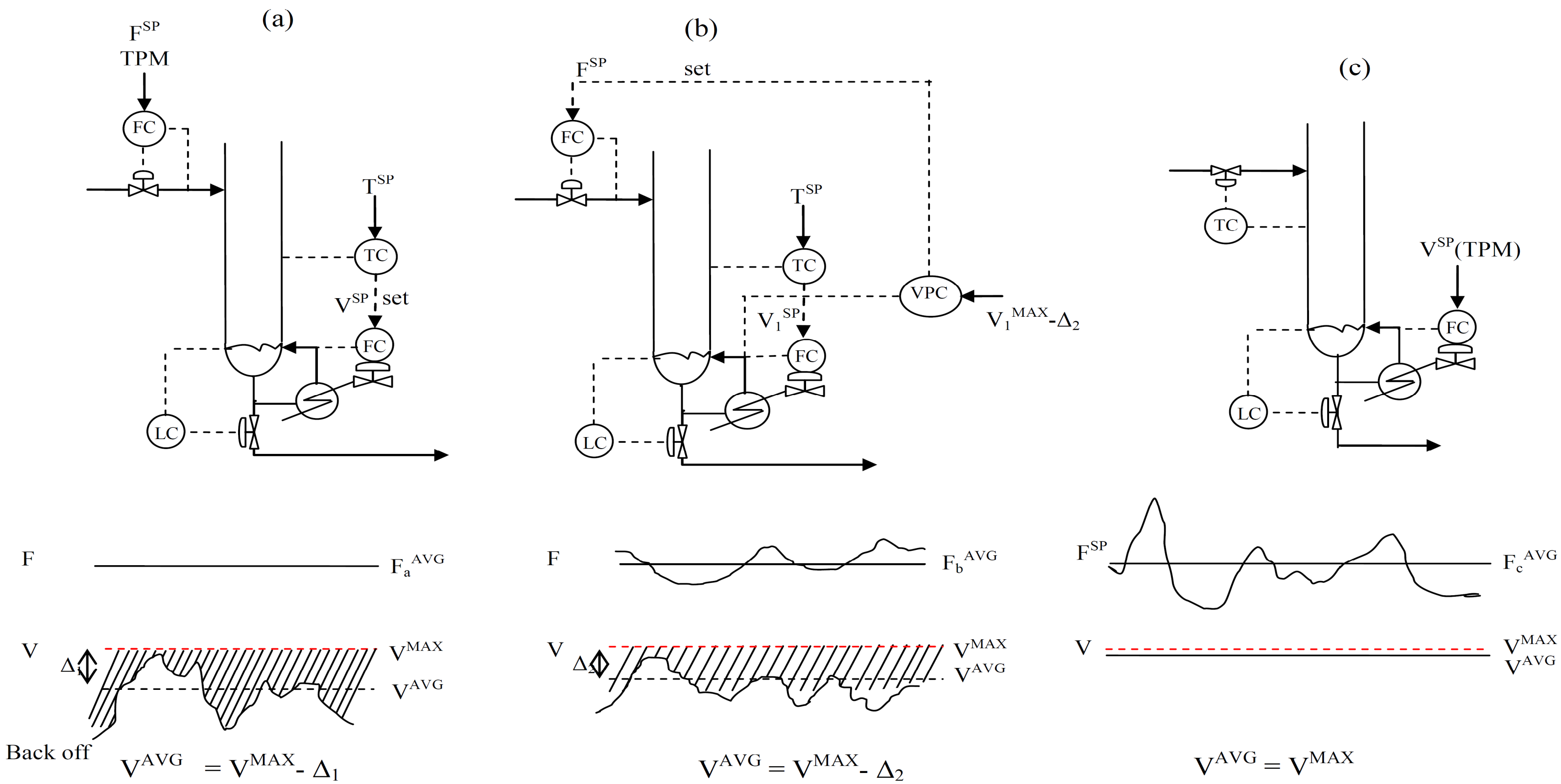
There is also the conventional approach of handling constraints using override controllers. The V^{MAX} constraint on a distillation column is conventionally handled by a slower override tray temperature controller with its setpoint slightly below the nominal setpoint and its output passing to the column feed valve through a low select, as shown in Figure 11.2(a). When V^{MAX} is inactive, the nominal temperature controller controls tray temperature close to the nominal setpoint. The tray temperature is then higher than the override temperature controller setpoint so that its output increases in an attempt to put more cold feed to reduce the tray temperature to its setpoint. The output is then high and the low select on the signal to the feed valve passes the desired feed throughput signal (column feed as TPM). When the V^{MAX} constraint goes active on eg sufficiently increasing column feed rate, the tray temperature would decrease causing a decrease in the override controller output with the low select eventually passing feed manipulation to the override temperature (column feed under temperature control). The override scheme thus alters the control structure from fixed feed – manipulated boilup to fixed boilup – manipulated feed.

In case the feed to the column is being set by an upstream process eg by the level controller of the upstream reactor, the temperature override taking up column feed manipulation would imply loss of level control on the reactor. The reactor level would then increase and an override level controller with its setpoint slightly higher than the nominal level controller setpoint must now take up manipulation of reactor feed to regulate its level. Appropriate overrides will have to be implemented all the way back to the process feed, as shown in Figure 11.2(b-c). Regardless of the number of intervening units between the process feed and the constrained unit, what the override scheme does is alter the material balance control structure from fixed process feed – varying constraint variable (boilup in the distillation example) to fixed constraint variable – varying process feed.

11.4.4. Using Constraint Variable as Throughput Manipulator

The use of overrides for altering the material balance control structure on hitting a constraint can be avoided as illustrated in Figure 11.3. Here, the constraint variable is the TPM and the material balance control loops are oriented around it using the radiation rule. Clearly, this gives a much simpler control system with no overrides. Also, no (minimum) back-off is needed from the active constraint limit. In contrast, a major disadvantage of using overrides is the need for appropriate offset in override controller setpoints. In the Figure 11.2 examples, the nominal reactor level setpoint would necessarily be lower than maximum implying that the nominal process operation would be at a lower than maximum single pass conversion due to lower than maximum holdup with consequent higher recycle cost. Similarly, the offset in the column temperature override controller would imply higher steady loss of the light-key down the bottoms once V^{MAX} goes active. The overrides also introduce an inherent dynamic disadvantage with the overrides taking time to take-over and give up control and also an element of on-off control with potential repeated misfiring causing unnecessary plantwide transients, particularly when the final steady state is not at the constraint limit but slightly below it. In our considered view, the use of overrides should be minimized as far as possible and using a (hard) equipment capacity constraint variable controller setpoint as the TPM and orienting the material balance control system around constitutes a simple and effective way of handling one such hard constraint variable for negligible back-off and consequent economic loss.

Typically the maximum throughput solution has multiple hard active constraints. The economic loss due to a back-off from these constraints would usually be the largest only with respect to a particular constraint. We refer to this constraint as the economically dominant constraint. For economic operation, we choose this constraint variable (or setpoint of the loop that controls it) as the TPM and put in place the total material balance control system around it. This minimizes the back-off in the economically dominant constraint mitigating the consequent economic loss. The loss in control dofs due to the remaining hard active constraints is then managed with sufficient back-off from the constraint limits which causes only an acceptably small steady economic loss, since these constraints are not economically dominant.



$\Delta_2 < \Delta_1 \qquad F_b^{AVG} > F_a^{AVG}$

$F_c^{AVG} > F_b^{AVG} > F_a^{AVG}$

Figure 11.1. Various control scheme for handling equipment capacity constraint

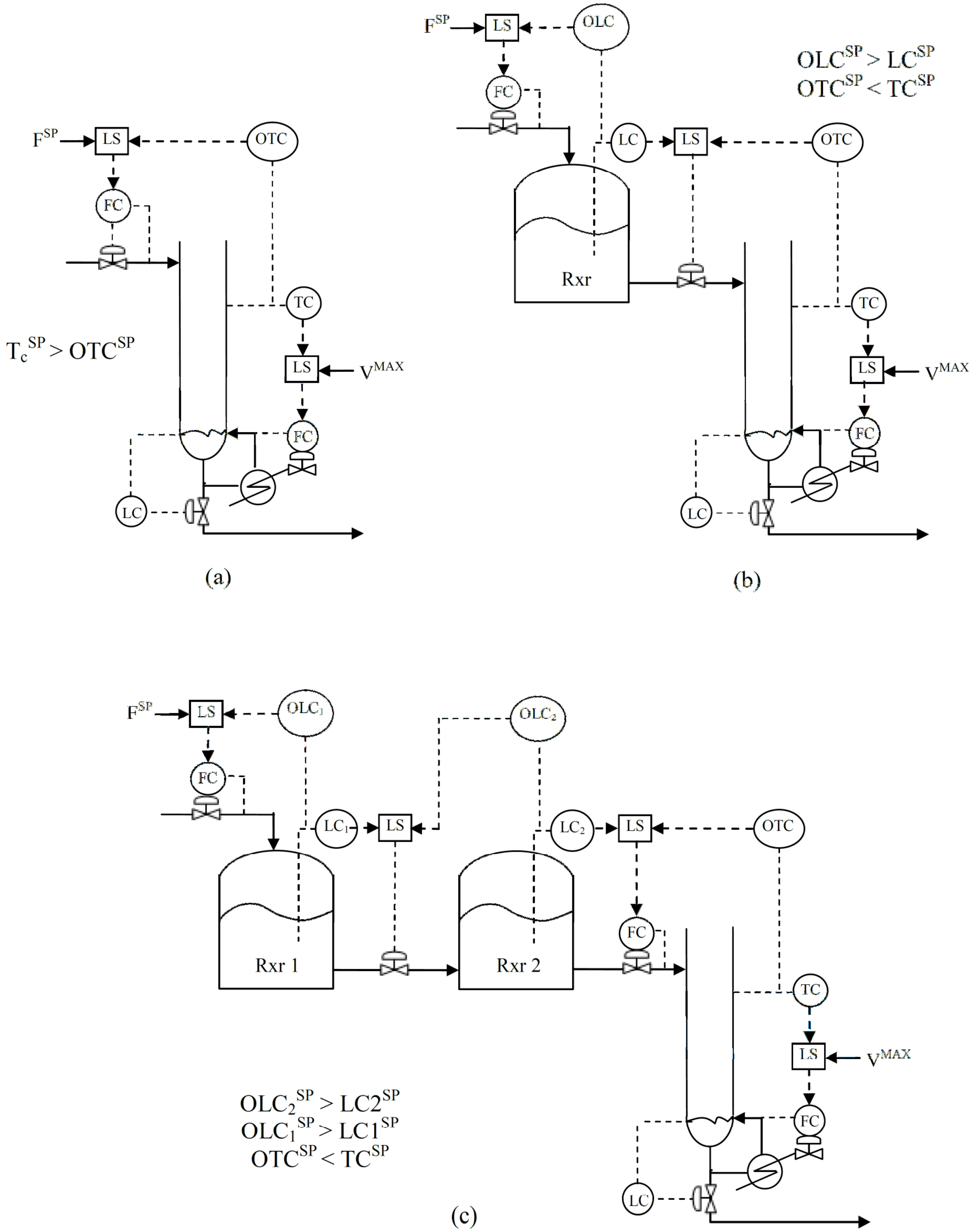


Figure 11.2. Override control scheme for handling capacity constraint

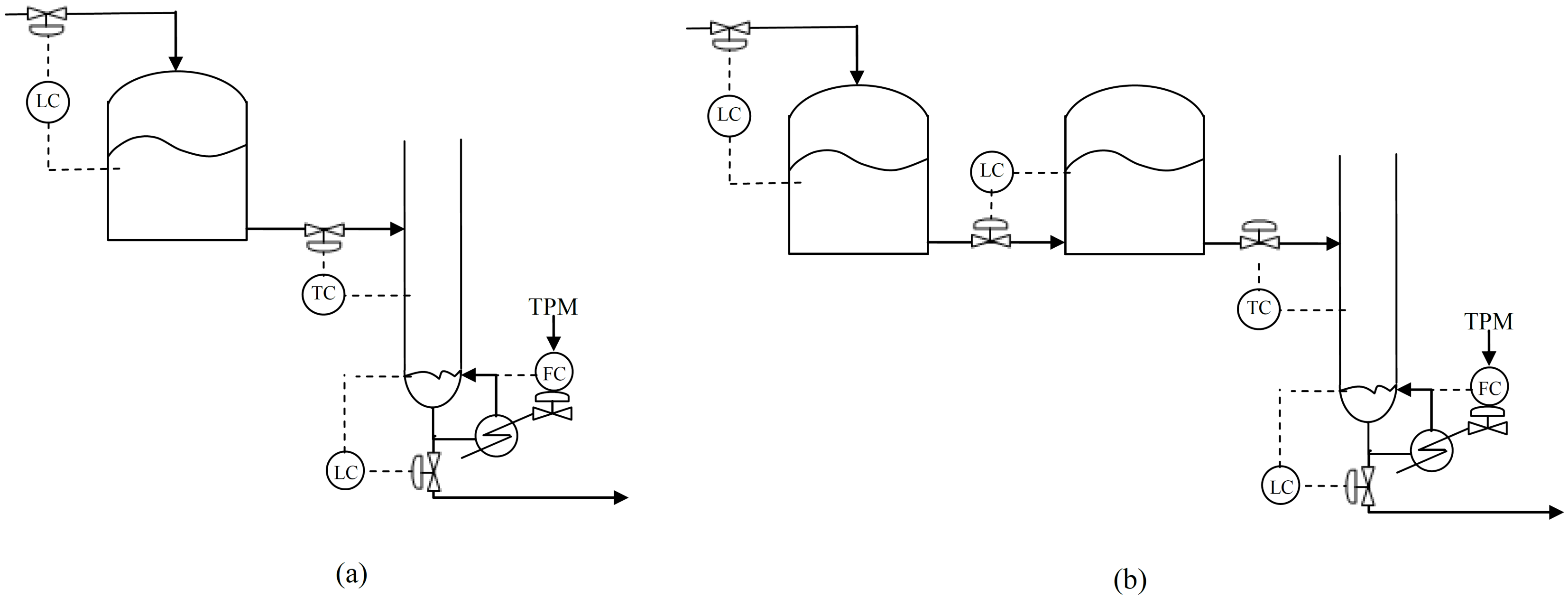


Figure 11.3. Choosing TPM at the constraint variable to avoid overrides

Chapter 12. Economic Plantwide Control Examples

We are now ready to synthesize a plantwide control structure for economic operation of the two example chemical processes in Figure 9.4 using the engineering heuristics discussed above.

12.1. Single Column Recycle Process

The material, component, phase and energy inventories have already been discussed previously. We now bring in economic considerations. The process has 6 steady state dofs. Since there are no side reactions in this toy-problem, economic operation corresponds to minimizing energy consumption (i.e. column reboiler duty). If the separation in the column is relatively easy (likely as C is formed by the addition of A to B and is therefore significantly heavier than both reactants), minimizing energy consumption per kg throughput would correspond to maximizing single pass conversion and hence minimizing the recycle load. Accordingly, the reactor should be operated at maximum level (LVL_{rxr}^{MAX}) and temperature (T_{rxr}^{MAX}). Also, no product give-away requires the B impurity in the product to be at its maximum allowed limit ($x_B^{B1\ MAX}$). These three constraints would be active regardless of throughput (ie both in Mode I and Mode II) and account for three steady state dofs.

In Mode I, the throughput (F_A) is specified leaving 2 unconstrained dofs. These correspond to the C leakage in the recycle stream and the B composition in the reactor (x_B^{rxr}) or more generally, in the recycle loop. If too little C leaks up the top (sharp separation), the boil-up increases (higher reflux for the sharper rectification). On the other hand, if too much C leaks up the top, the reactor gets diluted with the recycle C and the reactor reactant composition goes down for lower single pass conversion and consequent higher recycle cost. Sufficient reflux thus needs to be provided in the column so that too much C does not leak up the top. This is achieved by maintaining the reflux in ratio with the column feed (L_1/F_1) ensuring adequate C regulation at all throughputs.

With respect to x_B^{rxr}, we note that the conversion would be maximized for comparable reactor A and B mol fractions as the irreversible reaction kinetic expression is

$$r = k\, x_A^{rxr}\, x_B^{rxr}$$

Now since the reactor contains C (generated by reaction) and its amount varies with throughput (generation rate), the optimal value of x_B^{rxr} that ensures $x_B^{rxr} \approx x_A^{rxr}$, would vary with throughput. Care must then be exercised that the specified x_B^{rxr} setpoint is not infeasible due to the variation in x_C^{rxr}. The optimum x_B^{rxr} would be the smallest at maximum production (largest x_C^{rxr}) large. To ensure feasibility the desired setpoint over the entire throughput range, we may choose to implement this setpoint value at all throughputs. At low throughputs (x_C^{rxr} small due to low generation, x_B^{rxr} specified to be small), the reactor then gets operated in significant excess A environment implying higher than necessary reboiler duty.

One way around this problem is to realize that the recycle stream contains mostly A and B with only a small amount of C. If instead of holding x_B^{rxr} constant, we ensure that $x_B^{D1} \approx 50\%$ (ie comparable A and B in recycle stream), then x_B^{rxr} would automatically float to be comparable to x_A^{rxr}. Now since B is heavier than A and therefore requires more energy to boil-off, a reasonable specification for near optimal operation over the entire throughput range would be holding x_B^{D1} slightly but not too far below 50% (say at 45%). Such a choice would ensure reactor operation close to maximum achievable single pass conversion (an economic objective) across the entire throughput range.

As throughput is increased, let us say that the column approaches flooding. The maximum boilup (V^{MAX}) then limits the maximum achievable throughput (Mode II operation). We take the two regulatory plantwide control structures synthesized earlier (Figure 10.2) and adapt them for economic operation over the entire throughput range.

In Figure 12.1(a), we take the conventional plantwide control structure with F_B as the TPM and modify it for economic operation. The setpoints for T_{rxr} and LVL_{rxr} loops are specified to be T_{rxr}^{MAX} and LVL_{rxr}^{MAX} (for maximum single pass conversion). A slow x_B^{D1} controller is implemented that adjusts the x_B^{rxr} composition loop setpoint to hold x_B^{D1} at its (near) optimal value (chosen as 45% here) for the entire throughput range. Similarly, $L_1/F_1\ ^{SP}$ is set at an appropriate value for ensuring too much C does not leak in the recycle stream over the entire throughput range. For maximum throughput operation with V_1^{MAX} as the bottleneck constraint, an override scheme for altering the material balance control structure is implemented. Notice that the setpoint of the nominal and override temperature controllers on the column comes from the master x_B^{B1} (product B impurity) controller. The override temperature controller setpoint is always slightly lower than the nominal setpoint via the negative bias. When the temperature override gets triggered, the product impurity would increase (as override temperature setpoint is lower) and the action of the x_B^{B1} controller would slowly bring it back to the appropriate level. On the other hand, when the nominal controller takes up temperature control (V_1^{MAX} goes inactive), since its setpoint is higher than the override setpoint, the impurity leakage would decrease (below maximum allowed) and then get back to the desired value via the action of the x_B^{B1} controller. Clearly, product impurity control becomes loose due to the overrides 'taking over' or 'giving-up' control.

To avoid the disadvantages associated with overrides, one may insist on having a fixed control structure regardless of throughput. If the conventional regulatory control loops are already implemented and are not modifiable, the only free setpoint available for maintaining the constraint variable (V_1) at a desired value is F_B^{SP}. This loop is shown in Figure 12.1(b) and is a long one. When coupled with the snowball effect, V_1 would only get controlled loosely around the desired setpoint implying a large back-off from V_1^{MAX} and consequent throughput loss.

We may also take the regulatory control structure synthesized using Luyben's approach and adapt it for economic operation. Figure 12.2(a) shows the adapted control structure along with a material balance altering override scheme for handling the V_1^{MAX} constraint for maximum throughput operation. Figure 12.2(b) shows a long V_1 constraint control loop manipulating F_{rxr} to avoid the use of override controllers. These modifications to the basic regulatory control structure are very similar to those for the conventional control structure and are therefore not elaborated upon. It is however worth mentioning that tighter V_1 control by the long V_1-F_{rxr} loop would be achieved as the snowball effect is mitigated with the fresh reactants being fed as make-up streams. The back-off from V_1^{MAX} would then be lower and the control scheme would achieve higher maximum throughput than the one in Figure 12.1(b).

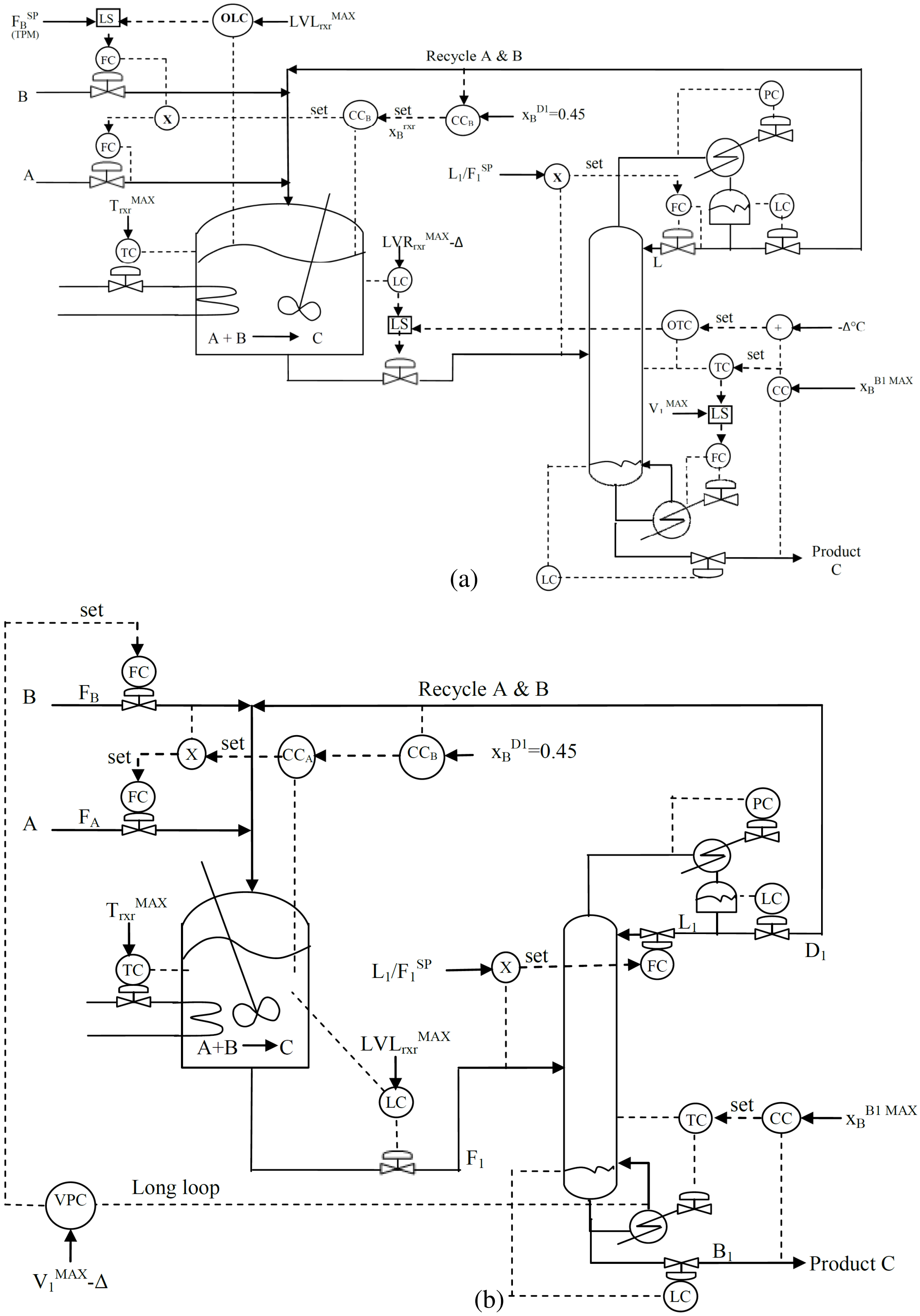


Figure 12.1. Handling capacity constraint in single column process (Conventional Process)
(a) Using overrides (b) Using long active constraint control loop

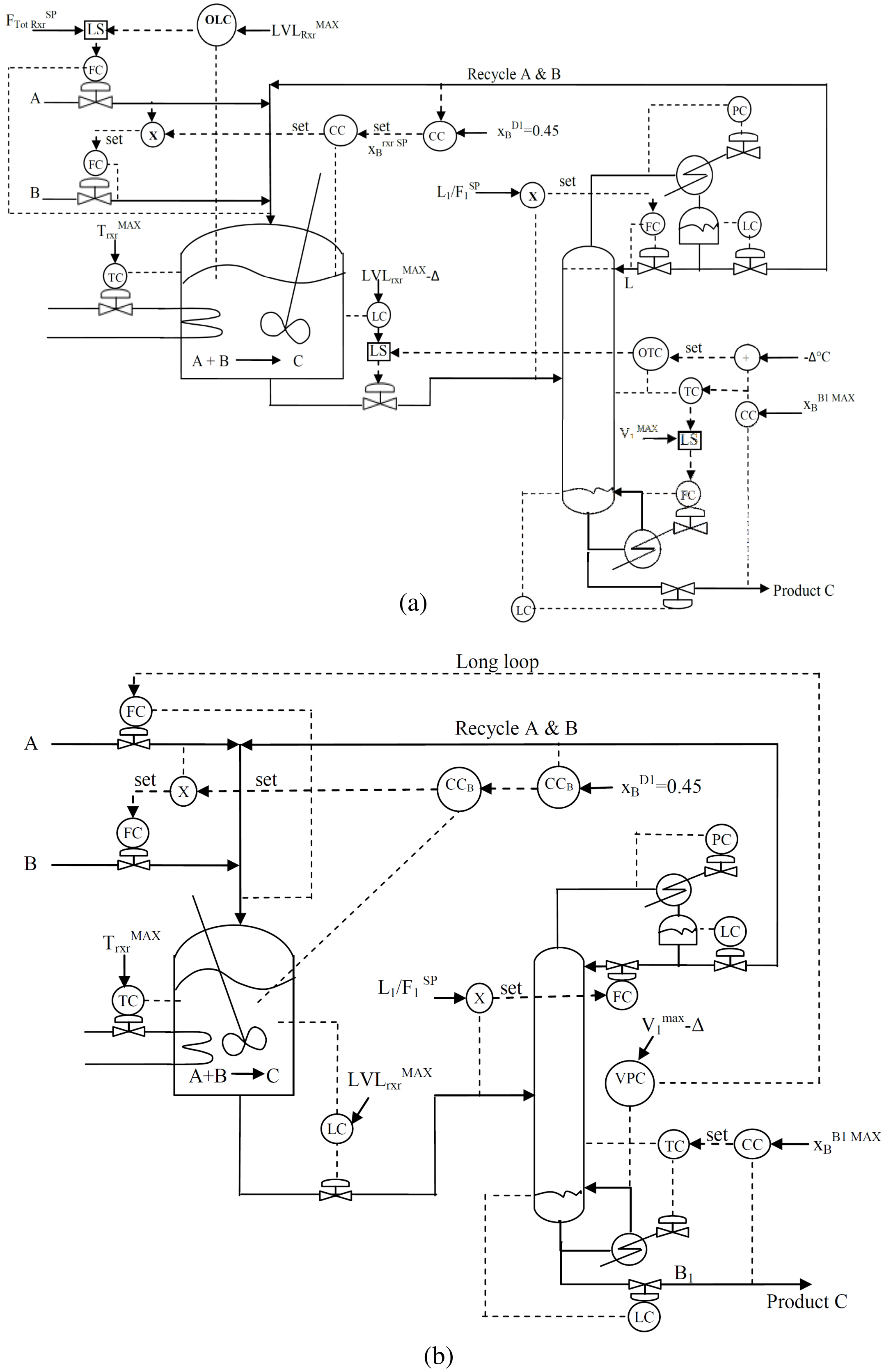


Figure 12.2. Handling capacity constraint in single column process (Luyben structure)
(a) Using override (b) Using long active constraint control loop

In Figure 12.3, we show the control system with V_1^{SP} as the TPM and the material balance control loops oriented around it. For economic operation, the reactor is operated at T_{rxr}^{MAX} and LVL_{rxr}^{MAX}. Also, a slow x_B^{D1} controller that cascades a setpoint to the x_B^{rxr} controller is implemented for ensuring near maximum reactor conversion at all throughputs. The control structure is particularly elegant in terms of the simplicity with which the V_1^{MAX} active constraint is handled with no overrides. The operator simply increases V_1^{SP} to V_1^{MAX} to transition to maximum throughput. More importantly, unlike the other control structures, the basic material balance control structure remains the same regardless of throughput. The only potential disadvantage is slightly more loose product impurity control at low throughputs (where V_1^{MAX} is inactive) as the boilup is not used for column temperature column. Appropriate detuning of other loops, in particular the surge level loops, to mitigate the transients propagated to the column can however be easily applied to ensure the product quality control is acceptably tight. Advanced control algorithms may also be applied to mitigate the variability in the product quality. The control structure is thus the simplest possible solution for economic process operation over the entire throughput range (low to maximum throughput).

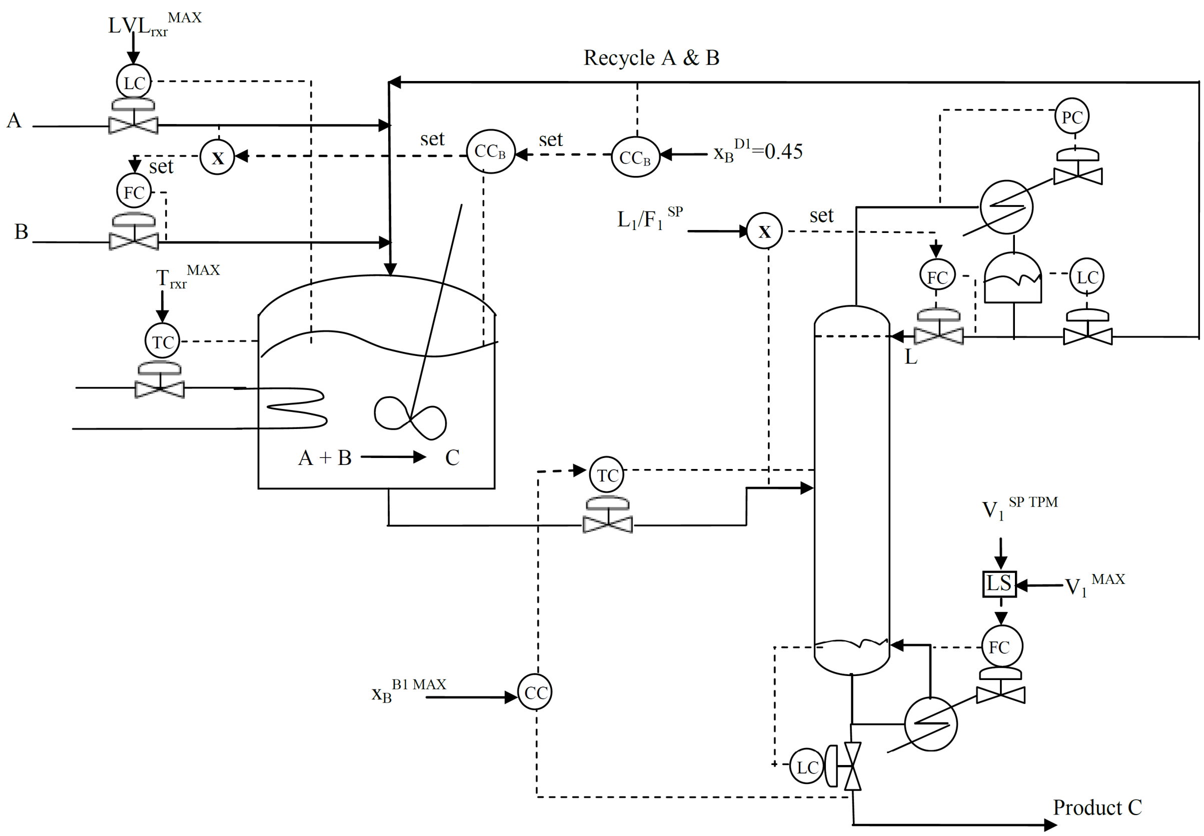
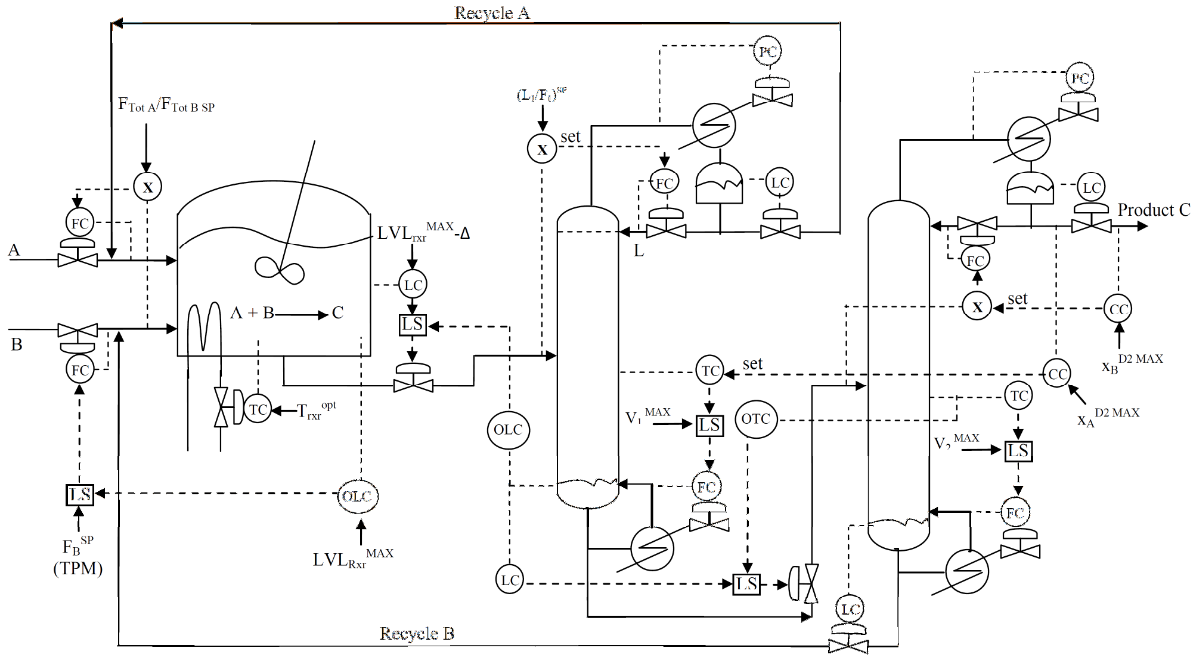


Figure 12.3 Using constraint as TPM to avoid overrides on the single column recycle process

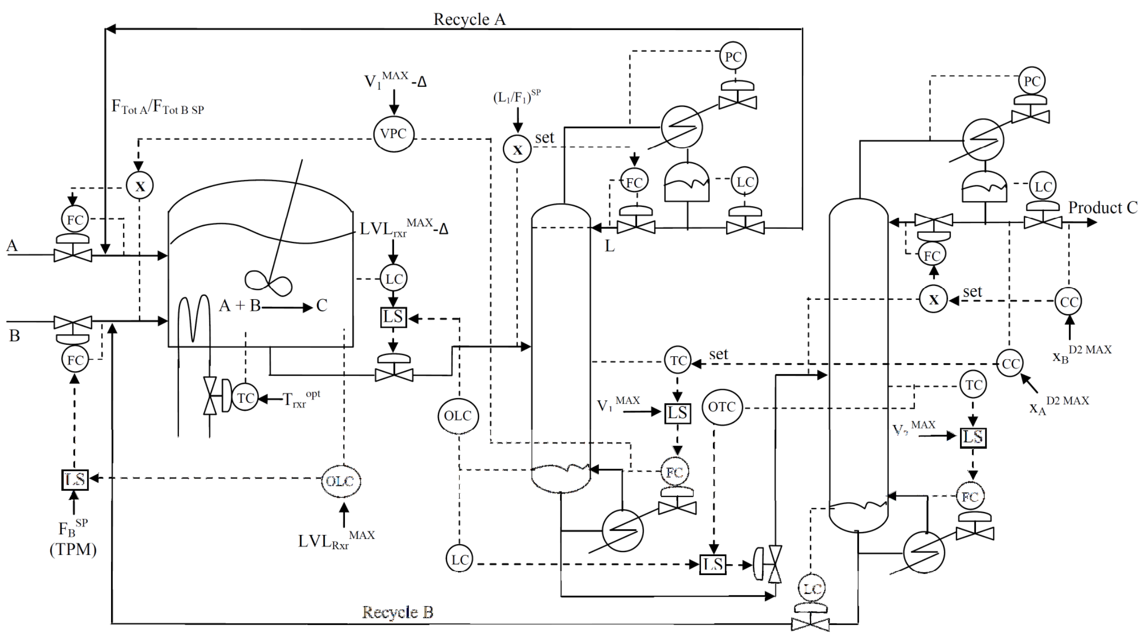
12.2. Two Column Recycle Process

This process has 8 steady state dofs, as discussed earlier. Purely for the sake of a more interesting discussion, let us assume that there is a side reaction (assume side product volatility is such that it leaves with product C stream) and that this side reaction is suppressed by operating the reactor in excess A environment (B limiting). Economic process operation then requires maximizing the reactor excess A environment, which requires operating the first column at maximum boilup (V_1^{MAX}) so that the A recycle rate is as high as possible. To maximize single-pass conversion with no yield penalty, it should be operated at maximum level (LVL_{rxr}^{MAX}). Also, the A and B impurities in the product should be at their maximum limits for no product give-away ($x_A^{D2\ MAX}$ and $x_B^{D2\ MAX}$). These four constraints are active at all throughputs. In Mode I (given throughput), we have a specified throughput leaving 3 unconstrained steady state dofs. These correspond to the optimum reactor temperature (conversion-yield trade-off) along with the C leakage in the A recycle stream and in the B recycle stream. This C leakage must be kept small enough at all throughputs. As throughput is increased, let us say the maximum boilup on the second column (V_2^{MAX}) constraint is hit, which fixes the maximum achievable throughput (Mode II).

We now adapt the conventional plantwide regulatory control structure (F_B TPM) for economic operation (Figure 10.3a). The adapted control structure is shown in Figure 12.4(a). In the regulatory control structure, the product impurity control loops are already in place and their setpoints are set at the maximum acceptable impurity level ($x_A^{D2\ MAX}$ and $x_B^{D2\ MAX}$). The reactor level setpoint is specified at LVL_{rxr}^{MAX}. To operate close to V_1^{MAX}, a V_1 controller is implemented which manipulates F_{TotA}/F_{TotB}^{SP} in a long loop. Its setpoint will require sufficient back-off from V_1^{MAX} to ensure A impurity regulation is never lost. The reactor temperature setpoint is specified at an appropriate value that ensures the yield is always sufficiently high. On the first column, L_1/F_1 setpoint is fixed at a value that ensures too much C does not leak up the top over the entire throughput range. On the second column, the stripping tray temperature setpoint is chosen to regulate C leakage down the bottoms at an acceptably small value. For handling the bottleneck V_2^{MAX} constraint that limits maximum throughput, a material balance altering control scheme with overrides from the second column back to the fresh A feed is implemented. Note that V_2^{MAX} represents a capacity constraint on the amount of product C that can be boiled off. If too much C is generated in the reactor than can be boiled off in the second column, the extra C would necessarily accumulate in the B recycle stream. The override scheme acts to cut the fresh B feed to the appropriate value so that the C generation in the reactor exactly matches what is boiled off in the second column. If the override scheme for altering material balance structure is to be avoided, F_B^{SP} must get adjusted to hold V_2 (constraint variable) in a long loop. While it may be acceptable to let the C impurity in the recycle stream float for short durations till the long V_2 loop sufficiently reduces F_B^{SP} after V_2^{MAX} goes active, large plantwide transients due to adjustment in F_B (snowball effect) are likely and conservative operators may simply back-off V_2^{SP} sufficiently to ensure V_2^{MAX} never goes active.



(a)



(b)

Figure 12.4 Use of overrides for handling capacity constraints for the two column recycle process. (a) Conventional structure (b) Luyben's structure

Figure 12.4(b) shows the adapted control structure for economic operation with regulatory plantwide control structure from Luyben's approach. The adaptations are very similar to the conventional structure (Figure 12.4a). Note that the L_2/B_1 ratio controller must be specified to a value that ensures too much C does leak down the second column bottoms over the entire throughput range. To avoid the override scheme for altering material balance control when V_2^{MAX} goes active, one can adjust F_{TotB}^{SP} to maintain V_2 in a long loop. The plantwide transients are expected to be smooth as F_{TotB} is inside the recycle loop so that F_B is always fed as a makeup stream mitigating the snowball effect and the back-off from V_2^{MAX} would be smaller.

In this example, we have two hard equipment capacity constraints, V_1^{MAX} and V_2^{MAX}. In the synthesized control structures, some back-off from V_1^{MAX} and V_2^{MAX} is needed to avoid loss of product quality control and snowballing issues. The back-off from V_1^{MAX} causes a loss in selectivity while and back-off from V_2^{MAX} causes throughput loss. The latter can be a significant economic loss and to avoid the same we may use V_2^{SP} (last constraint to go active) as the TPM and orient the material balance control system around it as shown in Figure 12.5. T^S_{col2} is controlled using B_1, LVL_{bot1} is controlled using F_{col1} and LVL_{rxr} is controlled using $F_{TotB.}$ As before, F_{TotA} is maintained in ratio with F_{TotB} to ensure the reactor feed composition does not vary too much. The ratio controller also ensures tight reactor level control with the total reactor feed varying in response to a change in its level. The rest of the control system is self explanatory.

Can we further alter the control structure to ensure the back-off from V_1^{MAX} is also eliminated. We show one possible control structure (there are other possibilities too) in Figure 12.6. Here, V_2^{SP} is used as the TPM as before. Since V_1^{MAX} is active, it is not used for controlling T^S_{col1} and F_{col1} is adjusted instead to ensure the A impurity in the product is always regulated. LVL_{bot1} is then controlled using B_1 and LVL_{RD1} is controlled using D_1. Similarly LVL_{RD2} and LVL_{bot2} are regulated using D_2 and B_2 respectively. LVL_{rxr} is controlled using F_{TotA} with F_{TotB} maintained in ratio to ensure the proper A excess in the feed to the reactor. The column pressures are controlled using the respective condenser duty valves. For product impurity control, the x_A^{D2} controller adjusts the T^S_{col1} controller setpoint while the x_B^{D2} controller adjusts L_2/B_1, as before. On the second column, no close by valves are available for stripping tray temperature control and the C leakage in B_2 remains unregulated. V_2^{SP} (TPM) fixes the product C boil-off from the second column and if more C is being generated in the reactor than what is boiled-off, it would drop down the second column and B_2 can show a very large increase (snowballing). To mitigate the same, B_2 is loosely regulated by adjusting the $F_{TotB}/F_{TotA}{}^{SP}$. If B_2 increases, the ratio setpoint is increased causing a decrease in F_B with F_A also eventually decreasing so that only as much C is produced in the reactor as is being boiled off in the second column. Loose control of B_2 flow rate is acceptable as it is a recycle stream and not an exit (product, byproduct or purge) stream. This example illustrates that economic considerations, in particular, tight control of equipment capacity constraints, results in a plantwide control structure that is very different from structures synthesized using the conventional approach or Luyben's approach.

The two toy problems considered here illustrate how economic considerations impact plantwide control structure design. We also hope that the elaborate discussion for the two case studies convinces the readers that common sense based process engineering principles clearly bring out the major considerations in economic / efficient process operation, at least at the qualitative level. These economic considerations, including equipment capacity constraints, translate to economic control objectives, which then govern the pairings to be implemented for achieving economic plantwide control. In the next Chapter, we consolidate the qualitative discussions here into a systematic step-by-step procedure for synthesizing an economic plantwide control system. The application of the procedure to five example processes with rigorous dynamic simulation results is presented in the subsequent chapters.

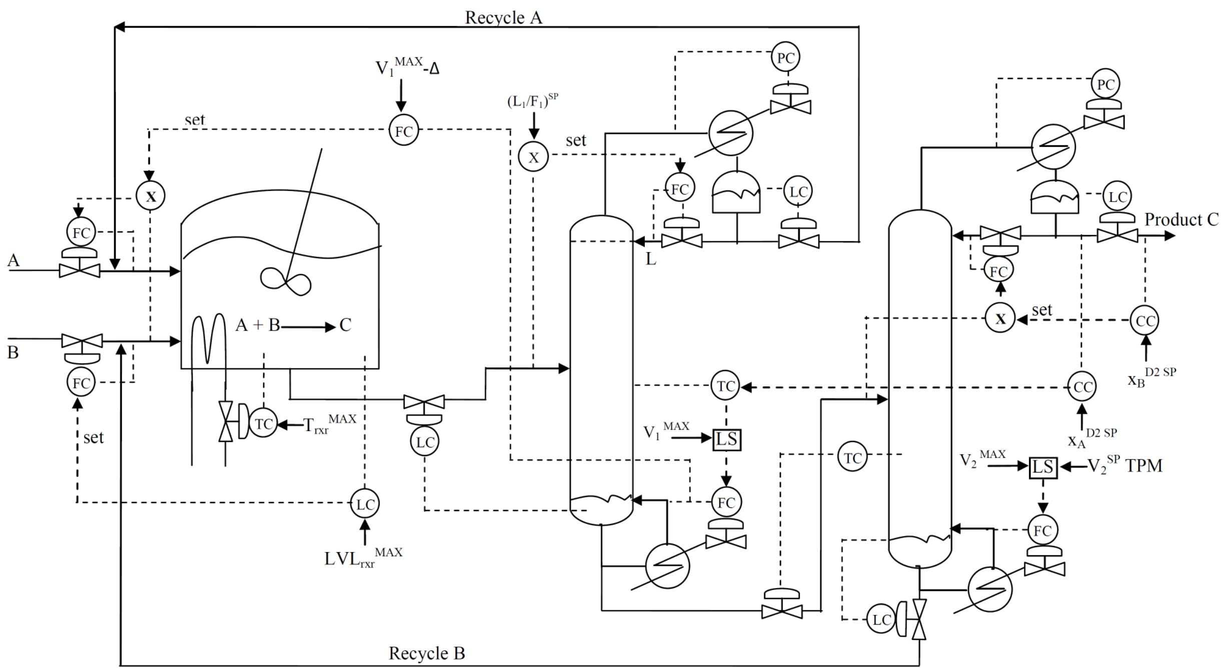


Figure 12.5. Use of bottleneck constraint as TPM to reduce overrides in the two column recycle process example

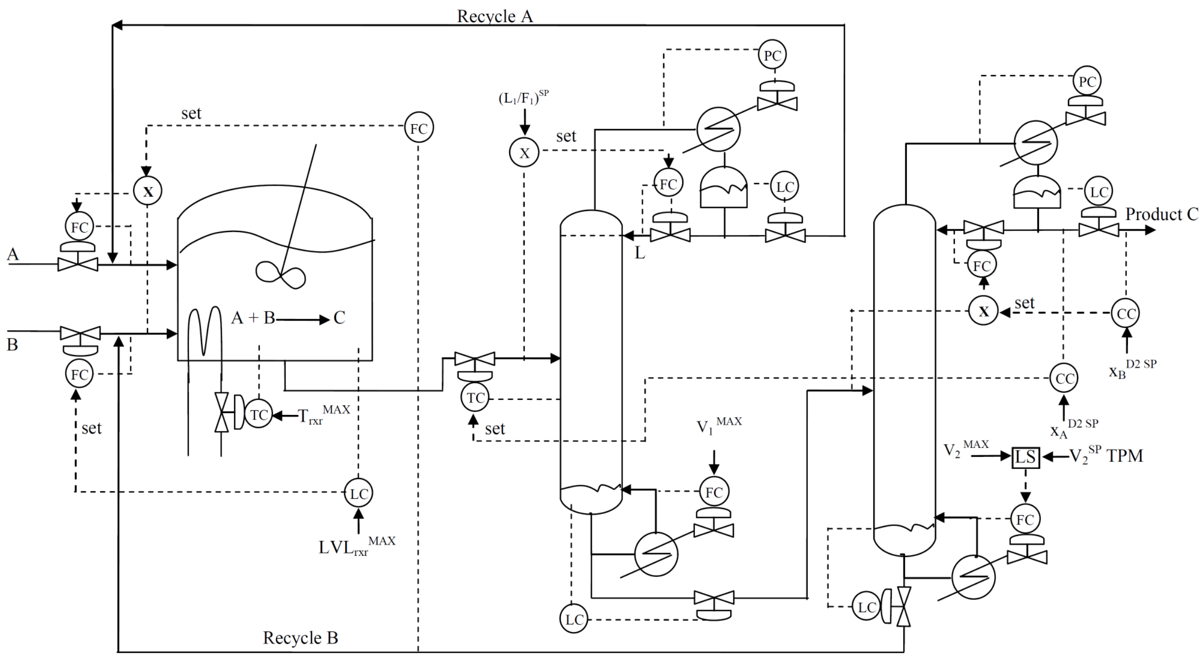


Figure 12.6. A control structure for the two column recycle process that allows operation at V_1^{MAX} and V_2^{MAX} with no back-off

MODULE IV

ECONOMIC PLANTWIDE CONTROL DESIGN PROCEDURE AND CASE STUDIES

With an appreciation of the regulatory and economic considerations in plantwide control system design, we are now ready to develop a systematic plantwide control system design procedure. We develop and present such a design procedure, which is a natural extension of the pioneering work of Page Buckley (DuPont), William Luyben (Lehigh), Jim Downs (Eastman) and Charlie Moore (Tennessee). Its application to four realistic processes, namely, a recycle process with side reaction, an ethyl benzene process, a cumene process and a C_4 isomerization process is also demonstrated. The last two examples are very comprehensive in that the performance of the economic plantwide control structure synthesized from our procedure is compared with a conventional plantwide control structure.

Chapter 13. Systematic Economic Plantwide Control Design Procedure

With the preliminaries on regulatory and economic operation considerations in plantwide control, we are now ready to develop a systematic procedure for designing an economic plantwide control system for integrated chemical processes. For completeness, we review the major contributors to plantwide control research before developing the procedure.

The design of effective plantwide control systems for safe, stable and economic process operation of complex chemical processes with material and energy recycle has been actively researched over the last two decades. The ready availability of dynamic process simulators has been crucial in fostering the research. Over the years, Luyben and co-workers have done seminal work in highlighting key regulatory control issues such as the snowball effect [15] in reactor-separator recycle systems and suggesting practical control system structuring guidelines (Luyben's rules [16]) for ensuring robust process stabilization in light of the same. Based on several case-studies, a nine-step general procedure has been developed for synthesizing effective plantwide control structures for integrated chemical processes [14]. In their procedure, economic concerns are addressed indirectly in the form of requiring 'tight' control of expected economic variables such as product impurity, process yield etc. The control objectives are obtained using engineering insights and heuristics.

Skogestad [24] has developed a more systematic steady state optimization based approach for obtaining the control objectives. Typically, at the optimum steady state, multiple process constraints are active so that these constraints must be controlled tightly. For managing the remaining unconstrained steady state degrees of freedom, the control of self-optimizing controlled variables [23] (CVs) is recommended. By definition, when self-optimizing variables are held constant at appropriate values, near-optimal operation is achieved in spite of disturbances. The quest for the best self-optimizing CV set is however not always straight-forward.

The combinatorial nature of the control structure design problem results in several possible structures that provide safe and stable process operation. A very simple example is a single-inlet single-outlet surge tank with two possible orientations for its level controller. In a simple distillation column, assuming the feed is fixed, the two orientations each for the reflux drum and bottom sump level controllers results in the well-known four basic regulatory control configurations. Other control configurations are possible if instead of the process feed, one of the other associated streams (distillate, bottoms, reflux or reboiler steam) is kept fixed. In a multi-unit chemical process, there would clearly be several possible reasonable control configurations. An obvious question then is which one is best for realizing economically (near) optimal process operation with robust stabilization over the expected process operating space. Further, is there a systematic methodology for synthesizing such an 'optimal' control structure?

A careful evaluation of the plantwide control literature reveals that most of the reported case studies consider process operation around the design steady state (see these example case studies [1,18,27]), although more recently, also at maximum throughput [2,3,11,22]. Around the base-case design steady state, usually all the process units are sufficiently away from any capacity constraints while at maximum throughput, typically, multiple units hit (hard) capacity constraints. The active constraint set progressively expands with throughput to the full set at maximum throughput. The expanding set partitions the throughput range into distinct regions. Much of the open plantwide control literature addresses control system design only for a fixed active constraint set, that is, only for a distinct region. This is surprising given that a plant must be operated over a wide throughput range with different active constraints over its life-span.

In this work, we develop a systematic approach for designing a simple and robust plantwide control system for near-optimal process operation over a wide throughput range with an expanding active constraint set. The approach has evolved out of very recent comprehensive case-studies from our group [7-9]. While the principles on which it is based may be well-known, our main contribution is in bringing these scattered principles together into a meaningful, holistic and practical top-down plantwide control system design framework. The application of the proposed framework is demonstrated on three realistic example processes.

13.1. Degrees of Freedom (DOFs) and Plantwide Control Structures

The plantwide control system design problem may be viewed as seeking the best possible way of managing the available control valves (control DOFs) for ensuring safe, stable and economic process operation in the face of principal disturbances that include large changes in the production rate (throughput) as well as variability in raw material quality, ambient conditions, equipment characteristics and economic conditions (e.g. volatility in the energy prices etc). If we discount the valves used to control nonreactive material inventories (surge tank levels, given column pressures etc), the number of independent control valves remaining equals the steady state operational DOFs for the process, which by definition, is the number of independent specifications necessary to solve for the steady state solution. For a given process, one may use alternative sets of independent specification variables. From the control perspective, each such DOF specification variable is an independent CV (excluding non-reactive material inventory controllers) in the plantwide control system. Note that one setpoint gets used to set the process throughput and is referred to as the throughput manipulator (TPM).

Figure 13.1 provides an illustration of the one-to-one correspondence between the independent CV setpoints (including TPM; excluding non-reactive material inventory controllers) and the steady state DOF specification variable set for a simple reactor-recycle process with five steady-state operation DOFs. The 5 DOFs are related to 1 fresh feed, 2 reactor specifications (level and temperature) and 2 specifications for the column. Four alternative DOF specification sets are shown in Figure 13.1. Implicit in each set is an inventory control system for balancing of the process material and energy inventories as well as appropriate pairings for controlling the specification variable. We have used the radiation rule [20] for material inventory control which gives the orientation of the level controllers upstream and downstream of the TPM respectively, opposite and in the direction of process flow, respectively. Note that for a given DOF specification set, multiple possibilities exist for the choice of the pairings for controlling the specification variables as well as for the inventory loops. Lastly, there exists flexibility in the choice of the DOF specification variable set (CV set) itself. There thus exists tremendous flexibility in designing the plantwide control system which must be gainfully exploited for achieving the twin objectives of robust stabilization and economic operation.

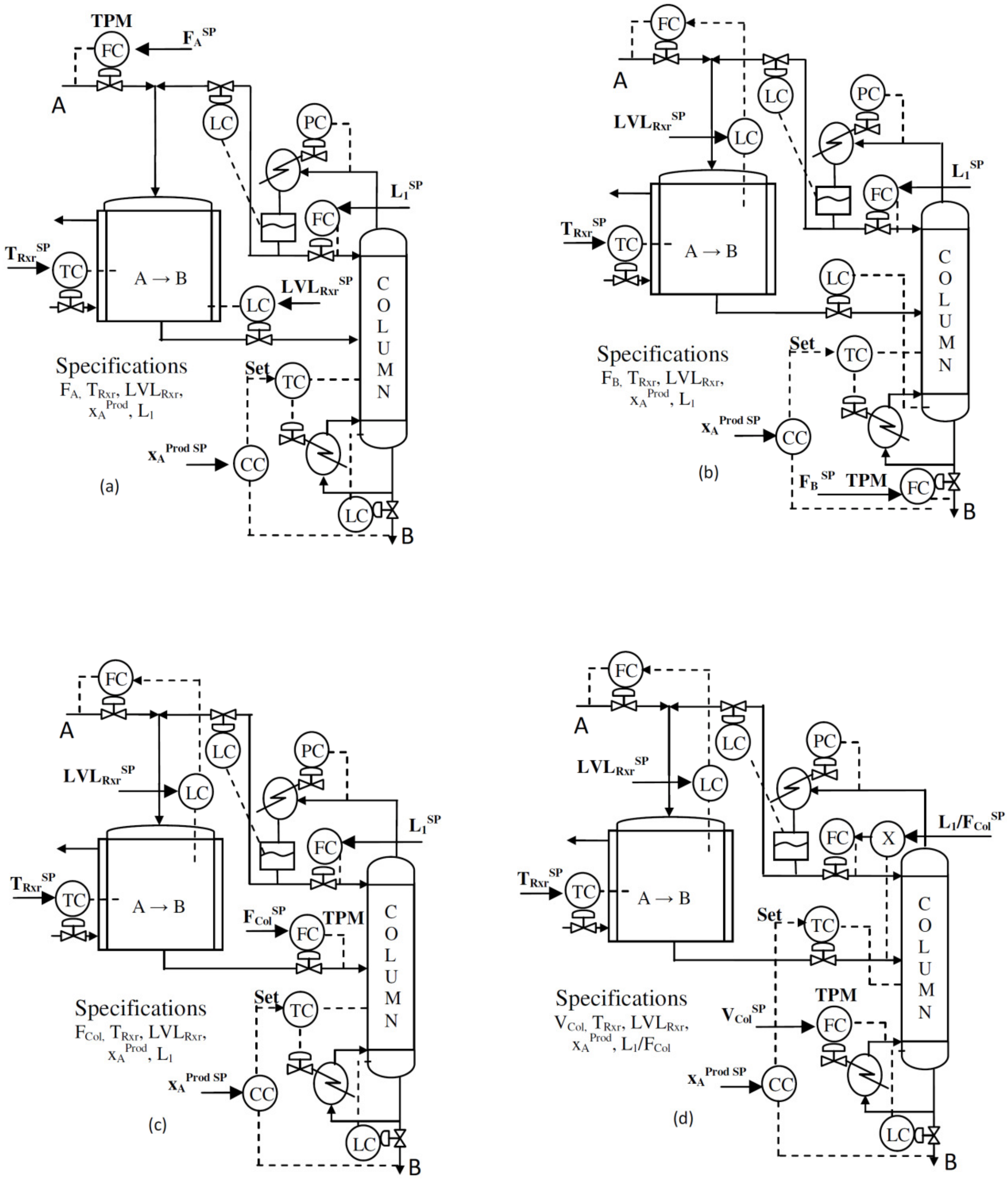


Figure 13.1. One-to-one correspondence between CV setpoints and steady state specification variables for a simple recycle process

13.2. Two-Tier Plantwide Control System Design Framework

The control system of a process plant has two main objectives:

1. Optimal economic operation: Control economic CVs
2. Stable operation: Control drifting inventories (i.e. material balance control)

'Inventory' is interpreted here in its most general sense to include material, phase, component and energy inventories in the different units as well as the overall process. The CVs for process inventory regulation (material balance control) are usually obvious. They typically include liquid levels and pressures, as well as selected temperatures, for example, a sensitive temperature in a distillation column. The best CVs for economic operation at a given throughput may be obtained from steady state optimization. Alternatively, process insight or operating experience may also suggest economically sound CVs that should be controlled.

Optimal operation requires operating the process at the optimal point, that is, *at* all the optimally active constraints as well as at the optimum value for decision variables corresponding to any remaining unconstrained DOFs. Typically, multiple constraints are active at the optimum solution. The choice of the unconstrained decision variable (CV) should be such that its optimum value is relatively insensitive to disturbances, for example, in feed rate or composition. This is the idea of 'self-optimizing' control where the economic loss due to no reoptimization for the disturbance is acceptably small. Purely from the steady state operation perspective, a constant setpoint operating policy with such CVs provides near-optimal operation in the face of disturbances. In summary, the economic CVs for optimal operation are the active constraints at the optimum plus the self-optimizing CVs corresponding to any unconstrained DOFs.

Once the set of economic CVs for a specified throughput are known (tier 1), either from economic optimization or from heuristics, the economic and regulatory loop pairings must be selected (tier 2). Which one of the two objectives (economic control or regulatory control) should have priority when designing the control system pairings (structure)? In the commonly used 'bottom-up' approach, process regulation is given priority over economic control. A 'basic' or 'regulatory' control layer with focus on inventory control (stabilization), usually with the feed rate as the throughput manipulator (TPM), is first designed. On top of this, one adds an 'advanced' or 'supervisory' control layer, often implemented using model predictive control, which aims at achieving optimal economic operation by adjusting the setpoints into the regulatory layer.

A problem with the 'bottom-up' approach is that it can yield slow control of the economic variables due to unfavorable pairings, since control valves are already paired up for regulatory control. This results in economic losses mainly because slow control requires back-off from hard active constraint limits, which can be especially costly when it is optimal to maximize throughput. As illustrated in Figure 13.2, the back-off and consequent economic penalty is primarily determined by the severity of transients in the active constraint for the worst-case disturbance. Even if the constraint is a soft one, tight regulation of the same may be desirable due to the often very non-linear nature of the process with highly skewed deviations in only one direction.

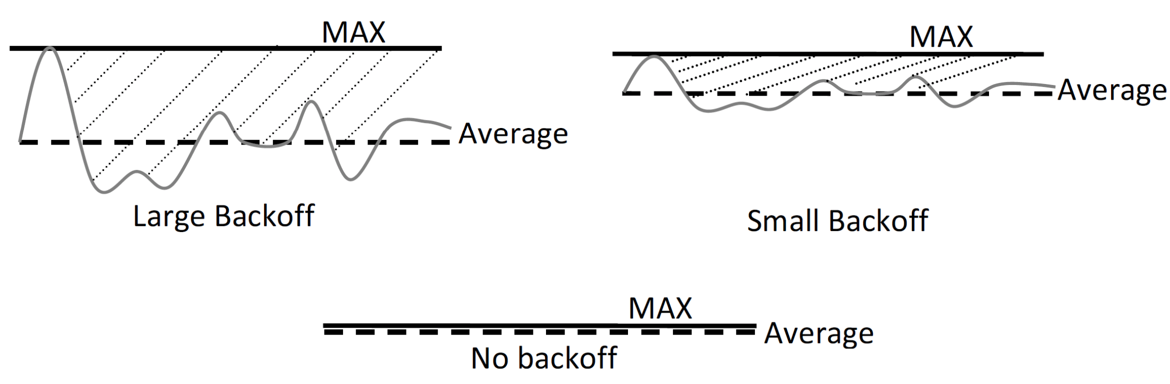


Figure 13.2. Illustration of tightness of active constraint control and back off

In this work, we consider the alternative 'top-down' approach for selecting the control pairings with higher priority to economic control over regulatory control. Such a reprioritization is natural in light of the global push towards green / sustainable / efficient process operation. In this approach, the best possible pairings for tight control of the economic CVs are obtained first followed by pairings for inventory (material balance) control. It attempts to accomplish economic and regulatory control in a single layer. The same is made possible as many-a-times controlling an economic CV accomplishes a regulatory task (and vice versa). Also, processes are designed to have sufficient number of surge capacities and the associated control valves remain available for dynamic control (including inventory control) with no steady state economic impact.

Regardless of the specific pairing philosophy (bottom-up or top-down), the application of the two-tiered framework is relatively straightforward for a given active constraint set, implying a fixed set of economic CVs that must be controlled. For most plants however, the active constraint set expands or contracts depending primarily on the plant throughput. The best economic CV set would then depend on the active constraint set (operating region) and conflicts can arise with a control valve being most suitable for robust inventory control in one region and economic CV control in another. Also, pairings done without considering the impact of a constraint going active can result in loss of crucial control functions such as product quality control or component inventory control with consequent snowballing. Additional override controllers that alter the material balance control structure may need to be configured to ensure a seamless transition and stable operation in the different regions. Alternatively, one can exploit *apriori* knowledge of the full active constraint set to devise a plantwide control system that ensures control of all critical economic and regulatory control objectives regardless of which constraints in the full active constraint set are active. Such a control system is appealing in that its basic regulatory structure remains fixed regardless of the operating region while also avoiding the need for complex over-ride controllers. The two-tiered framework must be appropriately modified to systematically devise such a control structure.

13.3. Active Constraint Regions for a Wide Throughput Range

A process is typically designed for a design throughput, where no hard constraints are active due to over-design of the different processing units. Over its life span, economic considerations necessitate sustained operation at throughputs much below and above the design throughput, usually including operation at maximum achievable throughput. As throughput increases above the design throughput, different processing units reach their (typically hard) capacity constraints, usually one after the other. These active constraints partition the entire throughput range into distinct regions. There are many disturbances in a plant, but throughput is usually considered the principal disturbance because of its wide range encompassing multiple active constraints. A control system that works well for such a large throughput range would also handle other routine disturbances well.

Figure 13.3 illustrates active constraint regions with respect to throughput for a process with 5 steady state DOFs. The active constraints divide the entire throughput range into three regions corresponding to low (2 active constraints), intermediate (3 active constraints) and high throughputs (4 active constraints). At the maximum achievable throughput (5 active constraints), all the steady state DOFs are used up to drive as many constraints active in this hypothetical example. Alternatively, one may have unconstrained DOFs remaining at maximum throughput (i.e. throughput decreases on moving the unconstrained variable away from its optimum value).

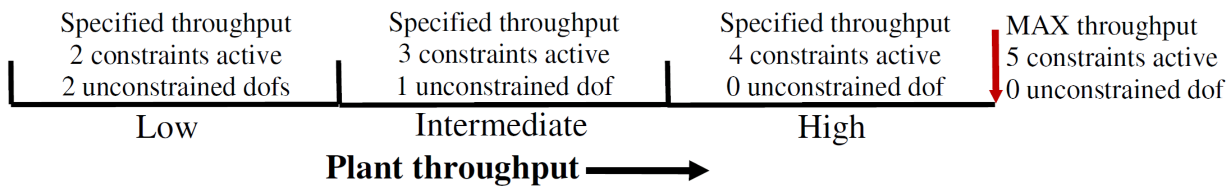


Figure 13.3. Active constraint regions with respect to throughput

Let us assume that the full active constraint set, corresponding to maximum throughput operation, does not change for a given process [a]. To design a truly top-down control system where economic objectives are given the highest priority, loops for the tightest possible control of all the active constraints would first be designed. We would then have the fewest number of control valves left for process regulation, specifically material (total, component and phase) and energy inventory control of the different units and the plant as a whole. If we can achieve effective inventory regulation for maximum throughput operation along with the tightest possible control of the economic CVs, the control system would most certainly work at lower throughputs with additional DOFs (setpoints) available for control due to constraints becoming (optimally) inactive. The reason we emphasize tight economic CV control at maximum throughput is that this is where the economic benefits of improved operation are usually the largest.

13.4. Systematic Control System Design Procedure

Based on the above arguments, the two-tier plantwide control system design framework is modified to designing a robust control system for process operation at maximum achievable throughput with tight economic CV control, arguably the most difficult to stabilize due to the highest number of active constraints, and then designing loops for taking up additional control tasks using constraints (setpoints) that become optimally inactive at lower throughputs. The additional control task may be economic CV control or throughput manipulation A step-by-step 'top-down' procedure for designing the overall control system for near optimum operation over a wide throughput range is then:

Step 0: Obtain active constraint regions for the wide throughput range
Step 1: Pair loops for tight control of economic CVs at maximum throughput
Step 2: Design the inventory (regulatory) control system
Step 3: Design loops for 'taking up' additional economic CV control at lower throughputs along with appropriate throughput manipulation strategy
Step 4: Modify structure for better robustness / operator acceptability

Each of these distinct steps is now elaborated upon.

[a] This appears to be a reasonable assumption.

13.4.1. Step 0: Obtain active constraint regions for the wide throughput range

Steady state optimization of the available steady state DOFs is performed to obtain the expanding set of active constraints with increasing throughput. A wide throughput range, from below design throughput to the maximum achievable, is considered. The active constraints partition the entire throughput range into distinct regions. To assess the economic impact of a back-off in any hard active constraints, obtain the economic sensitivity of the hard active constraints at maximum throughput, which corresponds to the full active constraint set. The sensitivities dictate the prioritization as to which constraints must be controlled the tightest.

Corresponding to the unconstrained DOFs in an active constraint region (including maximum throughput), propose self-optimizing CVs that give near-optimal operation with constant setpoint. Sometimes such self-optimizing CVs are not forthcoming. This is acceptable with the implicit understanding that these setpoints are adjusted by a real-time optimizer.

13.4.2. Step 1: Pair loops for tight maximum throughput economic CV control

The economic CVs at maximum throughput are all the active constraints (full active constraint set) and self-optimizing CVs corresponding to any unconstrained steady state DOFs. Typically constraints on maximum allowable product impurity, maximum allowable effluent discharge etc. would be active along with hard capacity constraints such as column operation at flooding limit, furnace operation at maximum duty etc. The full active constraint set may include direct MVs (e.g. a fully open valve). Direct MVs that are optimally at a constraint limit should be left alone at the limit and not used for conventional control tasks. Other active output constraints should be selected as CVs and tightly controlled using close-by MVs that are not active (saturated). For direct MV active constraints, the back-off is then eliminated while for active output constraints, the back-off is mitigated by the tight control.

After implementing loops for tight active constraint control (including leaving a direct MV at its limit), design loops for tight control of self-optimizing CVs. The economic optimum with respect to these unconstrained variables is often 'flat' so that the economic penalty for small deviations from the optimum setpoint is likely to be smaller than for a back-off from an active constraint limit. The loops for self-optimizing CV control are therefore implemented only *after* the loops for tight active constraint control. The flexibility in the input-output (IO) pairings then gets utilized for the tightest control of the economically most important CVs.

There may be situations where the best self-optimizing CV exhibits extremely slow and difficult dynamics. The control implementation may then be decomposed into a faster loop that controls a dynamically better behaved close-by secondary CV, which is not the best self-optimizing CV, with a cascade loop above adjusting its setpoint to ensure that the best self-optimizing CV is maintained close to its (optimum) setpoint over the long-term.

We also note that economic optimality usually requires maximizing reactive inventory hold up, for example, liquid (gas) phase reactor operation at maximum level (pressure). The best pairings for tight control of these inventories should be implemented in this step itself with the remainder of the inventory control system being synthesized in the next step (Step 2).

13.4.3. Step 2: Design the inventory (regulatory) control system

Given loops for tight economic CV control at maximum throughput, implement appropriate loops for consistent inventory control [4] of the different units and the overall process. Inventory is interpreted in its most general sense to include total amount of material, phases (e.g. liquid or vapour), components as well as energy held within the individual units and the overall process. Ensuring consistency of the inventory control system then accounts for tricky regulatory plantwide issues such as the snowball effect due to the integrating nature of component inventories in recycle systems. As recommended in Luyben et al. [14, 16], a 'Downs Drill' must be performed to ensure the control system guarantees that no chemical component (and energy) builds up within the process.

We note that processes are designed with sufficient number of surge capacities to smoothen flow imbalances and facilitate start-up / shut-down. Thus, even if all steady state DOFs are exhausted at maximum throughput to drive as many constraints active, these surge capacities with their associated independent control valves ensure availability of control valves for inventory regulation. An example is a simple distillation column with two steady state DOFs and five control valves (excluding feed). Let us say that to minimize energy consumption, the light key and heavy key in respectively the bottoms and distillate should be at their maximum limits. The 2 steady state DOFs thus get exhausted in driving as many constraints active. If two valves (e.g. reflux and reboiler steam) are paired for maintaining the light-key and heavy key impurities in the two product streams at their maximum limits, three valves (e.g. distillate, bottoms and condenser duty) remain available for controlling the three inventories (reflux drum level, bottom sump level and column pressure).

In a top-down sense, inventory regulation (stabilization) is a lower objective than economic control. The economic CV control loops are therefore put in place first (Step 1) followed by the inventory control system (Step 2). In the inventory loops, local unit specific pairings should be used \to the extent possible. However since valves already paired in Step 1 for tight economic CV control are unavailable, some of the inventory loop pairings may possibly be unconventional non-local 'long' loops.

It is important that, at least in the first pass, a truly 'top-down' plant-wide control structure with such unconventional inventory loops be synthesized. In situations where the inventory control turns out to be fragile due to these unconventional loops, the economic CV loop and inventory loop pairings can always be appropriately revised (this is Step 4 of the procedure). Many a times, these unconventional and seemingly unworkable inventory loops actually work surprisingly well in practice. An example is bottom sump level control of a column with a very small bottoms stream, akin to a leak compared to the internal column flows. Conventional wisdom would suggest using such a leak stream for bottoms level control is unworkable and therefore ill-advised. If however a stripping section tray temperature is well controlled e.g. by adjusting the boilup or feed, the seemingly unworkable pairing provides acceptable sump level control [25]. Level control would be lost only when the temperature loop is put on manual. In our opinion, the unconventional level controller pairing is acceptable with the caveat that the stripping temperature loop be viewed as part of the overall inventory control system and never put on manual. One of the case-studies provides another example where an unconventional inventory control loop pairing works surprisingly well.

13.4.4. Step 3: *Design loops for additional economic CV control at lower throughputs along with throughput manipulation strategy*

In the control structure for process operation at maximum throughput, one setpoint (TPM) must be used to reduce the process throughput below maximum. Usually, the setpoint for the last constraint to go active is an immediate choice for the TPM. Moving this TPM setpoint away from its active constraint limit would reduce the throughput. As throughput is reduced, additional active constraints become optimally inactive, typically, one after the other. The unconstrained setpoints of the corresponding constraint controllers are now MVs that may be used to control additional self-optimizing CVs for near-optimal operation at lower throughputs. For dynamic reasons, the new CV should be close to the MV (constraint controller setpoint) that becomes available. If such a close-by pairing is not forthcoming, the new unconstrained setpoint may alternatively be considered for use as the TPM in that active constraint region, while using the 'old' TPM (from the more constrained higher throughput region) to control the new CV. The best throughput manipulation strategy across the wide throughput range would then depend on the specific full active constraint set.

To develop such a scheme, list the MV setpoints that become unconstrained along with close-by CVs whose control can be taken-up for more economical operation. Usually, conventional control tasks are best taken up by these MV setpoints. An example is a column moving away from its flooding limit and the resulting unconstrained boilup (MV) taking up column tray temperature control for better energy efficiency. In this list, the unconstrained MV setpoint that gives the dynamically poorest economic CV control may be used as the TPM. In the special case where this MV setpoint is the last constraint to go active and its optimal variation with throughput is monotonic, this single setpoint can be used as the TPM over the entire throughput range. If optimality requires holding this MV setpoint constant in a lower throughput region, the TPM must be shifted to the setpoint of the constraint variable that becomes inactive in that lower throughput region. The shifting may have to be repeated depending on the nature of the next constraint that goes inactive on decreasing throughput.

Referring back to Figure 13.3, we note that the next constraint to become active as throughput is increased can always be used as the TPM in that operating region. If we keep shifting the TPM to the next constraint to go active as throughput is increased, the back-off from the active constraint limit is mitigated. In particular, using the unconstrained setpoint of a constraint control loop as the TPM allows the setpoint to be left closest to its active limit with the least back-off. If the constraint is economically dominant (i.e. large economic penalty per unit back-off), both throughput manipulation and reduced economic penalty due to mitigated back-off get achieved. Another pairing possibility that allows the same is using the unconstrained setpoint of the constraint control loop to control a self-optimizing CV, and not a critical CV such as product quality (critical for economic reasons) or a process inventory (critical for process stabilization). When the constraint limit is reached (e.g. when throughput is increased), control of the non-critical self-optimizing CV is simply given up and the constraint variable setpoint is left closest to the constraint limit with the least back-off. In the special case where the active constraint is a saturated valve, the valve gets left at its saturated position with no back-off.

The point is that there is nothing sacrosanct about fixing the TPM location, although it may be desirable that operators have a single handle to adjust the throughput. This flexibility should be gainfully exploited for eliminating / mitigating the back-off in economically dominant active constraints, obtaining pairings for tight control of the additional unconstrained economic

CVs at lower throughputs as well as simplifying the overall plantwide control system. The throughput manipulation strategy is therefore best considered along with the additional unconstrained economic CV loop pairings in a single step. The best throughput manipulation strategy usually becomes self evident in light of the particular full active constraint set.

13.4.5. Step 4: Modify structure for better robustness / operator acceptance

The control structure obtained from Step 1-3 corresponds to a fully top-down design approach where tight economic CV control at maximum throughput is given precedence over regulatory inventory control, for which control valves are typically available by the design of the process. Through carefully chosen input-output (IO) pairings, the structure attempts to transform all the process variability to the surge capacities and utilities, while maintaining economic CVs at their constrained / optimum setpoints. In such a structure, we may have inventory control loops that are quite unconventional with long loops across units. These may result in fragile inventory (including energy inventory) control.

A surge drum overflowing or drying for even moderately large flow disturbances is a typical result of inventory control fragility. Another example is temperature control of a highly exothermic CSTR with maximum reactor cooling duty being an active constraint. If the cooling duty is left alone at maximum (as it is active) and the CSTR temperature is controlled using the reactor feed, there is the possibility of a thermal runaway with reactants slowly building up inside the reactor when the temperature is below setpoint and the accumulated reactants lighting up once the temperature starts to rise back-up due to the exponential dependence of reaction rate on temperature. The energy inventory inside the reactor then blows up, which is unacceptable. The IO pairings must then be revised to improve inventory control robustness.

To revise the pairings, in the control structure obtained for maximum throughput operation (Step 1-3), tight control of one or more economic CVs must first be given up to free appropriate control valves that then get paired for robust / conventional inventory control. The valves (or setpoints) that become available in lieu may be used for less tight or loose control of the economic CVs whose control was earlier given up. In this exchange of economic CV and unconventional inventory loop MVs for a more robust / conventional inventory control system, it is preferable that the economic CV with the least economic impact (lowest sensitivity) be used to minimize the economic penalty. Instead of unconventional 'long' inventory loops, the revised structure would then have more conventional inventory loops with 'long' economic CV loops.

In most chemical processes, only a few active constraints are dominant with a large economic penalty per unit back-off. With appropriate iteration between Step 1-3, it should be possible to synthesize a control system for tight control of the few dominant active constraints with a not-too-unconventional (i.e. acceptable) and robust inventory control system along with well-behaved additional unconstrained economic CV loops at lower throughputs.

The application of the systematic approach for economic plantwide control system design is demonstrated on four realistic process examples. The first example process is a hypothetical reactor-separator-recycle process with side reaction. The second example process is a C_4 isomerization process. The ethyl benzene manufacturing process is the third example considered. We finally consider two alternative processes for cumene manufacture.

Chapter 14. Economic Plantwide Control of Recycle Process with Side Reaction

14.1. Process Description

The process flowsheet is shown in Figure 14.1 and consists of a cooled liquid phase CSTR followed by a stripper and a distillation column. The main reaction A + B → C and the minor side reaction C + B → D occur in the CSTR. Reaction kinetics and other modelling details are available in Jagtap et al. [7]. The unreacted A and B in the reactor effluent are stripped, condensed and recycled along with some C. The stripper bottoms is fractionated to recover 99% pure C as the distillate (main product) and D with some C as the bottoms (side product). The process has 7 steady state DOFs (2 fresh feeds, reactor level and temperature, 1 stripper DOF and 2 column DOFs) and there are 13 independent control valves. Thus even if all steady state DOFs are exhausted at maximum throughput, 6 valves would still remain available for dynamic control, including inventory control.

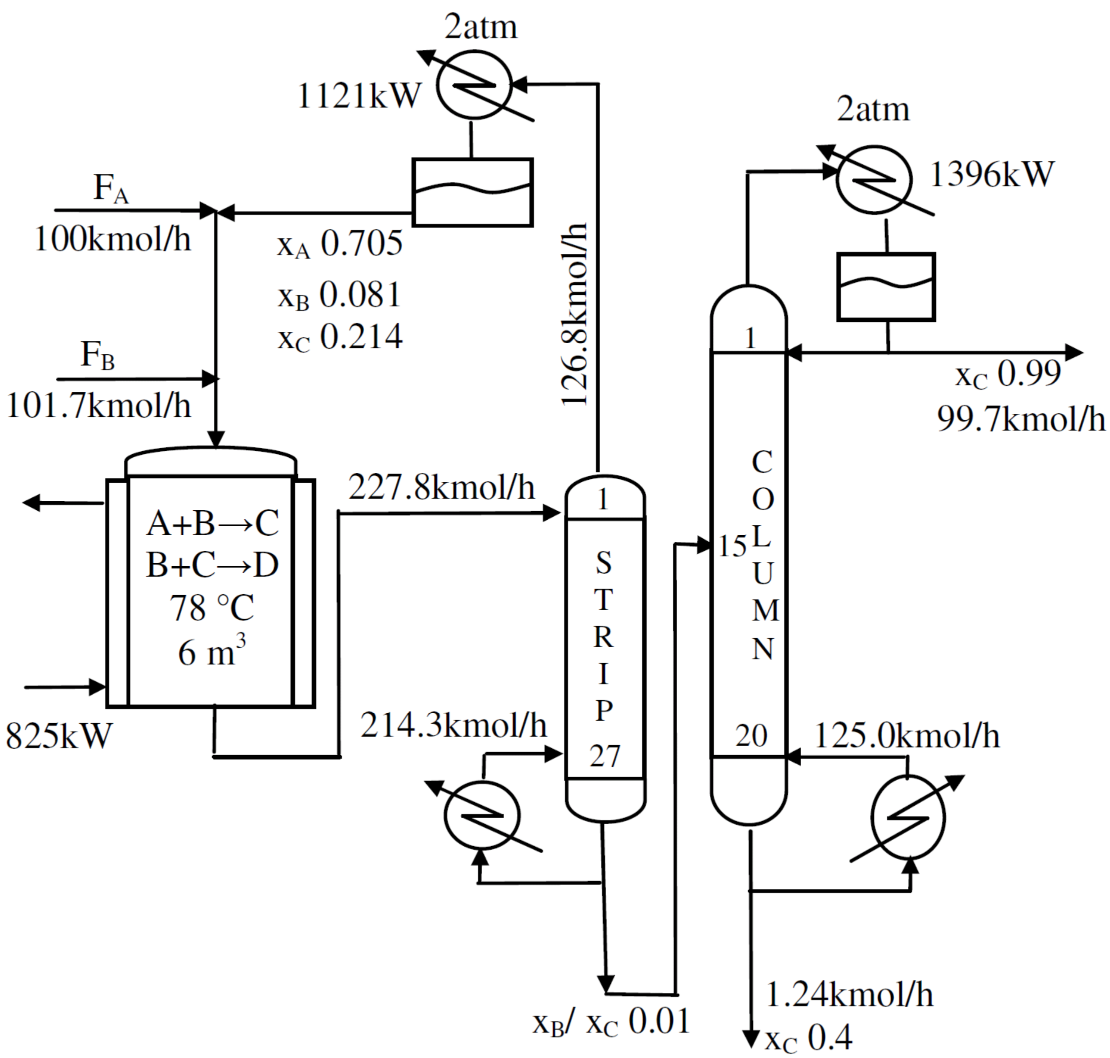


Figure 14.1. Schematic of recycle process with design and base operating conditions

14.2. Economic Plantwide Control System Design

Table 14.1 neatly summarizes the step-by-step implementation of the four-step economic plantwide control system design procedure to this process. A reasonably detailed explanation of the steps is provided in the following.

Table 14.1. Economic Plantwide Control Structure Synthesis for Recycle Process

Step 0: Active Constraint Regions and Economic CV's

Region	I	II	III	Max Throughput
Additional Active Constraints*	-	V_1^{MAX}	V_1^{MAX} T_{Rxr}^{MAX}	V_1^{MAX} T_{Rxr}^{MAX} V_2^{MAX}
Unconstrained DOF's	2	1	0	0
Self-Optimizing CV's	x_B^{Rxr}, T_{Rxr}	x_B^{Rxr}	-	-

Step 1: Maximum Throughput Economic Control Loops

Active Constraint Control Loops	$T_{Rxr}^{MAX} \leftrightarrow Q_{Rxr}$	$V_1^{MAX} \leftrightarrow Q_{Reb1}$	$V_2^{MAX} \leftrightarrow Q_{Reb2}$	$T_S^{Col} \leftrightarrow B_1$
	$x_B^{ColD} \leftrightarrow T_{Stp}^{SP} \leftrightarrow F_{Stp}^{SP}$	$x_D^{ColD} \leftrightarrow L_2/B_1^{SP} \leftrightarrow L_2^{SP}$		$LVL_{Rxr}^{MAX} \leftrightarrow F_{Tot}^{Rxr} \leftrightarrow F_A$
Self-Optimizing Loops	none			

Step 2: Maximum Throughput Inventory Loops

$LVL_{Reb2} \leftrightarrow B_1$	$LVL_{Cnd1} \leftrightarrow F_{Rcy}$	$P_{Cnd1} \leftrightarrow Q_{Cnd1}$
$LVL_{Reb1} \leftrightarrow x_B^{Rxr\ SP} \leftrightarrow (F_B/F_{Tot}^{Rxr})^{SP} \leftrightarrow F_B$	$LVL_{Cnd2} \leftrightarrow D_2$	$P_{Cnd2} \leftrightarrow Q_{Cnd2}$

Step 3: Additional Self-Optimizing CV Loops at Reduced Throughput

Region III	Region II	Region I
TPM: V_2^{SP}	TPM: V_2^{SP} $x_B^{Rxr\ SP\#} \leftrightarrow (F_B/F_{Tot}^{Rxr})^{SP} \leftrightarrow F_B$ $LVL_{Reb1} \leftrightarrow T_{Rxr}^{SP} \leftrightarrow Q_{Rxr}$	TPM: V_2^{SP} $T_{Rxr}^{SP\#} \leftrightarrow Q_{Rxr}$ $x_B^{Rxr\ SP\#} \leftrightarrow (F_B/F_{Tot}^{Rxr})^{SP} \leftrightarrow F_B$ $LVL_{Reb1} \leftrightarrow V_1^{SP} \leftrightarrow Q_{Reb1}$

Step 4: Modifications for Conventional Inventory Control Loop

$LVL_{Reb1} \leftrightarrow B_1$; $T_S^{Col2} \leftrightarrow V_2^{SP}$(with sufficient back-off in V_2^{SP})

Region III	Region II	Region I
TPM: $x_B^{Rxr\ SP}$	TPM: T_{Rxr}^{SP} $x_B^{Rxr\ SP\#}$	TPM: V_1^{SP} $T_{Rxr}^{SP\#}$ $x_B^{Rxr\ SP\#}$

*: LVL_{Rxr}^{MAX}, x_B^{ColD}, x_D^{ColD}, T_S^{Col} are always active; #: Set point value is the optimized value

14.2.1. Step 0: Active Constraint Regions and Economic Operation

To avoid product give-away, the product C impurity mol fractions are fixed at their specified upper limits of 0.98% B (x_B^{ColD}) and 0.02% D (x_D^{ColD}) for the desired 99 mol% pure C (x_C^{ColD}) product. At maximum throughput, the active constraints are maximum column boilup (V_2^{MAX}), reactor temperature (T_{Rxr}^{MAX}), stripper boilup (V_1^{MAX}) and reactor level (LVL_{Rxr}^{MAX}). Further, to prevent loss of precious C with the side product, the average temperature of three adjacent sensitive stripping trays (T_S^{Col}) is maintained [a]. The four equipment capacity constraints, the two product impurity mol fractions and the product column stripping section temperature specification exhaust all 7 steady state DOFs.

At lower throughputs, it is economically near optimal to hold the two product impurity mol fractions and the column stripping section temperature at their maximum throughput values. Also, the LVL_{Rxr}^{MAX} constraint is active at all throughputs as it maximizes the reaction conversion at a given reactor temperature. As throughput is reduced below maximum, the capacity constraints become optimally inactive in the order V_2^{MAX}, T_{Rxr}^{MAX} and V_1^{MAX}. The entire throughput range thus gets partitioned into three active constraint regions (see Table 14.1, Step 0). The number of unconstrained steady state DOFs corresponding to the low throughput (only LVL_{Rxr}^{MAX} active), intermediate throughput (LVL_{Rxr}^{MAX} and V_1^{MAX} active) and high throughput (LVL_{Rxr}^{MAX}, V_1^{MAX} and T_{Rxr}^{MAX} active) regions is respectively, 2, 1 and 0. The V_2^{MAX} constraint going active represents the loss of DOF corresponding to specifying the throughput. The process throughput is then determined by the actual 7 equality / inequality constraint variable values. Jagtap et al. [11] have shown that in the low throughput region, holding the reactor temperature (T_{Rxr}) and the CSTR inlet B (limiting reactant) concentration (x_B^{Rxr}) at appropriate constant values provides near-optimal steady operation. In other words, T_{Rxr} and x_B^{Rxr} are self-optimzing CVs corresponding to the two unconstrained DOFs. In the intermediate throughput region, holding x_B^{Rxr} constant ensures near optimum steady operation (T_{Rxr}^{SP} is not held constant and adjusted for either active constraint control or throughput manipulation). In the high throughput region, there are no unconstrained steady state DOFs left.

14.2.2. Step 1: Loops for Tight Control of Full Active Constraint Set

We now design the control system for maximum throughput operation, where all constraints in the full active constraint set are active. At maximum throughput, there is no TPM as all steady state DOFs are exhausted implying the DOF related to throughput is used for active constraint control. V_2^{MAX} and V_1^{MAX} are active hard constraints with significant economic penalty. Any back-off from V_2^{MAX} causes a large loss in throughput and any back-off in V_1 causes a reduction in the recycle rate and hence a loss in selectivity. Accordingly, V_1 and V_2 are controlled tightly using the respective reboiler steam valves. The back-off necessary from V_1^{MAX} and V_2^{MAX} is then almost negligible.

It is economically important to have tight control of the impurities in the product. The product impurity D mol fraction (x_D^{ColD}) is controlled using the column reflux. The composition controller manipulates the reflux-to-feed ratio setpoint [b]. Maintaining product impurity B mol

---

[a] This ensures that C composition in the byproduct stream remains small

[b] In practice, the composition controller would cascade a setpoint to a rectifying tray temperature controller which manipulates the L/F ratio setpoint.

fraction (x_B^{ColD}) requires tight control of the B dropping down the stripper as all of it ends up in the product. Since V_1^{MAX} is active, V_1 cannot be used for stripper tray temperature control. The stripper temperature (T_{Stp}) controller then manipulates the stripper feed (F_{Stp}), which provides tight temperature control. The temperature setpoint is adjusted by a cascade x_B^{ColD} controller.

LVL_{Rxr}^{MAX} and T_{Rxr}^{MAX}, the other active equipment capacity constraints imply LVL_{Rxr} and T_{Rxr} must be controlled tightly. Controlling LVL_{Rxr} and T_{Rxr} (at their maximum limits) would also stabilize the reactor material and energy inventories, respectively. For tight control, T_{Rxr} is controlled using reactor cooling duty (Q_{Rxr}), the MV with the best dynamic response (fast dynamics and high open loop gain). We assume T_{Rxr}^{MAX} to be a soft constraint and set $T_{Rxr}^{SP} = T_{Rxr}^{MAX}$. The orientation of the reactor level controller must be opposite to process flow since the reactor effluent (F_{Stp}) is already paired for stripper temperature control. The total flow to the reactor (F_{Tot}^{Rxr}) is a good MV for tight reactor level control. Accordingly, LVL_{Rxr} is controlled by adjusting $F_{Tot}^{Rxr\ SP}$, which in turn is maintained by manipulating the fresh A feed (F_A).

Lastly, it is economically important to maintain an appropriate column stripping section temperature (T_S^{Col}) to ensure loss of precious C in the bottoms is kept small. The active V_2^{MAX} constraint implies column boilup is unavailable for temperature control. Accordingly, the column feed (B_1) is manipulated for the purpose. The active constraint control loops are shown in Figure 14.2. The constrained setpoints at maximum throughput are highlighted in brown.

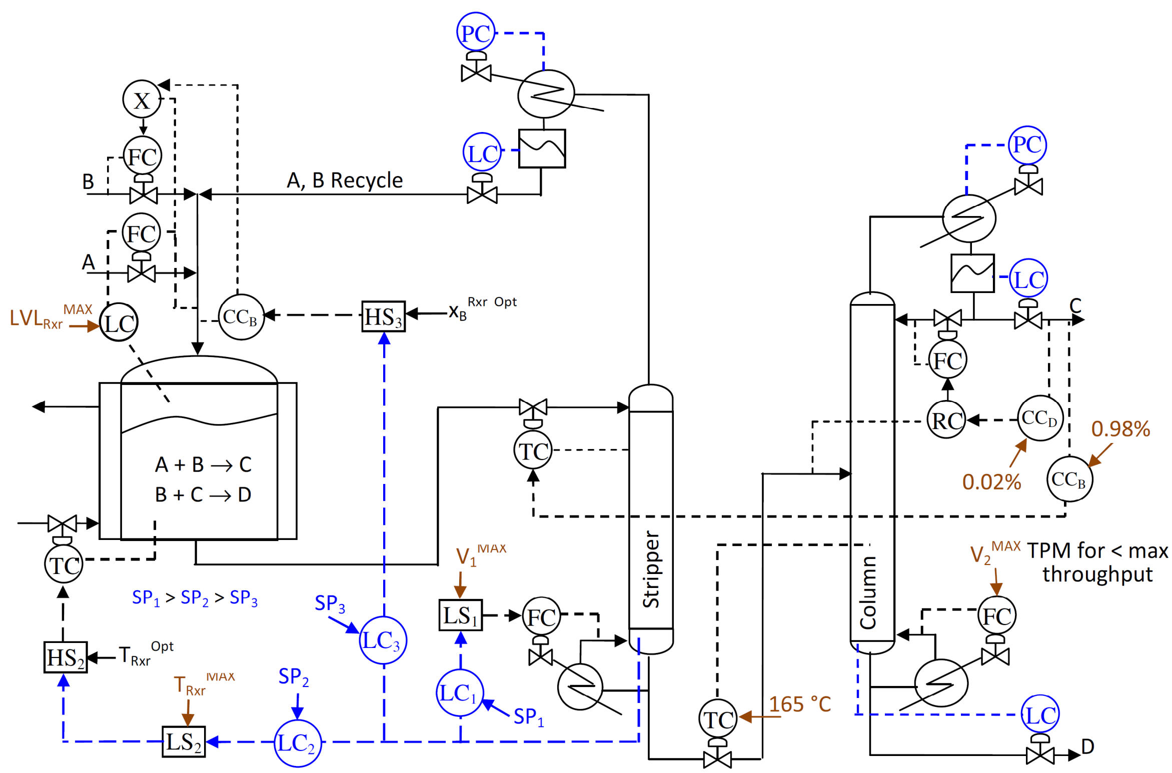


Figure 14.2. Plantwide control structure for maximum throughput operation of recycle

14.2.3. Step 2: Inventory (Regulatory) Control System

Control loops to stabilize the liquid, vapour and component inventories in the process are now implemented using the available unpaired valves (reactor level and energy is already stabilized by the LVL_{Rxr} and T_{Rxr} loops). The inventory loops are shown in blue in Figure 14.2. We need to control the column reflux drum and sump levels, the stripper sump level and the recycle condenser level. The column and the recycle condenser pressures also need to be controlled.

The existing loops for tight active constraint control in Figure 14.2 imply obvious loop pairings for inventory control. The column reflux drum level (LVL_{Cnd2}) is controlled using the distillate (D_1). The recycle and column condenser pressures (P_{Cnd1} and P_{Cnd2}) are controlled using the respective cooling duty valves (Q_{Cnd1} and Q_{Cnd2}). The column sump level (LVL_{Bot}) is controlled using the feed from the stripper (B_1). To mitigate transients in the reactor composition, F_B is maintained in ratio with F_{Tot}^{Rxr}. To ensure A or B component inventory does not build up inside the recycle loop (snowball effect), the B mol fraction in the reactor inlet (x_B^{Rxr}) is maintained by adjusting the F_B to F_{Tot}^{Rxr} ratio setpoint ($F_B/F_{Tot}^{Rxr\ SP}$).

With these pairings, no close-by valves are left for controlling stripper sump level (LVL_{Stp}). The only available option is to adjust the $x_B^{Rxr\ SP}$. The pairing makes sense in that the reaction products accumulate in the stripper sump for downstream separation. The sump level is then an indirect indication of the reactor production rate. If this level is falling, the reactor production needs to be increased. Increasing the $x_B^{Rxr\ SP}$ causes the limiting reactant B composition in the reactor to increase with consequent increase in generation of product C and hence in the stripper sump level.

The stripper level controller is the most unconventional in the scheme. Will it work in practice? That depends on the hold up in the CSTR. If the reactor is too big, the dynamic effect of a change in the $x_B^{Rxr\ SP}$ on stripper sump level would be slow and it may run dry or overflow during worst case transients. The robustness of the control system is tested for a ±5 5% step bias in the F_B sensor (control system tuning details in Appendix A). In the transient response, all the levels are well controlled with the maximum deviation in the stripper sump level being < 4%. The inventory control scheme, though unconventional, is quite robust and acceptable.

14.2.4. Step 3: Additional Economic CV Control Loops and Throughput Manipulation

At lower throughputs, the additional unconstrained economic CVs whose control must be taken up are x_B^{Rxr} and T_{Rxr}. Both are associated with the reactor. Since maximum column boilup (V_2^{MAX}) is the last constraint to go active and its optimal variation with throughput is monotonic, we consider using it as the TPM over the entire throughput range. Now as V_2^{SP} is reduced below V_2^{MAX}, the production rate would decrease below maximum with x_B^{Rxr} reducing. The excess A inside the reactor then increases to further suppress the side reaction for improved yield to the desired product. When x_B^{Rxr} reduces to its optimal value, it must be held constant for optimal operation. LVL_{Stp} then gets controlled using T_{Rxr}^{SP}, in lieu of x_B^{Rxr}. T_{Rxr}^{SP} would reduce below T_{Rxr}^{MAX} as V_2^{SP} is decreased. When T_{Rxr}^{SP} decreases to its optimum value, it must be held constant. LVL_{Stp} then gets controlled using V_1^{SP} in lieu of T_{Rxr}^{SP}). V_1^{SP} would reduce below V_1^{MAX} as V_2^{SP} is reduced to decrease the throughput. The stripper bottom sump level controller pairing thus switches from $x_B^{Rxr\ SP}$ to T_{Rxr}^{SP} to V_1^{SP} as throughput is reduced. Referring to the throughput regions in Table 14.1, at high throughputs, x_B^{Rxr} floats to the appropriate value determined by V_2^{SP} via the action of the inventory control system. At intermediate throughputs, x_B^{Rxr} is maintained at its optimum and T_{Rxr} floats to the appropriate value. Finally, at low throughputs, x_B^{Rxr} and T_{Rxr} are held at their near optimum values and V_1^{SP} floats to the appropriate value.

A simple override scheme to accomplish the switching between the operating regions with three separate PI stripper sump level controllers (LC_1, LC_2 and LC_3) is shown in Figure 14.2. The MVs for LC_1, LC_2 and LC_3 are respectively, V_1^{SP}, T_{Rxr}^{SP} and $x_B^{Rxr\ SP}$. At maximum throughput, since T_{Rxr}^{MAX} and V_1^{MAX} are active, LC_1 and LC_2 are inactive and sump level control is performed by LC_3. As V_2^{SP} (TPM) is reduced below V_2^{MAX}, LC_3 decreases $x_B^{Rxr\ SP}$. When $x_B^{Rxr\ SP}$ reduces below its optimum value, the high select block, HS_3, passes the optimum value to the x_B^{Rxr} controller. LC_3 then becomes inactive and stripper sump level control is lost. The level then increases beyond LC_2 setpoint and the LC_2 output starts to decrease. When the output decreases below T_{Rxr}^{MAX}, level control is taken over by LC_2. When T_{Rxr}^{SP} decreases below its optimum value, the high select block, HS_2, passes the optimum value and LC_2 becomes inactive and the stripper sump level again rises beyond LC_1 setpoint. LC_1 output then reduces and on decreasing below V_1^{MAX}, the low select block, LS_1, causes LC_1 to take over level control. A complementary logic causes proper switching from LC_1 to LC_2 to LC_3 as throughput is increased.

Note that the decreasing level setpoint order ($LC_1 > LC_2 > LC_3$) is necessary to enforce the proper switching order. For example, when LC_1 is active, the level would be close to LC_1 setpoint and the I action in LC_2 and LC_3 would cause the respective controller output signals to be sufficiently high ensuring the respective (high) select blocks pass the appropriate signal (optimum T_{Rxr}^{SP} and $x_B^{Rxr\ SP}$ respectively). It is also highlighted that in the given scheme, LC_1 is reverse acting and nested with the stripper temperature loop. As LVL_{Stp} decreases, V_1^{SP} increases (reverse action) which causes the stripper temperature to increase. The temperature controller then increases the stripper feed which causes the LVL_{Stp} to return to setpoint.

Rigorous dynamic simulations are performed to test the synthesized control structure in Hysys. Unless specified otherwise, all flow / pressure PI controllers are tuned tight for a fast and snappy servo response. The non-reactive level controllers are P-only with a gain of 2. The only exception is the unconventional stripper sump level controller with overrides. For the three different pairings in the three operating regions, distinct conservative (non-aggressive) tunings are used to dampen flow variability. The CSTR level is controlled using a PI controller for offset free level tracking. The approximate controller tuning is first obtained using the Hysys autotuner and then adjusted for a fast and not-too-oscillatory servo response at maximum throughput. All temperature measurements are lagged by 2 mins to account for sensor and cooling / heating circuit dynamics. To tune the temperature loops, the open loop step response at maximum throughput is obtained and the reset time set to 1/3rd of the approximate 95% response completion time. The gain is then adjusted for a slightly underdamped servo response with mild oscillations. The composition controllers are similarly tuned. A sampling time and delay time of 5 mins each is applied to all composition measurements. Salient controller parameters are reported in Table 14.2.

The dynamic response of salient process variables of this control system to a throughput transition from the base-case throughput (F_A = 100 kmol/h) to the maximum throughput (F_A = 188.7 kmol/h) and back is shown in Figure 14.3. Tight product purity control is achieved along with smooth plantwide transients. The control system is also tested for a ±5% step bias in the F_B measurement signal at maximum throughput operation. The dynamic response is plotted in

Figure 14.4. Notice the tight control of the product impurities as well the C loss in the by-product stream. The synthesized plantwide control system is thus suitable for economic process operation across the wide throughput range.

If a conventional control system with the TPM at the fresh feed were to be implemented, the need for a back-off from V_1^{MAX} and V_2^{MAX} during worst case transients results in significant throughput (economic) loss (~4-7%) [8]. The synthesized plantwide control system thus achieves significantly superior economic operation for the same plant equipment.

Table 14.2. Salient controller tuning parameter for recycle process

CV	K_C	τ_i (min)	Sensor Span
x_B^{Rxr}	0.8	400	0 – 1
T_{Rxr}^*	1	10	60 – 130 ºC
LVL_{Rxr}	0.5	25	0-100%
T_{Stp}	0.5	15	100 – 160 ºC
T_S^{Col}	0.6	25	140 – 180 ºC
x_B^{ColD}	0.1	40	0 – 0.02
x_D^{ColD}	0.1	30	0 0.0004
Tuning for LVL_{Reb1} override control			
LVL_{Reb1}^1	0.8	200	0-100%
LVL_{Reb1}^2	0.6	250	0-100%
LVL_{Reb1}^3	0.5	400	0-100%

All level loops use K_C = 2 unless otherwise specified
Pressure/flow controllers tuned for tight control
All composition measurements: deadtime = 5 min; sampling time = 2 min;
*: Derivative action used with τ_D = 2 min
All temperatures measurements lagged by 2 mins
1: MV= V_1; 2: MV= T_{Rxr},; 3: MV= x_B^{Rxr}

14.2.5. Step 4: Modifications for a More Conventional Inventory Control System

Given that the control system works well with the unconventional stripper bottoms level control loop, Step 4 (control system modification for a more conventional inventory control system) is not necessary. It is however instructive to develop a control system with conventional local inventory control loops.

The stripper sump level control loop in Figure 14.2 is arguably the most controversial inventory control loop. For a more conventional local pairing, the column stripping section temperature (T_S^{Col}) loop is broken to free the stripper bottoms valve, which is then paired to control the stripper sump level. T_S^{Col} may then be maintained by adjusting $x_B^{Rxr\ SP}$ in a long loop. Even as the steady state economic penalty with such a long economic loop is small, the penalty during transients is likely to be severe. Due to the V_2^{MAX} active constraint, the precious C that could not be boiled off would accumulate at the bottom of the product column and get discharged in the by-product stream by the action of the column sump level controller. Since the optimum C leakage in the bottom stream is very small to begin with, one would expect transient deviations in the direction of higher than optimum C leakage to be significantly more severe than in the opposite (lower than optimum C leakage) direction, where there is little / no leeway. The long column stripping section temperature loop is then susceptible to large loss of precious C during transients. To mitigate the same, a local temperature control loop is needed. Accordingly,

T_S^{Col} is controlled using the column boilup (V_2^{SP}). For maximum throughput operation without loss of control of C leaking down the product column bottoms, the $x_B^{Rxr\ SP}$ would be set at a value such that V_2^{MAX} constraint is just hit during the worst case transient. The back-off from V_2^{MAX} then represents an unrecoverable economic loss, which is the price that must be paid for a more conventional inventory control system.

In the original control system (Figure 14.2), V_2^{SP} was used as the TPM in all regions. With the revised pairings where V_2^{SP} is used for T_S^{Col} control, an alternative throughput manipulation strategy is needed. To reduce throughput below maximum (Region III), $x_B^{Rxr\ SP}$ gets used as the TPM. Once $x_B^{Rxr\ SP}$ is reduced to its optimum value, the TPM shifts to T_{Rxr}^{SP} which is reduced below T_{Rxr}^{MAX} (Region II). Once T_{Rxr}^{SP} is reduced to its optimum value, the TPM shifts to V_1^{SP}, which is reduced below V_1^{MAX} (Region I). Note that in this TPM shifting scheme, the back-off from V_1^{MAX} is negligible. Also, the transient variability in T_{Rxr} for operation at T_{Rxr}^{MAX} is minimal as T_{Rxr}^{SP} is not adjusted by any master cascade loop once T_{Rxr}^{MAX} is hit. The revised control system is shown in Figure 14.5 (Step 4 in Table 14.1).

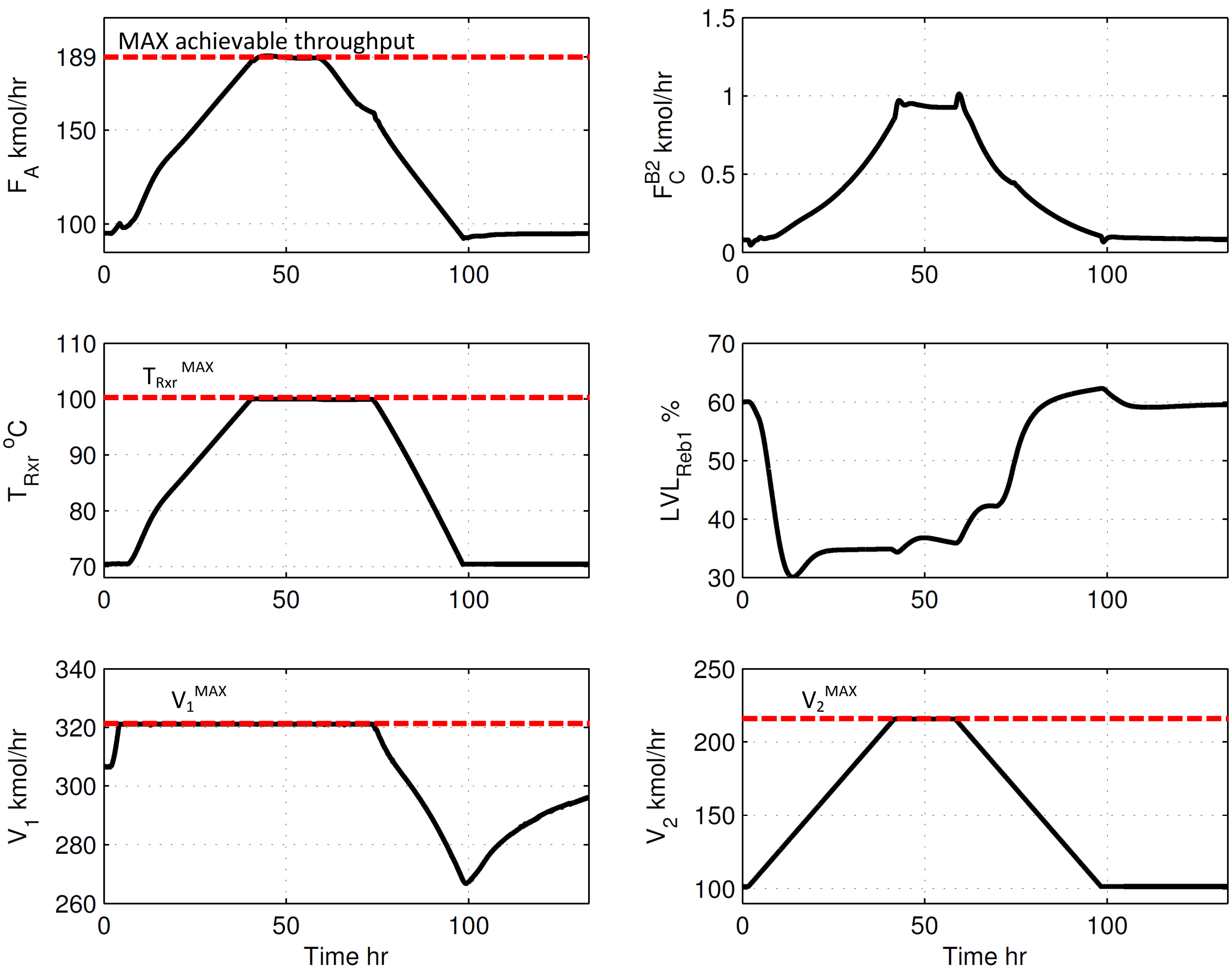


Figure 14.3. Throughput transition with stripper sump level override control scheme

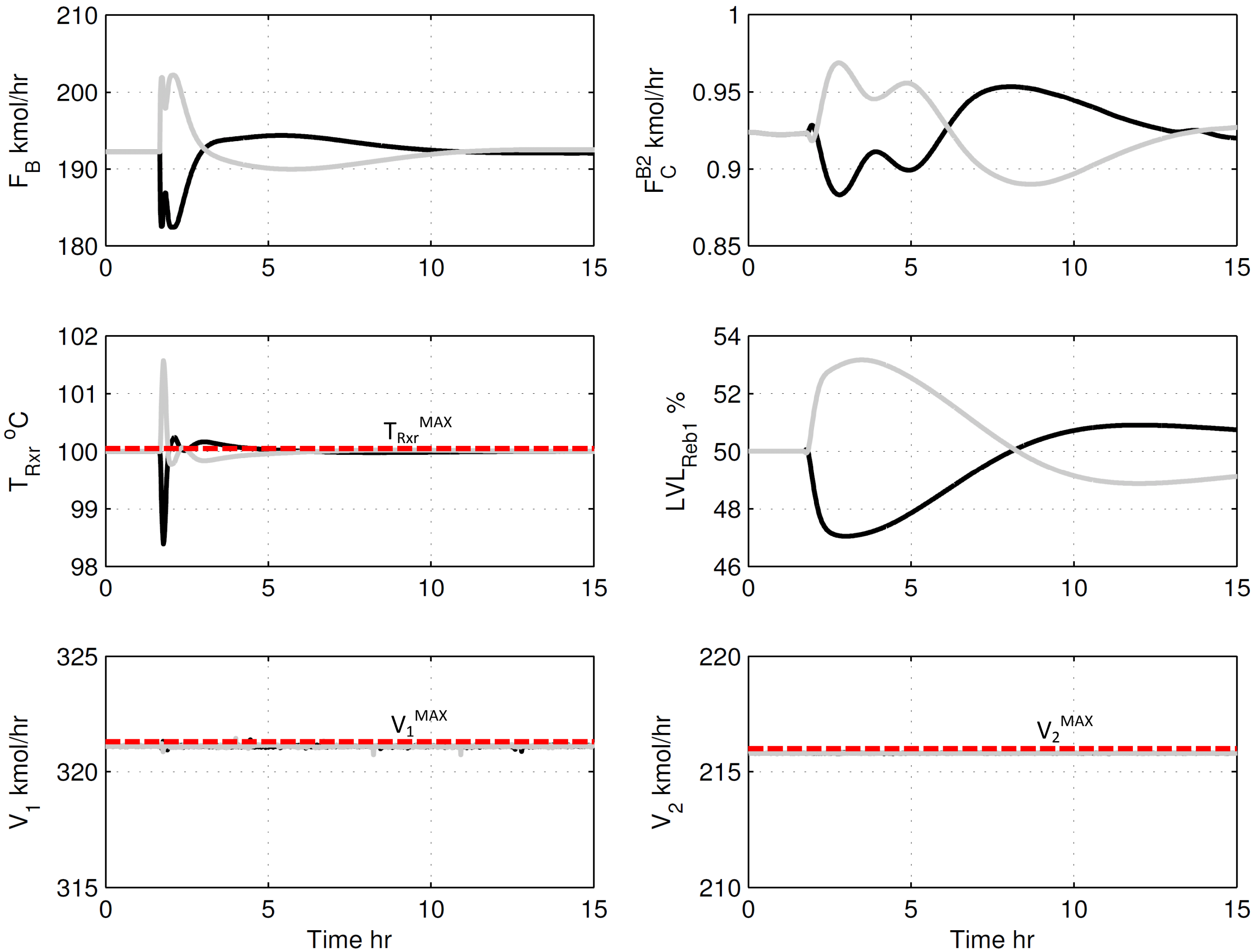


Figure 14.4. Transient response for ±5% step bias in F_B flow sensor

: +5% bias; : -5% bias

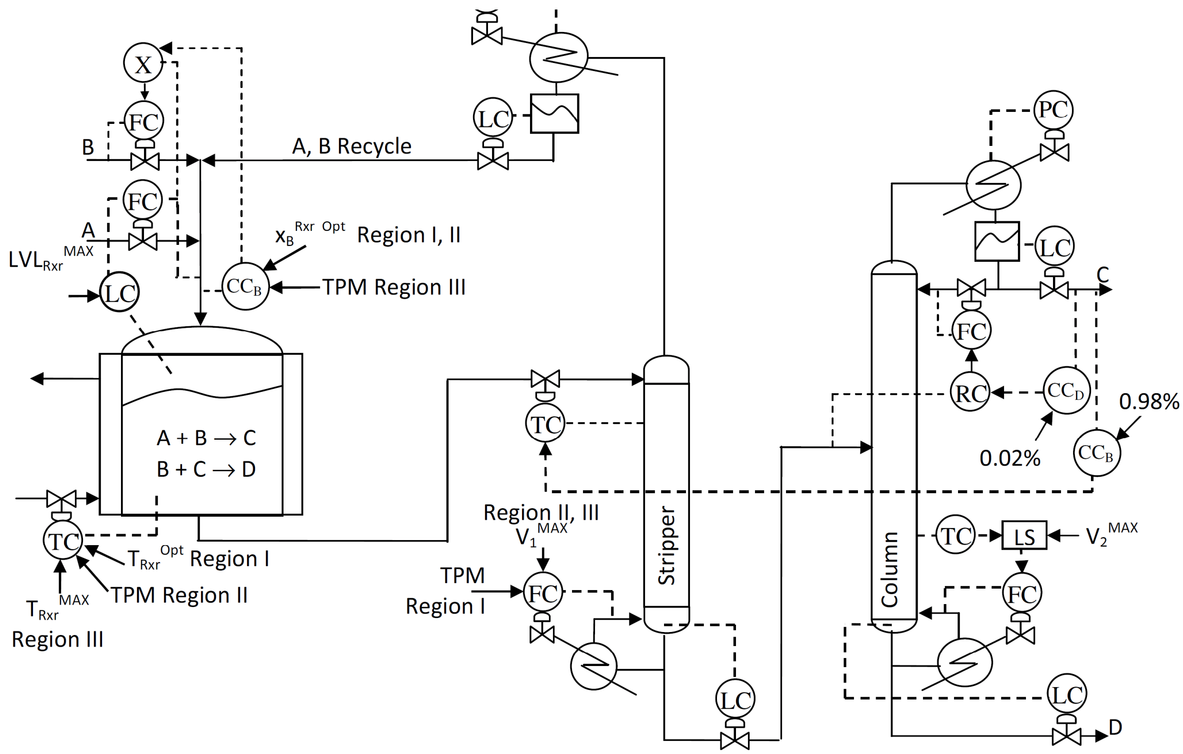


Figure 14.5. Recycle process modified control structure for conventional inventory control

Chapter 15. Economic Plantwide Control of Ethyl Benzene Process

15.1. Process Description

The process consists of two reactors and two columns along with two liquid recycle streams, as in Figure 15.1. The reaction chemistry consists of three reactions

C_6H_6	+	C_2H_4	→	C_8H_{10}		Main Reaction
Benzene		Ethylene		Ethyl Benzene		
C_8H_{10}	+	C_2H_4	→	$C_{10}H_{14}$		Side Reaction
Ethyl Benzene		Ethylene		Diethyl Benzene		
$C_{10}H_{14}$	+	C_6H_6	→	2 C_8H_{10}		Transalkylation
Diethyl Benzene		Benzene		Ethyl Benzene		

The reaction kinetics and other modeling details are available in Jagtap and Kaistha [8]. The first two reactions occur primarily in the first coil cooled CSTR while transalkylation primarily occurs in the second adiabatic CSTR. Near complete ethylene conversion occurs in the two CSTRs. The reaction section effluent is fractionated in the recycle column to recover and recycle unreacted benzene back to the first CSTR. The bottoms is fractionated in the product column to recover 99.9 mol% pure ethyl benzene (EB) as the distillate. The diethyl benzene (DEB) drops down the bottoms and is recycled to the second CSTR. The DEB is allowed to build in the recycle loop so that the DEB formation rate by the side reaction exactly matches the DEB transalkylation rate for no net DEB formation. The DEB is thus recycled to extinction.

15.2. Economic Plantwide Control System Design

The step-by-step synthesis of the economic plantwide control system is summarized in Table 15.1. The major steps are briefly described below.

15.2.1. Step 0: Active Constraint Regions and Optimal Operation

With fixed pressures, the process has nine steady state degrees of freedom: 2 fresh feeds, 2 DOFs for the first reactor (level and temperature), 1 for the second reactor (level) and 4 DOFs for the two columns. At maximum throughput, there are 8 active constraints: maximum recycle column boilup (V_1^{MAX}) and reflux (L_1^{MAX}), maximum product column boilup (V_2^{MAX}), first reactor maximum temperature (T_{rxr1}^{MAX}) and level (LVL_{rxr1}^{MAX}), second reactor maximum level (LVL_{rxr2}^{MAX}) plus maximum product impurity levels $x_{Bz}^{D2\ MAX}$ (benzene mol fraction) and $x_{DEB}^{D2\ MAX}$ (DEB mol fraction) for no product give-away. This leaves one unconstrained steady state DOF at maximum throughput, which is related to the optimal DEB recycle (L_1^{MAX} fixes benzene recycle). Of the active constraints, T_{rxr1}^{MAX}, LVL_{rxr1}^{MAX} and LVL_{rxr2}^{MAX} are active regardless of throughputs. As throughput is increased, L_1^{MAX}, V_2^{MAX} and V_1^{MAX} become active, in that order. These three active constraints are treated as hard while the remaining ones are treated as soft.

In this process, unlike previous examples, an unconstrained DOF remains at maximum throughput. The DEB recycle flow rate (B_2) is considered as a self-optimizing CV. We have shown that holding B_2 fixed at its optimal maximum throughput value results in only a maximum 0.35% operating profit loss at lower throughputs [8]. The loss is deemed acceptable and is a consequence of energy being significantly cheaper than products or raw material (Douglas' doctrine [5]). At lower throughputs, overrefluxing in the two columns is mitigated by maintaining L_1 in ratio with the recycle column feed (F_{col1}) and maintaining a sensitive stripping tray temperature (T_S^{col2}) using V_2. The self-optimizing CVs corresponding to unconstrained L_1 and and V_2 are L_1/F_{col1} and T_S^{col2} respectively.

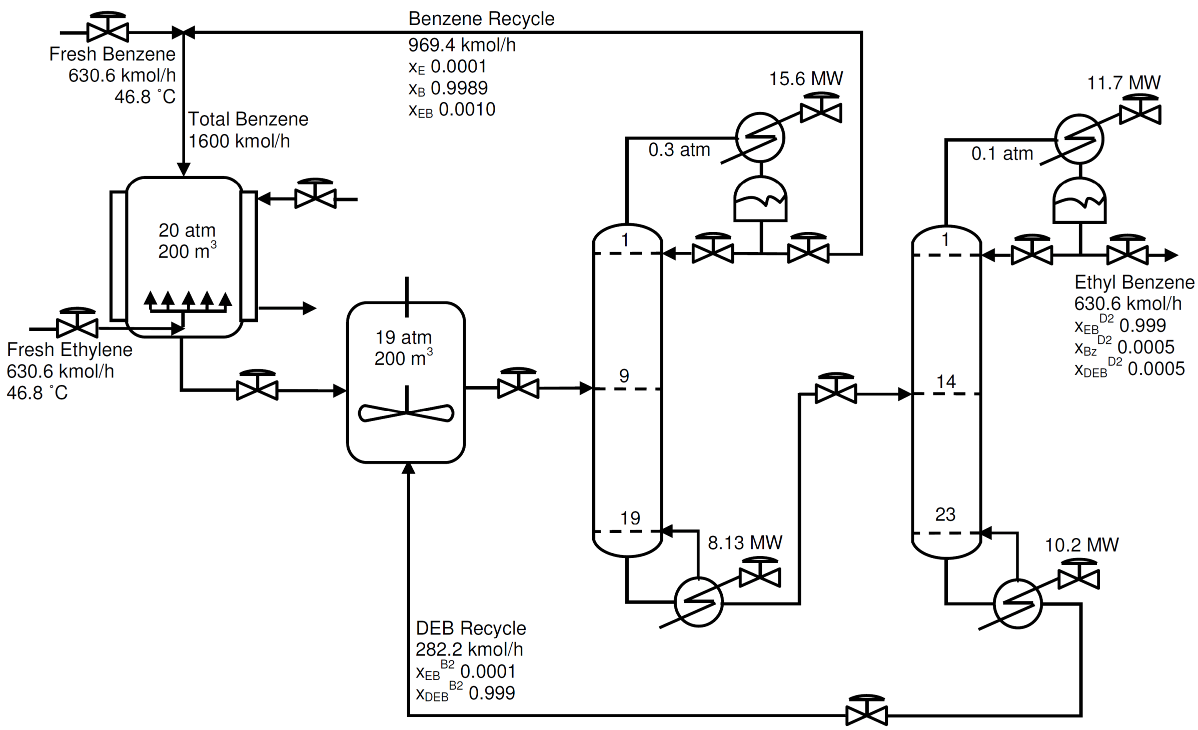


Figure 15.1. Schematic of ethyl benzene process with design and operating conditions

15.2.2. Step 1: Loops for Maximum Throughput Economic CV Control

The full active constraint set consists of LVL_{rxr1}^{MAX}, T_{rxr1}^{MAX}, LVL_{rxr2}^{MAX}, L_1^{MAX}, V_2^{MAX}, V_1^{MAX} $x_{DEB}^{D2\ MAX}$ and $x_{Bz}^{D2\ MAX}$. Of these, L_1^{MAX}, V_2^{MAX} and V_1^{MAX} are hard constraints. For negligible back-off from their hard constraint limits, V_1 and V_2 are controlled using the respective reboiler steam valves (Q_{reb1} and Q_{reb2}) while L_1 is flow controlled. T_{rxr1}^{MAX} is controlled using the reactor cooling duty (Q_{rxr}), a conventional pairing for tight temperature control. For tight control of x_{DEB}^{D2} (product impurity), the column reflux to feed ratio is adjusted. For tight control of x_{Bz}^{D2} (product impurity) another cascade loop arrangement is implemented where the composition controller adjusts a sensitive recycle column stripping tray temperature controller setpoint, which in turn manipulates the column feed (F_{col1}). With the recycle column feed (F_{Col1}) paired for temperature control, the level controllers in the two reactors must be oriented opposite to the process flow. Accordingly, LVL_{rxr2} is controlled using its feed (F_{rxr2}). Similarly, for tight level control of the first reactor (LVL_{rxr1}), the reactor liquid feed (fresh + recycle benzene, F_{TotBz}) is adjusted. F_{TotBz} is maintained by adjusting the fresh benzene so that that the fresh benzene is fed as a make-up stream (Luybens' rule). Lastly, B_2 (self optimizing CV) is flow controlled.

Table 15.1. Economic Plantwide Control Structure Synthesis for Ethyl Benzene Process

Step 0: Active Constraint Regions and Economic CV's

Region	I	II	III	Max Throughput
Additional Active Constraints*	-	L_1^{MAX}	V_2^{MAX} L_1^{MAX}	V_1^{MAX} V_2^{MAX} L_1^{MAX}
Unconstrained DOF's	3	2	1	1
Self-Optimizing CV's	B_2, L_1/F_1, T_S^{col2}	B_2, T_S^{col2}	B_2	B_2

Step 1: Maximum Throughput Economic Control Loops

Active Constraint Control Loops	$T_{rxr1}^{MAX} \leftrightarrow Q_{rxr1}$ $V_1^{MAX} \leftrightarrow Q_{reb1}$ $V_2^{MAX} \leftrightarrow Q_{reb2}$ $LVL_{rxr1}^{MAX} \leftrightarrow F_{TotBz} \leftrightarrow F_{Bz}$ $x_{Bz}^{D2} \leftrightarrow T_S^{col1\ SP} \leftrightarrow F_{col1}^{SP}$ $x_{DEB}^{D2} \leftrightarrow L_2/B_1^{SP} \leftrightarrow L_2^{SP}$ $LVL_{rxr2}^{MAX} \leftrightarrow F_{rxr2}$
Self-Optimizing Loops	none

Step 2: Maximum Throughput Inventory Loops

$LVL_{cnd1} \leftrightarrow D_1$	$LVL_{reb1} \leftrightarrow F_{C2}/F_{TotBz}^{SP} \leftrightarrow F_{C2}$	$P_{cnd1} \leftrightarrow Q_{cnd1}$
$LVL_{cnd2} \leftrightarrow D_2$	$LVL_{reb2} \leftrightarrow B_1$	$P_{cnd2} \leftrightarrow Q_{cnd2}$

Step 3: Additional Self-Optimizing CV Loops at Reduced Throughput

Region III	Region II	Region I
TPM: V_1^{SP}	TPM: V_1^{SP} $T_S^{col2} \leftrightarrow V_2^{SP\ \#}$	TPM: V_1^{SP} $T_S^{col2} \leftrightarrow V_2^{SP\ \#}$ $L_1/F_1 \leftrightarrow L_1^{\#}$

Step 4: Modifications for Conventional LVL_{Reb1} Control Loop

$LVL_{reb1} \leftrightarrow B_1$

Region III	Region II	Region I
TPM: V_1^{SP} $B_2 \leftrightarrow F_{TotBz}/F_{C2}^{SP}$	TPM: V_1^{SP} $T_S^{col2} \leftrightarrow V_2^{SP\ \#}$ $B_2 \leftrightarrow F_{TotBz}/F_{C2}^{SP\ \#}$	TPM: V_1^{SP} $T_S^{col2} \leftrightarrow V_2^{SP\#}$ $B_2 \leftrightarrow F_{TotBz}/F_{C2}^{SP} \leftrightarrow F_{C2}$ $L_1/F_1 \leftrightarrow L_1^{\#}$

*: T_{rxr1}^{MAX}, LVL_{rxr1}^{MAX}, LVL_{rxr2}^{MAX}, $x_{Bz}^{D2\ MAX}$, $x_{DEB}^{D2\ MAX}$ are always active; #: Is unconstrained from MAX limit

15.2.3. Step 2: Inventory (Regulatory) Control System

The remaining inventories to be controlled include the four column levels (LVL_{cnd1}, LVL_{cnd2}, LVL_{bot1}, LVL_{bot2}) and the two column pressures (P_{cnd1} and P_{cnd2}). The column pressures are controlled conventionally using the respective condenser duty valves (Q_{cnd1} and Q_{cnd2}). The reflux drum levels of the two columns (LVL_{cnd1} and LVL_{cnd2}) are controlled using the respective distillate stream (D_1 and D_2). On the product column, since the B_2 is under flow control as a self-optimizing variable and therefore unavailable, the sump level (LVL_{bot2}) is controlled using the product column feed (B_1). This leaves no close-by valves for controlling the recycle column sump level (LVL_{bot2}). The only pairing possibility is to adjust the fresh ethylene feed rate (F_{C2}). To mitigate the transients in the reactor composition, F_{C2} is maintained in ratio with the F_{TotBz} with the LVL_{bot2} controller adjusting the ratio setpoint, $F_{C2}/F_{TotBz}{}^{SP}$. As in the recycle process case study (Case Study 1), this is an unconventional long inventory loop and makes sense in that the reaction products (EB and DEB) accumulate in the bottom sump of the recycle column. LVL_{Bot2} thus indirectly indicates the production rate. A decreasing level implies the reaction production rate must be increased, which is accomplished by increasing F_{C2} (limiting reactant) via appropriate adjustment in $F_{C2}/F_{TotBz}{}^{SP}$ by the level controller.

15.2.4. Step 3: Additional Economic CV Loops and Throughput Manipulation

To reduce throughput below maximum, we consider using V_1^{SP} as the TPM across the entire throughput range as V_1^{MAX} is the last constraint to go active. When optimally inactive, L_1^{SP} is maintained in ratio with the recycle column feed to mitigate overrefluxing in the recycle column [e]. Similarly, V_2^{SP} takes up tight control of a sensitive product column stripping tray temperature, whenever feasible at lower throughputs.

15.2.5. Step 4: Modifications for a More Conventional Inventory Control System

The economic plantwide control structure synthesized by the application of Step 1-3 of our procedure is shown in Figure 15.2. In this control system, we have an unconventional and long loop for controlling the recycle column sump level. For this process, the total reactor residence time is ~2 hrs so that the dynamic response of LVL_{bot2} to a change in $F_{C2}/F_{TotBz}{}^{SP}$ (MV) is quite sluggish resulting in the recycle column sump overflowing or running dry even for the mildest of disturbances such as a 1% step change in B_2^{SP}. Clearly the inventory control system is very fragile so that the economic CV and inventory loop pairings must be appropriately revised.

To revise the pairings, we first consider giving up on tight control of the self-optimizing CV, B_2. The product column sump level (LVL_{bot2}) is then paired with B_2 which frees up the recycle column bottoms flow (B_1) which is then used for robust control of LVL_{bot1}. This frees up $F_{C2}/F_{TotBz}{}^{SP}$ which takes up 'loose' control of the self-optimizing variable, B_2. The long inventory loop, LVL_{bot1} - $F_{C2}/F_{TotBz}{}^{SP}$, in Figure 15.2 (Step 2 row in Table 15.1) thus gets replaced by a long B_2 - $F_{C2}/F_{TotBz}{}^{SP}$ loop after the re-pairing exercise to provide a conventional and robust inventory control system. The revised control system is shown in Figure 15.3.

---

[e] Alternatively, L_1^{SP} can take up rectifying temperature control for dual ended control.

To transition to lower throughputs, V_1^{SP}, the last constraint to go active is used as the TPM over the entire throughput range. Also, to prevent overrefluxing in the two columns at low throughputs, V_2^{SP} takes up product column stripping tray temperature control and L_1 is maintained in ratio with the recycle column feed (F_{col1}). These two loops take-up control as and when the controller output becomes implementable (i.e. $V_2^{SP} < V_2^{MAX}$ and $L_1^{SP} < L_1^{MAX}$).

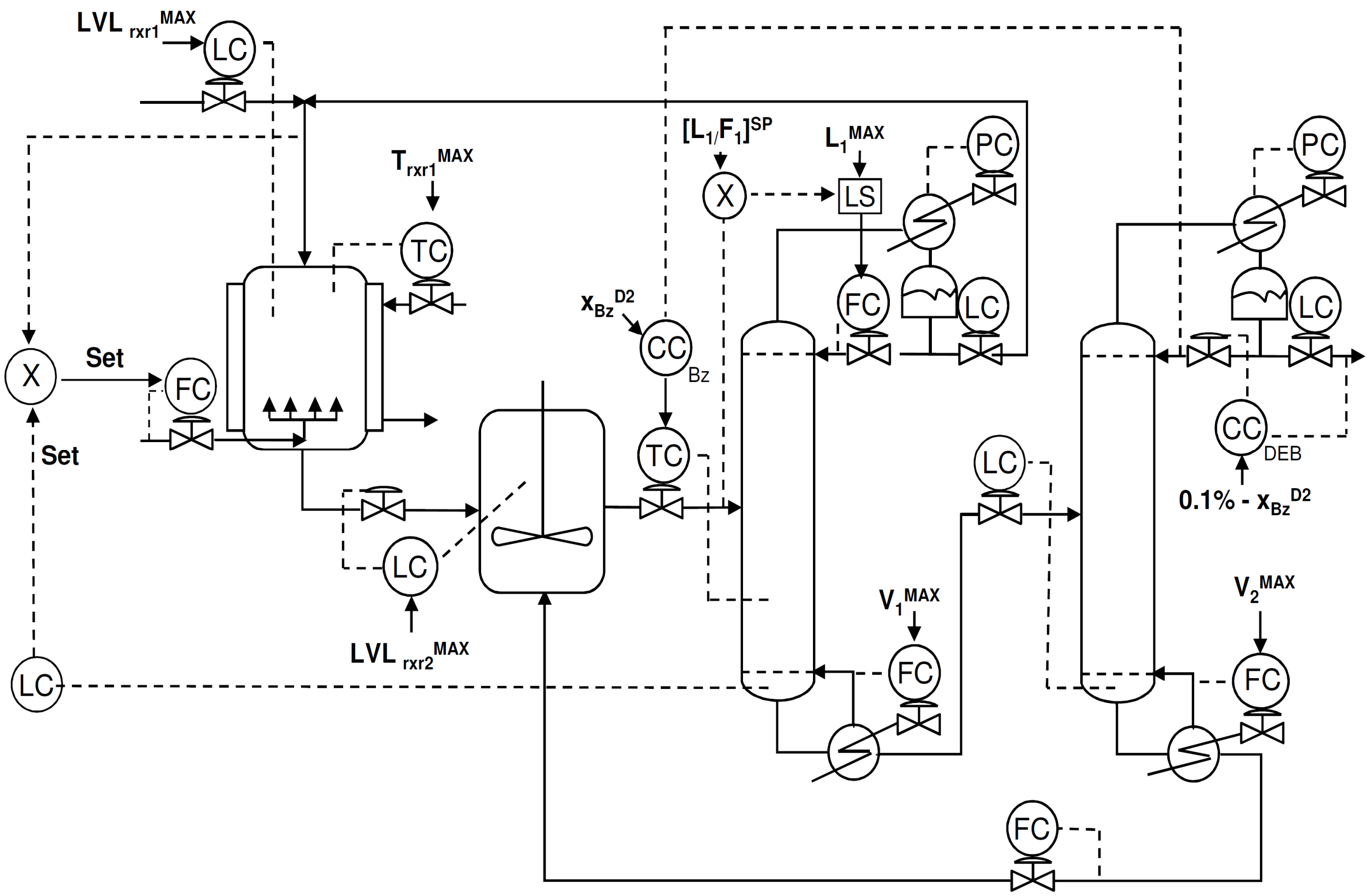


Figure 15.2. Ethyl benzene process economic plantwide control structure (with long inventory loop)

It is highlighted that in the revised pairings for more conventional inventory control (Step 4 in Table 15.1), B_2 must be controlled (by adjusting $F_{C2}/F_{TotBz}{}^{SP}$) and not allowed to float as it can result in a snowballing problem. This is because V_2^{MAX} is an active constraint at maximum throughput implying limited capacity to boil-off EB in the product column. Any EB that could not be boiled off in the product column would necessarily drop down the bottoms causing the DEB recycle rate (B_2) to slowly increase. To prevent this slow drift (snowballing), it must be ensured that only as much EB is produced in the reaction section as can be boiled off in the product column. This gets accomplished by adjusting the $F_{C2}/F_{TotBz}{}^{SP}$ to maintain B_2, which ensures the fresh ethylene feed to the process matches the EB boil-off rate. A seemingly innocuous recommendation of allowing a self-optimizing CV to float and accepting the consequent economic loss results in a very severe consequence of potential process instability. This highlights the importance of Down's drill in ensuring the recommended control structure does not suffer from such hidden instabilities due to slow accumulation of component inventories.

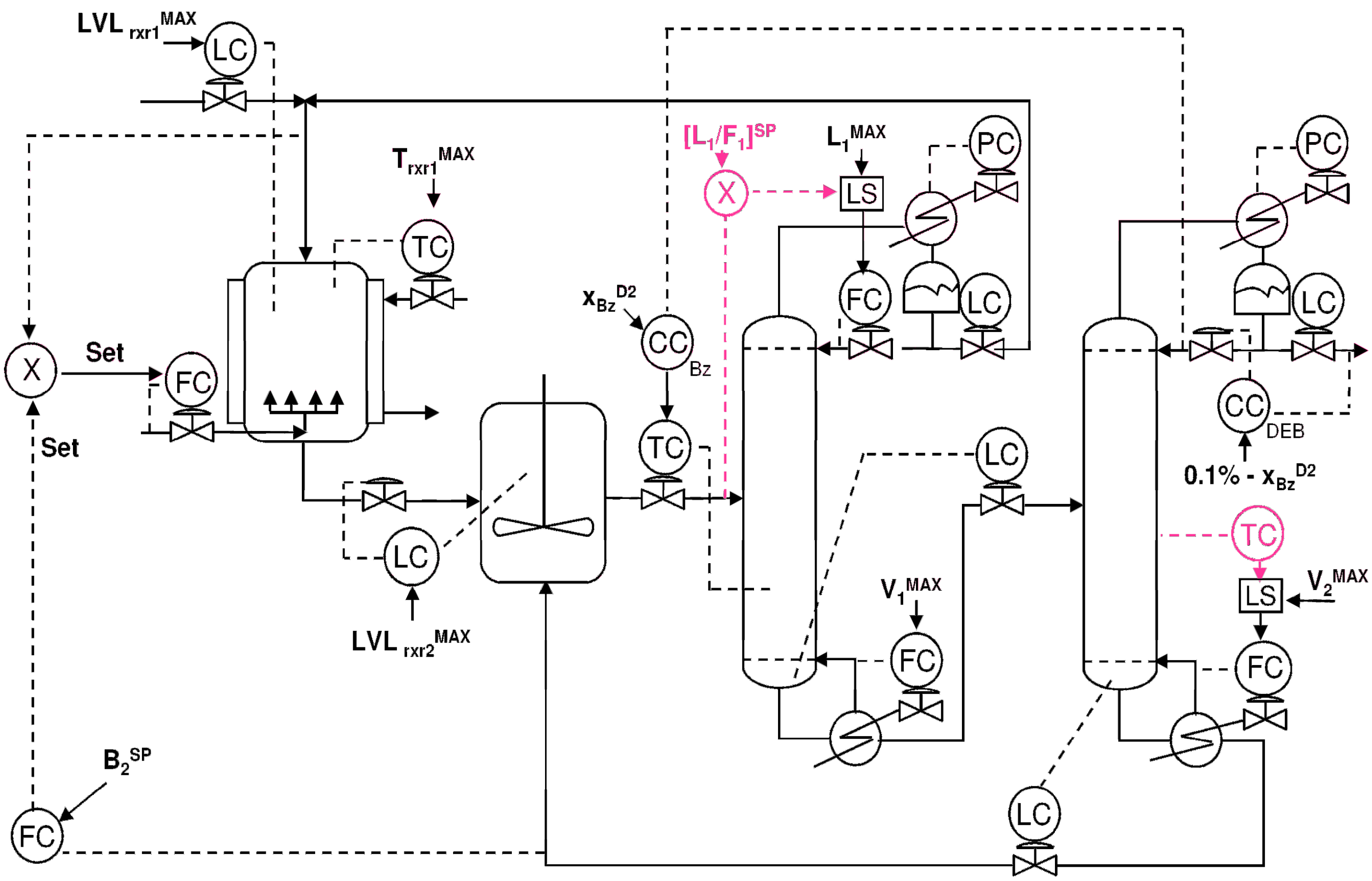


Figure 15.3. Modified economic plantwide control structure for ethyl benzene process

If a conventional control system was designed for process operation around the design condition, V_2 would get used for maintaining a product column stripping temperature. As long as the loop is functioning, the EB would get boiled-off and not accumulate in the DEB recycle loop. However, once V_2^{MAX} goes active, product column stripping temperature control would be lost. To ensure that the process does not succumb to snowballing in the DEB recycle loop, one would have to design an override scheme that alters the material balance structure all the way up to the process feed resulting in an inherently complicated scheme for constraint handling. In contrast, the synthesized control structure is much simpler with no overrides and appealing in that the way inventory is regulated remains the same regardless of the operating region.

Rigorous dynamic simulations are performed to test the synthesized control structure in in Aspen Plus. All flow / pressure PI controllers are tuned tight for a fast and snappy servo response, unless specified otherwise. The long B_2 loop is tuned by hit-and-trial for a smooth overall plantwide response. The non-reactive level controllers are P-only with a gain of 2. The CSTR levels are controlled using a PI controller for offset free level tracking. The relay feedback test feature with Tyreus-Luyben settings is used to obtain the CSTR level controller tuning parameters at maximum throughput. All temperature measurements are lagged by 2 mins to account for sensor and cooling / heating circuit dynamics. To tune the temperature loops, the open loop step response at maximum throughput is obtained and the reset time set to 1/3rd of the approximate 95% response completion time. The gain is then adjusted for a slightly underdamped servo response with mild oscillations. The composition controllers are similarly tuned. A sampling time and delay time of 5 mins each is applied to all composition measurements. The tuning parameters of salient loops are reported in Table 15.2.

The closed loop dynamic response of the synthesized plantwide control system to a throughput transition from the design throughput (F_{C2} = 630 kmol/h) to maximum throughput (F_{C2} = 970 kmol/h) is shown in Figure 15.4. The product impurity is tightly controlled and the transients in the process variables are smooth implying the suitability of the control structure for near optimal operation over the wide throughput range.

Table 15.2. Salient Controller tuning parameter for Ethyl Benzene process

Controlled Variable	K_C	τ_i (min)	Sensor Span
LVL_{rxr1}	5	250	0 – 100%
LVL_{rxr2}	5	250	0 – 100%
T_{rxr1}	4.8	25	0 – 400°C
T_{col1}	3.2	18.5	77 °C – 157 °C
T_{col2}	2	11	0 .0 – 244.7 °C
x_{Bz}^{D2}	0.3	100	0 – 0.0016
x_{DEB}^{D2}	0.8	88.5	0 0.002
B_2	0.2	1200	0 – 500 kmol/h

All level loops use K_C = 2 unless otherwise specified
Pressure/flow controllers tuned for tight control
All composition measurements use a deadtime of 5 minutes and a sampling time of 5 mins

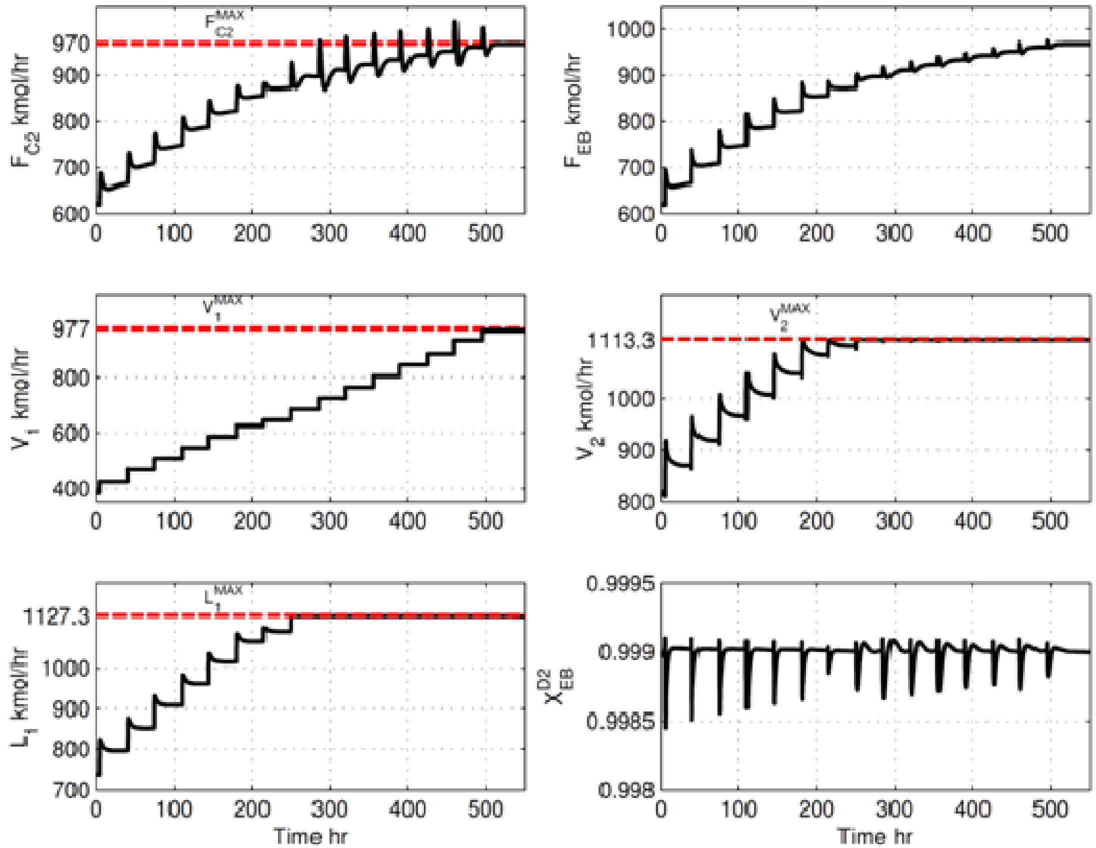


Figure 15.4. Low to maximum throughput transition of ethyl benzene process using modified economic plant-wide control structure

Chapter 16. Comprehensive Case Study I: Cumene Process

16.1. Process Description

Figure 16.1 provides a schematic of the cumene process along with the design and base-case salient operating conditions. Fresh benzene (C_6) and fresh propylene (0.95 propylene and 0.05 propane), mixed with recycle benzene are vaporized in a vaporizer. The vapor stream is preheated using the hot reactor effluent in a feed effluent heat exchanger (FEHE) before being heated to the reaction temperature in a furnace. The heated stream is fed into a packed bed reactor (PBR), a shell and tube heat exchanger with catalyst loaded tubes and pressurized coolant on the shell side. Propylene (C_3) and C_6 react in the vapor phase to produce cumene (C_9), which can further react with C_3 to produce a small amount of di-isopropyl benzene (C_{12} or DIPB) side product. The reactor effluent loses sensible heat in the FEHE and is partially condensed in a cooler. The cooled stream with C_9, C_{12}, unreacted reactants and inert propane is fed to a three column light-out-first distillation train. The purge column recovers inert propane and any unreacted propylene with some benzene as vapor distillate. The bottoms is sent to the recycle column which recovers the unreacted benzene as the distillate and recycles it. The recycle column bottoms is sent to the product column, which recovers nearly pure C_9 distillate and heavy C_{12} (+ some C_9) bottoms.

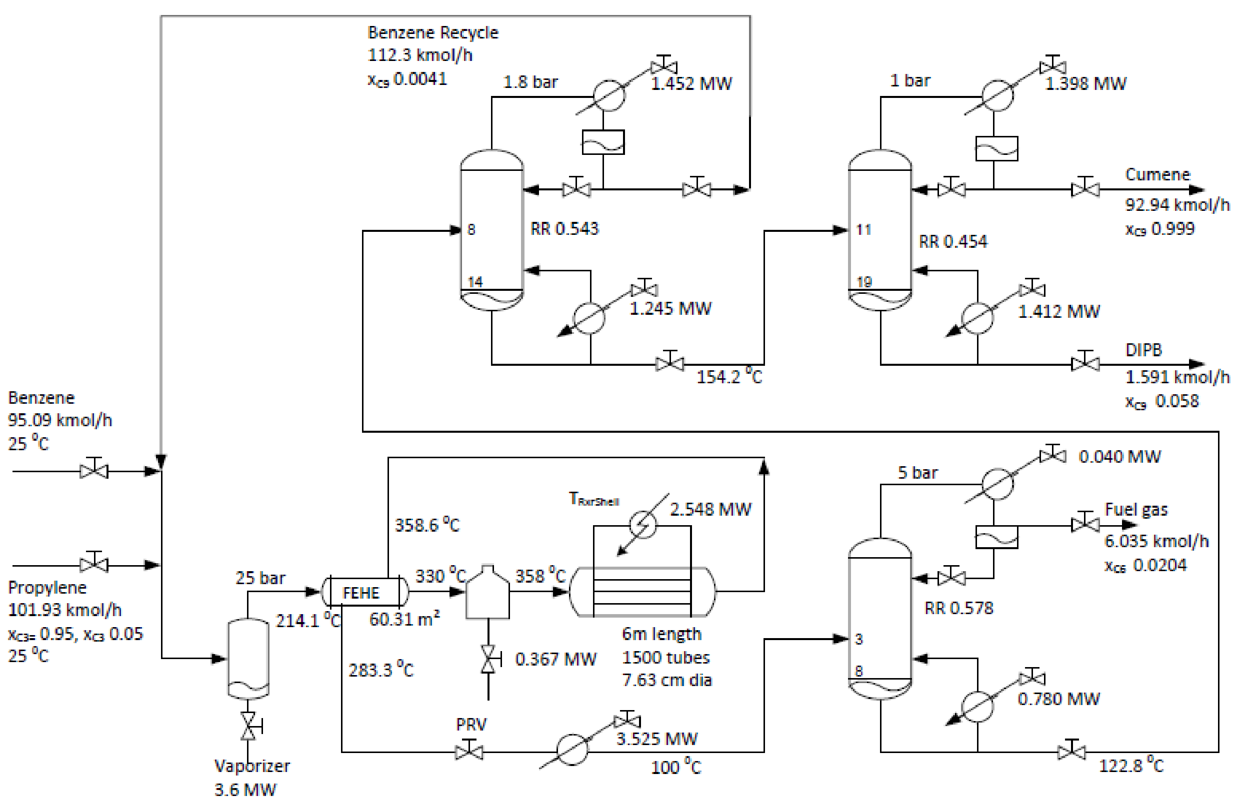


Figure 16.1. Cumene process schematic with salient design and base-case operating

The reaction chemistry and kinetics used to model the process are provided in Table 16.1. The NRTL physical property method is used to model thermodynamic properties. Steady state simulation was performed using UniSim Design R390 version 3.61.0.0 from Honeywell. Luyben [19] has studied the design and basic regulatory control of a very similar cumene process flowsheet with the same reaction kinetics. The flowsheet studied here differs in that the first distillation column replaces a flash tank to mitigate loss of precious benzene in the C_3 fuel gas stream. The optimized base-case process design and steady state operating conditions are also shown in Figure 16.1. This revised design gives 6.8% higher profit [6] than Luyben's flowsheet.

Table 16.1. Reaction chemistry and kinetics

i	Reaction	k_i	E_a^i *(kJ/kmol)*	Concentration terms $f_i(C_j)$
1	$C_6H_6 + C_3H_6 \rightarrow C_9H_{12}$	2.8 x 10^7	104174	$C_{C3}C_{C6}$
2	$C_9H_{12} + C_3H_6 \rightarrow C_{12}H_{18}$	2.32 x 10^9	146742	$C_{C3}C_{C9}$

Reaction rate $r_i = k_i.exp(-E_a^i/RT).f_i(C_j)$
C_j in kmol.m^{-3}; r_i in kmol.m^{-3}.s^{-1}

16.2. Economic Plantwide Control System (CS1) Design

16.2.1. Step 0: Optimal Steady State Process Operation

The plant has a total of 12 steady state operating degrees of freedom (DOFs): 1 each for the two fresh feeds, 1 for the furnace, 1 for reactor cooling, 1 for reactor pressure, 1 for reactor effluent cooler and 2 each for the three distillation columns. Specification variables corresponding to these degrees of freedom chosen for robust flowsheet convergence are: fresh propylene feed (F_{C3}), total benzene flow (F_{C6}^{Total}), reactor inlet temperature (T_{rxr}), reactor coolant temperature ($T_{RxrShell}$), reactor pressure (P_{Rxr}), reactor effluent cooler outlet temperature (T_{cooler}), first column vent temperature and bottoms propane mole fraction (T_{vent}^{D1} and x_{C3}^{B1}), the recycle column distillate cumene and the bottoms benzene mole fractions (x_{C9}^{D2} and x_{C6}^{B2}) and finally, the product column distillate cumene and the bottoms cumene mole fractions (x_{C9}^{D3} and x_{C9}^{B3}). These 12 specification variables can be adjusted to achieve a given objective such as maximum throughput/profit or maximum yield/selectivity.

In this work, the steady state hourly operating profit, P, defined as

$$P = [\text{Product Revenue} - \text{Raw Material Cost} - \text{Energy Cost}] \text{ per hour}$$

is used as a quantitative economic criterion that is maximized using the available steady state DOFs. We consider two modes of steady process operation. In Mode I, the desired throughput (production rate or feed processing rate) is specified, usually based on business considerations. For processes with undesirable side products, such as the cumene process considered here, the optimization typically attempts to maximize the yield to desired product. For processes with no undesirable side products (e.g. a separation train), the optimization attempts to minimize the energy consumption per kg product. In Mode II, the throughput itself is a decision variable for maximizing the economic criterion. Often, the Mode II solution corresponds to steady process operation at/near the maximum achievable throughput.

For the cumene process considered here, in Mode I, since the fresh propylene feed (F_{C3}) is fixed, only the remaining 11 DOFs need to be optimized. In Mode II, all 12 DOFs (including

F_{C3}) need to be optimized. The optimization is subject to physical and operational process constraints such as maximum / minimum material / energy flows, temperatures, pressures, product impurities etc.

Ideally all decision variables should be optimized simultaneously but this can result in an unwieldy problem with poor convergence. The optimization is therefore simplified by applying engineering reasoning to optimize only the dominant decision variables affecting the economic criterion with reasonable values for the remaining decision variables. For the cumene process, the reactor effluent cooler temperature (T_{cooler}) has very little impact on the economic objective function (P) and is therefore kept fixed at 100 °C, a reasonable value that ensures the reactor effluent vapor is condensed. Similarly, the yearly operating profit is insensitive to changes around the base design values of the propane mol fraction leaking down the first column bottoms (x_{C3}^{B1}) and the cumene mole fraction leaking up the second column distillate (x_{C9}^{D2}). These are therefore kept fixed at the base values. Also, the first column vapor vent stream temperature (T_{vent}^{D1}) is set by the cooling water at 32 °C.

These simple engineering arguments fix 4 specifications simplifying the optimization to 7 decision variables for Mode I (given F_{C3}) and 8 for Mode II. The optimization is performed using Matlab's *fmincon* routine with Unisim as the back-ground steady state flowsheet solver. The constrained optimization problem formulation (including price data and process constraints) and results for Mode I and Mode II are briefly summarized in Table 16.2.

The optimization results are interpreted as follows. The minimum product purity constraint ($x_{C9}^{D3\ MIN}$ = 99.9%) is active in both Mode I and Mode II, i.e. at all throughputs, for on-aim product quality with no product give-away. The maximum reactor operating pressure (P_{Rxr}^{MAX}) and maximum recycle (second) column boilup (V_2^{MAX}) constraints are active at all throughputs. Reactor operation at maximum operating pressure causes the reactor temperature to be lower for a given conversion improving selectivity (cumene product yield). Recycle column operation at maximum boilup causes the total (fresh + recycle) benzene to the reactor to be as high as possible, again enhancing selectivity with a higher reactor benzene to propylene ratio. As throughput is increased, the product column maximum boilup constraint, V_3^{MAX}, goes active. Even as the throughput may be further increased by e.g. reducing the recycle column reflux (i.e. x_{C9}^{D2} is increased) and adjusting T_{Rxr} and $T_{RxrShell}$ to maintain conversion and selectivity, the Q_{fur}^{MIN} constraint goes active after which the selectivity decreases dramatically. The increase in throughput achieved is very marginal at < 1 kmol/h. We therefore treat V_3^{MAX} going active as corresponding to the maximum economic throughput (Mode II) with F_{C3} = 169.96 kmol/h.

The three Mode I active constraints ($x_{C9}^{D3\ MIN}$, P_{Rxr}^{MAX} and V_2^{MAX}) along with the throughput specification (F_{C3}) leave four unconstrained DOFs. In Mode II, the throughput is not specified and gets determined by the value of the additional V_3^{MAX} constraint so that the number of unconstrained DOFs remains four. The unconstrained optimum values of the four decision variables, x_{C9}^{B3}, x_{C6}^{B2}, T_{Rxr} and $T_{RxrShell}$ are reported in Table 16.2 for Mode I and Mode II.

The low Mode I optimum x_{C9}^{B3} reduces the loss of precious cumene down the product column bottoms without a prohibitively high energy cost. The optimum Mode II x_{C9}^{B3} is much higher at 10%. This reduces the recycle column stripping load so that the V_3^{MAX} constraint goes active at higher throughputs for increased profit. Further loosening x_{C9}^{B3} however causes the profit to decrease due to excessive cumene loss in the side product stream.

The Mode I optimum benzene leakage down the recycle column bottoms, x_{C6}^{B2}, is on the higher side at 0.09% so that benzene is the principal cumene product impurity. This is reasonable as benzene is the cheaper product impurity with DIPB consuming 2 extra mols of propylene. The

Mode II optimum x_{C6}^{B2} value reduces to 0.05% so that the two product impurities are comparable. As shown in Figure 16.2, this balances throughput and selectivity with V_2^{MAX} and V_3^{MAX} active constraints. If x_{C6}^{B2} is too high, the DIPB leakage in the product column distillate is prohibitively small requiring high reflux so that the V_3^{MAX} constraint goes active at a significantly lower throughput. Similarly, if x_{C6}^{B2} is too low, the feed that can be processed by the recycle column maintaining its two separation specifications without violating the V_2^{MAX} constraint is lower implying a loss in throughput. Also, as x_{C6}^{B2} is loosened, with V_2^{MAX} active, the benzene recycle increases for better selectivity with lower DIPB formation. Comparable amounts of the two principal impurities in the product balances these two effects.

Table 16.2. Process optimization formulation and results' summary

Objective	Maximize(J) J: hourly operating profit*	
Process Constraints	*$0 \leq$ Material Flows ≤ 2 (base case)* *$0 \leq V_1, V_2, V_3 \leq 1.5$ (base case)* *Vent Temperature = 32 ^oC* *$0 \leq$ Energy Flows ≤ 1.7 (base case)* *1 bar $\leq P_{Rxr} \leq$ 25 bar* *Cumene Product Purity $\geq$ 0.999 mol fraction*	
Decision Variable	Mode I	Mode II
F_{C3}	101.93 kmol/h Fixed	169.96 kmol/h
F_{C6}^{Total}	294.16 kmol/h	316.2 kmol/h
T_{rxr}	322.26 °C	318.58 °C
$T_{RxrShell}$	368.95 °C	367.98 °C
P_{Rxr}	25 bar Max	25 bar Max
T_{cooler}	100 °C Fixed	100 °C Fixed
T_{vent}^{D1}	32 °C Fixed	32 °C Fixed
x_{C3}^{B1}	0.1 % Fixed	0.1 % Fixed
x_{C9}^{D2}	0.4 % Fixed	0.4 % Fixed
x_{C6}^{B2}	0.09 %	0.05 %
x_{C9}^{D3}	99.9 % Min	99.9 % Min
x_{C9}^{B3}	0.4 %	10 %
Optimum J	\$3.809x10^3 h^{-1}	\$5.879x10^3 h^{-1}
F_{C9}	93.59 kmol/h	150.045 kmol/h
Active Constraints	$x_{C9}^{D3\,MIN}$, P_{Rxr}^{MAX}, V_2^{MAX}	$x_{C9}^{D3\,MIN}$, P_{Rxr}^{MAX}, V_2^{MAX}, V_3^{MAX}

*: Heater duty \$16.8 GJ^{-1}; Steam \$9.83 GJ^{-1};Cooling water \$0.16 GJ^{-1};F_{C6} \$ 68.5kmol^{-1}; F_{C3} \$ 34.3kmol^{-1}; F_{C9} \$ 150.0kmol^{-1}

We now seek a simple steady state operating policy that ensures near optimal operation over the entire throughput range. For economically optimal operation, we would like tight control of the active constraints and appropriate management of the remaining unconstrained steady state DOFs using SOVs. Preferably, the CVs corresponding to the unconstrained steady state DOFs should be measurements that are cheap, reliable, fast, robust and dynamically well behaved with respect to the manipulated variables (MVs). These CVs should therefore be flow, pressure and temperature based avoiding cumbersome analytical measurements.

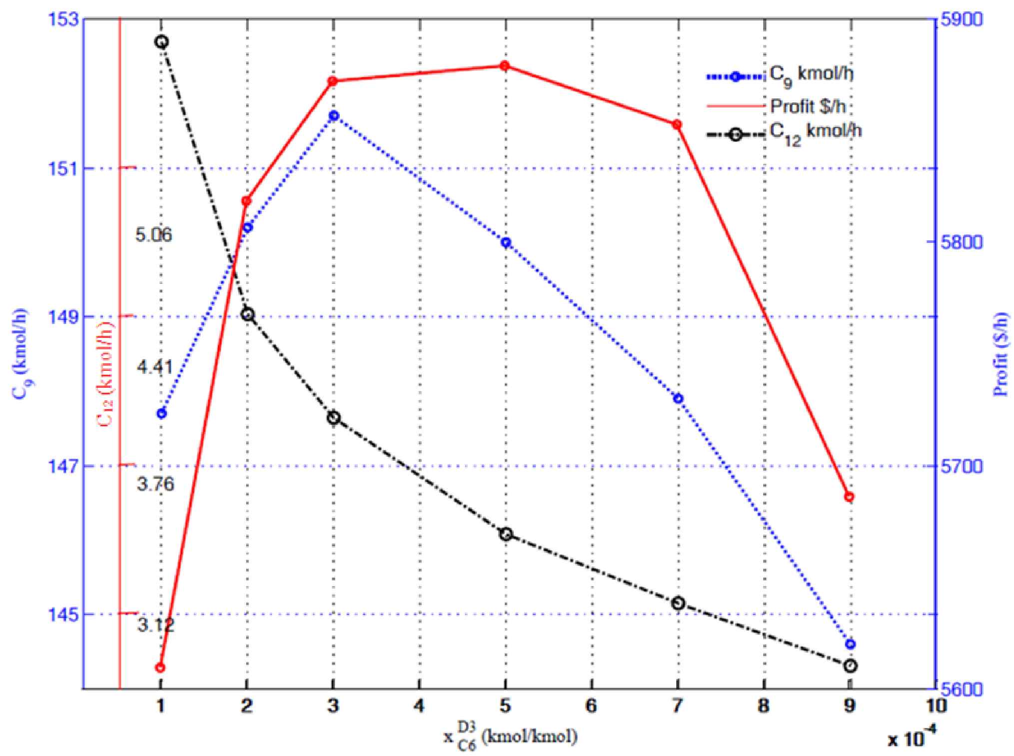


Figure 16.2. Optimum benzene impurity level in cumene product

Of the 12 decision variables in Table 16.2, 4 decision variables, T_{vent}, T_{Cooler}, $x_{C3}{}^{B1}$ and $x_{C9}{}^{D2}$ were fixed at reasonable values. In Mode I, there are three active constraints, $x_{C9}{}^{D3\ MIN}$, $P_{Rxr}{}^{MAX}$ and $V_2{}^{MAX}$ along with a specified F_{C3}. In Mode II, $V_3{}^{MAX}$ going active sets F_{C3}. Optimum values for the remaining 4 unconstrained decision variables in both modes, T_{Rxr}, $T_{RxrShell}$, $x_{C6}{}^{D3}$ and $x_{C9}{}^{B3}$ were obtained.

In the above set of variables, compositions not related to the product quality, i.e., $x_{C3}{}^{B1}$, $x_{C9}{}^{D2}$ and $x_{C9}{}^{B3}$ would usually not be available. Accordingly, we consider using appropriate temperature inferential measurements. On the purge and product columns, controlling appropriate sensitive stripping tray temperatures, $T^S{}_{Col1}$ and $T^S{}_{Col3}$, respectively, would regulate the light key leakage down the bottoms. This would indirectly maintain $x_{C3}{}^{B1}$ and $x_{C9}{}^{B3}$ within a small band. On the recycle column, maintaining the reflux (L_2) in ratio with the column feed (B_1) would regulate the distillate cumene leakage ($x_{C9}{}^{D2}$). The product DIPB impurity mol fraction ($x_{C12}{}^{D3}$) and benzene impurity mol fraction ($x_{C6}{}^{D3}$) measurements would usually be available in an industrial setting. For on-aim product cumene mol fraction ($x_{C9}{}^{D3} = x_{C9}{}^{D3\ MIN} = 99.9\%$), $x_{C6}{}^{D3} + x_{C12}{}^{D3} = 0.1\%$ so that only one of the impurity mol fractions is independent. We take $x_{C6}{}^{D3}$ to be independent with $x_{C12}{}^{D3} = 0.1\% - x_{C6}{}^{D3}$.

The revised practical CVs corresponding to the 12 steady state DOFs are tabulated in Table 16.3 along with their regulatory and economic significance. The CVs are the active constraints (or specifications) and four unconstrained CVs, T_{Rxr}, $T_{RxrShell}$, $x_{C6}{}^{D3}$ and $T^S{}_{Col3}$. Of the unconstrained CVs, the optimum reactor inlet temperature (T_{Rxr}) and reactor coolant temperature

($T_{RxrShell}$) are nearly the same for Mode I and Mode II (see Table 16.2). Holding these two variables constant would likely be near optimal across the wide throughput range. For the remaining two CVs, since economic losses per unit deviation away from the optimum values are usually the highest at maximum throughput, we consider implementing the Mode II optimum value at the lower throughputs. This gives a very simple constant setpoint policy across the entire throughput range. To quantify the economic loss entailed, Figure 16.3 compares the variation with throughput in the optimum operating profit and the operating profit using the constant Mode II setpoints for the above four CVs. The constant setpoint operating policy provides near optimal steady operation with the maximum profit loss being < 0.21%. These four CVs may thus be deemed as SOVs that provide near optimum steady operation across the entire throughput range.

Table 16.3. Revised practical CVs

SNo	*CV*	*Remarks on regulatory / economic significance*
1	F_{C3}	Determines process throughput. Maximum throughput limited by V_3^{MAX}
2	F_{C6}^{Total}	Increasing F_{C6Tot} improves selectivity. Maximum F_{C6Tot} limited by V_2^{MAX}.
3	T_{rxr}	Affects reactor conversion and selectivity. Stabilizes reaction heat recycle through FEHE.
4	$T_{RxrShell}$	Affects reactor conversion and selectivity. Stabilizes reaction heat removal.
5	P_{Rxr}	Operate at P_{Rxr}^{MAX} for maximum reactor conversion. Stabilizes gas inventory in reaction section.
6	x_{C6}^{D3}	Determines benzene impurity level in product. Fixed by benzene dropping down the recycle column.
7	x_{C12}^{D3}	Determines DIPB impurity level in product.
8	$T^S{}_{Col3}$	Regulates precious cumene lost with the DIPB by-product.
9	T_{cooler}	Ensures heat removal and condensation of hot reactor effluent.
10	T_{vent}^{D1}	Determines loss of precious benzene in the fuel gas. Should be as low as possible to minimize benzene loss. Fixed by cooling water temperature.
11	$T^S{}_{Col1}$	Regulates C_3 leakage down the purge column.
12	L_2 / B_1	Regulates C_9 leakage in the benzene recycle stream

16.2.2. Step 1: Loops for Tight Economic CV Control

The hard active constraints at maximum throughput are V_2^{MAX} and V_3^{MAX}. These are economically important as a back-off from V_2^{MAX} reduces the benzene recycle rate with loss in reactor selectivity while a back-off in V_3^{MAX} causes a loss in throughput. To minimize the back-off, V_2 and V_3 are controlled tightly using the respective reboiler duties (Q_{Reb2} and Q_{Reb3}).

P_{Rxr}^{MAX}, another economically important active constraint due to its impact on the reactor conversion, is considered a soft constraint. The reactor pressure is controlled tightly around its maximum value ($P_{Rxr}^{SP} = P_{Rxr}^{MAX}$) by manipulating the pressure regulatory valve (PRV) between the reaction and separation sections. The pairing would provide tight control.

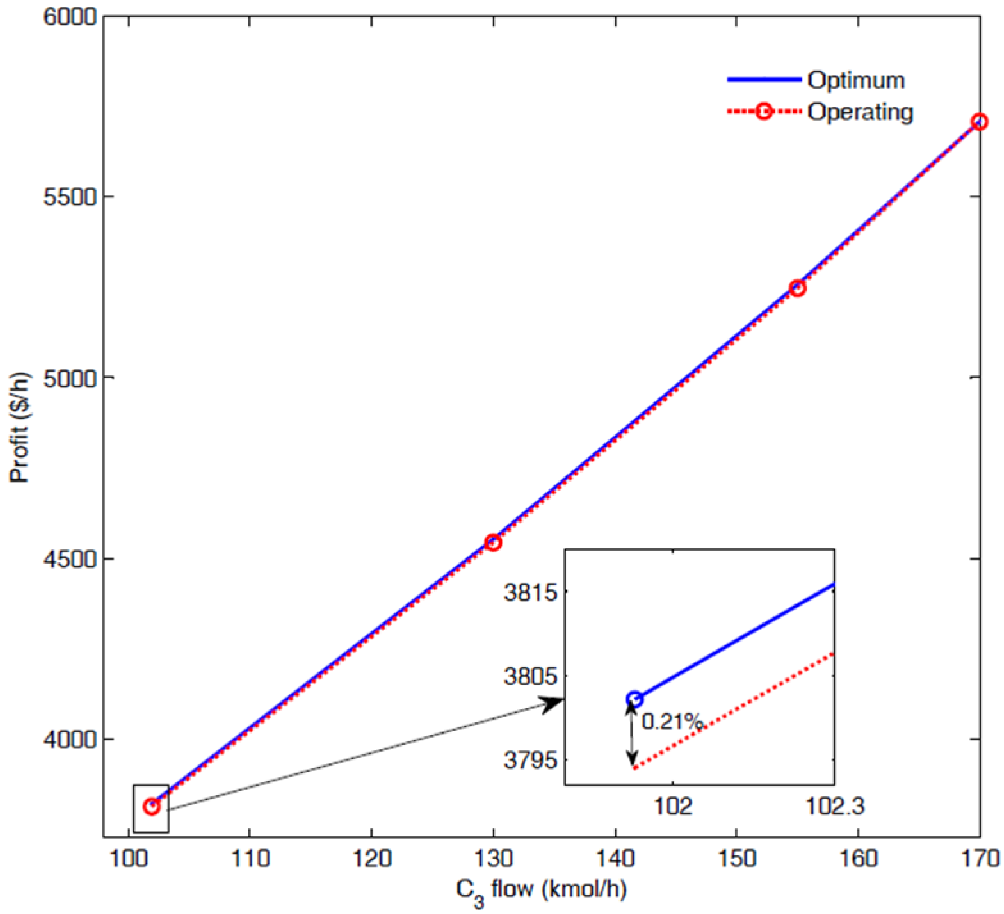


Figure 16.3. Comparison of optimum steady profit and achieved profit using simple constant setpoint operating policy at various throughputs

Economic operation requires tight control of the product impurity levels for on aim product purity of $x_{C9}^{D3\ MIN}$, a soft active constraint. For maintaining x_{C9}^{D3}, the two principal impurities in the product, C_{12} and C_6, must be maintained. Control of x_{C12}^{D3} is accomplished by adjusting the product column reflux to feed ratio (L_3/B_2). The ratio scheme helps mitigate the variability in x_{C12}^{D3} due to the feedforward action of the ratio controller to column feed flow disturbances. With regard to the C_6 impurity in the product, note that all the benzene that leaks down the recycle column ends up in the product. Tight regulation of the benzene leakage down the recycle column can be achieved by maintaining a stripping tray temperature (T^S_{Col2}). Since V_2^{MAX} constraint is active, we may use the feed to the recycle column (B_1) or the recycle column reflux rate (L_2) as the MV. The former would be effective for a mostly liquid feed and the latter must be used for a mostly vapor feed. For the specific choice of the design pressures of the purge and recycle columns, the B_1 vapor fraction is ~25% so that the T^S_{Col2}-B_1 pairing is selected. The $T^S_{Col2}{}^{SP}$ is adjusted by a x_{C6}^{D3} composition controller. The product impurity mol fraction setpoints are chosen as $x_{C6}^{D3\ SP}$ = 0.05% (Mode II optimum value) and $x_{C12}^{D3\ SP}$ = 0.1% - $x_{C6}^{D3\ SP}$ = 0.05%. These setpoints are held constant at lower throughputs for near optimal operation.

Economic operation requires the cumene leakage down the product column bottoms to be small. This is achieved by maintaining a product column stripping tray temperature (T^S_{Col3}). Since V_3^{MAX} is active and the column feed (B_2) is mostly liquid, the T^S_{Col3}-B_2 pairing is chosen.

Lastly, maintaining a high reactor conversion for a small propylene loss in the fuel gas stream as well as a high reactor selectivity for small loss of precious raw materials as DIPB by-product are economically important objectives. Holding the reactor inlet temperature constant at 322 °C and the reactor shell side coolant temperature at 367 °C ensure that the reactor conversion and selectivity are maintained at high values across the entire throughput range. T_{Rxr} is controlled tightly by manipulating the furnace duty (Q_{fur}) for tight control. $T_{RxrShell}$ = 367 °C is a direct input (MV) to the process as the constant coolant temperature model is used in the simulations. In practice, since the reactor temperature is high, a proprietary heating oil such as Dowtherm would be used as the coolant with high pressure steam being generated in a downstream Dowtherm heated boiler. $T_{RxrShell}$ then is controlled by adjusting the boiler pressure setpoint with the boiler pressure being controlled by the exit steam flow.

16.2.3. Step 2: Inventory Control System Design

We now pair loops for inventory regulation, inventory being interpreted in its most comprehensive sense to include total material, phase, components and energy. Of the 12 steady state DOFs, 8 loops have already been implemented in Step 1. This leaves 4 additional loops that need to be configured plus loops for regulating the reflux drum and bottom sump levels on the three columns along with the column pressures and the feed vaporizer level.

The 4 additional loops correspond to holding L_2/B_1, T_{vent}, T^S_{Col1} and T_{Cooler} at their design values. Maintaining L_2/B_1 using a feed to reflux ratio controller regulates the C_9 leakage in the benzene recycle stream. The purge column condenser temperature is controlled by manipulating its condenser duty (Q_{Cnd1}). This regulates the loss of precious benzene in the fuel gas stream. The purge column stripping tray temperature (T^S_{Col1}) is controlled using its boilup (V_1) to regulate the C_3 leakage down the bottoms. The reactor effluent condensate temperature (T_{Cooler}) is controlled by manipulating the effluent cooler duty (Q_{Cooler}). This ensures proper regulation of the gas/vapor inventory in the reaction section in conjunction with the P_{Rxr} control loop.

The recycle and product column pressures (P_{Cnd1} and P_{Cnd2}) are regulated by the respective condenser duty valves, Q_{Cnd2} and Q_{Cnd2}. The purge column pressure (P_{Col1}) is regulated by the vent rate, D_1. Its reflux drum level (LVL_{RD1}) is regulated by manipulating the reflux (L_1). The feed vaporizer level (LVL_{Vap}) is regulated by the vaporizer duty (Q_{Vap}). The recycle column and product column reflux drum levels (LVL_{RD2} and LVL_{RD3}) are regulated using the respective distillate rates (D_2 and D_3). The product column bottom sump level (LVL_{Bot3}) is regulated using its bottoms rate (B_3). With these pairings, no close-by valves are left for regulating the purge column and recycle column bottom sump levels (LVL_{Bot1} and LVL_{Bot2}). The only option is to manipulate the two fresh feeds, F_{C3} and F_{C6}. C_3 is the limiting reactant with near complete single-pass conversion so that F_{C3} determines the cumene and DIPB production in the reactor. Since the cumene and DIPB accumulate at the bottom of the recycle column, the LVL_{Bot2}-F_{C3} pairing is implemented for recycle column sump level control with the LVL_{Bot1}-F_{C6} pairing being implemented for purge column sump level control.

16.2.4. Step 3: Throughput Manipulation and Additional Economic Loops

In this example, there is only one active constraint region corresponding to V_3^{MAX} going active at maximum throughput with the other constraints / specifications being fixed at their Mode II values at lower throughputs. The throughput may be reduced by reducing V_3 below V_3^{MAX}. V_3^{SP} is then the throughput manipulator (TPM) adjusted to operate the plant at the desired throughput below maximum. There are no additional SOVs whose control needs to be taken up at lower throughputs as no additional constraints become inactive at lower throughputs.

The economic plantwide control structure, labeled CS1, obtained by the application of Step 1-3 is shown in Figure 16.4 with the economic loops in blue. CS1 has been designed for the tightest possible control of the economic CVs using close by MVs. Since control valves get used up in these loops, in the inventory control system, the MVs of the bottom sump level loops for the purge and recycle columns are not local to the respective units but away at the fresh feeds and thus very unconventional. Even so, acceptable level regulation is expected as the lag associated with the reaction section is small with the material essentially flowing through a long pipe with small vaporizer and the reactor effluent cooler lags. The acceptable level regulation and overall process stabilization was confirmed from rigorous dynamic simulations. With the unconventional long level loops, the control structure attempts tight control of the economic CVs with loose level control. In other words, the structure attempts tight control of the economic CVs by transforming the transients to the surge levels that have no steady state economic impact.

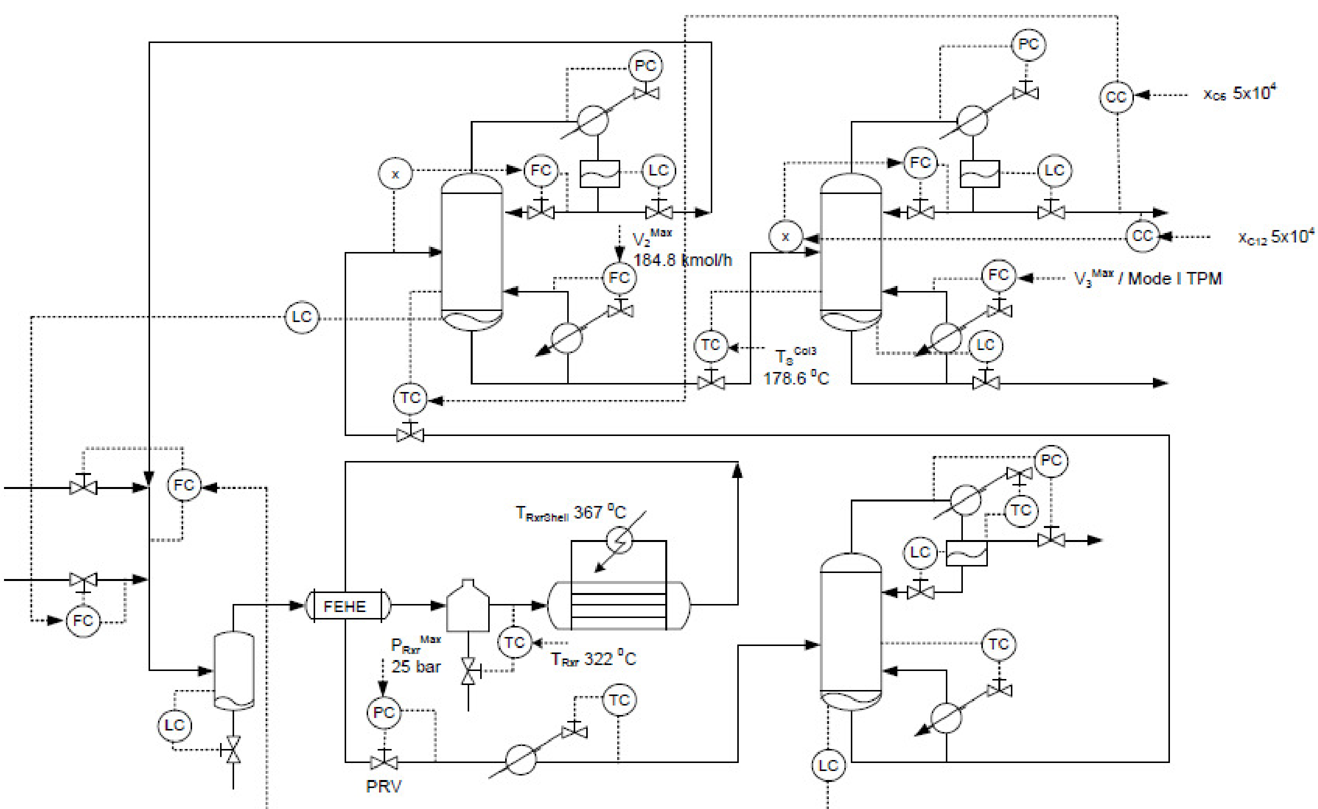


Figure 16.4. Economic plantwide control structure (CS1)

16.3. Conventional Plantwide Control Structure (CS2)

The conventional plantwide control structure, CS2, with the TPM at the C_3 (limiting reactant) feed is shown in Figure 16.5. The total benzene (fresh + recycle) is maintained by F_{C6Tot} to prevent snowballing in the benzene recycle loop. In the reaction section, LVL_{Vap} is controlled by Q_{Vap}, T_{Rxr} is controlled by Q_{Fur}, $T_{RxrShell}$ is set at its near optimum value, P_{Rxr} is controlled at P_{Rxr}^{MAX} by the PRV and the partially condensed reactant effluent temperature (T_{Cooler}) is maintained by its cooling duty, Q_{Cooler}. In the separation train, the recycle and product column pressures are controlled by the respective condenser duties, the reflux drum levels using the respective distillate streams and the bottom sump levels using the respective bottoms streams. On the purge column, the column pressure is controlled by the vapor vent, the overhead condenser temperature is maintained by the condenser duty and the reflux drum level is controlled by the reflux. To regulate the C_3 leakage down the bottoms, T^S_{Col1} is maintained by V_1. On the recycle column, L_2 is maintained in ratio with the column feed (B_1) and T^S_{Col2} is maintained by V_2 with $T^S_{Col2}{}^{SP}$ being adjusted to maintain the product impurity $x_{C6}{}^{D3}$. On the product column, the reflux (L_3) is maintained in ratio with the feed (B_2) and $L_3/B_2{}^{SP}$ is adjusted to maintain the product impurity $x_{C12}{}^{D3}$. T^S_{Col3} is maintained by adjusting V_3.

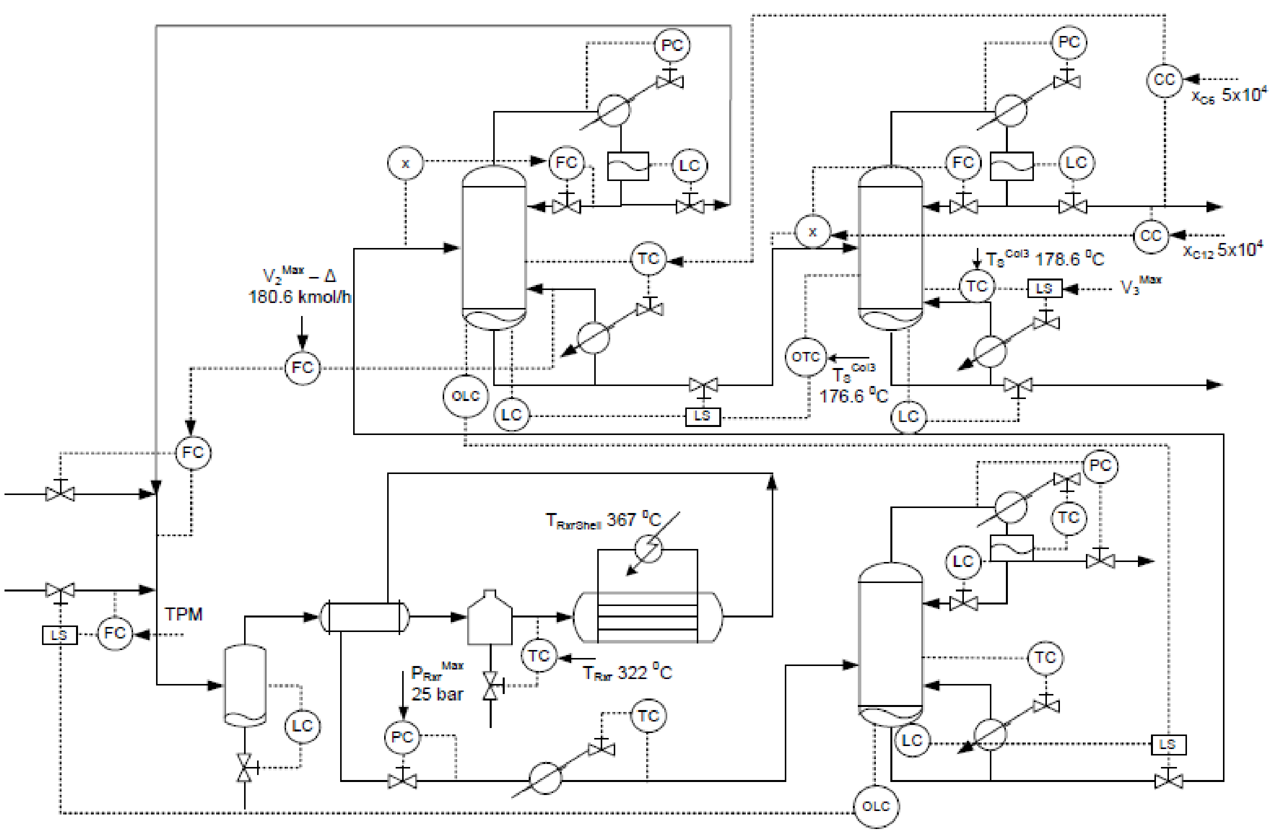


Figure 16.5. Conventional plantwide control structure, CS2, with overrides

Since optimal operation requires running the process at V_2^{MAX} at all throughputs, a supervisory controller is installed that adjusts the total benzene setpoint ($F_{C6Tot}{}^{SP}$) to maintain V_2

at its setpoint. Since V_2^{MAX} is a hard constraint corresponding to the initiation of recycle column flooding and since control of the stripping tray temperature (T^S_{Col2}) must never be lost to ensure the product benzene impurity level is always regulated, some back-off from the V_2^{MAX} limit would be needed to ensure the hard constraint is not violated during worst case transients.

The other hard constraint that must be handled is V_3^{MAX}, the bottleneck constraint, which goes active as throughput is increased towards maximum. When V_3^{MAX} goes active, product column temperature control (T^S_{Col3}) is lost implying loss of precious cumene down the bottoms with a severe economic penalty. To avoid the same, an override control system is put in place that alters the material balance control structure all the way up to the C_3 feed to ensure that column temperature control is not lost when V_3^{MAX} goes active, as in Figure 16.5.

The override scheme works as follows. The override temperature controller on the product column is direct acting and has its setpoint slightly below the T^S_{Col3}-V_3 loop setpoint. Thus when V_3^{MAX} is inactive, its output is high (usually saturated) and B_2 controls the recycle column sump level. When V_3^{MAX} goes active, product column temperature decreases below the second temperature controller setpoint and its output ultimately decreases below the LVL_{Bot2} controller output with the low select passing the manipulation of B_2 from the LVL_{Bot2} controller to the override temperature controller. Once this occurs, LVL_{Bot2} control is lost and it rises. The second LVL_{Bot2} override controller then takes over manipulation of B_1 via the low select in a manner similar to the product column temperature override scheme. This causes LVL_{Bot1} control to be lost and the second LVL_{Bot1} override controller ultimately takes over F_{C3} manipulation. The override scheme thus works to cut down on the fresh propylene feed on V_3^{MAX} going active.

16.4. Dynamic Simulation Results and Discussion

Rigorous dynamic simulations are performed in Unisim to evaluate and compare the performance of the synthesized economic plantwide control structure, CS1, with the conventional plantwide control structure, CS2.

16.4.1. Controller Tuning

A consistent procedure is used to tune the various controllers. All flow and pressure controllers are PI and tuned for a fast and snappy response. All conventional level controllers with local unit specific pairings are P only and use a gain of 2 to smooth out flow transients. The temperature controllers are PI with a 45 s sensor lag. The Unisim autotuner is used to obtain a reasonable value of the reset time and controller gain (K_C). The K_C is then adjusted for a fast but not-too-oscillatory servo response. All composition controllers use a sensor dead-time and sampling time of 5 mins. The autotuner does not provide reasonable initial tuning parameters so that the open loop response is first obtained and the reset time set to 2/3rd open loop response completion time and K_C set to the inverse of the process gain. These tunings work well for the two product impurity controllers in both CS1 and CS2.

In CS1, the unconventional non-local LVL_{Bot1} and LVL_{Bot2} controllers are P only and are tuned initially by hit and trial to stabilize the process. The temperature and composition loops are then tuned as discussed above. Finally, the non-local level controller tunings are further refined for a smooth overall plantwide response to the principal disturbances. In CS2, the product column override temperature controller setpoint is chosen to the highest possible value so that the over-ride controller never goes active for the different disturbance scenarios. This gives a setpoint that is 2 °C below nominal. The LVL_{Bot1} and LVL_{Bot2} override setpoints are chosen 10% above the nominal setpoint of 50%. Also, aggressive tuning is attempted to ensure F_{C3} is cut quickly when V_3^{MAX} goes active to mitigate the loss of precious cumene down the product column bottoms during the transient. Both the over ride level controllers are P only. Finally the supervisory recycle column boilup controller is tuned for a not-too-oscillatory servo response. The salient controller tuning parameters and setpoints thus obtained are reported in Table 16.4 for CS1 and CS2.

Table 16.4. CS1 and CS2 controller parameters*#

CV attributes			CS1			CS2		
CV	Set-point	Sensor Span	MV	K_C	τ_i (min)	MV	K_C	τ_i (min)
T^S_{Col1}	140 °C	115-175 °C	Q_{Reb1}	0.2	8	Q_{Reb1}	0.2	8
T^S_{Col3}	178.64 °C	150-200 °C	B_2	0.18	20	Q_{Reb3}	0.5	15
T_{rxr}	322 °C	301-360 °C	Q_{Fur}	0.3	2	Q_{Fur}	0.3	2
T_{Cooler}	100 °C	70-130 °C	Q_{Cooler}	0.4	8	Q_{Cooler}	0.4	8
x_{C6}^{D3}	0.0005	.0001-.0015	T^S_{Col2}	0.40	40	T^S_{Col2}	0.4	40
x_{C12}^{D3}	0.0005	.0001-.0030	L_3/B_2	0.08	30	L_3/B_2	0.08	30
V_2	184.8 kmol/h	0-250 kmol/h	Q_{Reb2}	0.5	0.3	F_{C6}^{Total}	0.4	60
$T^S_{Col3}{}^{OR}$	176.64 °C	150-200 °C	-	-	-	B_2	0.4	20
LC_{Col2}^{OR}	45%	0-100%	-	-	-	B_1	4	-
LC_{Col1}^{OR}	70%	0-100%	-	-	-	F_{C3}	0.5	-

*: All level loops use K_C = 2 unless otherwise specified
#: Pressure/flow controllers tuned for tight control

16.4.2. Closed Loop Results

CS1 and CS2 are dynamically tested for different disturbance scenarios. First, the dynamic transition from Mode I to Mode II is simulated. The dynamic response is also obtained for a ±10% throughput step change and a ±3% step change in the feed propylene mol fraction for Mode I (F_{C3} = 101.93 kmol/h) operation. For Mode II, the dynamic response is obtained for the latter as well as a ±5% step bias in the F_{C3} flow sensor. For convenience, the CS2, supervisory V_2 controller setpoint is set at V_2^{MAX} even as in practice sufficient back-off would be provided to ensure the hard V_2^{MAX} constraint is never violated during worst case transients and benzene impurity control in the product cumene is never lost.

We first consider throughput transition using CS1 and CS2, from Mode I (low throughput) to Mode II (maximum throughput) and back. In both structures, the TPM is ramped at a rate that causes F_{C3} to change by ~10 kmol in 15 hrs. This ensures that the severity of the throughput transition disturbance is comparable in both the structures. For the throughput transition in CS1, V_3^{SP}, is ramped up at a rate of 0.79 kmol/h to V_3^{MAX}, held constant for 20 hours and then ramped back down at the same rate. In CS2, F_{C3}^{SP} is ramped at a rate of 0.74 kmol/h till 184 kmol/h (or lower if override takes over F_{C3} manipulation), held there for about 30 hours to allow for the over-rides to take over and stabilize and then ramped back down to 101.93 kmol/h. As recommended by Shinskey [21], we use external reset on the PI T^S_{Col3} override controller to ensure it takes up B_2 manipulation at the earliest once V_3^{MAX} goes active.

The CS1 and CS2 transient response of salient process variables is plotted in Figure 16.6. Tight product purity control as well as smooth plantwide transients are observed for both CS1 and CS2. In CS2, the major events of V_3^{MAX} going active (P_1), the ethylene feed being cut by the LVL_{Bot1} override (P_2) and beginning of the F_{C3}^{SP} (TPM) ramp down (P_3) are shown. In the CS2 dynamic response, oscillations post LVL_{Bot1} override controller taking over F_{C3} manipulation are seen. Also it takes about 5 hrs between V_3^{MAX} going active and F_{C3}^{SP} manipulation passing to the LVL_{Bot1} override. The transient x_{C9}^{B3} response for CS1 and CS2 also shows that once V_3^{MAX} goes active, the cumene leakage in the DIPB stream remains well regulated in CS1 while in CS2 the leakage increases due to the lower T^S_{pur} override setpoint. In the entire transient period, LVL_{Bot1} and LVL_{Bot2} vary within a band of 15% and 24% respectively, in CS1. The corresponding figures for CS2 are comparable at 16% and 24% respectively.

To compare the structures for Mode II operation, Figure 16.7 plots the dynamic response of important process variables to a ±5% step bias in the F_{C3} measurement for CS1 and CS2. The dynamic response for CS1 achieves tight product purity control with a settling time of about 10 hours. Similarly, the CS2 transient response also completes in about 10 hours. Note that since V_3^{MAX} is active, the CS2 T^S_{Col3}, LVL_{Bot2} and LVL_{Bot1} overrides are on and the material balance control structure is oriented in the reverse direction of process flow.

To compare the structures for Mode I operation, Figure 16.8 plots the plantwide dynamic response of important process variables to a step change in the TPM for a ±10% throughput change. In CS1, to bring about a 10% increase and decrease in F_{C3}, the V_3^{SP} must be changed by +22.1 kmol/h and -21.9 kmol/h, respectively. In CS2, F_{C3} is directly set by F_{C3}^{SP} (TPM). The product purity and DIPB cumene loss control in CS2 is not as tight as in CS1 as the TPM for CS1 is located at the product column. In CS2, on the other hand, the TPM is at a process feed and the downstream product column gets subjected to a less severe transient due to filtering by the intermediate units. Overall, a smooth plantwide response is observed in both structures. The response completion time for CS1 and CS2 is slightly above and below 10 hrs, respectively.

Figure 16.9 compares the plantwide response of important process variables to a ±3% step change in the C_3 feed propane (inert) impurity in Mode I operation. Both structures handle the disturbance well with the product purity being tightly controlled. The overall plantwide response is also smooth with a response settling time of about 15 hrs for CS1 and about 10 hrs for CS2.

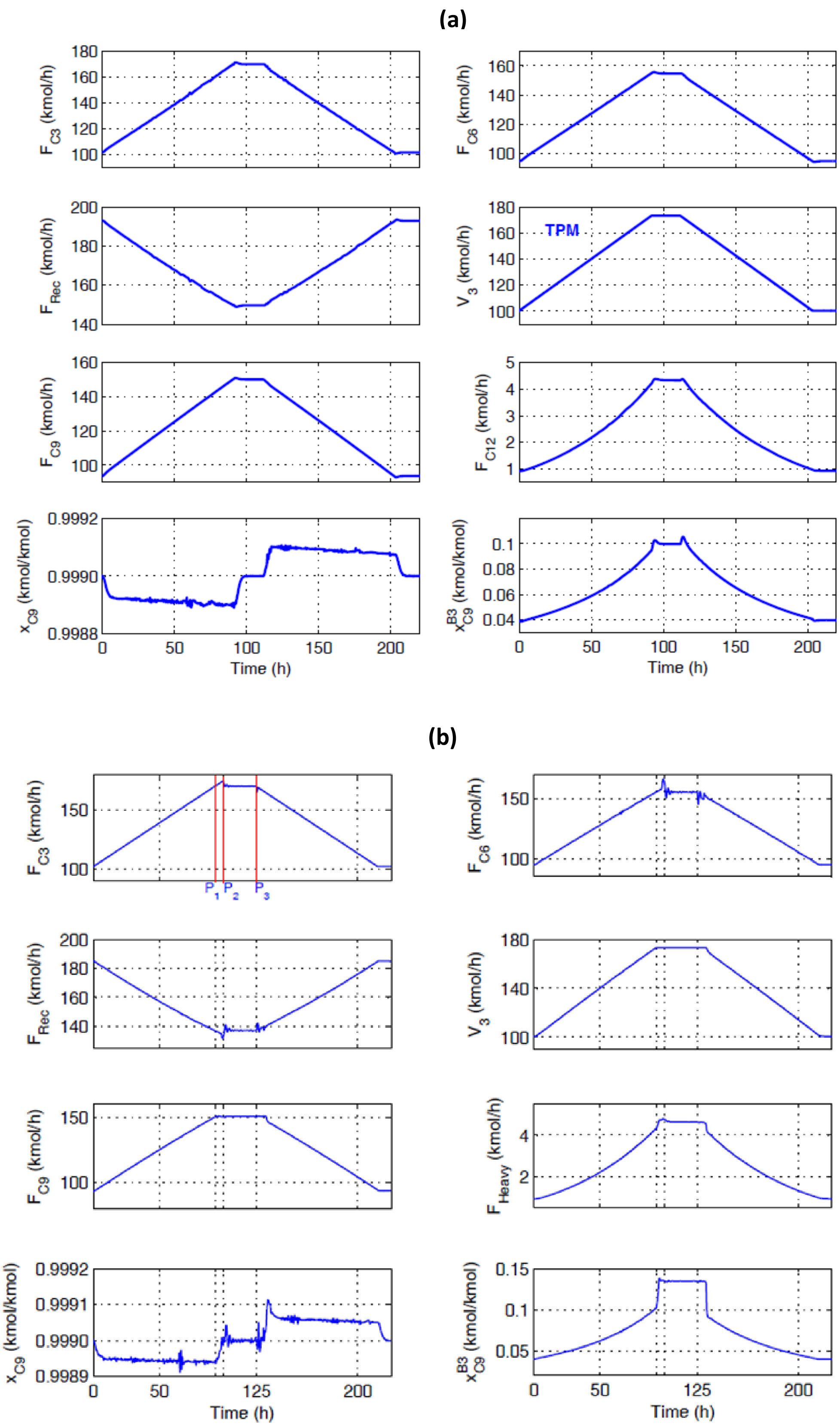


Figure 16.6. Transient response for throughput transition. (a) CS1; (b) CS2

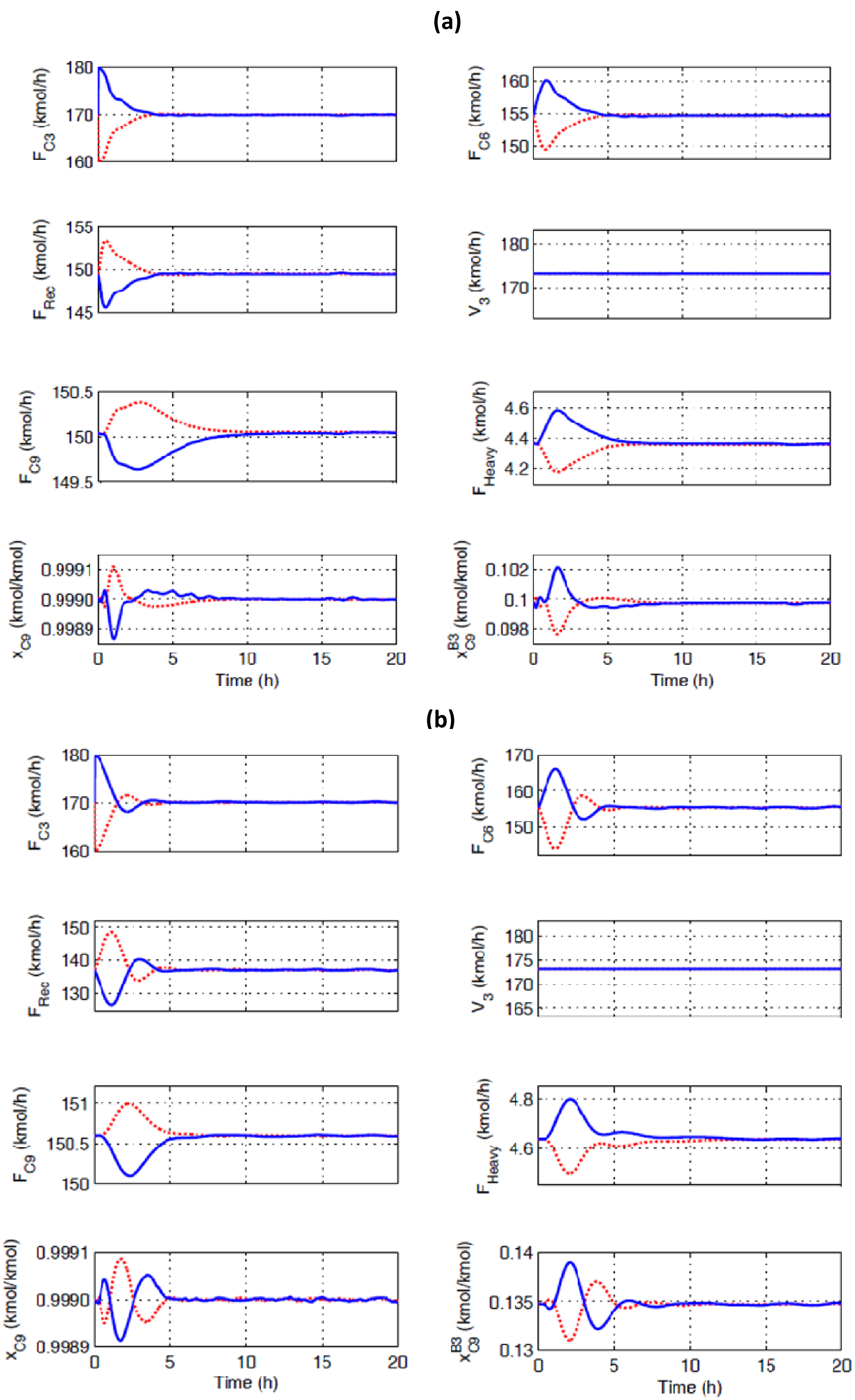
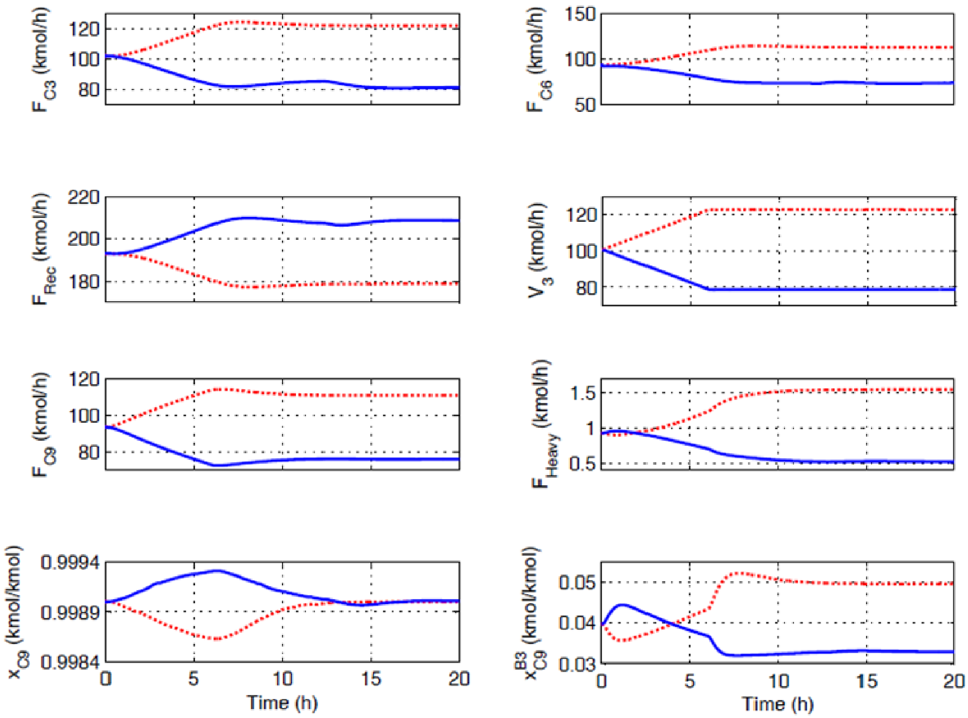


Figure 16.7. Maximum throughput transient response to ±5% step bias in F_{C3} sensor .
(a) CS1; (b) CS2
—: -5% bias; ⋯: +5% bias

(a)



(b)

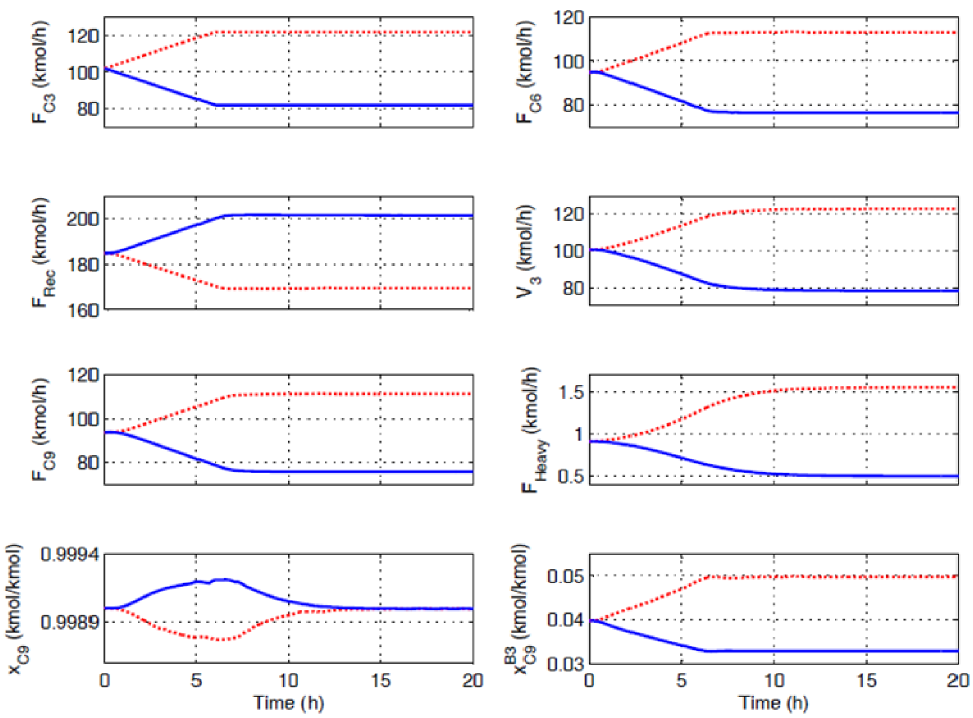
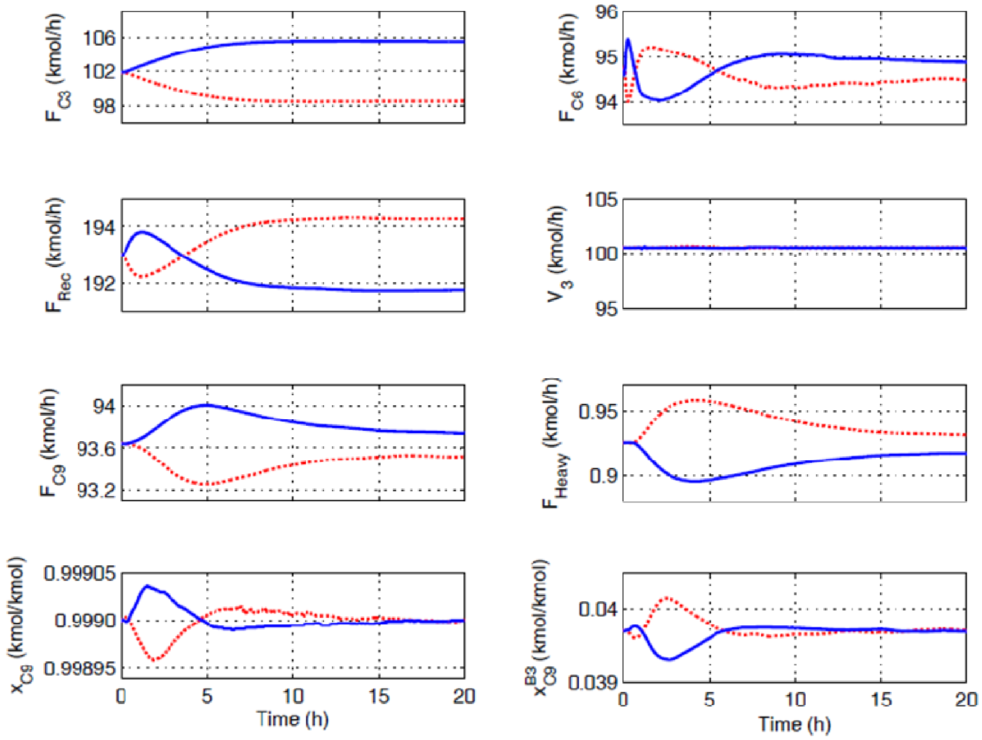


Figure 16.8. Mode I transient response to ±10% throughput change. (a) CS1; (b) CS2
—: -10%; ⋯: +10%

(a)



(b)

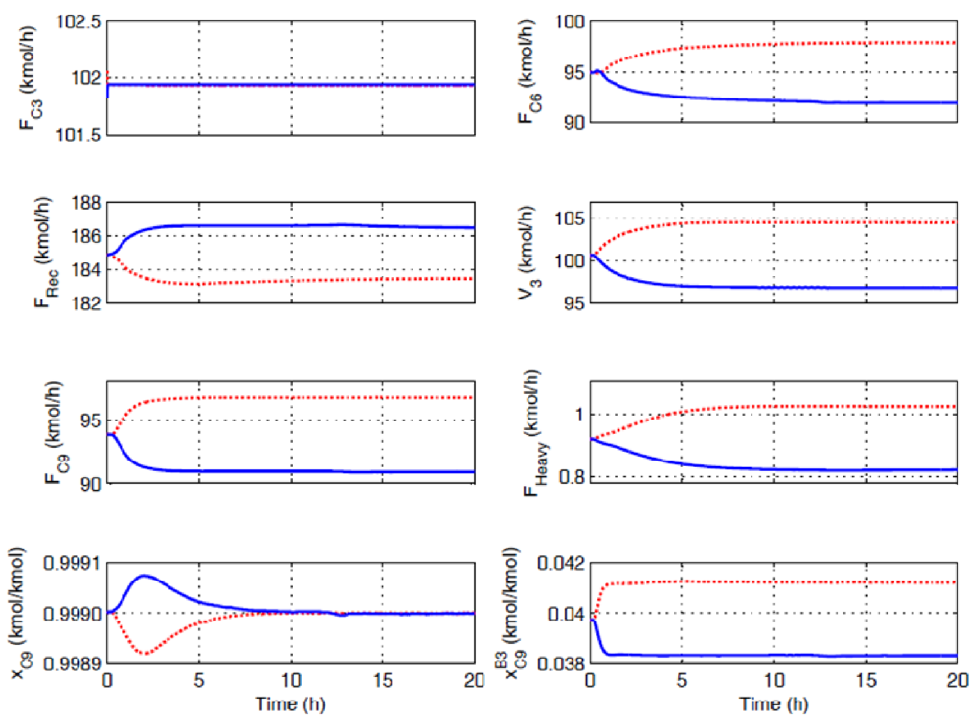


Figure 16.9. Mode I transient response to ±3% step in F_{C3} propylene mol fraction.
(a) CS1; (b) CS2

—: -3% ; ···: +3%

16.4.3. Quantitative Dynamic and Economic Comparison of CS1 and CS2

In this subsection, the dynamic and economic performance of CS1 and CS2 is quantitatively compared. In addition to the disturbance scenarios already considered, we consider a -5% step bias in F_{C3} measurement with the initial steady state corresponding to V_3 - V_3^{MAX} approaching 0 (Mode II). The overrides in CS2 are then 'ready to be triggered'.

To quantify the dynamic performance, the IAE values for x_{C9}^{D3} and x_{C9}^{B3} for the 10 h transient period post disturbance are reported in Table 16.5. From the data, it is evident that both structures provide comparable regulation of product purity and the cumene loss in the byproduct stream in Mode I (V_3^{MAX} inactive) for a feed propylene composition change. For a ramped throughput change, even as the regulation of x_{C9}^{B3} is significantly poorer in CS1, it is acceptably small. As already noted, the larger x_{C9}^{B3} variability in CS1 is because the CS1 TPM (V_3^{SP}) is located at the product column. The Mode I throughput change data (row 1) also suggests that CS2 achieves slightly tighter product purity control. For Mode II operation, the data (rows 3 and 4) suggests that CS1 and CS2 provide comparable dynamic regulation of x_{C9}^{D3} and x_{C9}^{B3} for process feed disturbances, namely, a 3% step change in the propylene feed composition or a 5% step bias in the F_{C3} sensor. The IAE values for x_{C9}^{B3} with the T^S_{Col3} override about to be triggered (last two rows) with and without external reset suggest that Shinskey's simple external reset scheme significantly improves the tightness of control by ensuring that the unselected output does not deviate too far away from the selected output due to reset windup.

Table 16.5. IAE values for x_{C9}^{D3} and x_{C9}^{B3} for 10 h transient post disturbance

Disturbance Scenarios			*CS1*		*CS2*	
*ISS**	*Description*	*Magnitude*	x_{C9}^{D3} (10^{-3})	x_{C9}^{B3} (10^{-2})	x_{C9}^{D3} (10^{-3})	x_{C9}^{B3} (10^{-2})
Mode I	Throughput	+10%&	2.180	7.490	1.380	3.60
		-10%&	2.068	5.294	1.318	2.12
	C_3feed composition	+3%	0.140	0.139	0.254	0.098
		-3%	0.118	0.125	0.263	0.073
Mode II	F_{C3} sensor bias	+5%	0.171	0.341	0.187	0.808
		-5%	0.180	0.383	0.195	0.971
	C_3 feed composition	+3%	0.154	0.329	0.119	0.610
		-3%	0.152	0.305	0.114	0.524
$V_3^{MAX}-\delta$#	F_{C3} sensor bias%	+5%	0.171	0.341	0.868	1.326
		-5%	0.180	0.383	0.550	24.247
	F_{C3} sensor bias@	+5%	0.171	0.341	0.876	1.058
		-5%	0.180	0.383	0.370	3.602

*: Initial steady state
&: TPM setpoint ramped over 6 h. IAE calculated over 15 h period
#: CS2 overrides are 'ready to be triggered'
%: No external reset in CS2 T^S_{pur} override
@: External reset in CS2 T^S_{pur} override

To quantify the economic performance, the Mode I and Mode II steady state hourly profit is reported in Table 16.6. In CS2, V_2^{SP} is backed-off from V_2^{MAX} by the least amount for which the V_2^{MAX} constraint does not get violated for the worst-case disturbance scenario, which is a -5% step bias in F_{C3}, requiring the maximum back-off from V_2^{MAX}. Negligible back-off is needed in

CS1 which is designed for process operation at V_2^{MAX}. Due to the back-off from V_2^{MAX} in CS2, its steady profit is slightly lower (up to >0.1% in Mode II) than CS1.

Table 16.6. Steady state and transient profit data for CS1 and CS2

Steady state hourly profit data

Mode of Operation	*CS1 (10^3 \$/h)*	*CS2 (10^3 \$/h)*
Mode I	3.8082	3.8059
Mode II	5.8790	5.8527

Transient profit data (IE_P^{Av} and ΔIE_P^{Av} values)

Disturbance Scenarios			*CS1*		*CS2*	
*ISS**	*Description*	*Magnitude*	IE_P^{Av} (\$/h)	ΔIE_P^{Av} (\$/h)	IE_P^{Av} (\$/h)	ΔIE_P^{Av} (\$/h)
Mode I	Throughput	+10% -10%	132.76 -126.84	5.91	-277.15 274.94	-2.21
	C_3feed composition	+3% -3%	-59.46 72.93	13.47	11.45 -17.94	-6.49
Mode II	F_{C3} sensor bias	+5% -5%	119.08 -131.07	-11.99	125.51 -113.10	12.41
	C_3 feed composition	+3% -3%	-17.46 17.01	-0.45	-22.26 23.95	1.69
V_3^{MAX}–δ#	F_{C3}sensor bias%	+5% -5%	119.08 -131.07	-11.99	98.38 -383.60	-285.22
	F_{C3} sensor bias@	+5% -5%	119.08 -131.07	-11.99	101.42 -364.36	-262.94

*: Initial steady state
&: TPM setpoint ramped over 6 h. IAE calculated over 15 h period
#: CS2 overrides are 'ready to be triggered'
%: No external reset in CS2 T^S_{pur} override
@: External reset in CS2 T^S_{pur} override

To quantify economic losses during transients, Table 16.6 also reports the time average integral error for the 10 hour transient period (T) post disturbance defined as

$$IE_P^{Av} = \frac{\int_0^T \left(P_t - P_f^{SS}\right) dt}{T}$$

where P_t is the instantaneous hourly profit and P_f^{SS} is the final steady state hourly profit for a disturbance. The metric is thus the time average cumulative transient profit deviation from the final steady state profit. Positive (negative) values indicate the extra hourly profit (loss) over the final steady state profit in the transient period. One would expect that any transient profit for a disturbance in one direction would be nullified by a similar transient loss for the same disturbance in the opposite direction. The IE_P^{Av} values for a given disturbance in either direction should thus be approximately the same magnitude but opposite signs. A large negative difference between the two corresponds to an unrecoverable transient economic loss. Table 16.6 also reports this difference

$$\Delta IE_P^{Av} = IE_P^{Av+} - IE_P^{Av-}$$

where IE_P^{Av+} and IE_P^{Av-} correspond to an increase and decrease, respectively, in the disturbance magnitude. As expected, in all but one disturbance scenario, ΔIE_P^{Av} is small for both CS1 and CS2. For a ±5% step change in the F_{C3} measurement with the CS2 overrides 'ready-to-be-triggered', the ΔIE_P^{Av} is large negative implying significant unrecoverable transient losses. These losses are attributed to the excessive leakage of precious cumene in B_3 between V_3^{MAX} going active and T^S_{Col3} override taking over B_2 manipulation. Every extra mol of lost cumene consumes expensive reactants that cost twice the product to raw material price difference. Regardless of whether external reset is used or not on the T^S_{pur} override, the transient profit loss is significant at >4.5% of the steady state Mode II profit. The transient loss figures with and without external reset are comparable as the oscillatory x_{C9}^{B3} response for the no external reset leads to cancellation of errors in the undershoots and overshoots.

If the CS2 overrides are switched off (e.g. by an operator), F_{C3}^{SP} must be sufficiently reduced from the maximum achievable throughput so that the V_3^{MAX} constraint does not get violated during the worst-case transient, which is a -5% step change in the F_{C3} measurement. This back-off results in a significant steady hourly profit loss of >4% due to lower maximum throughput. The results demonstrate that CS2 with overrides or backed-off operation results in non-negligible economic loss.

16.4.4. Discussion

The results for the case study suggest that the economic plantwide control structure, CS1, designed for tightest possible control of the economically important hard active constraints (V_3^{MAX} and V_2^{MAX}), achieves superior economic process operation particularly in Mode II, compared to the conventional control structure, CS2. CS1 is also simpler than CS2 in that the inventory management strategy remains fixed regardless of whether the V_3^{MAX} constraint is active or not. CS2 on the other hand is more complicated requiring 3 additional override controllers to alter the material balance control structure all the way up to the C_3 feed, once the V_3^{MAX} constraint goes active. Proper tuning and setpoint selection of these override controllers is necessary to ensure that they get activated in the proper order without too much time elapsing between when V_3^{MAX} goes active and the overrides 'take-over' control. Proper design of the override scheme can be tricky and for severe enough transients, the correct override order may get violated and large plantwide transients can occur due to the overrides 'taking-over' and 'giving-up' control, similar to 'on-off' control. One such occurrence and operators would be inclined to turn the scheme off and resort to the more conservative backed-off process operation with a significantly more severe economic penalty.

It is also worth noting that in our analysis, we have considered only a single disturbance to be active at a time and the hard maximum boilup constraints (V_2^{MAX} and V_3^{MAX}) to be constant. In practice, multiple disturbances are active all the time. More importantly, the hard maximum boil-up constraint limits themselves are transient, depending on the feed flow and reflux flow as well as other factors such as impurities that build-up over time inside the column. The CS2 economic performance is therefore likely to be significantly inferior to CS1 due to the need for a higher back-off in V_2^{MAX} as well as unrecoverable transient cumene loss in the DIPB stream with the override scheme switching on and off due to variability in the V_3^{MAX} limit.

The major difference between CS1 and CS2 is in the location of the TPM; V_3^{SP} for CS1 and F_{C3}^{SP} for CS2. Since V_3^{SP} is the last constraint to go active (i.e. the bottleneck constraint) and also economically important with any back-off resulting in reduced throughput, it makes sense to use it as the TPM and not for the conventional control task of tray temperature control. Typically, due to the high sensitivity of recycle flows to throughput changes (snowball effect), the bottleneck constraint is usually inside the recycle loop. The case study results support the heuristic of locating the TPM at the bottleneck constraint for economic operation.

Lastly, we highlight that the conventional practice in control structure design is to implement inventory control loops with their MVs being 'local' to the specific unit containing the inventory. The basic idea is to ensure that the inventory loops are robust. This case study illustrates that it is possible to develop control structures with seemingly unworkable 'long' inventory control loops that provide acceptable regulation with tight control of the economic CVs over the entire throughput range. The top-down pairing philosophy, as illustrated here should be applied to come up with such unconventional but workable economic plantwide control structures, in the knowledge that should the inventory control be fragile, the pairings can always be revised towards 'local' inventory loops and 'long' economic loops in lieu.

16.5. Conclusions

In conclusion, this article demonstrates through a case-study, the crucial role of economically important maximum throughput hard active constraints in determining the input-output pairings for economic plantwide control. The approach demonstrated here leads to a simple control structure with unconventional inventory loops for process operation over the entire throughput range. Conventional control systems that do not take into consideration the active constraints on the other hand must resort to complicated overrides for constraint handling at high throughputs, with overall inferior economic performance.

Chapter 17. C_4 Isomerization Process

17.1. Process Description

Figure 17.1 shows a schematic of the C_4 isomerization process studied in this work. A fresh C_4 stream containing n-C_4 and i-C_4 with some C_3 and i-C_5 impurities is fed to a deisobutanizer (DIB) column that recovers i-C_4 with some n-C_4 (heavy key) impurity as the distillate. All the C_3 in the fresh C_4 feed leaves in the distillate. The DIB bottoms consisting of n-C_4, i-C_5 and some i-C_4 (light key) impurity is fed to a purge column that recovers i-C_5 with some n-C_4 (light key) as the bottoms. The purge column distillate consisting of C_4's and some i-C_5 (heavy key) is fed to an adiabatic packed bed reactor (PBR) after preheating in a feed effluent heat exchanger (FEHE) followed by heating to the reaction temperature in a heater. The n-C_4 isomerizes in the PBR to i-C_4. The hot reactor effluent preheats the cold reactor feed in the FEHE and is then condensed in a flooded cooler. The subcooled liquid is rich in i-C_4 and is fed to the DIB column above the relatively i-C_4 lean fresh C_4 feed. The base-case process design and steady state operating conditions (adapted from Luyben et al. [17]) are shown in Figure 17.1. The irreversible reaction kinetic model in their work is used along with the SRK equation of state to model the thermodynamic properties. Aspen Hysys is used for steady state and dynamic process simulation. Hysys uses the sequential approach for steady state solution of flowsheets with Wegstein updation at the recycle tear. The inside-outside algorithm is used on the distillation columns with the light key and heavy key impurity mol fractions in respectively the bottoms and distillate as the 2 column specifications. For robust recycle-tear convergence, the total benzene flow (recycle + fresh) is specified so that the fresh benzene gets calculated at the end of each recycle tear iteration.

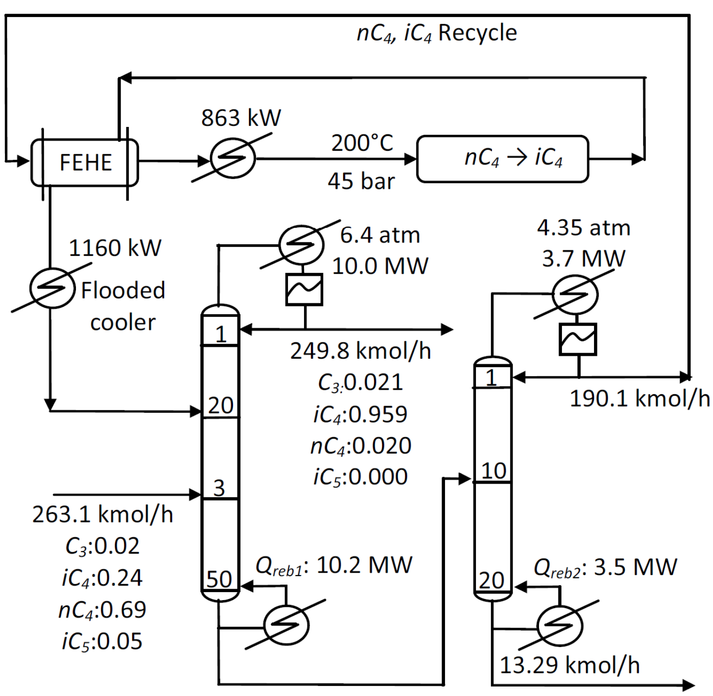


Figure 17.1. Isomerization process schematic with salient design and base operating conditions

17.2. Economic Plantwide Control System (CS1) Design

17.2.1. Step 0: Active Constraint Regions and Economic Operation

The process has 14 independent control valves. Of these, 4 valves must be used to control surge levels, namely, two reflux drum levels and two sump levels on the columns. Also, two valves will get used to maintain the columns at their design pressures There are then 8 steady state operating dofs for the process; 1 for the fresh feed, 2 each for the two columns, 1 for the reactor feed heater, 1 for the reactor effluent cooler and 1 for the reactor pressure. For robust flowsheet convergence, the chosen 8 specification variables are: the fresh C_4 feed (F_{C4}), the DIB distillate $n\text{-}C_4$ and bottoms $i\text{-}C_4$ mol fractions (x_{nC4}^{D1} and x_{iC4}^{B1}), the purge column distillate $i\text{-}C_5$ and bottoms $n\text{-}C_4$ mol fractions (x_{iC5}^{D2} and x_{nC4}^{B2}), the reactor inlet temperature (T_{rxr}) and pressure (P_{rxr}) and the cooler outlet temperature (T_{cool}).

Of the 8 steady state dofs, T_{rxr} and P_{rxr} are assumed fixed at their design values and not considered for optimization. This is done as the kinetic parameters were adapted by Luyben et al.[17] to match the operating conditions of an existing industrial reactor and are therefore artificial. Also, in industrial processes, gas phase reactors are usually operated at the design pressure and not lower so the reaction kinetics are as fast as possible. Also there is usually a very limited recommended catalyst temperature range for which the technology licensor guarantees catalyst life. Holding reactor temperature and pressure constant is therefore a reasonable assumption. The remaining 6 dofs can and should be adjusted for optimizing an economic criterion such as the steady hourly profit or steam consumption per kg product etc. We consider two process operation modes; Mode I where the throughput is fixed (eg by market demand-supply considerations) and Mode II where the market conditions are such that it is optimal to operate the process at maximum throughput.

For Mode I, the optimized economic criterion is the yearly profit, P, defined as

P = [Product Sale – Raw Material Cost – Energy Cost] per year.

The fresh C_4 feed (F_{C4}) is fixed at its base case design value (263.1 kmol/h) and the remaining 5 dofs are to be optimized. For Mode II, the objective is to maximize F_{C4} using all 6 dofs (including F_{C4}) as decision variables. The optimization is performed subject to process constraints on the maximum and minimum material / energy flows, maximum column boilup, maximum product impurity and the maximum allowed reactor temperature.

To simplify the optimization, engineering common sense is applied to reduce the number of decision variables. To minimize the loss of precious $n\text{-}C_4$ down the purge column bottoms, x_{nC4}^{B2} is chosen to be small at 1% (base-case design value). In addition, the maximum product impurity constraint ($x_{nC4}^{D1\ MAX}$) should be active for no product give-away. Finally, the cooler outlet temperature, T_{cool}, has almost no impact on the economic objective function and is therefore fixed at a reasonable value of 53 ºC to ensure the reactor effluent vapor is fully condensed using cooling water. These simple engineering arguments leave 2 decision variables, x_{iC4}^{B1} and x_{iC5}^{D2}, for Mode I (F_{C4} given) optimization. In Mode II (maximum F_{C4}), F_{C4} is an additional third decision variable.

The optimization is performed using the *fmincon* subroutine in Matlab with AspenHysys 2006 as the background steady state flowsheet solver. The optimization problem formulation and its results are summarized in Table 17.1. In Mode I, the specified F_{C4}, x_{nC4}^{B2}, T_{cool} , T_{rxr} and P_{rxr} values along with $x_{nC4}^{D1\ MAX}$ active constraint leaves two unconstrained steady state dofs corresponding to x_{iC4}^{B1} = 0.0565 and x_{iC5}^{D2} = 0.02. To maximize throughput (Mode II), these two unconstrained dofs along with the additional dof corresponding to F_{C4} are exhausted to drive the maximum preheater duty (Q_{htr}^{MAX}), maximum purge column boilup (V_2^{MAX}) and maximum *DIB* boilup (V_1^{MAX}) constraints active. At maximum throughput, all steady state dofs get exhausted.

Table 17.1. Isomerization process optimization summary

J	Mode I: Maximum yearly profit* Mode II: Maximum throughput (F_{C4})	
Process Constraints	$160\ °C \le T_{rxr} \le 200\ °C$ $0 \le$ Feed/product flows $\le$ 2(base-case) $0 \le V_1 \le 1.3$(base-case) $0 \le Q_{htr} \le 1.3$(base-case) $x_{nC4}^{B2} = 0.01$ $P_{rxr} = 45$bar	$x_{nC4}^{D1} \le 0.02$ $0 \le$ Recycle loop flows $\le$ 3(base-case) $0 \le V_2 \le 1.5$(base-case) $0 \le$ Other energy flows $\le$ 2(base-case) $T_{cool} = 53$°C
Case	Mode I	Mode II
F_{C4}	263.1 kmol/hr&	334.5 kmol/h#
T_{rxr}	200 °C $_{\text{Max}}$	200 °C $_{\text{Max}}$
T_{cool}	53 °C $_{\text{Fixed}}$	53 °C $_{\text{Fixed}}$
x_{nC4}^{D1}	0.02 $_{\text{Max}}$	0.02 $_{\text{Max}}$
x_{iC4}^{B1}	0.0565	0.0125
x_{iC5}^{D2}	0.020	0.00022
x_{nC4}^{B2}	0.01 $_{\text{Fixed}}$	0.01 $_{\text{Fixed}}$
Optimum J	\$17.84x10^6 yr^{-1}	334.5 kmol/h
Active Constraints^	T_{rxr}^{MAX}	T_{rxr}^{MAX}, Q_{htr}^{MAX}, V_1^{MAX}, V_2^{MAX}

*: Heater duty \$9.83 GJ^{-1}; Steam \$4.83 GJ^{-1};Cooling water \$0.16 GJ^{-1};F_{C4} \$ 32.5kmol^{-1}; F_{iC4} \$ 42.0kmol^{-1}; F_{iC5} \$ 22.0kmol^{-1}

&: F_{C4} is specified ; ^: Active constraint; #: F_{C4} is optimized for maximum throughput

As the throughput is increased from Mode I (F_{C4} = 263.1 kmol/h), the optimization of the two unconstrained dofs using *fmincon* shows that Q_{htr}^{MAX} is the first constraint that becomes active at an F_{C4} of about 320 kmol/h. A further increase in throughput to 334 kmol/h F_{C4} drives V_1^{MAX} active followed by V_2^{MAX} becoming active at the maximum throughput of 334.5 kmol/h. The increase in throughput over what is achieved when Q_{htr}^{MAX} becomes active is quite small at ~4.5%. We therefore assume that once Q_{htr}^{MAX} becomes optimally active, incrementally higher throughput is achieved by driving V_1^{MAX} and V_2^{MAX} constraints active.

The large throughput range from 263.1 kmol/h to the maximum throughput of 334.5 kmol/h witnesses Q_{htr}^{MAX}, V_1^{MAX} and V_2^{MAX} becoming active. These constraints are in addition to the other always active constraint $x_{nC4}^{D1\ MAX}$ and specifications for T_{rxr}, P_{rxr}, T_{cool} and x_{nC4}^{B2}, the latter specification being economically significant. If we assume that Q_{htr} is adjusted for a desired reactor inlet temperature of T_{rxr}, then once the Q_{htr}^{MAX} constraint becomes active at a high throughput, a further increase in throughput is made possible by reducing the *i-C$_5$* leaking up the purge column distillate and the *i-C$_4$* leaking down the DIB column distillate. The reduced *i-C$_4$/C$_5$*

circulating around the plant causes the flow through the reactor to reduce allowing more F_{C4} to be processed while keeping the Q_{htr}^{MAX} constraint active.

17.2.2. Step 1: Loops for Tight Economic CV Control

At maximum throughput, Q_{htr}^{MAX}, V_1^{MAX} and V_2^{MAX} are process inputs (potential MVs) constrained to be active. These are hard active constraints and back-off in these must be minimized for process operation at the maximum possible throughput. In addition, $x_{nC4}^{D1\ MAX}$ constraint, which is a process output (CV), is active along with output specifications for T_{rxr}, P_{rxr}, x_{nC4}^{B2} and T_{cool}. Of these, tight control of $x_{nC4}^{D1\ MAX}$ and x_{nC4}^{B2} is desirable for respectively, on-aim product quality and small loss of precious n-C_4 in the purge column bottoms. The analytical measurement x_{nC4}^{B2} is not related to the product quality and therefore unlikely to be available in practice. As the purge column temperature profile is quite sharp, the average temperature of sensitive stripping tray temperatures, T^S_{pur} (14th-16th tray from top) is therefore controlled as an inferential measure of x_{nC4}^{B2}. Due to their economic significance, we first pair loops for tight control of Q_{htr}, V_2 , V_1 and x_{nC4}^{D1} at their maximum limits as well as tight control of T^S_{pur}.

The Q_{htr} valve is left fully open for process operation at Q_{htr}^{MAX}. For operating the columns close to their maximum boil-up limits (i.e. close to flooding limit) with negligible back-off, the respective reboiler steam valves are used to control the boilups. Thus V_1 is paired with Q_{reb1} and V_2 is paired with Q_{reb2}. Tight control of the product impurity x_{nC4}^{D1} is achieved by manipulating the DIB column reflux (L_1). Because V_2^{MAX} is active, T^S_{pur} cannot be controlled conventionally using boilup, V_2, and the feed to the purge column (B_1) is used as the MV instead.

For effective stabilization of the reactor, its pressure and temperature must be controlled tightly. Since Q_{htr}^{MAX} is active, the reactor inlet temperature is maintained at its setpoint using the reactor feed flow stream (D_2). Note that the degree-of-tightness of control in this arrangement would be comparable to Q_{htr} as the MV since the open loop dynamic response time constants are likely to be comparable. The reactor pressure is controlled at its design value by manipulating the cooler outlet valve. To ensure proper condensation of the reactor effluent, the cooler duty (Q_{cool}) is manipulated to maintain T_{cool}.

17.2.3. Step 2: Inventory Control System

We now pair loops for remaining inventories that are not important from the economic standpoint. The two column pressures (P_{col1} and P_{col2}) are controlled at their specified values conventionally using the respective condenser duties (Q_{cnd1} and Q_{cnd2}). Lastly, we pair loops for the four surge levels on the two columns. Since the purge column distillate is already paired with the T_{rxr} controller, its reflux drum level (LVL_{RD2}) is controlled using the reflux rate (L_2). The purge column sump level (LVL_{Bot2}) is controlled using the column bottoms (B_2). Note that even as B_2 is a very small stream, effective level control will be achieved as long as T^S_{pur} is controlled, an economic loop already paired. The DIB reflux drum level (LVL_{RD1}) is controlled using the distillate (D_1). Since B_1 is already paired for purge column temperature control, the DIB column sump level (LVL_{Bot1}) is controlled using the fresh C_4 feed (F_{C4}). It is highlighted that in the control structure for maximum throughput operation, the light key i-C_4 impurity leaking down the DIB bottoms and the heavy key i-C_5 impurity leaking up the purge column distillate are not controlled and float at appropriate values determined by the values of V_1^{MAX} and V_2^{MAX} as well as the other setpoints.

17.2.4. Step 3: Throughput Manipulation and Additional Economic Loops

We now seek an appropriate strategy for reducing throughput while ensuring (near) optimal operation at lower throughputs. From the optimal Mode I and Mode II results in the previous section, V_2^{MAX} is the last constraint to go active. On reducing throughput, V_1^{MAX} is the next constraint to go inactive followed by Q_{htr}^{MAX}. The sensitivity of throughput with respect to the constraint variables decreases in order Q_{htr}, V_1 and V_2. As explained previously, once Q_{htr}^{MAX} goes active, only an incremental increase in throughput is achieved by reducing the *i*-C_4 leaking down DIB column (this causes V_1^{MAX} to go active) and the *i*-C_5 leaking up the purge column (this causes V_2^{MAX} to go active).

The simplest way to reduce throughput (Option 1) would be to maintain the boilups at V_1^{MAX} and V_2^{MAX} and reduce Q_{htr}^{MAX}. Even as throughput would reduce, the operation would be suboptimal due to overrefluxing in the two columns (unnecessarily high boilups). For near optimal operation at low throughputs, this overrefluxing must be mitigated. One simple possibility (Option 2) is to hold V_2 and V_1 in ratio with the respective column feeds, with the Mode I optimum ratio as their setpoint. Another possibility (Option 3) is to hold the difference between two appropriate DIB column stripping tray temperatures ($\Delta T_{DIB} = T_{37} - T_{32}$) constant by adjusting V_1 and holding V_2 in ratio with B_1. The setpoint for these two controllers would be the Mode I optimum value. Note that ΔT_{DIB} is controlled instead of a tray temperature as the DIB temperature profile is quite flat. The last option (Option 4) is to maintain x_{iC4}^{B1} and x_{iC5}^{D2} at their Mode I optimum values by adjusting respectively V_1 and V_2. This however requires two additional composition analyzers, an unlikely scenario in an industrial setting.

Figure 17.2 compares the optimum steady state profit at various throughputs with the profit achieved using the four different options: (1) process operation at V_1^{MAX} and V_2^{MAX} at all throughputs; (2) $V_1/(F_{C4} + D_2)$ and V_2/B_1 held constant at Mode I optimum till V_1^{MAX} and V_2^{MAX} become active; (3) ΔT_{DIB} and V_2/B_1 held constant at Mode I optimum till V_1^{MAX} and V_2^{MAX} become active and (4) x_{iC4}^{B1} and x_{iC5}^{D2} held constant at its Mode I optimum till V_1^{MAX} and V_2^{MAX} become active. Note that for the price data used, the operating profit decreases for a throughput increase beyond F_{C4} ~332 kmol/h. This point then represents an economic bottleneck and one would operate below this throughput. The economic scenario may however change with significantly higher margins for the product, in which case it may become optimal to operate the process at maximum throughput.

Of the various options considered, Option 4 is economically the best with almost no economic loss from optimum till a throughout of F_{C4} ~ 320 kmol/h, where V_1^{MAX} becomes active. The simpler Option 3 with no additional composition analyzers is comparable to Option 4. The still simpler Option 3 using ratio controllers gives slightly higher profit loss (~1%) at low throughputs. The simplest Option 1 is economically the worst with a significantly higher economic loss between of up to 8% over the throughput range. These results suggest that Option 2 represents a good compromise between simplicity and minimizing the steady state economic loss. It is therefore considered for implementation.

The overall throughput manipulation scheme in Option 2 is then as follows. At low throughputs, Q_{htr} is used as the throughput manipulator (TPM). Once Q_{htr}^{MAX} goes active to increase throughput, throughput manipulation is shifted to ΔT_{DIB}^{SP}, which must be increased for a higher throughput. Once V_1^{MAX} goes active, the TPM is shifted to $V_2/B_1{}^{SP}$, which must again be increased to enhance throughput. Once the V_2^{MAX} limit is reached, the process operates at the maximum achievable throughput. A reverse logic applies for reducing throughput below maximum. The TPM for the entire throughput range is then a split range controller, its output shifting from Q_{htr} to ΔT_{DIB}^{SP} to $V_2/B_1{}^{SP}$ to increase throughput from low to maximum and vice

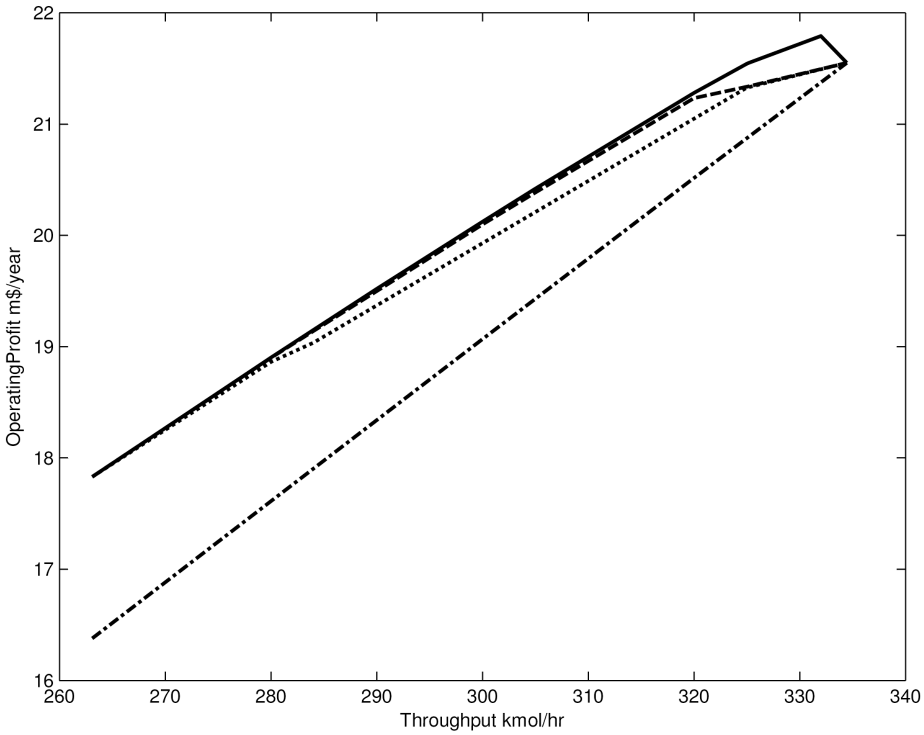


Figure 17.2. Profit for alternative ways of managing the two unconstrained dofs

__ : Optimum profit

_ _ : Constant $x_{iC4}{}^{B1}$ and $x_{iC5}{}^{D2}$

• • • • : Constant $V_1/(F_{C4} + D_2)$ and V_2/B_1

_ • _ : Process operation at V_1^{MAX} and V_2^{MAX}

versa. Figure 17.3 depicts the economic plantwide control structure, labeled CS1 for convenient reference, including the split-range throughput manipulation scheme. Note that low and high limits are applied on ΔT_{DIB}^{SP} and $V_2/B_1{}^{SP}$ for throughput manipulation. The low limit for both corresponds to the Mode I optimum values. The high limits for ΔT_{DIB}^{SP} and $V_2/B_1{}^{SP}$ are chosen slightly above the values for which V_1^{MAX} and V_2^{MAX} go active, respectively. In Table 17.2(a), the sequence in which the different pairings are implemented to obtain CS1 is also listed.

17.3. Conventional Plantwide Control Structure (CS2)

Conventionally, the feed to a process is used as the throughput manipulator and the plantwide control system is configured with the inventory control loops oriented in the direction of process flow. Such a TPM choice is often dictated in integrated chemical complexes with the plant feed being set by an upstream process. Figure 17.4 shows such a conventional plantwide control structure, labeled CS2, for the isomerization process. To contrast with CS1, the sequence in which the pairings are obtained for CS2 are noted in Table 17.2(b).

In CS2, the column level and pressure controllers are first implemented along with the reactor pressure and temperature loops (material and energy balance control). On the two columns, the top and bottom levels are controlled using respectively the reflux and bottoms. The two column pressures are controlled using the respective condenser duties. The reactor inlet temperature is controlled using the furnace duty. The reactor pressure is controlled using the reactor effluent condenser outlet valve while the condensed reactor effluent temperature is controlled using its condenser duty.

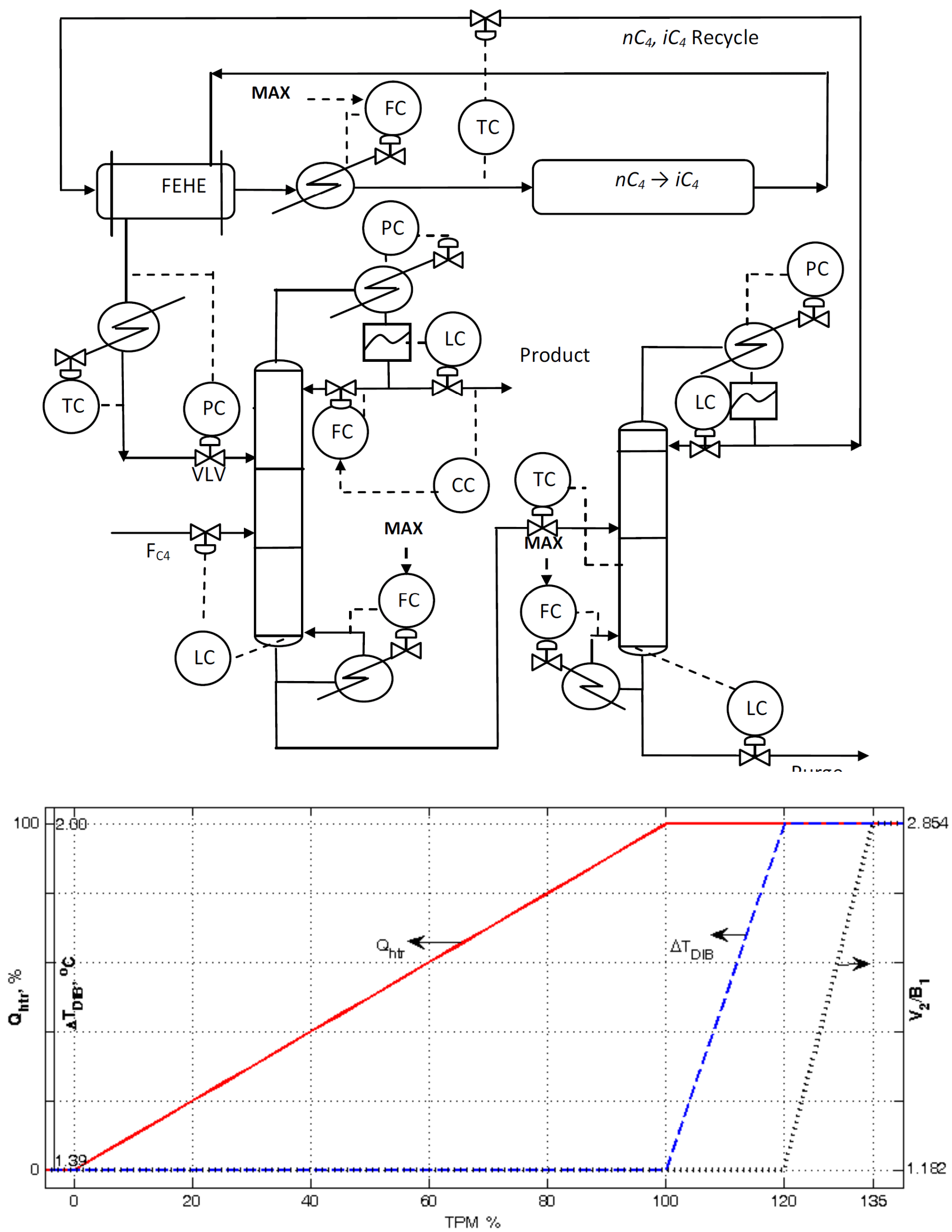


Figure 17.3. Economic Plantwide control structure CS1 with split range throughput manipulator for maximum throughput operation

Table 17.2. Loop pairing sequence followed for CS1 and CS2

(a) CS1			*(b) CS2*		
Description	*CV*	*MV*	*Description*	*CV*	*MV*
Hard active constraint control loops	Q_{htr}^{MAX}	Q_{htr}	TPM	F_{C4}	F_{C4} valve
	V_1^{MAX}	Q_{reb1}	Material balance loops	LVL_{RD1}	L_1
	V_2^{MAX}	Q_{reb1}		LVL_{RD2}	L_2
Other economic control loops	x_{nC4}^{D1}	D_1/L_1		LVL_{Bot1}	B_1
	T^S_{pur}	B_1		LVL_{Bot2}	B_2
Other loops with steady state impact	T_{rxr}	D_2	Column vapor inventory loops	P_{DIB}	Q_{cnd1}
	P_{rxr}	VLV		P_{pur}	Q_{cnd2}
	P_{DIB}	Q_{cnd1}	Reactor stabilization loops	T_{rxr}	Q_{htr}
	P_{pur}	Q_{cnd2}		P_{rxr}	VLV
Material balance loops	LVL_{RD1}	L_1	Column separation regulatory loops	x_{nC4}^{D1}	D_1/L_1
	LVL_{RD2}	L_2		ΔT_{DIB}	V_1
	LVL_{Bot1}	F_{C4}		T^S_{pur}	V_2
	LVL_{Bot2}	B_2		D_2/L_2	D_2

With the basic material/energy balance loops in place, pairings for component inventory control are implemented next. The product n-C_4 impurity leaking up the DIB column is controlled by adjusting D_1/L_1. The boilup, V_1, is adjusted to maintain ΔT_{DIB}. The purge column distillate is maintained in ratio with its reflux while the bottoms is used control T^S_{pur}. With the T^S_{pur} loop, the small purge column bottoms stream would provide acceptable sump level control. With these pairings, the control structure would provide stable unconstrained operation ie Mode I operation. The operation would be near optimal for appropriate choice of the steady state dof setpoints. Upon hitting constraints such as Q_{htr}^{MAX} on increasing throughput, appropriate overrides are needed to ensure control of crucial CVs is not lost. These overrides are also shown in Figure 17.4 and are briefly explained below.

On increasing the F_{C4}^{SP} to increase throughput, the Q_{htr}^{MAX} constraint would be hit implying loss in control of T_{rxr}. Losing T_{rxr} control is not acceptable and an alternative manipulation handle for maintaining T_{rxr} is needed. The closest manipulation handle that would provide tight T_{rxr} control is D_2. An override T_{rxr} controller is therefore implemented with its setpoint slightly below the nominal setpoint. When Q_{htr} is unconstrained, T_{rxr} would be above the override controller temperature setpoint and the override controller output would increase. This output would then be high and the low select block would pass the D_2/L_2 ratio controller output to D_2^{SP} (i.e. D_2^{SP} under ratio control). When Q_{htr}^{MAX} is hit, T_{rxr} would start decreasing and go below the override controller setpoint, whose output would decrease till the low select ultimately passes this signal to D_2^{SP} (i.e. D_2^{SP} under T_{rxr} control).

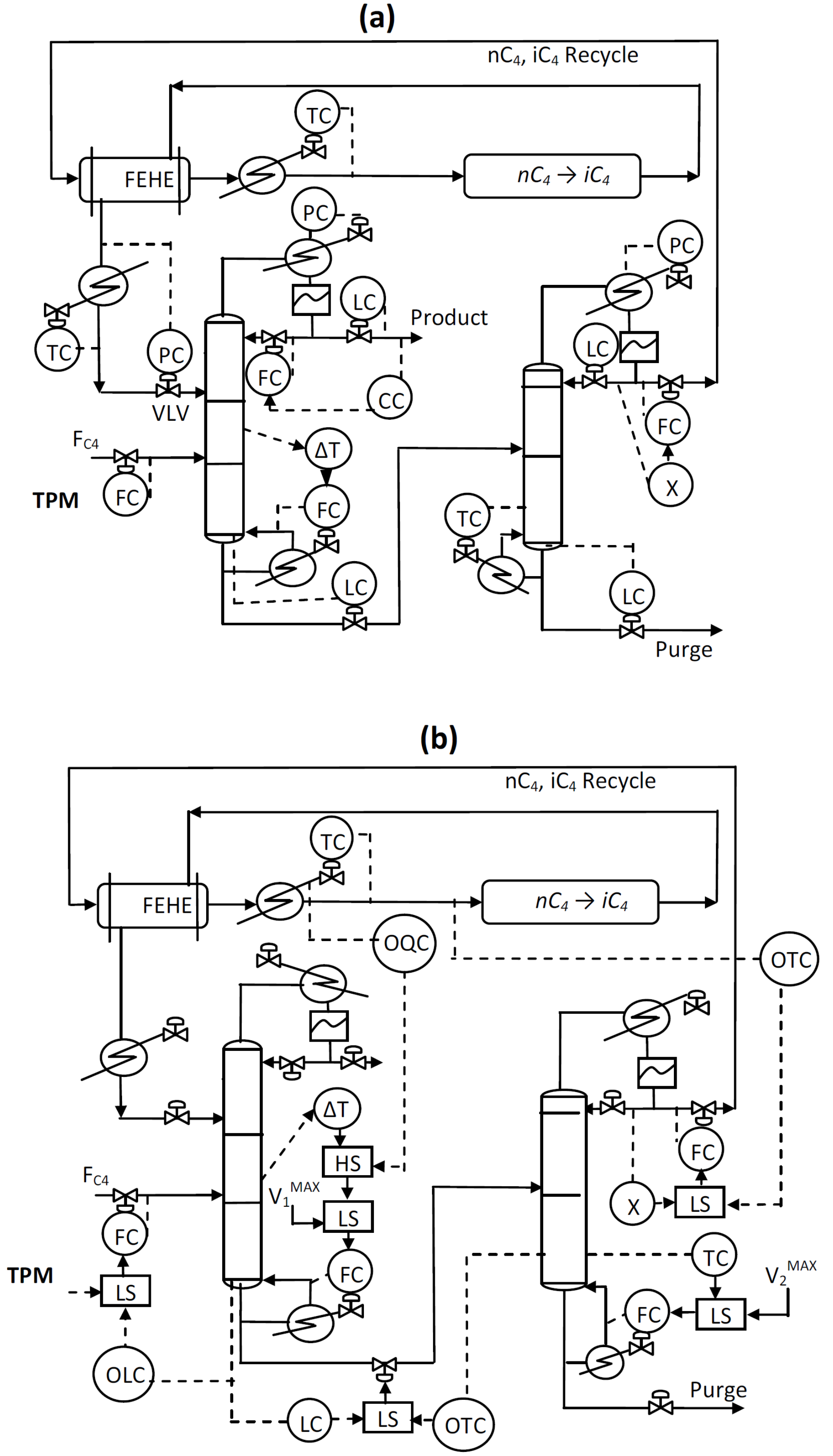


Figure 17.4. Conventional plantwide control structure, CS2
(a) Basic pairings for Mode I (unconstrained) operation
(b) Overrides for handling constraints

It is possible to bring about a near optimal increase in throughput with Q_{hr}^{MAX} active by driving V_1^{MAX} and V_2^{MAX} active, in that order. To do so, a PI Q_{htr} override controller with its setpoint very close to the Q_{htr}^{MAX} limit is implemented. The high select on the Q_{htr} override output and the ΔT_{DIB} controller output, selects the greater of the two signals. The selected signal is sent as the setpoint to the V_1 controller through a low select that ensures V_1^{SP} does not ever exceed V_1^{MAX}. At low throughputs (F_{C4} low, $Q_{htr} < Q_{htr}^{MAX}$) the direct acting Q_{htr} override controller output would decrease and the high select would pass the ΔT_{DIB} controller output. On sufficiently increasing F_{C4}, Q_{htr} would increase above the override controller setpoint, and the controller output would start to increase. The high select would ultimately pass V_1^{SP} manipulation to the Q_{htr} override, which would cause V_1^{SP} to increase. If F_{C4} is high enough (or increased fast enough), V_1^{SP} would reach V_1^{MAX}. The T^S_{pur} controller would increase V_2^{SP} to ensure that the n-C_4 does not leak out the purge column bottoms. V_2^{MAX} going active would signal that fresh n-C_4 beyond the processing capacity of the plant is being fed. To automatically reduce F_{C4} to the maximum processing capacity limit, an override scheme for altering the material balance structure from V_2^{MAX} all the way back to the process fresh feed is implemented.

When V_2^{MAX} goes active, T^S_{pur} control is lost implying excessive leakage of precious n-C_4 down the purge column bottoms and consequent economic loss. To prevent the same, an alternative manipulation handle for T^S_{pur} is needed. The feed to the purge column would provide reasonably tight tray temperature control. A PI T^S_{pur} override controller with its setpoint slightly below the nominal setpoint is implemented. When V_2^{MAX} is inactive, the tray temperature would be higher than the override controller setpoint so that its output would increase. The low select on LVL_{Bot1} controller output and the T^S_{pur} override controller output would pass the former signal to B_1^{SP} (purge column feed under LVL_{Bot1} control). When V_2^{MAX} goes active, T^S_{pur} control would be lost and it would decrease below the override controller setpoint. The controller output would then decrease and the low select would ultimately pass B_1^{SP} manipulation to the override controller (purge column feed under T^S_{pur} control). LVL_{Bot1} control is now lost and it would increase. A reverse acting LVL_{Bot1} override controller with a setpoint slightly higher than the nominal setpoint is implemented. As LVL_{Bot1} increases, its output would decrease (reverse action). The low select on this signal and operator specified F_{C4}^{SP} would ultimately pass the former signal as the setpoint to the fresh C_4 feed flow controller causing the fresh feed to be cut by the appropriate amount once V_2^{MAX} goes active. As recommended by Shinskey [21], external reset on all PI controllers whose output passes through a low/high select block is used to ensure that when inactive, the output is not too far from the selected signal due to reset windup. This ensures quick 'taking over' of control so that the duration for which a CV remains unregulated is as small as possible. The external reset is implemented internally in AspenHysys.

17.4. Dynamic Simulations and Closed Loop Results

17.4.1. Tuning of Controllers

The performance of the two control structures, CS1 and CS2, is evaluated using rigorous dynamic simulations in AspenHysys 2006. To ensure that any differences in the performances are largely attributable to the structure, a consistent tuning procedure is followed for tuning the loops in both the structures. All flow controllers are tuned with a gain of 0.5 and a reset time of 0.5 mins. All pressure controllers are tuned for tight pressure control, which is any way necessary for stabilizing the pressure driven dynamic simulation. All level controllers are P only with a gain of 2. The only exception is the DIB sump level controller in CS1 where a lower gain of 1 is used since the lag between the sump and the fresh C_4 feed is significant due to the intervening 20 stripping trays. In all temperature loops, the temperature measurement is lagged by 1 minute to account for sensor dynamics. Also, the controller output signal is lagged by 2 mins to account for heat transfer equipment dynamics. The only exception is the cooler temperature controller where a higher 8 min lag is applied to account for the slow dynamics of a flooded condenser. All temperature controllers are PI(D) and tuned using the autotuner with minor refinement for a not-too-oscillatory closed loop servo response, if necessary. In the PI product composition control loop, a 5 minute dead time and a 5 minute measurement sampling time is applied. The autotuner does not give reasonable tuning and the open loop step response is used to set the reset time at the 2/3rd response completion time and the controller gain adjusted for a not-too-oscillatory servo response. In both structures, the product composition loop is tuned first with the ΔT_{DIB} loop on manual followed by tuning of the ΔT_{DIB} loop with the composition loop on automatic. This ensures that all the detuning due to multivariable interaction gets taken in the ΔT_{DIB} loop and not the product purity loop. This gives tight product purity control, an economically important control objective.

In the CS2 override scheme, the override setpoint for T_{rxr} and T^S_{pur} cannot be chosen too close to the corresponding nominal controller setpoint as that would lead to unnecessary controller output switching during routine transients causing further transients. Accordingly the override controller setpoint is chosen as close as possible to the corresponding nominal controller setpoint for the disturbance that causes the worst-case transients. It is also highlighted that the Q_{htr} override controller that manipulates V_1 is a long loop with slow dynamics. Since its setpoint must be close to Q_{htr}^{MAX}, a P only controller would require a large gain to ensure V_1 gets driven to V_1^{MAX} for achieving maximum throughput. The large gain leads to on-off control for routine disturbances at a high but below maximum throughput with the override taking over and giving up V_1 manipulation. A loose PI Q_{htr} override controller is therefore implemented to ensure its setpoint is close to Q_{htr}^{MAX} and on-off control is avoided. Table 17.3 lists the salient controller tuning parameters for CS1 and CS2 using the above procedure.

Table 17.3. Controller tuning parameters

Regulatory controllers

	CS1				CS2				SP	Sensor Span
CV	MV	K_C	τ_i (min)	τ_d (min)	MV	K_C	τ_i (min)	τ_d (min)		
T_{rxr}	D_2	2	1.5	*0.2*	Q_{htr}	2	1	0.1	200°C	160 – 240 ºC
T_{cool}	Q_{cool}	0.2	20	*2*	Q_{cool}	0.3	20	2	53°C	40 –60 ºC
T^S_{pur}	B_1	0.1	20	*1.5*	V_2	0.2	15	1.5	63.8°C	40 – 80 ºC
x_{nC4}^{D1}	L_1	0.2	120	-	L_1	0.15	150	-	0.02	0-0.04
ΔT_{DIB}	V_1	0.2	150	-	V_1	0.3	150	-	1.39	0-0.03

CS2 override controllers

CV	MV	K_C	τ_i (mins)	SP	Sensor Span
Q_{htr}	V_1	0.05	150	1230kW	0-1294kW
T_{rxr}	D_1	0.4	10	199.5 °C	160-240°C
T^S_{pur}	B_1	0.5	40	58°C	40-80°C
LVL_{Bot1}	F_{C4}	2	-	70%	0-50%

17.4.2. Closed Loop Results

The plantwide transient response of the two control structures, CS1 and CS2, is obtained for principal disturbances for Mode I and Mode II operation. In Mode I, a ±5 mol% step change in the fresh C_4 feed $i\text{-}C_4$ mol fraction with a complementary change in the $n\text{-}C_4$ mol fraction and a ±20 kmol/h F_{C4} (throughput change) are considered the principal disturbances. In Mode II, only the feed composition step change is considered the principal disturbances as the throughput gets fixed by the active constraints. The dynamic response is also obtained for a throughput transition from Mode I to Mode II and back.

Figure 17.5 plots the dynamic response of salient process variables to a feed composition step disturbance in Mode I for CS1 and CS2. Both structures are observed to effectively reject the disturbance with tight control of the $n\text{-}C_4$ impurity in the product. In CS1, F_{C4} gets adjusted and the flow to the reactor settles to the appropriate value for maintaining T_{rxr} for the set Q_{htr}, the TPM. In CS2 on the other hand, the F_{C4} (TPM) remains fixed and the $i\text{-}C_4$ production changes in proportion to the $n\text{-}C_4$ in the fresh feed. In both structures, the leakage of $n\text{-}C_4$ down the purge column bottoms is well regulated via the action of the T^S_{pur} controller.

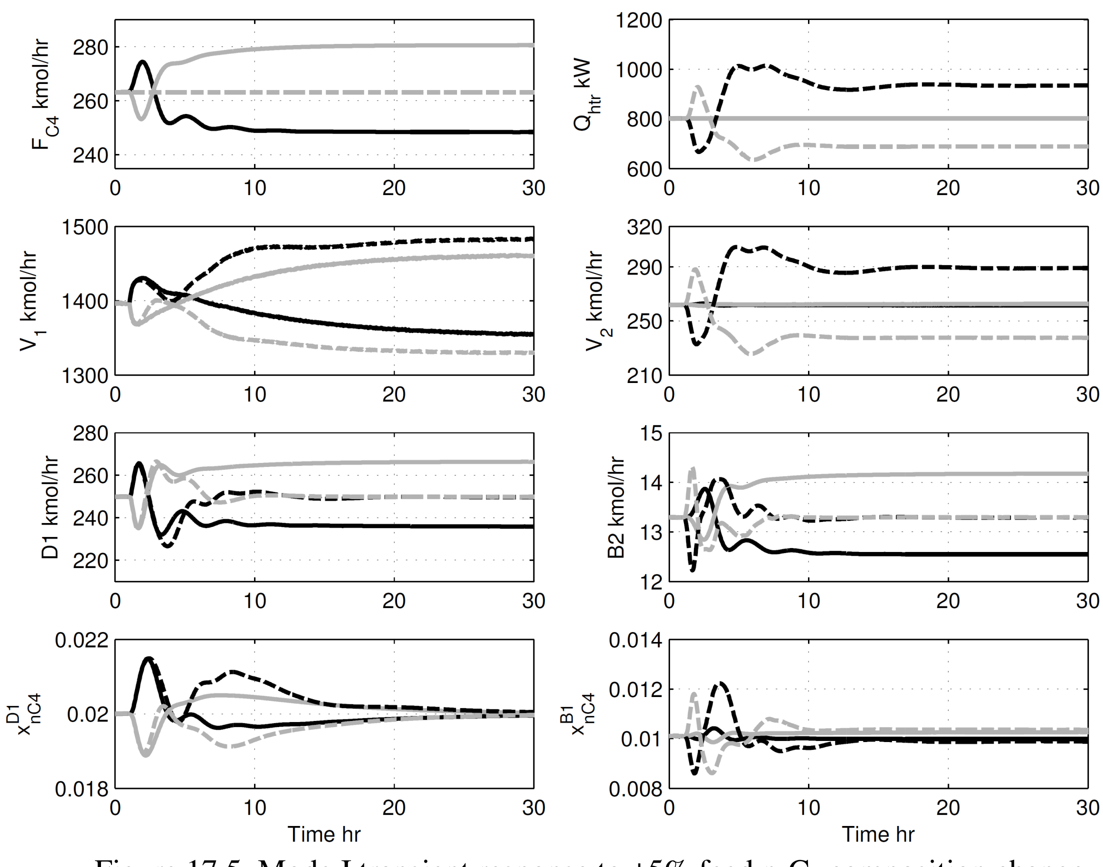


Figure 17.5. Mode I transient response to ±5% feed n-C_4 composition change

: +5% CS1 : -5% CS1 : +5% CS2 : -5% CS2

Figure 17.6 plots the Mode I dynamic response for a ±20 kmol/h change in F_{C4}. In CS1, the Q_{htr} setpoint must be increased (decreased) by 169 kW (~21% of base-case Q_{htr}) to bring about a 20 kmol/h (~7.6% of base-case F_{C4}) increase in F_{C4}. Similarly, Q_{htr} must be decreased by 138 kW (~17.2%) for achieving the decrease in F_{C4}. For the throughput change disturbance, the product impurity is well controlled in the transient period in both CS1 and CS2. The transient deviations in CS1 are slightly lower than in CS2 due to more severe transients in the recycle loop in the latter. In CS1 on the other hand, the recycle loop transients are less severe (smooth response). In addition to tight product impurity control, both the structures achieve tight regulation of the *n-*C_4 leakage in the purge column bottoms via the action of the T^S_{pur} controller. The transient variability in x_{nC4}^{B2} is significantly higher in CS1 as a large change in Q_{htr} (TPM) causes a large change in D_2 which severely disturbs the purge column material balance.

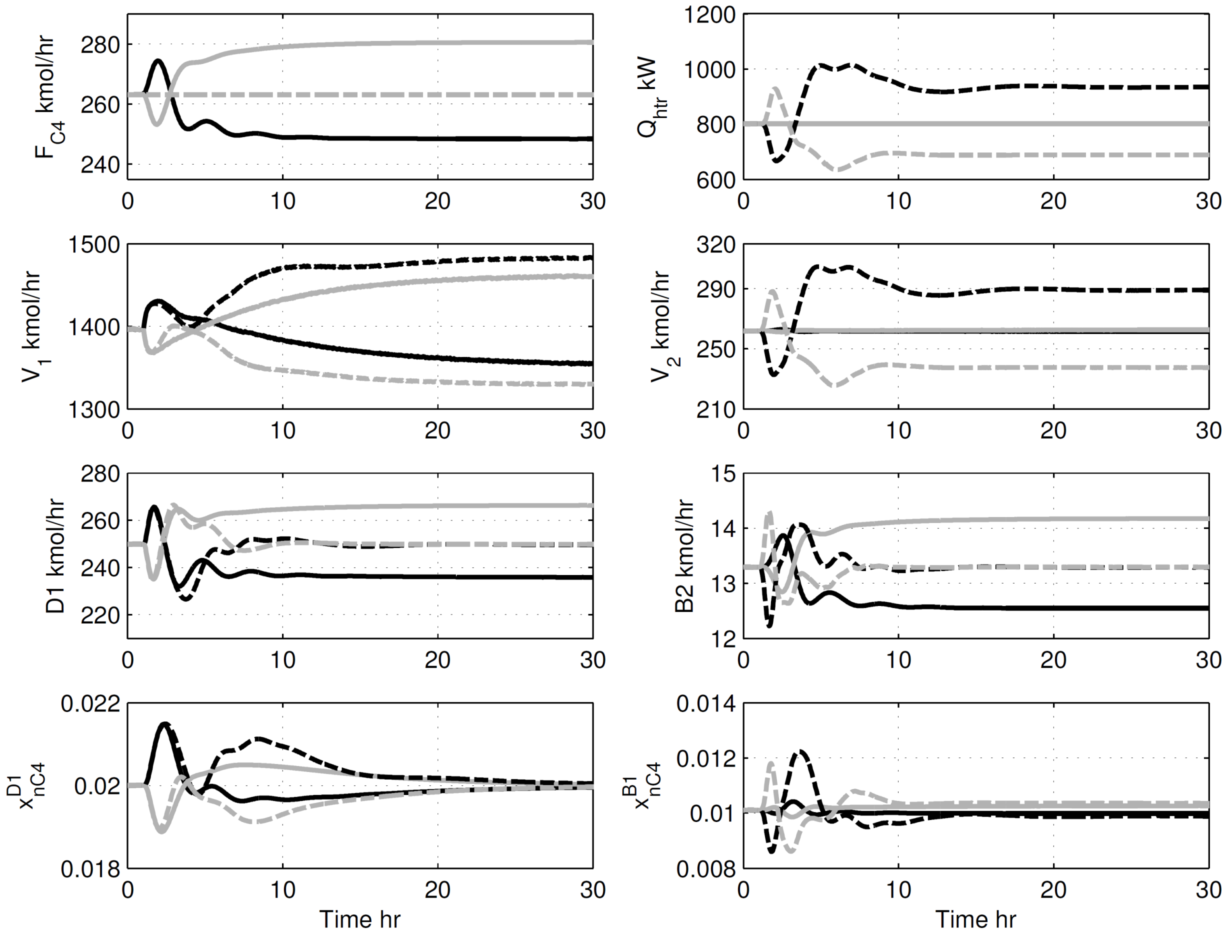


Figure 17.6. Mode I transient response to ±5% feed n-C_4 composition change

: +5% CS1 : -5% CS1 : +5% CS2 : -5% CS2

Figure 17.7 plots the Mode II dynamic response to a ±5% feed composition step change. All override controllers in CS2 are active so that structurally, CS1 and CS2 are very similar. The only significant difference is that the setpoint of the T_{rxr} and T^S_{pur} override controllers in CS2 is slightly lower than the corresponding nominal setpoint values. In CS1, on the other hand, the setpoint values are held at their nominal values. As seen from the dynamic responses, the plantwide transient response is smooth in both the structures. Also, tight control of product impurity and the $n\text{-}C_4$ leakage down the purge column bottoms is achieved. In CS2 however, the production of $i\text{-}C_4$ at the initial and final steady state is slightly lower than in CS1 due to the slightly lower T_{rxr} setpoint which causes a slight reduction in single pass reactor conversion as well as higher $n\text{-}C_4$ leakage in the purge column bottoms due to the lower T^S_{pur} setpoint.

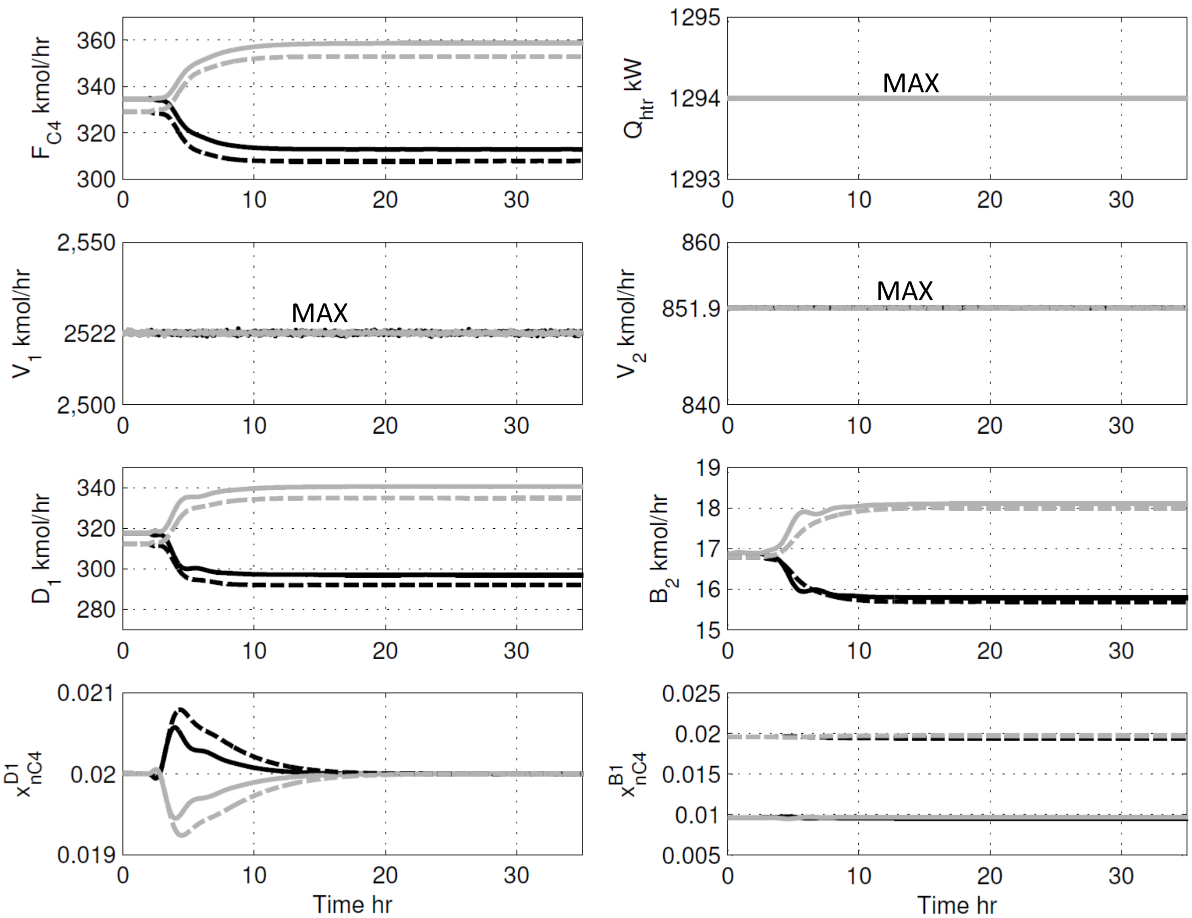


Figure 17.7. Mode II transient response to ±5% feed n-C_4 composition change

: +5% CS1 : -5% CS1 : +5% CS2 : -5% CS2

The synthesized control structures are also tested for a large throughput transition from the design throughput (F_{C4} = 263.1 kmol/h) to the maximum achievable throughput and back. The transient response is shown in Figure 17.8. In CS1, to increase throughput, the split range scheme switches the TPM from $Q_{htr}{}^{SP}$ to $\Delta T_{DIB}{}^{SP}$ and then to $V_2/B_1{}^{SP}$. The switching order gets reversed for decreasing the throughput. The transient response shows that tight product impurity control is achieved across the entire throughput range. The loss of precious $n\text{-}C_4$ down B_2 is also regulated at a small value. Most importantly, the plantwide transients are smooth and not too severe.

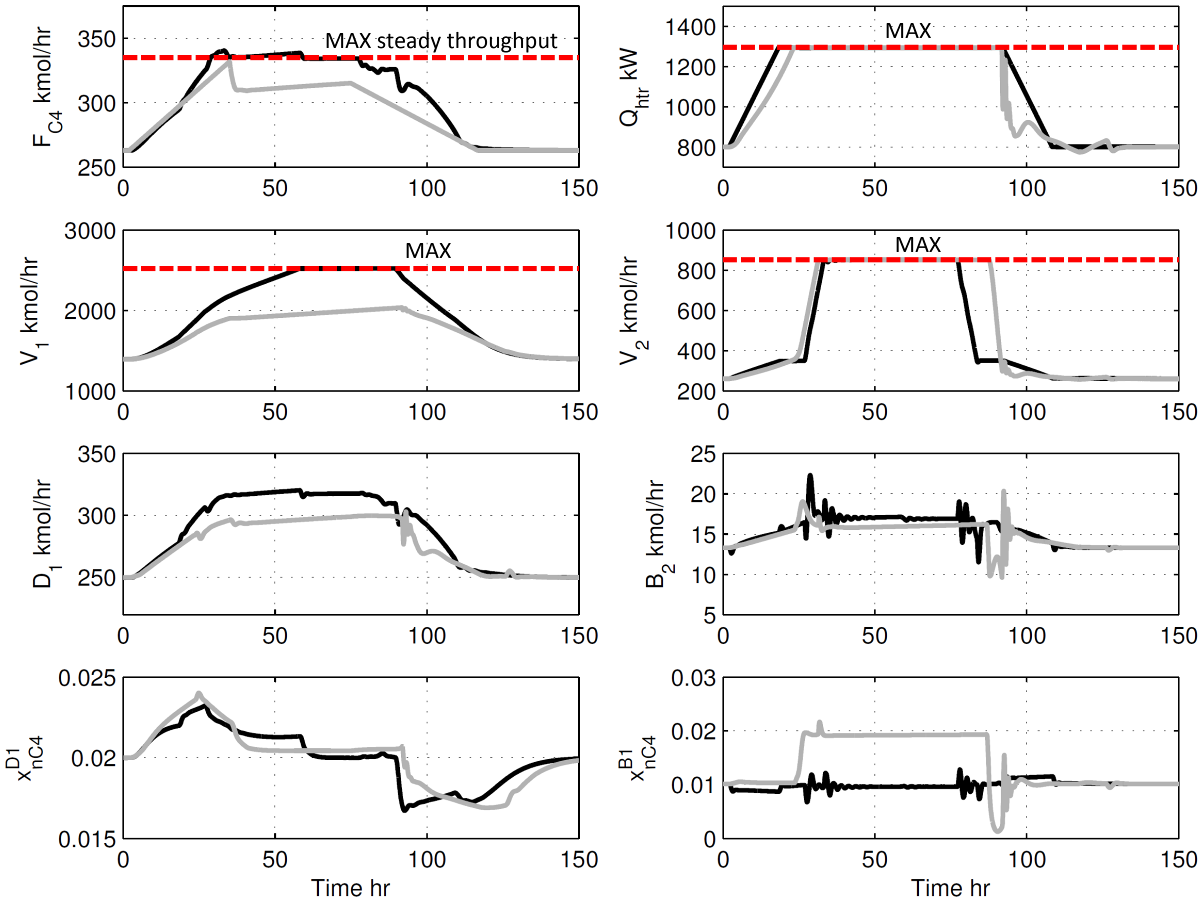


Figure 17.8. Throughput transition for CS1 and CS2

——: CS1 ——: CS2

In CS2, F_{C4}^{SP} is ramped up causing Q_{htr} to increase and as it crosses the Q_{htr} override controller setpoint (chosen setpoint is 95% of Q_{htr}^{MAX}), the override output increases above the ΔT_{DIB} controller output passing V_1^{SP} manipulation to the Q_{htr} override, which slowly keeps on increasing V_1^{SP} to V_1^{MAX}. As and when Q_{htr}^{MAX} is reached, T_{rxr} decreases and the override T_{rxr} controller takes over D_2 manipulation. Meanwhile, V_2^{SP} increases rapidly and hits V_2^{MAX} as more $n\text{-}C_4$ is being fed in than being consumed in the reactor. This causes T^S_{pur} to decrease and the override scheme for altering the material balance structure gets activated to cut the F_{C4} feed. Since the Q_{htr} override is a long loop, the increase in V_1 is slow and even after 75 hrs, the V_1^{MAX} constraint is not approached and the product rate, D_1, is about 299 kmol/h (~20 kmol/h < maximum steady D_1). Even as D_1 reaches its maximum steady value, it takes a very long time. After 75 hrs, F_{C4}^{SP} is ramped down to its base value (263.1 kmol/h) and a smooth transition occurs. From the CS2 response in Figure 17.8, notice that in the small period where V_2^{MAX} goes active and T^S_{pur} override starts manipulating B_1, large transient loss of precious n-C_4 down the purge column bottoms occurs. Also, the steady n-C_4 loss is higher due to the lower than nominal setpoint of the T^S_{pur} override.

Another pertinent comparison is the transients caused due to overrides taking over / giving up control during routine disturbances. We consider a worst-case step disturbance in the fresh feed composition, where the n-C_4 composition increases by 5% with initial steady operation at F_{C4} = 293.1 kmol/h, where none of the constraints are active. The transient response of CS1 and CS2 to this disturbance is shown in Figure 17.9. CS1 effectively rejects the disturbance with tight product purity control and regulation of n-C_4 in the purge column bottoms with the plant settling down at the new steady state in about 30 hrs. In CS2, on n-C_4 composition increasing by 5%, a large transient increase occurs in Q_{htr} due to the snowball effect [12], which triggers the Q_{htr} override. V_1 is then slowly driven towards V_1^{MAX} while the additional n-C_4 causes V_2 to increase. The slow increase in V_2 causes the i-C_5 circulating in the plant and hence D_2 to decrease. For the lower D_2 (reactor feed), T_{rxr} control eventually passes back to Q_{htr} and the plant settles at the new steady state in about 75 hrs, which is more than twice the time for CS1. If the Q_{htr} override controller is made aggressive by increasing the proportional gain by a factor of 2, oscillations due to the T_{rxr} override successively going active and inactive are observed (see Figure 17.9). The dynamic performance thus degrades significantly at high throughputs where the overrides get activated. It is then not surprising at all that operators tend to switch the overrides off and make the necessary adjustments manually.

17.4.3. Quantitative Economic Performance Comparison

A quantitative economic comparison of the two control structures is performed for maximum throughput (Mode II) operation. We consider a +5% feed n-C_4 composition step change as the worst case disturbance. Table 17.4 compares the maximum achieved steady throughput (F_{C4}) along with the corresponding n-C_4 component flow (loss) in the purge column bottoms, the i-C_4 product rate and the operating yearly profit for CS1 and CS2. Expectedly, no back-off and throughput loss is observed for CS1, which has been designed for process operation with all the hard active constraints at their maximum limits. In contrast, in CS2, due to the need for the T_{rxr} and T^S_{pur} override setpoints to be lower than nominal, an yearly profit loss of \$0.45x10^6 (~2%) occurs compared to CS1. The override controller setpoint offsets have been chosen to be as small as possible at 1 °C for T_{rxr} and 5 °C for T^S_{pur} to ensure that the overrides do not get triggered during routine transients. CS2, which was obtained without any consideration of the constraints that go active at higher throughputs, thus is economically and dynamically inferior to CS1 regardless of the approach used to handle constraints (back-off or overrides). Overall, these results demonstrate that the full active constraint set plays a key role in economic plantwide control system design.

17.5. Conclusions

In conclusion, this case study on plantwide control of the C_4 isomerization process demonstrates that a simple decentralized plantwide control system for achieving near optimal and smooth process operation over a wide throughput range can be synthesized. The active constraints at maximum throughput form the key to devising the control system. These constraints dictate the pairings for tight control of these active constraints and the consequent pairings for inventory regulation as well as the throughput manipulation strategy. Quantitative results show that a conventional control structure with the TPM at the process feed with overrides for handling constraints is economically inferior with a steady profit loss of ~2% at maximum throughput due to the offset needed in the override controller setpoints. The conventional scheme is also found to be dynamically inferior. The case study demonstrates the crucial role of the active constraints in economic plantwide control structure synthesis.

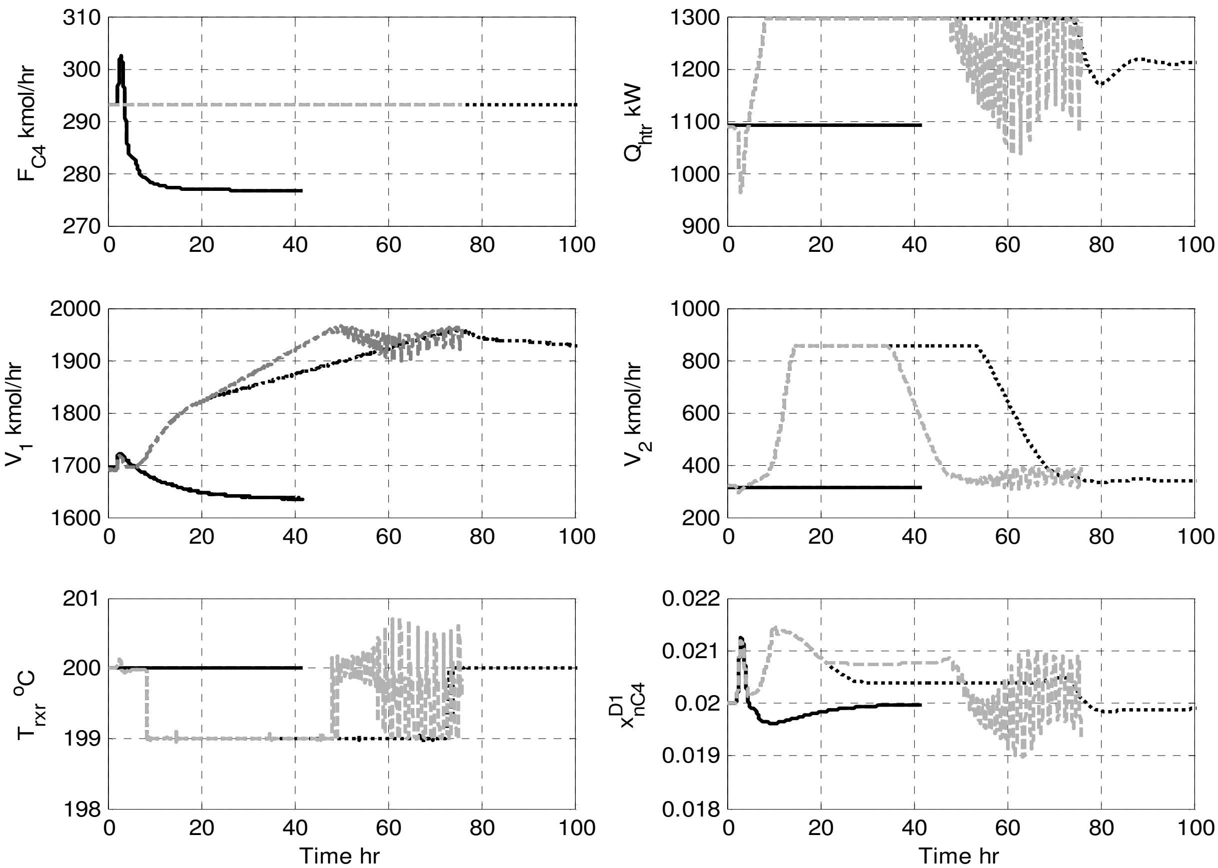


Figure 17.9. Transient response for +5% feed n-C_4 composition change at F_{C4} = 293.1kmol/hr

: CS1 : CS2 aggressive Q_{htr} override : CS2 loose Q_{htr} override

Table 17.4. Mode II throughput loss comparison for +5 mol% feed composition step change

	CS1	*CS2*
F_{C4}	334.5 kmol/hr	329 kmol/hr
Product	317.6 kmol/hr	312.3 kmol/hr
F_{nC4}^{B1}	0.16 kmol/hr	0.33 kmol/hr
Profit	21.51m$/yr	21.1m$/yr
% Loss	0	1.8

Bibliography

1. Al-Arfaj MA, Luyben WL. Plantwide control for TAME production using reactive distillation. *AIChE J.* 2004;50(7):1462-1473.
2. Araujo A, Skogestad S. Control structure design for the ammonia synthesis process. *Comp Chem Eng*. 2008;32(12):2920-2932.
3. Aske EMB, Strand S, Skogestad S. Coordinator MPC for maximizing plant throughput. *Comp Chem Eng*. 2008;32:195-204.
4. Aske EMB, Skogestad S. Consistent inventory control. *Ind Eng Chem Res.* 2009;48(44): 10892-10902.
5. Douglas JM. *Conceptual Design of Chemical Processes*. New York: McGraw Hill, 1988.
6. Gera V, Kaistha N, Panahi M, Skogestad S. Plantwide control of a cumene manufacture process. *Computer Aided Chemical Engineering*, 2011, *29* (8), 522-526.
7. Jagtap R, Kaistha N, Skogestad S. Plantwide control for economic optimum operation of a recycle process with side reaction. *Ind Eng Chem Res.* 2011;50(14):8571-8584.
8. Jagtap R, Kaistha N. Economic plantwide control of the ethyl benzene process. *AIChE J.* 2012; submitted.
9. Jagtap R, Kaistha N. Economic plantwide control of the C_4 isomerization process. *Ind Eng Chem Res*. 2012; submitted.
10. Jagtap R, Kaistha N. Throughput manipulator location selection for economic plantwide control. In Rangaiah GP, Kariwala VA. *Advances in Plantwide Control*. Upper Saddle River NJ: John Wiley and Sons, 2012 in press.
11. Kanodia R, Kaistha N. Plantwide control for throughput maximization: A case study. *Ind Eng Chem Res.* 2010;49(1):210-221.
12. Luyben M.L, Luyben W.L. Design and control of a complex process involving two reaction steps, three distillation columns, and two recycle streams. *Ind. Eng. Chem. Res.* 1995, *34* (11), 3885-3898.
13. Luyben M.L, Tyreus B.D, Luyben W.L. Analysis of control structures for reaction/separation/recycle processes with second order reactions. *Ind. Eng. Chem. Res.* 1996, *35* (3), 758-771.
14. Luyben ML, Tyreus BD, Luyben WL. Plantwide control design procedure. *AIChE J.* 1997;43(12):3161-3174.
15. Luyben WL. Snowball effects in reactor/separator processes with recycle. *Ind Eng Chem Res.* 1994;33(2):299-305.
16. Luyben WL, Tyreus BD, Luyben ML. *Plantwide Process Control*. New York: McGraw Hill, 1999.
17. Luyben WL, Tyreus BD, Luyben ML. Isomerization process, *Plantwide Process Control*, McGraw Hill: New York, 1999, 273-293.
18. Luyben WL. Plantwide control of an isopropyl alcohol dehydration process. *AIChE J.* 2006;52(6):2290-2296.
19. Luyben WL. Design and control of the cumene process. *Ind. Eng. Chem. Res.* 2010, *49* (2), 719.
20. Price RM, Lyman PR, Georgakis C. Throughput manipulation in plantwide control structures. *Ind Eng Chem Res.* 1994;33(5):1197-1207.
21. Shinskey FG. *Process Control Systems: Application, Design and Tuning*. New York: McGraw Hill, 1996.

22. Singh S, Lal S, Kaistha N. Case study on tubular reactor hot-spot temperature control for throughput maximization. *Ind Eng Chem Res.* 2008;47(19):7257-7263.
23. Skogestad S. Plantwide control: The search for the self-optimizing control structure. *J Proc Cont.* 2000, 10(5), 487-507.
24. Skogestad S. Control structure design for complete chemical plants. *Comp Chem Eng*. 2004;28(1-2):219-234.
25. Skogestad S. Do's and dont's of distillation control. *Chem Eng Res Des (Trans I ChemE, Part A)*. 2007;85(A1):13-23.
26. Tyreus BD, Luyben WL. Dynamics and control of recycle systems 4. Ternary systems with one or two recycle stream. *Ind. Eng. Chem. Res.* 1993, *32* (6), 1154-1162.
27. Zhang C, Vasudevan S, Rangaiah GP. Plantwide control system design and performance evaluation for ammonia synthesis process. *Ind Eng Chem Res.* 2010;49(24):12538-12547.