

CONTROL TO ECONOMIC OPTIMUM

By

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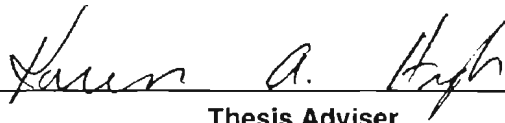
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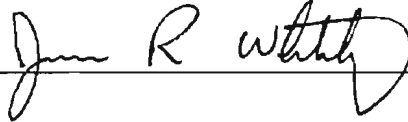
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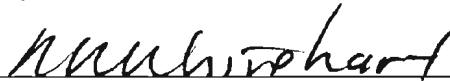
CONTROL TO ECONOMIC OPTIMUM

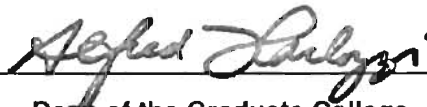
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Nomenclature

English

B	Bottoms flow rate (mol/hr)
B^*	Matrix of measurements and gross errors (online optimization)
C_F	Cost of feed (\$/mol)
C_S	Cost of steam (\$ /mol)
d	Vector of disturbances
D	Distillate flow rate (mol/hr)
$e(t)$	Error between current value of variable and its set point
F	Feed flow rate (mol/hr)
F	Weighting factor in model predictive control to measure relative importance of each control variable
g'	Set of equality constraints
g''	Set of inequality constraints
h	Enthalpy (BTU/mol)
h'	Set of equality constraints relating process output to x and u
H	Weir height for trays (in.)
$h_{acc,max}$	Maximum level for reflux drum (in.)
$h_{acc,min}$	Minimum level for reflux drum (in.)
$h_{bot,max}$	Maximum level for bottom sump (in.)
$h_{bot,min}$	Minimum level for bottom sump (in.)
J	Performance measure to be optimized

k	Particular time instant in MPC
K	Collocation point in orthogonal collocation
K_c	Controller gain (mol/hr)
L	Liquid flow on a tray (mol/hr)
M	Inventory on a given tray (mol/hr)
$NCOL$	Number of collocation points
NE	Number of finite elements
N_t	Number of trays in distillation column
$o(t)$	Operating value of a variable at time t
P	Pressure in distillation column (psia)
PMM	Process Model Mismatch
$p(t)$	Bias value of proportional controller
q	Set of inequality constraints
Q_c	Heat input in reboiler (BTU/hr)
R	Reflux flow rate (mol/hr)
R	Weighting factor in model predictive control to measure relative importance of control variable changes
S	Steam flow rate (mol/hr)
$s(t)$	Setpoint
t	Continuous time (hr)
t_i	Discrete time (hr)
t_o	Time scale for regulatory control

T_o	Time scale for optimizing control
$u(k), u(t), u$	Vector of control variables
V	Vapor flow on a tray (mol/hr)
V (with subscript	Product values (\$/mol)
$B, D)$	
W	Weighting factor matrix in optimization problems
w_{len}	Weir length for trays
x	Vector of state variables
x_0	Initial condition for state variable x
\tilde{x}_i	Approximate value of x from collocation model
X_b	Minimum purity for bottoms (mol fraction light key)
X_d	Minimum purity of distillate (mol fraction light key)
$X_{corrected}$	Value of state variable x corrected for process-model mismatch
x_{est}	Estimated value of state variable x
x_{mes}	Measured value of state variable x
$x_{process}$	Values of state variable x from process measurements
$x_{predicted}$	Predicted value of state variable x
y_i	Vapor phase compositions on i th tray
\tilde{y}_i	Approximate value of y from collocation model
y^*	Desired trajectory for process output in MPC
y'	Vector of process outputs
	Set of process measurements in online optimization

z_f	Feed composition (mol fraction light key)
Z	Pricing function for bottoms and distillate values as a function of purity

Greek

α	Relative volatility
β	Hydraulic tray time constant (s)
Γ	Weighting factor for error residual term in Model predictive control
γ	Activity coefficient
δ	Residuum of the material and energy balances
ε	Gross error in a measurement
ε_r	Residual error vector for Model predictive control
θ	Vector of model parameters in nonlinear MPC
ρ	Liquid density (ft ³ /lb)
τ_D	Derivative time for PID controller (hr)
τ_i	Scaled discrete time in orthogonal collocation
τ_I	Reset time for PI controller (hr)
Φ	Lagrange polynomial in orthogonal collocation for state variable
Φ, φ	Performance measure to be optimized
ψ	Lagrange polynomial in orthogonal collocation for control variable

Superscripts

*	Optimal values of a variable
ρ	Time horizon for model predictive control
L	Lower bound for variable
l	Relating to liquid phase
U	Upper bound for variable
v	Relating to vapor phase

Subscripts

n	Tray number
i	i^{th} component; i^{th} finite element
j	j^{th} collocation point
F	Relating to the feed
d, D	Relating to the distillate stream
b, B	Relating to the bottoms stream

Chapter 1

Introduction

1.1 Control and Optimization

“Control” traditionally has been regarded as the problem of maintaining the process at setpoints so as to ensure stability – if the process deviates from the desired setpoints determined at the design stage, the departures must be corrected as quickly, smoothly and effortlessly as possible. This follows from the axiom that *any* system be it electrical, mechanical, biological, will need continuous monitoring and correction if it is to remain stable.

However, from the mid 20th century increasing attention has been directed to realizing more specific goals, while also maintaining stability of the process. Control rules are chosen to minimize a cost function over a time horizon, which penalizes deviation from setpoint and excessive control action. That is, the control problem is now formulated as an *optimization problem*. This formulation has virtues in that it leads to a sharpening of focus towards the goals of a process. However, such a formulation may suffer from the drawback that the model behind the optimization may be so idealized that it leads to a non-robust solution – a solution that does not take into account the reality of the process, but relies on an *idealized process model*.

Why are idealized models chosen for optimization? The answer to this lies in the fact that early attempts at optimization suffered from lack of computational facilities which could handle nonlinearities in the process and which were limited in the number of variables they could handle. In addition, these primitive optimization methods could not

handle optimization problems within a feasible length of time. Today, we possess computational tools that can handle non-ideality in the process; which are swift and accurate; and, which can handle complex constraints and process disturbances, and optimize in a reasonable amount of time. In the context of the tools available today, it is therefore possible for us to address better the basic motive behind industrial operations – **“maximizing profit.”**

1.2 Conventional Methods of Maximizing Profitability

As mentioned before, the aim of a control system is to maintain the process in a profitable state of operation, while respecting safety, stability and quality constraints of the process. Thus, if we wish to produce a product of uniform quality, process control must compensate for the effects of disturbances and hold the product quality constant (Buckley 1964). In conventional control, maximizing the profit is achieved by deciding an optimal operating value for each process variable in the plant for a certain condition of the plant. These operating values are *setpoints*, and the aim of the control system then, is of holding each process variable at its setpoint. However, these setpoints represent optimal operating points for the design condition for which they have been calculated. As the plant continually changes from one state to another, its optimal conditions change. Thus, the basic motive of maximizing profit mentioned above is addressed only at particular conditions. Control systems include conventional feedback control systems, and new schemes such as Model Predictive Control (MPC) are being used; however, these methods rely on linearized dynamic models.

The next layer of control consists of updating these setpoints at prescribed intervals based on objective techniques so that the process is kept in profitable operation. Online optimization is the strategy currently used to optimize processes using

nonlinear steady state models. Here an optimizer, based on its search on the model “dictates” the direction that the process has to take to minimize the process cost function. This is implemented by the local controllers. As will be discussed later, the model equations for the optimization problem are algebraic equations representing steady state operation, which are not accurate representations of the reality of the process. Obviously, the optimum is only as good as the model. If the model closely matches the process, the optimum found on the model is nearly the true optimum. However, steady state models do not account for the process dynamics and transience in process behavior again lead to off-optimal operation.

1.3 *The Next Step*

The logical next step would be to consider the limitations of conventional control – by the introduction of process dynamics into the optimization models to address the question of maximizing profitability at every step of the process and by including better, more realistic nonlinear models. An ideal dynamic controller would:

- dynamically determine the “best” operating point for the process, which maximizes a particular performance criterion – preferably the profit made by the process to reflect the operational objective
- determine the time-optimal path to these operating conditions
- respect the safety, environment, design, and product quality constraints of the process along the optimal path

With such a controller, the necessity of using setpoints for control variables to be a reflection of the process profit can be eliminated. A scheme can be developed wherein a dynamic controller addresses the question of maximizing profit every step of the way. This is a problem of dynamic nonlinear optimization. It is only recently that

simple and effective numerical methods for dynamic optimization that can be easily implemented on a computer have been developed. The ultimate goal of these optimization schemes is *plantwide optimization*, which involves effective control and optimization of an entire sequence of unit operations and not simply individual units. This consists of implementing nine aspects of plant operation effectively, viz.: energy management; production rate; product quality; operational, environmental and safety constraints; inventories; component balances; and economic optimization (Luyben et al. 1998).

1.4 Purpose and Significance of the Study

Several mathematical methods have been developed for solving dynamic optimization problems, and these have been tested on example processes, such as batch reactors (Vassiliadis et. al 1994, Cuthrell and Biegler 1987). However, these remain confined to academic studies. The use of optimal control strategies for profit maximization using rigorous economic models has not been widely observed in industry. It is the aim of this study to demonstrate the efficacy of this method to improve the bottomline profitability of the process. An optimization scheme, which looks at profit maximization every step of the way and looks at production rates, energy conservation opportunities and process constraints in its search for its optimum, should necessarily lead to improved profit and palpable dollar savings.

This work attempts to start the journey to realize this ultimate objective of plantwide optimization using the powerful computational tools available. As a first step, an industrially important process was chosen to implement a dynamic optimization and control scheme, which realizes the three desirables mentioned above. The process under consideration to test this concept is a simple distillation column. Distillation

remains the most widely used separation method in chemical and petroleum industries. Distillation columns contribute sometimes to as much as 50% of the plant operating costs. Distillation operations consume about 10% of the total energy in the industrial sector in the US. Hence, there is a significant economic incentive in effective control and optimization of distillation columns. Besides this, the distillation process has just enough complexity and size to be a challenging example process to demonstrate a new concept. Proof that dollars can be saved by a new optimization strategy on a distillation process would give a good impetus for future research on processes that are more complex. Hence, distillation is a good first step to test a new concept.

The distillation column model and simulation were developed starting from first principles. The optimization problem is a nonlinear problem (NLP) which is constrained by the material and energy balances ("model"), physical limitations, and design limitations of the column. The problem of controlling the column was formulated as an optimization problem of maximizing the profit made by the column subject to constraints, which "restrain" the process from becoming unstable. Thus, a control strategy is developed which continually steers the process to an economically optimal operating point. Comparisons for profit over time, disturbance rejection and stability have been made with conventional PI control and steady state online optimization. It is hoped that this will be the first step towards realizing a dynamic control strategy for an integrated plant.

1.5 Scope and Limitations

As mentioned previously, this study is merely a first step in the path to achieving plantwide control and optimization. The implementation of this proposed strategy has

been simulated on a simple binary distillation column. Comparisons have been made with simple PI control and online optimization schemes for simple disturbances.

Simple dynamic models were used. The dynamic optimization algorithm, which will be described later, is developed in a restricted demonstration version of GAMS/CONOPT (a nonlinear optimization package), and hence it is simplified. Further fine-tuning and testing is necessary to ensure complete robustness. Other issues such as sensitivity to model parameters and more rigorous economics must be explored. The distillation column represents a starting point for extending this algorithm to more complex systems. The next step should be to implement and test the performance of this strategy on a more complex three-unit process, such as a Fluidized Catalytic Cracking unit or the Flotation process in the IMC Agrico plant. The performance on actual plant data and more severe disturbances must be evaluated before this strategy becomes functional.

1.6 Outline of Work

Chapter 2 examines the conventional schemes for control, such as PI control and multivariable control. Chapter 3 introduces optimization methods and discusses the currently prevalent optimization schemes. The drawbacks of these schemes will be pointed out and dynamic optimization will be introduced. Chapter 4 focuses on developing the setup on which this new approach will be tested: the distillation column model and simulation and the optimization program. Chapter 5 provides information on the steps taken to code this setup. Chapter 6 analyzes the results of the study and provides a comparison with conventional control schemes. Finally, Chapter 7 summarizes the results and outlines future recommendations.

Chapter 2

Background

This chapter reviews some of the conventional schemes of control that are in use in industry today. Review of these schemes, their applications and drawbacks provides the basis of this study. The gradual transition of simple PI control to advanced control schemes is tracked. The chapter begins with a discussion of some control fundamental aspects of control schemes. Following this, optimization concepts and conventional methods of optimization will be reviewed.

2.1 *Fundamental Aspects of Control Schemes*

A control structure consists of the following elements (Morari et al 1980):

- A set of variables to be controlled to achieve a set of specified objectives, which are usually derived from economic considerations
- A set of variables which can be measured for control purposes
- A set of manipulated variables that can directly be “adjusted” to affect the control variables, and
- A structure interconnecting measured and manipulated variables

Any control structure must specify the above elements. Morari et al. (1980) discuss each of these in detail:

Control objectives:

Control objectives can be *twofold*. In the *first* category of objectives, are those related to operational feasibility. This involves keeping process variables within desired bounds, in spite of uncontrolled influences on the process, called disturbances. These take into

account product quality specifications, safety considerations, operational requirements, environmental regulations, etc. These objectives are termed regulatory objectives. Typically, these are realized by keeping certain “controlled variables” at desired values called “set points.” (Smith and Corripio 1985)

The *second* category is derived from economic considerations. These enter only if, after satisfying the first class of objectives, there is freedom to adapt the operating conditions to stay at the most profitable point of operation. These objectives are termed optimizing objectives. Control schemes or laws determine how these objectives will be realized. These will be discussed in greater detail in the next section.

Measurements:

The first class of objectives dictates directly the measurements that need to be made to regulate the process. The second class needs additional measurements, which can affect economic performance. Sometimes some measurements cannot be made directly and need to be inferred from secondary measurements. The method of selection of these measurements is dealt with in Morari et al. (1980). The relation between primary and secondary measurements is given by the *process model*.

Selection of manipulated variables:

Manipulated variables are those that are used to maintain controlled variables at their set points. Selecting the manipulated variables affects the response to external disturbances. The more the manipulated variables, the better is the control of the process. The way the manipulated variables are chosen is an important aspect of control. The selection of a control structure is a complex problem, which requires looking at the column from several perspectives (Moore 1992):

- A local perspective considering the steady-state characteristics of the column
- A local perspective considering the dynamic characteristics of the column
- A global perspective considering the interaction of the column with other unit operations in the plant

Interconnecting the measured and manipulated variables:

Solutions to this problem are dependent on the answers to the above three issues. Based on the three perspectives mentioned above, a sensor-valve pairing is done, and pairings, which minimize the interaction between individual control loops, are identified. Naraway et al. (1993) propose a method of selecting the measured and manipulated variables based on economic criteria. Proper pairing is necessary for effective control of the process. When this issue is addressed, we obtain a complete control structure.

2.2 Optimizing and Regulatory Control

The basic goal in operating a plant is to optimize an economic measure of plant operation (e.g., minimize operating cost or maximize profit), while satisfying certain constraints, and in the presence of external disturbances (Morari et al. 1980). This optimization problem is formulated by Morari et al. as follows:

(Minimize specified performance criterion – profit, squared error of deviations etc. – a function of process variables, subject to process constraints)

Minimize $J = \int_0^T \phi(y, u, d) dt$

Subject to

$$\dot{x} = g'(x, u, d)$$

State equations

$$x(0) = x_0$$

$$g''(x, u, d) \leq 0$$

Feasibility constraints

$$y' = h'(x, u, d)$$

Outputs from process

(Problem 1)

(2-1)

where, x is the vector state (dependent) variables; u is the vector of manipulated (independent) variables; d is the vector of external disturbances; y' is the vector of process outputs; Φ is the performance criterion of the process; g' is the set of equality constraints; g'' is the set of inequality constraints of the process; and h' is the set of equality constraints relating the process output to the dependent and independent variables.

Control is required because of external disturbances, d , whose stochastic nature makes it difficult to keep the process at a desired point. If we define implicitly two time-scales, which describe control activities of a plant, we can partition the disturbance d into a stationary part (d_1) and a non-stationary part (d_2). The component d_2 defined on a time scale t_1 (a small enough time scale where transient disturbances affect dynamics), comprises of disturbances that are “fast” in nature, which affect the short term dynamics of the process. These are irrelevant to the long-term optimization of the process, because their value becomes zero. The component d_1 , defined on a much larger time scale T_0 comprises of persistent disturbances which have to be included in the long term optimization of the plant. Thus, conventionally, the control objectives have been partitioned into two optimization problems as:

1) Optimizing control

(Minimize operating cost (performance criterion) of the process)

Minimize $J_1 = \int \varphi(y, u, d_1) dt$

Subject to

$$g'(x, u, d_1) = 0$$

$$g''(x, u, d_1) \leq 0$$

$$y' = h'(x, u, d_1) \quad (2-2)$$

[Problem 2a]

where $d_1 = f(T_0)$, and T_0 is large enough for plant dynamics to be negligible

The optimum solution to the above problem is given by:

$$\dot{x}^* = x(\dot{u}^*, d_1) \text{ and,}$$

$$\dot{y}^* = y(\dot{u}^*, d_1) \quad (2-3)$$

Where the superscript asterisk denotes optimal values, the solution to the optimization problem.

These optimal points are the set points provided to the regulatory system.

2) Regulatory control (Morari et al. 1980)

(Minimize deviation between optimal points and the current operating points)

$$\text{Minimize } J_2 = \int_{t_0}^{t_1} \left\{ (y - y^*)^T \left(\frac{\partial^2 \varphi}{\partial y^2} \right)_{y^*, u^*, d_1} (y - y^*) + (u - u^*)^T \left(\frac{\partial^2 \varphi}{\partial u^2} \right)_{y^*, u^*, d_1} (u - u^*) \right\} dt$$

Subject to

$$x = g'(x, u, d)$$

$$x(t_0) = x_0; \quad x(t_1) = \dot{x}^*(t_1)$$

$$g'(x, u, d) \leq 0$$

$$y = h(x, u, d)$$

where, $0 \leq t_0 \leq t_1 \leq T_0$

(2-4)

[Problem 2b]

This implies that the time horizon for regulation is significantly shorter than for optimization. The above objective function says that the basic function of the regulatory controller is to minimize the deviation between the set points and the operating point.

The focus of this work is to look at this partitioning of the control objectives and to analyze the necessity and validity of this partition. In other words, the work aims at looking at the complete plant control problem 1 instead of partitioning it into two separate optimization problems 2a and 2b. The main aspects to be considered are economic performance and performance in the face of transient disturbances.

Regulatory control strategies will be considered below, and their merits and demerits explained. Before that, the following remarks about optimizing control are worth noting:

Set points, as mentioned previously, are solutions to the optimizing control problem. These are first established in the design stage, based on economic, safety, environmental impact, product quality and other considerations. Thus, a set point represents an optimum operating point with regard to design conditions with maximum possible economic benefit, maximum safety, minimal environmental impact and perfect product quality. However, these setpoints reflect only the design conditions. In conventional control, typically, these are re-estimated whenever there are major

changes to the plant, or based upon operator experience. They are typically updated at intervals of greater than a day and in some plants even every few weeks. Consequently, in the face of the changing state of a plant, the set points are not up to date. A regulatory controller is not “aware” of this and its function is to merely keep variables at these set points. This approach leads to several issues that will be dealt with later.

2.3 *Some Conventional Regulatory Control Schemes*

The objective of regulatory control schemes, as pointed out earlier, is to keep controlled variables at their set points by adjusting the manipulated variables (Luyben, 1990). The various schemes of adjusting manipulated variables are given below:

2.3.1 Feedback Control

The most popular and simple way of manipulating variables is using a simple feedback control strategy. In feedback control, the process variable to be controlled is measured and the measurement is used to adjust another process variable, which can be manipulated (Seaborg, Edgar & Mellichamp 1989). Feedback control involves three stages (Smith and Corripio 1985):

Measurement – done by a sensor and transmitter

Decision – done by controller, which decides what to do to maintain a variable at its desired value.

Action – done by a final control element, usually a control valve

A simple feedback loop is shown in Fig 2.1.

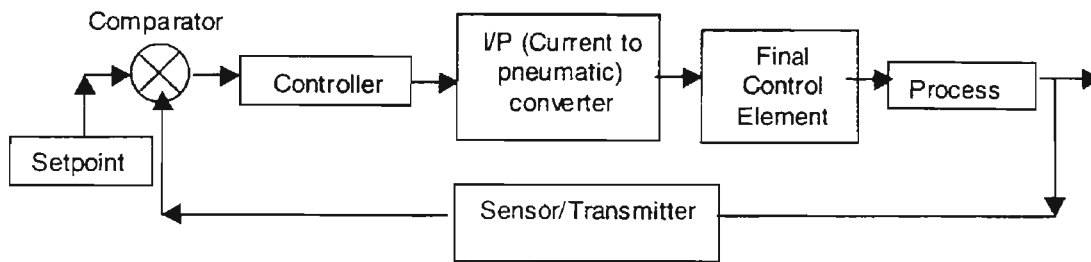


Fig 2.1: Feedback control loop

The above figure illustrates the basic components of a feedback loop: the controller, the sensor, transmitter, and the process being controlled. The controller here makes a decision to manipulate the control valve, and it can be digital or analog. Analog controllers use continuous electric or pneumatic signals. The controllers see transmitter signals continuously, and control valves are changed continuously (Luyben 1990). Digital controllers are discontinuous in operation, looking at a number of loops sequentially. Each individual loop is only looked at every sampling period. Analog signals from transmitters have to be converted to digital signals by A/D converters and fed to computers. Similarly, computer signals have to be transformed into analog signals by D/A converters before implementation in a control valve. There are three basic control laws that are used for continuous feedback control:

Proportional Control:

In proportional control, the controller output is proportional to the error, where the error $e(t)$ is defined by:

$$e(t) = s(t) - o(t) \quad (2-5)$$

$$\text{and, } p(t) = p_0 + K_c \cdot e(t) \quad (2-6)$$

where, $e(t)$ represents the deviation between the setpoint $s(t)$ and the current operating point $o(t)$; $p(t)$ is the controller output; p_0 is the bias value and K_c the controller gain. It is seen that the set point $s(t)$, is shown to be time-varying, but, in most process control problems, it is kept constant for long periods of time. An inherent disadvantage of proportional control is its inability to eliminate the steady-state errors that occur after a set point change or a sustained load disturbance (Seaborg, Edgar, Mellichamp 1989).

Proportional-Integral Control

Here the controller output depends on the integral of the error signal over time,

$$p(t) = p_0 + K_c \left[e(t) + \frac{1}{\tau_I} \int_0^t e(t) dt \right] \quad (2-7)$$

where, τ_I is the integral reset time

Proportional-integral control has the important advantage of elimination of offset and also combines the advantage of proportional control of responding rapidly to error changes. However, integral control has the disadvantage of producing oscillatory response of the controlled process and reduces system stability (Seaborg, Edgar and Mellichamp 1989).

Proportional-Integral-Derivative Control

Derivative action is used in conjunction with a PI strategy to provide anticipatory control of processes. This is done by measuring constantly the rate of change of the controlled variable and anticipating its future course. If there is a large rate of change, corrective action may be taken in advance to overcome future instability. By providing anticipatory control, the derivative mode tends to stabilize the process. The controller output for a PID controller is given by:

$$p(t) = p_0 + K_c \left[e(t) + \frac{1}{T_i} \int_0^t e(t) dt + T_D \frac{de}{dt} \right] \quad (2-8)$$

To summarize, feedback control provides:

- corrective action as soon as the controlled variable deviates from the set point
- control with minimal knowledge of the process
- simple and versatile control

However, it has the following disadvantages:

- No corrective action is taken until after the deviation in the controlled variable occurs
- No predictive control to compensate for the effects of known or measurable disturbances is possible
- Set points are seldom a reflection of the actual state of the process and hence do not represent the optimal operating point. The feedback controller is completely “unaware” of economic considerations

2.3.2 Feedforward, Ratio and Cascade Control - Simple Predictive Control Schemes

Process control can be significantly improved, if "predictive control," i.e. control to compensate for known disturbances, can be provided. Also, optimization using the degrees of freedom available for manipulation can lead to increased profits.

Feedforward control allows for some predictive action. For this, disturbances must be measured online, which requires knowledge of the process model.

Feedforward control involves measuring the process disturbances and taking corrective action based on the process model by calculating the manipulated variable required to maintain the controlled variable at its setpoint (Smith and Corripio 1985). Another way to

think about it is that it involves adjusting the material and energy that must be delivered to the process against the demands of the load (Shinsky 1988).

Ratio control is a special type of feedforward control, where the objective is to maintain the ratio of two variables at a specific value (Seaborg, Edgar and Mellichamp 1989). Thus, the actual ratio of two process variables is controlled rather than the two variables.

One of the disadvantages of feedforward control, mentioned in the previous section, is that it can only be used to compensate for measurable disturbances. An alternative strategy, which improves the dynamic performance is to utilize a secondary measurement point and a secondary feedback controller, which is so located that it recognizes the upset condition sooner than the controlled variable (Seaborg, Edgar and Mellichamp 1989). Thus predictive control is achieved through multiple feedback loops. This is called cascade control. This requires more than one control loop. The controller that keeps the primary variable at its set point is called the *master controller* and that used to keep the secondary variable at the set point required by the master controller is called the *slave controller* (Smith and Corripio 1989).

To summarize, the above controllers provide,

- Predictive control for known disturbances. For immeasurable disturbances, feedback control uses feedback compensation has to be used to “blindly” control the process. Quicker response to known, unmeasured disturbances affecting manipulated variables can be obtained using cascade control.
- Control based on the specific process being controlled

The various drawbacks are:

- No “awareness” of process economics
- Idealized models used do not provide proper control of the process

2.3.3 Multivariable Control – Advanced Predictive Control

The PID controller has been the workhorse in process industries for the past 40 years. PID controllers are routinely used in SISO (single input single output) applications with good results but success with this controller for multivariable systems has been limited (Deshpande 1989, Ogunnaike and Ray 1994).

A multivariable system is one in which one input not only affects its own output but also one or more other outputs in the plant. These processes are difficult to control because of the presence of interactions. The problem is further complicated by the presence of long time delays, process nonlinearities, and operating constraints. Such processes cannot be handled by the PID controller because of its inherent characteristics (Deshpande 1989). With the advent of digital computers, better designs can be produced without any consideration for hardware realizability. This has spurred better control strategies for process systems. Comparisons for PI control schemes and multivariable schemes obviously favor multivariable schemes, as they take into effect interactions and the actual process model.

The following step-by-step procedure may be employed to solve a multivariable problem, (Deshpande 1989):

1. Determine the best pairings of controlled and manipulated variables, from competing sets, by *interaction analysis*

2. If interaction is modest, one may consider SISO controllers for multivariable systems.
3. If interaction is significant, it may be possible to use decouplers to reduce interaction in conjunction with PID controllers
4. An alternative to steps 3 and 4 is to use a full multivariable scheme that inherently compensates for interaction such as model predictive control (MPC)

Each of these issues is addressed in several references (Ogunnaike and Ray 1994, Luyben 1986). The general elements of MPC are given below, to aid the discussion that follows (Ogunnaike and Ray 1994):

1. *Reference Trajectory Specification* – The first element in MPC is the definition of a desired target trajectory for the process output, $y^*(k)$. This can be simply a step to the new set point value or more commonly, it can be a desired reference trajectory that is less abrupt than a step.
2. *Process Output Prediction* – Some appropriate model, M , is used to predict the process output over a predetermined, extended time horizon (with the current time as the origin) in the absence of further control action.
3. *Control Action Sequence Computation* – The same model, M , is used to calculate the sequence of control moves that will achieve some specified optimization objective such as minimizing the predicted deviation of the process output from target over the predicted time horizon, or, minimizing the expenditure of control effort in driving the process output to target, subject to some operating constraints
4. *Error Prediction Update* – In recognition of the fact that no model accurately represents reality, plant measurement, $y_m(k)$, is compared with the model prediction and the prediction error $e(k) = y_m(k) - y(k)$ is used to update future predictions.

There are issues with the above control sequence:

- In conventional control, the models chosen for MPC are *linear*, a major simplification of reality. Although there is nothing in the basic MPC structure that fundamentally forbids the use of a nonlinear model, the following serious practical difficulties prevent the use of nonlinear models:
 - Difficulty in the development of nonlinear models
 - Difficulty in nonlinear model solution
- For many processes, steady states may not exist. There is severe transience in the process due to the presence of disturbances. The nonlinearities even around steady state may be so severe that no linear model can be an adequate representation of reality. However, recently advances have been made to make use of the computational power available to incorporate and solve nonlinear models. In the face of disturbances, an open-loop back-off calculation is used to maintain optimality and feasibility by calculating the optimal back-off from the nominal optimum point. (Bahri et al., 1996)
- As with other control schemes, this approach does not inherently possess any “awareness” of economics, concerned mainly with maintaining a reference state of operation. The way this reference state is determined is of no “concern” to the MPC.
- The control problem contains a large number of tuning parameters – and it is not always obvious how these parameters should be chosen.
- The model prediction updating strategy is often extremely inadequate as it assumes that the currently observed discrepancy between the model prediction and the plant measurement is due only to unmodeled disturbances, and more importantly, that such discrepancy will remain constant over the prediction horizon. This often leads to poor performance, especially in disturbance rejection.

Conventional regulatory control schemes, which aim at maintaining process variables at their setpoints have been discussed. Their inherent drawbacks were mentioned. Optimization methods, which determine setpoints for the regulatory controllers, will be discussed in the next section.

2.4 Optimization Schemes

This section discusses some essentials of optimization methods used to generate setpoints to the conventional regulatory control systems. These can be broadly classified as static and dynamic optimization. Online optimization, currently in use in industry uses steady-state models and the various aspects of online optimization and its drawbacks are discussed. In the next chapter, numerical methods for the reformulation and solution of dynamic optimization problems will be dealt with.

2.4.1 Static and Dynamic Optimization

The goal of optimization is to find the values of the variables in a process that yield the best value of a performance criterion of the process (profit, operating costs, efficiency, operating time etc) (Edgar and Himmelblau 1988).

Static optimization refers to the optimization wherein the performance index does not involve the evolution of the controlled system in time, i.e, if it defines a property of the system that may be considered as instantaneous with respect to the time scale of the process. The optimization problem constraints then can be described by steady state algebraic equations. The cost function typically used for static optimization would be:

$$J = \phi(x, u, d)$$

The model for the process is usually a steady state model and these algebraic equations are the equality constraints. Algebraic inequalities, which represent design limits and product quality constraints, constitute the other constraints.

Optimization becomes dynamic if time is explicitly involved in the performance index (Naslin 1968). Use is often made of cost functions of the following type,

$$J = \int_{t_0}^{t_1} \phi(x, u, d, t) dt$$

The problem then consists in controlling the process from its initial to its final time in such a manner as to minimize the performance criterion. Typically solution to dynamic optimization problems involves determination of the optimum values of the control variables (or “*optimum control policy*”) which will take the system as quickly as possible from a given state to a new desired operating state, while minimizing the *performance criterion* (Pollard et al., 1970). The constraints for this optimization problem are, typically, differential equations representing unsteady state material and energy balances, and other algebraic equalities and inequalities, thus giving rise to a *differential-algebraic equation* (DAE) system. The necessity and the advantages of dynamic optimization are discussed in Chapter 3.

2.4.2 Steady State Online Optimization

The control activities of a firm are typically grouped into various levels. These levels range from the actual production goals to the individual single loop controllers in the plant that “blindly” try to keep the process variables at their setpoints.

Online optimization, the next level in the control hierarchy to regulatory controllers, involves providing these setpoints to the plant’s distributed control system.

These setpoints are arrived at by a solution of an economic optimization problem. These setpoints determined at this higher level, as mentioned above, are implemented in the lower levels by single loop controllers, or more aptly, regulators. Regulators, as was emphasized in the previous section perform regulatory control, and these typically have no knowledge of economic considerations. It is the optimizer which “knows” the process economics. This optimization, until recently, was done off-line by various analytical and numerical methods and provided updates to setpoints at fairly infrequent intervals (e.g., Pollard et al. 1970, Maarleveld et al. 1969).

However, in modern plants the steady state optimization is carried out online at regular intervals (Glemmestad et al 1997). This means that setpoints are provided in a time scale of hours. Thus setpoint changes are carried more frequently and these appear as “economic disturbances” that the regulatory control system has to accommodate (Ogunnaike and Ray 1994, Smith and Corripio 1985). The actual implementation is discussed below:

2.4.2.1 Implementation

Online optimization provides a means of maintaining a plant near its optimal operating conditions by providing setpoints to the regulatory control system (Zhang et al. 1995, Chen et al. 1998). In order to perform a meaningful on-line optimization, it is required that there is at least one extra degree of freedom during operation. Thus, if there is one degree of freedom, it means that we can choose a value for this so as to minimize cost (Glemmestad et al. 1997). Online optimization requires the solution of three nonlinear programming problems (NLPs) similar to Eq. 2-11:

For gross error detection and data reconciliation –

Measurements are subject to random errors. Therefore, they have to be adjusted so that appropriate heat and mass balances are satisfied and random errors eliminated. This is referred to as data reconciliation. The main aim of data reconciliation is to improve the data from plants using a model of the plant (Dempf et al., 1998). Similarly, process data sometimes contains errors caused by non-random events, such as instrument bias or malfunction.

The presence of any such gross errors invalidates the statistical basis of data reconciliation and hence they must be detected and eliminated before data reconciliation is carried out. If a gross error is identified in a measurement, it is defined as:

$$x_{mes} = x_{est} + \varepsilon + B^* \Delta \varepsilon \quad (3-1)$$

where x_{mes} is the measured value of a variable with an estimated value of x_{est} ; B^* is the matrix containing as many rows as there are measurements and a column for each gross error; ε is the gross error in the measurement; . The elements containing measurements with gross errors contain the value 1 and others have value 0.

The data reconciliation problem is formulated as an NLP (Nooraii et al. 1998):
(Minimize weighted squared error sum of the deviation between measured and estimated values)

$$\text{Minimize} \quad (x_{mes} - x_{est})^T W (x_{mes} - x_{est})$$

Subject to

$$Ax = 0 ; \delta = A(x_{mes} - x_{est}) = A(\varepsilon + B^* \Delta \varepsilon) \quad (3-2)$$

where δ is the residuum of the material and energy balances and Eq. 3-2 represents the equality constraints of the process.

It must be noted that the model used in data reconciliation is initially chosen to be of reduced order to avoid complexity. After matching this basic plant model and the plant data with an accuracy of 10%, model complexity can be enhanced (Dempf et al., 1998)

Parameter Estimation –

Model parameters such as catalyst activities, heat exchanger fouling factors, and heat transfer coefficients do not remain constant with time and these need to be updated based on prevalent process conditions. The number and type of parameters depend on the process being optimized. Parameter estimation algorithms are also least square NLPs.

Process Optimization –

This is the “main” part of the optimizer, in which an economic model of the process is used to describe a performance criterion to be optimized. This can be done analytically (e.g., Moore et al., 1991), but typically solved numerically using an optimization package. The process model gives the constraint equations (in other words, the equality constraints for the optimization problem) for the mass and energy, chemical reaction kinetics and equilibrium relationships. Other specifications such as design limits and minimum product quality specifications constitute the inequality constraints. The process model is usually chosen to be a linearized steady state model at the design conditions, which is one of the issues to be discussed. In steady state optimization, the process has to reach a new steady state before the next optimization loop is carried out. This provides a lower bound for the optimization (Loeblein et. al 1998).

2.4.2.2 Issues with Online Optimization

The above scheme of optimization based on a steady state linearized model raises two important issues. These are addressed below:

1. *Linearized Models* –

Verne et al. (1999) consider some of the reasons why linearized models are chosen:

- The first principles nonlinear models should be converted to a form understood by the optimizer. This is a complex problem involving conversion of nonlinear implicit equations to explicit equality constraints.
- Nonlinear equations require sophisticated optimization software, with possible requirements of new computer hardware
- Ensuring a valid interface between the regulatory controller (which runs every minute) and the upper-level optimizer (which typically runs one or two hours) is required, which may be a complex task.
- The likely cost of implementation of a rigorous optimizer is quite substantial and may not be cost-justified.
- For some processes, with few disturbances and upsets, the plant operates in and around the desired steady state for which the optimizer is designed. By supplementing the optimizer with feedback from the process, the simple linear models “get the job done.” Small errors in model gains are corrected by comparing the predicted process response to what is observed. The important assumptions are that model gains are at least the correct sign and that the relative magnitudes between gains are correct.

However, linear models have the following drawbacks:

- The simple linear model is not a close representation of reality. Most processes are nonlinear and even feedback from the process is not enough to provide an optimal solution, especially in the face of transient conditions. This is the main argument in favor of using a nonlinear process mode, which produces consistent performance even in the face of upsets and disturbances. The oversimplification in a linear model often produces sub-optimal results
- The process models used in the controller and the optimizer differ considerably. Hence, there is no single accountability for the optimum operating performance.

2. *The Steady State Assumption –*

The traditional Optimizer, as mentioned above relies on a steady state model. The steady state assumption gives it a basis for optimization. However, for most processes, it is rare to encounter steady state operation. Model parameters change, upsets occur or equipment may undergo modifications. The validity of the setpoint calculated by the Optimizer based on the steady state is questionable. The invalidity of the above assumptions causes sub-optimal solutions, and the eventual upshot is that the Optimizer is turned “off.” which is to say it is removed from the line.

In addition to these, White (1998) discusses some of the reasons why Optimizers are turned “off”:

- a) *Optimization solution does not change* – Optimization systems push the operating point of the plant to the point of intersection of certain constraints and try to hold it there. Plant operators quickly observe this result and are able to duplicate it without the Optimizer by adjusting the action of the multivariable controller. Eventually, the Optimizer is turned “off.” The same ensues if the process being optimized is relatively stable, and encounters few disturbances, in which case the Optimizer

solution does not vary with time. For such situations, most of the optimization can be obtained by offline studies.

- b) *Disturbance frequency too high* – The setpoints from the Optimizer are downloaded to the system and the plant adjusts to new steady state conditions. Generally, the time this process takes is of the order of the settling time of the process. However, if major disturbances occur more rapidly than the plant's settling time, then it is seldom at steady state and the optimization fails. This can be partially offset by using a dynamic model in the Optimizer.
- c) *Poor parameter updating and data reconciliation algorithms* – Successful optimization algorithms incorporate online model auto-calibration procedures that use plant data to update model parameters. Similarly, the plant data being used for the optimization may be subject to random errors, which a robust data reconciliation algorithm can “filter.” If these are not available, then sub-optimal solutions result.
- d) *Pricing coefficients* – The price coefficients used are typically updated on a monthly basis. Use of incorrect coefficients causes sub-optimal solutions, which may result in the Optimizer being turned “off.”

Most of the above drawbacks can be eliminated if the optimization is made more frequent and dynamic (White 1998, Henry et al. 1998). This will help realize the objective of realizing flexible and dynamic optimization and control based on current process conditions. A dynamic optimization algorithm can be used to predict an optimal control path to the desired point of maximum profit.

It is thus obvious that a dynamic optimization algorithm should be the first step to realize the objectives of control mentioned in the previous chapter. A review of numerical methods to solve dynamic optimization problems follows in the next chapter.

Chapter 3

Dynamic Optimization

The previous chapter provided background information on the conventional control and optimization schemes. It was pointed out that dynamic optimization *to maximize economic benefit* could address some of the drawbacks of the conventional control schemes. This chapter takes an overview of the numerical methods for dynamic optimization, and their relative merits. However, it will be useful to appreciate where these dynamic optimization methods fit in into the overall control structure. Hence the first part of this chapter presents an overview of the proposed strategy for dynamic optimization. The next sections discuss the numerical methods of dynamic optimization.

3.1 *Proposed Strategy*

In Chapter 1, the desirable characteristics of a controller were discussed.

These are recounted below for discussion:

An ideal dynamic controller would:

- Determine setpoints for the optimal point of operation and evolve them with time to best reflect current operating conditions
- determine the fastest path to these optimal conditions, based on economic considerations instead of least squares minimization techniques
- respect the safety, environment, design, and product quality constraints of the process along the optimal path

In mathematical terms, the objective function of such a controller would be to *maximize profit over a time horizon, subject to safety, environmental, design and product*

quality constraints. This is a dynamic optimization problem, the methods of solution for which will be discussed below.

The performance criterion for the general dynamic optimization problem (3-3) should then be the profit made by the process over a time horizon, the interval (a,b). The solution to this optimization problem is then the control and state variable profiles to be “followed” by the process if it is to make the maximum profit. Since the control is based on economic considerations as well, this strategy will be termed *Control to Economic Optimum*. This can be mathematically represented as:

$$\text{Max } J = \Sigma(\Sigma\text{value}(x) - \Sigma\text{cost}(u, \Delta u))\Delta t$$

Where, Δt is the interval (a,b) $\equiv \alpha_{\text{TOTAL}}$

The proposed optimization is similar to a nonlinear model predictive optimization algorithm in constraint handling and solution methods, but the objective function for the optimization is maximizing profit made by the process instead of minimizing the deviation from setpoints. This setup would then determine economically optimum points of operation and evolve them with time. This translates to dynamic determination of setpoints for state (“controlled”) variables. The process maintains these setpoints for a “control step” before the Optimizer is re-run and new setpoints are found. During this control step, the manipulated variables are kept at the values dictated by the Optimizer. Thus, the optimization and regulatory control stages are “unified” in the sense that there is just a single stage, which keeps the process under control and determines the optimum operating point. The actual method of implementation will be discussed in Chapter 5.

In summary, the features of the dynamic optimizer are proposed as follows:

- Objective is to maximize profitability over a future horizon
- Provides predictive control based on a mechanistic, nonlinear process model
- Takes into account current process conditions and unexpected disturbances, which necessitates that the optimizer 'runs' frequently (once every few minutes) and "re-optimizes" based on current conditions
- Determines optimal conditions which do not simply optimize process for a particular instant, but over a control horizon
- Determines optimal path to these optimum conditions based on economic considerations instead of least squares optimizations or subjective operator tuning
- Respects process constraints
- Maintains stability of process by not taking too aggressive control actions

This proposed strategy would be, for reasons mentioned in Chapter 1, implemented and tested on a binary distillation column. Chapter 4 describes the modeling, simulation and the optimization program formulation for the distillation column for implementation of the concept.

The next section discusses the numerical methods for dynamic optimization.

3.2 *Dynamic Optimization*

A general dynamic optimization problem, as mentioned previously, contains time as a variable in the optimization. The general form of a dynamic optimization problem is given by:

(Minimize a specified performance criterion over the time horizon (a,b))

Minimize

$$\Psi(x(b)) + \int_a^b \Phi(x(t), u(t)) dt$$

Subject to

$$\begin{aligned} \frac{dx}{dt} &= h'(x(t), u(t)) && \text{(equality model constraints)} \\ g''(u(t), x(t)) &\leq 0 && \text{(inequality constraints)} \\ g^*(x(b)) &\leq 0 && \text{(inequality constraint at the end condition)} \\ x(a) &= x_0 && \text{(initial conditions)} \\ x(t)^L &\leq x(t) \leq x(t)^U && \text{(bounds on state variables)} \\ u(t)^L &\leq u(t) \leq u(t)^U && \text{(bounds on control variables)} \end{aligned} \quad (3-3)$$

Where, a and b represent the beginning and ending time for optimization; $\Psi(x(b))$ is the component of the objective function at the end condition; $x(t)$ is the state profile vector and $u(t)$ the control profile vector; g'' is the set of inequality design constraints; the superscripts L and U represent lower and upper bounds; x_0 is the initial condition for the state vector (Logsdon et al. 1989). In fact, this is a more general version of the nonlinear model predictive control discussed in the previous chapter.

The optimization problem such as the one for the binary distillation column are complicated by the presence of model differential and algebraic equations, which must be solved by the optimizer to determine the optimum operating point. Such a system of equations is called a DAE (differential algebraic equation) system. The model equations are usually differential, and the algebraic equations are constituted by the physical and design constraints that ensure the thermodynamic consistency and physical meaningfulness (Tanartkit and Biegler 1995). Typically, these are solved by

transforming them into nonlinear optimization programs (Tanartkit and Biegler 1996, Sistu et al. 1993).

Numerical techniques for dynamic optimization problems can be classified into three approaches (Barton et al. 1998): *dynamic programming based* approaches; *indirect* approaches, and *direct* approaches. The dynamic programming approach was first described by Luus (1990) and consists of including constraints on state and control variables in the objective function as penalties, and solution is obtained by using the Bellman principle of optimality (Fikar et al. 1998) without transforming the original problem as in the other approaches described below. Indirect approaches or variational approaches consist of transforming the optimization program into a two-point boundary value problem (Tanartkit and Biegler 1996). Recent studies have focussed on the third category of approaches called the direct approaches for their generality and ease of implementation. These direct approaches can be further classified as the sequential or *control vector parameterization* approach and the simultaneous or the *collocation* method. In these approaches, the original optimal control problem is converted to a nonlinear programming problem.

A discussion of these direct approaches follows.

3.2.1 Control Vector Parameterization

Control vector parameterization reduces the infinite dimensional dynamic optimization problem to a finite dimensional problem through approximation of *only* the control variable profiles (Barton et al. 1998). This is also called the *feasible path* approach. Basically this consists of discretizing the control variables $u(t)$ in the time horizon of interest. For given $u(t)$, it is then possible to integrate the underlying DAE

system using standard integration algorithms (Vassiliadis et al., 1994) so as to evaluate the objective function and the constraints that have to be satisfied by the solution. This control vector parameterization thus corresponds to a *feasible path* approach since the DAEs are satisfied at each step of the optimization algorithm. The problem is thus converted into a nonlinear programming problem, for which the objective function and the constraint functions are evaluated by the integration of the system equations, and their gradients with respect to the optimization parameters via the integration of the sensitivity equations (Pantelides et al., 1994). Thus the integration (of the model and the sensitivity equations) is done by any standard integration algorithm independent of the optimization algorithm, and the evaluation of the objective function and the inequalities is done subsequent to the integration (Vassiliadis et al. 1994) for given values of control variables, which are the decision variables in the optimizer.

Mathematically, the general dynamic optimization problem (3-2) is converted into a sequence of approximate problems such that the solution of each of the approximation problems is a sub-optimal solution to the above problem (Goh and Teo 1988). Approximation is carried out by sub-dividing the time horizon of control into finite control intervals as shown in Fig 3-1.

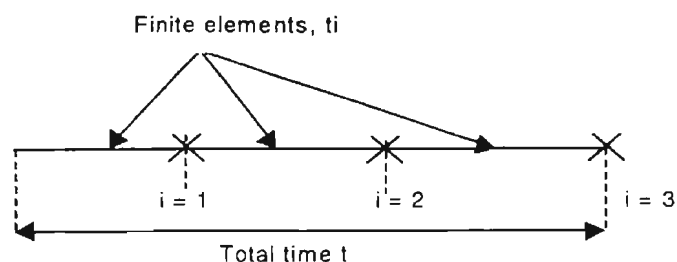


Fig 3-1: Division of time into finite elements

A low order polynomial form is assumed for the control variables $u(t)$. Thus, control profiles are discretized (as order K polynomials) as follows (Vassiliadis et al. 1994):

$$u(t) = \sum_{i=1}^K u_{ik} \psi_i^K(t)$$

Where,

$$\psi_i^K(t) = 1, \quad (K=1)$$

$$\psi_i^K(t) = \prod_{\substack{j=1 \\ j \neq i}}^K \frac{t - t_j}{t_i - t_j} \quad (K \geq 2) \quad (3-4)$$

and i and j represent finite points in time, demarcating control intervals

$K = 1$ corresponds to a piecewise constant control profile, $K = 2$ to a piecewise linear, $K = 3$ to piecewise quadratic and so on. For some applications, continuity may be enforced on control profiles by suitable junction conditions.

This type of approach to solving dynamic optimization problems is called the *sequential approach*. In addition to the smaller size of the optimization problem, this approach has the advantage of controlling the discretization error by adjusting the step size by adjusting the order and size of the integration steps using well-established ODE/DAE integration techniques (Vassiliadis et al. 1994). The disadvantage of this approach lies in the treatment of profile constraints as well as eliminating the need to obtain expensive and possibly infeasible intermediate solutions (Tanartkit and Biegler 1996). Also, since the model and sensitivity equations are solved at each iteration, it is found that 85% of the system time is spent on the integration of the equations that provide gradient information. If the integration could be accomplished with the

optimization, computational times can be reduced significantly (Renfro et al. 1987). This leads us to consider the simultaneous optimization and solution of dynamic systems.

3.2.2 Orthogonal Collocation

An alternative to the above approach is the simultaneous approach in which *both state and control variables are discretized*. This is called the infeasible path approach as the discretized constraints are, in general, satisfied at the solution to the optimization problem only (Vassiliadis et al. 1994). The result of discretizing both the control and state profiles is to convert the model differential equations into algebraic equations that can be directly embedded as equality constraints in the optimization problem along with other constraints (Cuthrell and Biegler 1989, Tjoa and Biegler 1991).

The numerical discretization of ordinary differential equations representing the model is accomplished through polynomial approximation of time varying profiles. In theory, any polynomial can be used to approximate the state and control profiles. A low order polynomial is usually found to be sufficient to give good accuracy while keeping the dimension of the NLP problem low (Renfro et al. 1987). Early approaches (Tsang et al. 1975) used arbitrary approximating polynomials, of usually linear or quadratic order. Biegler (1984) proposed the use of Lagrange polynomials to approximate the time-varying independent variables, which have several desirable properties: using these polynomials forces the polynomial coefficient to be equal to the value of the variable itself at certain points of evaluation called the collocation points. This technique is called global orthogonal collocation (Cuthrell and Biegler 1989).

To overcome the disadvantage of global collocation which fails to approximate sharply varying variable profiles (which would require the number of collocation points to

be very large), Cuthrell and Biegler (1987) proposed the use of orthogonal collocation on finite elements, where the time horizon is partitioned into finite elements and control profile discontinuity is allowed across the elements. As in control vector parameterization, the discretization is carried out by sub-dividing the time into finite elements. However, another layer of sub-division is carried out by dividing each finite element into collocation points as shown in Fig 3-2. Thus, the state and control vectors are approximated by piecewise polynomials over each finite element.

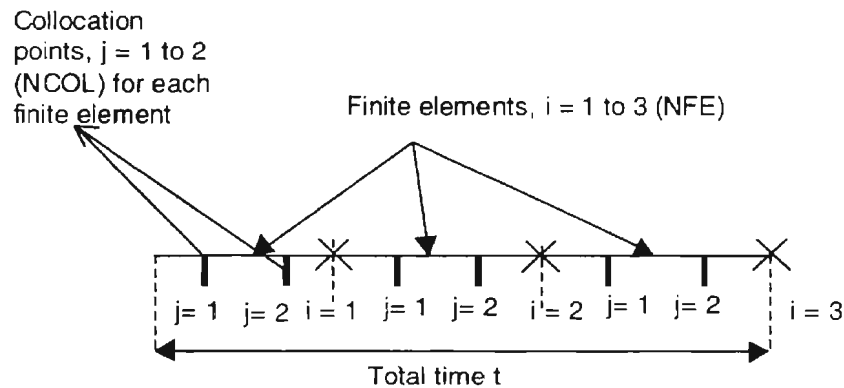


Fig 3-2: Division of time into finite elements and collocation points

Using these collocation points provides an extra level of definition of state and control variables is obtained. Boundaries between finite elements are defined as the points of discontinuity for control variable profiles. These discontinuities help approximate steep bang-bang type profiles. As will be described below, discontinuities are not allowed in state variable profiles. Tieu et al. (1995) also consider an endpoint collocation method, where the final point at $t = t_f$ is also treated as a collocation point, avoiding the interpolation of the state variables to the end condition. This improves the stability of the optimization. Certain conjunction equations are used to artificially enforce

continuity in state profiles. The control and state profiles are defined by polynomials with constant coefficients.

The state and control vectors are thus determined if the coefficients of these polynomials are evaluated at collocation points (see Appendix C). The polynomial basis functions are usually chosen as the Lagrange polynomial functions, which are given by:

$$\Phi_{[ij]}(\tau) = \prod_{\substack{k=0 \\ k \neq j}}^{NCOL} \frac{(\tau - \tau_k)}{(\tau_j - \tau_k)} \text{ for state variables} \quad (3-5a)$$

$$\text{and } \psi_{[ij]}(\tau) = \prod_{\substack{k=1 \\ k \neq j}}^{NCOL} \frac{(\tau - \tau_k)}{(\tau_j - \tau_k)} \text{ for control profiles} \quad (3-5b)$$

where NCOL is the number of collocation points

j represents the piecewise polynomial coefficient

i represents the i^{th} finite element

$\phi_{[ij]}$, $\psi_{[ij]}$ represent the j^{th} polynomial basis function in the i^{th} finite element at time

$t_{[ij]}$

and $[ij] \equiv (i+1)(j-1)$

In the above equations, the τ 's are defined as follows:

$$t_{[ij]} = \alpha_i + \tau_j (\alpha_{i+1} - \alpha_i), \quad 0 \leq \tau \leq 1 \quad (3-6)$$

where α_i is the i^{th} finite element length

Thus the state and control vectors can be discretized as follows:

$$\begin{aligned} x^i(t) &= \sum_{j=0}^{NCOL} x_{[ij]} \Phi_{[ij]}(t) \\ u^i(t) &= \sum_{j=1}^{NCOL} u_{[ij]} \psi_{[ij]}(t) \end{aligned} \quad (3-7)$$

where $x^i(t)$ represents the state variable in the i^{th} finite element

and $u^i(t)$ represents a control variable in the i^{th} finite element

Discontinuities are allowed in control profiles, but not allowed in state profiles.

Continuity is enforced on state profiles using conjunction equations as follows:

$$x_{[i0]} = \sum_{j=0}^{N_{COL}} x_{[i-1,j]} \Phi_j(\tau=1) \quad i=2,3,\dots,NE \quad (3-8)$$

where NE is the number of finite elements

Thus, the optimization problem becomes:

Minimize

$$\varphi(x_f) + \sum_{i=1}^{NE} \sum_{j=1}^K \varphi(x_{[ij]}, u_{[ij]}, \Delta\alpha_i)$$

subject to

$$r(t_{[ij]}) = \dot{x}(t_{[ij]}) - F(x_{[ij]}, u_{[ij]}, \Delta\alpha_i, t_{[ij]}) = 0$$

$$g(x_{[ij]}, u_{[ij]}, \Delta\alpha_i) \leq 0$$

$$g_f(x_f) \leq 0$$

$$x_{[10]} - x_0 = 0$$

$$x_{[i0]} = \sum_{j=0}^{N_{COL}} x_{[i-1,j]} \Phi_j(\tau=1), \quad i=2,3,\dots,NE$$

$$x_f - x^{i-1}(\alpha_{NE+1}) = 0$$

$$x_{[ij]}^L \leq x_{[ij]} \leq x_{[ij]}^U$$

$$u_{[ij]}^L \leq u_{[ij]} \leq u_{[ij]}^U$$

(3-9)

$$\sum_{i=1}^{NE} \Delta\alpha_i = \alpha_{TOTAL}$$

where α_{TOTAL} is the time horizon for optimization

These concepts are explained through an example in Appendix C. The reader is directed to Appendix C for further details.

The advantage of the complete discretization approach is that it does not waste valuable computational effort trying to obtain feasible solutions away from the solution to the optimization problem (Vassiliadis et al 1994). However, the difficulty is the formidable size of the optimization problem. This and other difficulties will be discussed later. Due to its inherent advantages mentioned above, the simultaneous approach would be used in the solution of the problem of dynamic optimization of the performance of the distillation column chosen in this study.

This chapter discussed the numerical methods for dynamic optimization. The next chapter introduces the binary distillation process on which the above concepts would be implemented. The actual implementation of the strategy and its comparison with conventional control schemes form the focus of Chapter 5.

Chapter 4

Modeling, Simulation and Optimization Problem Formulation

This chapter deals with the modeling, simulation and the development of the optimization program for the distillation column. Fundamental aspects of the model development are first discussed, as outlined in commonly used textbooks such as Luyben (1990). This is followed by a description of the method for a first principles simulation of the distillation column. Finally, the economic objective function for the distillation column and the constraints for the optimization problem are developed.

Before beginning, the following points are in order:

The proposed concept involves an *Optimizer* dictating optimal control policies over a time horizon to a *Process*. The Optimizer uses a model for itself to verify that the control policy it dictates does not violate the process constraints. Since this study is carried out on a simulation, the “Process” on which the Optimizer works is also a simulation in itself. Thus, there are two models in use:

1. For the Process (simulation)
2. For the Optimizer model constraints

The reason why different models are chosen for the Process and the Optimizer is as follows:

No model can adequately represent the reality of the process. Hence, when implemented this setup would obviously have a different model, which would behave differently from the process. Hence, the Process model is chosen to be different from the Optimizer model. The Process model uses a simple tray model, and assumes equimolar overflow. The Optimizer uses a reduced order model, where all the enriching

section trays are lumped into two collocation points in the enriching section (not to be confused with the orthogonal collocation technique used in the Optimizer), and all the stripping section trays are lumped into two points in the stripping section. The reboiler and the reflux drum represent the other two collocation points, with the result that the column is approximated by equations at 7 “lumping” or collocation points.

The development of both the models will be discussed. The general aspects of distillation modeling will be discussed first.

4.1 *Distillation Column Modeling*

Distillation is one of the most important separation processes in industry. Modeling of distillation columns has been dealt with in several texts (Luyben 1990, Luyben et al. 1992). These involve writing mass and energy balances over various modules of the distillation column and applying simplifying assumptions while appropriate.

For the purpose of modeling, a simple binary distillation column with feed flow rate F , feed composition z_F as shown in Fig. 4-1 is chosen. The overhead vapors are condensed in the condenser and these flow into a reflux drum, whose holdup is M_d . The liquid in the drum is at its bubble point. Reflux is pumped back at rate R to the top tray. Overhead product is removed at a rate D . Liquid bottoms product is removed at a rate B . The column consists of N_T trays. Two models will be developed – one a rigorous model and the other a simplification based on certain assumptions.

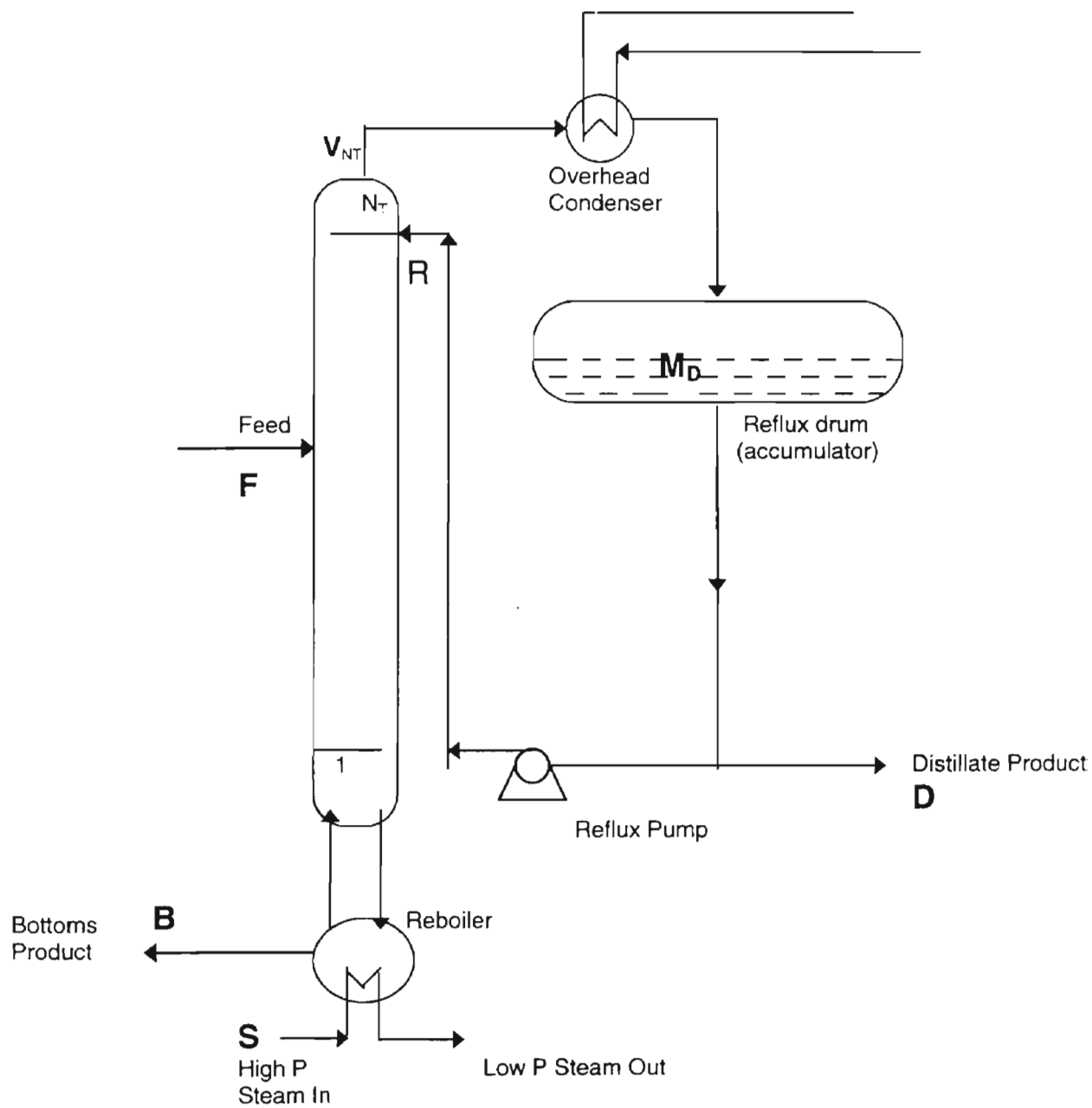


Fig. 4-1 Binary Distillation Column

4.1.1 Tray Model

The equations for material and energy balances can be derived by defining the streams that enter and leave the tray. These are shown in Fig 4-2 below:

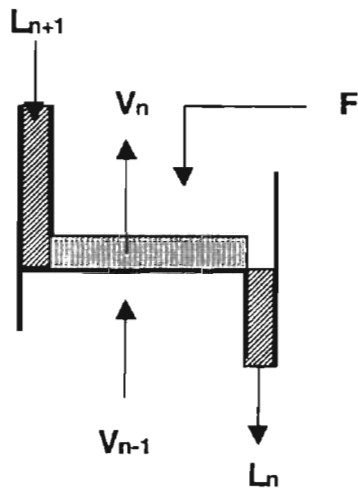


Fig. 4-2 Tray Model

Applying material and energy balance for the trays gives rise to the following equations, where:

F = feed flow rate

L_n = Liquid flow rates on the n^{th} tray, $n=1,2,\dots,N_T$

V_n = Vapor flow rates on the n^{th} tray

M_n = Inventory on the n^{th} tray

X_i = liquid phase composition of the i^{th} component; $i = 1, 2, \dots, N_c$

N_c = number of components

Y_i = Vapor phase composition of the i^{th} component;

h_n^l = Liquid phase enthalpy on the n^{th} tray

h_n^v = Vapor phase enthalpy on the n^{th} tray

Material Balance for nth tray

$$\frac{dM_n}{dt} = F + L_{n+1} + V_{n-1} - L_n - V_n \quad (4-1)$$

Component Balance for ith component from nth tray

$$\frac{d(x_i M_n)}{dt} = z_i F + x_{i,n+1} L_{n+1} + y_{i,n-1} V_{n-1} - x_{i,n} L_n - y_{i,n} V_n \quad (4-2)$$

Energy Balance for ith tray

$$\frac{d(h_n^l M_n)}{dt} = h_F F + h_{n+1}^l L_{n+1} + h_{n-1}^l V_{n-1} - h_n^l L_n - h_n^v V_n, \text{ where } \frac{d(h_n^l)}{dt} = 0 \quad (4-3)$$

The key assumptions involved in this model are listed below:

- Negligible vapor hold up
- Negligible specific enthalpy change
- Constant pressure or tray pressure drop

This model is reported to be successful in 95% of industrial distillation problems (Grassi II 1992). However, further assumptions are made to simplify the problem.

Usually, the major simplification is of equimolal overflow. If the molal heats of vaporization of the two components are about the same, whenever one mole of vapor condenses, it vaporizes a mole of liquid. Assuming heat losses up the tray are negligible and the feed is a saturated liquid, the vapor rates on all trays may be assumed to be the same, so that

$$V = V_1 = V_2 = V_3 = \dots = V_{NT}$$

The mathematical effect of this is that the energy balance on each tray can be neglected.

4.1.2 Condenser and Reflux Drum

Total Continuity

$$\frac{dM_D}{dt} = V_{NT} - R - D \quad (4-4)$$

where R = reflux flow rate

D = Distillate flow rate

Component Continuity (More volatile component)

$$\frac{d(M_D x_D)}{dt} = V_{NT} y_{NT} - (R + D) x_D \quad (4-5)$$

where x_D is the distillate composition

Energy Balance

The energy dynamics of the condenser are small relative to the column composition dynamics (Grassi II 1992). The condenser duty is equal to the latent heat required to condense the overhead vapor to its bubble point liquid plus the sensible heat for any subcooling of the liquid.

This is given by:

$$Q_c = V_{NT} h_{NT} - (R + D) h_D \quad (4-6)$$

Where Q_c is the cooling load of the condenser

Usually, a simplification that is made is that the inventory in the accumulator is constant and that there is perfect level control. Hence the first equation vanishes and in the second equation, the term M_D can be removed from the derivative.

4.1.3 Column Base and Reboiler

Total Continuity

$$\frac{dM_B}{dt} = L_1 - V_0 - B \quad (4-7)$$

where M_B is the material in the reboiler

and B is the bottoms flow rate

Component Continuity

$$\frac{d(x_{B,i} M_B)}{dt} = x_{1,i} L_1 - y_{0,i} V_0 - x_{B,i} B \quad (4-8)$$

where x_b is the bottom composition

Energy Balance

$$\frac{d(h_{B,i}^l M_B)}{dt} = h_1^l L_1 - h_0^v V_0 - h_B^l B + Q_R \quad (4-9)$$

The usual simplification is of constant base inventory which eliminates the first equation.

Also, neglecting the changes in the specific enthalpy gives a simple relation between the reboiler heat duty Q_R and the vapor flow rate V .

4.1.4 Simple Tray Hydraulic Model

A simple linear relationship between the liquid leaving the tray, L_n and the liquid holdup on a tray, M_n is used as follows:

$$L_n = \bar{L}_n + \frac{M_n - \bar{M}_n}{\beta} \quad (4-10)$$

L_n is the liquid leaving the nth tray;

\bar{L}_n is the initial liquid flow rate (at the start of the simulation);

M_n is the holdup of the nth tray;

\bar{M}_n is the initial holdup on the nth tray;

β is the hydraulic tray time constant, typically between 3 to 6 s per tray

4.1.5 Vapor-Liquid Equilibrium Model

The following equation is used to represent equilibrium:

$$y_n = \alpha x_n / (1 + (1-\alpha)x_n) \quad (4-11)$$

where α is the relative volatility, which is assumed constant throughout the column.

4.2 *Developing the Process Model*

Although there are distillation column simulations available in simulation packages such as ASPEN and HYSYS, a rigorous simulation of the distillation column was developed from first principles. The reasons for doing so are that a rigorous dynamic model would be readily available for later use with the Optimizer. Also that the nonlinear Optimizer used in the study (GAMS – General Algebraic Modeling System) is Visual Basic compatible.

To summarize, the assumptions made in the model to be used for the distillation column *Process* are as follows (Luyben 1992) –

- There is one feed plate onto which a saturated liquid feed is introduced
- Pressure is constant and is known on each tray. It varies linearly up the column from P_B at the bottom to P_D at the top
- Equimolal overflow is assumed, so that the vapor flows on all trays is equal
- Coolant and steam dynamics are negligible in the condenser and the reboiler
- Dynamics of vapor space in the reflux drum and throughout the column are negligible
- Liquid hydraulics are calculated by the simple hydraulic relation (4-10)
- Volumetric liquid holdups in the reflux drum and the column base are held perfectly constant
- There is negligible specific enthalpy change, as a result of which the energy balance is purely algebraic

The simulation is fairly straightforward if the model equations established above are available. It mainly involves solving material and energy balances for each tray, and looping back at the end of a time step after integrating the process equations. The integration procedure used is the Euler's method, chosen for its simplicity and reasonable accuracy.

The main issue is of developing a consistent initial condition from which the simulator can move forward. This is simple if consistent input data from an experiment are available. However, this not being the case, the initial convergence procedure followed is given below:

- An input file is prepared with feed stream information, reflux, heat input (which gives the vapor boilup) and product compositions
- Tray liquid compositions are initialized using a linear profile from top to bottom
- A constant vapor rate based on the heat input is computed
- The liquid rate is initialized to be equal to the reflux in the trays above the feed tray and the reflux rate plus the feed rate for the feed tray and the trays below it
- The dynamic simulation is run from these conditions until it converges to a bona fide steady state

Once an initial convergence is obtained, then the following steps are used to move forward in time –

1. An input file is created with relevant physical property data
2. The initial convergence simulation results are used as the bona fide input conditions to the simulator

3. The equilibrium vapor composition is calculated from liquid composition using the equilibrium equation
4. The liquid rate leaving the stage is obtained using Eq. 4 -10
5. The total and component mass balance derivatives are computed using the model equations
6. All the ODEs using are integrated using Euler's method and the procedure loops to step 3.

Since the simulation is in Visual Basic, which is a partial object-oriented programming language, this can be easily converted to an object-oriented simulation by declaring trays and fluids as classes. The main advantage of object-oriented simulations is that they are extremely flexible and generic and they can be easily modified for any system. Also, they support reusability and require less computer requirements.

4.3 *Developing the Collocation Model for the Optimizer*

The procedure followed is the one described by Papadourakis and Rijnsdorp (1992), in which the authors develop a reduced order model of a distillation column, by approximating the dynamics of a number of stages by the dynamics of a fewer number of pseudostages. In the collocation model, certain grid points, which are the zeroes of suitable polynomials are chosen as locations where material and energy balances are written. The advantages of these models are that they retain the nonlinear nature of the original model; allow for free choice of the thermodynamic subroutines; can be implemented without the full order solution; and reduce the computational time significantly. Their main disadvantage is that the nonretention of the original model's gain in an exact manner. However, the gain predicted by the collocation model is usually in good agreement with that of the full model.

The development of the collocation model is detailed in Appendix A. In the Appendix, the method of choosing collocation points and the development of model equations is elaborated. The reader is directed to Appendix A for details regarding model development.

Using the method detailed in Appendix A, the model for the distillation column used in the study was determined as follows:

Reboiler

$$M_{LB} \frac{d\tilde{x}_1}{dt} = (R + F)[(1/2)\tilde{x}_1 + (1/2)\tilde{x}_2] - B\tilde{x}_1 - V\tilde{y}_1 \quad (4-12a)$$

Stripping Section Trays

$$M_L \frac{d\tilde{x}_2}{dt} = (R + F)[(5/8)\tilde{x}_2 + (5/8)\tilde{x}_3 + (-1/4)\tilde{x}_4] - (R + F)\tilde{x}_2 + V[(5/12)\tilde{y}_1 + (5/8)\tilde{y}_2 + (-1/24)\tilde{y}_3] - V\tilde{y}_2 \quad (4-12b)$$

$$M_L \frac{d\tilde{x}_3}{dt} = (R + F)[(-1/24)\tilde{x}_2 + (5/8)\tilde{x}_3 + (5/12)\tilde{x}_4] - (R + F)\tilde{x}_3 + V[(-1/4)\tilde{y}_1 + (5/8)\tilde{y}_2 + (5/8)\tilde{y}_3] - V\tilde{y}_3 \quad (4-12c)$$

Feed Tray

$$M_L \frac{d\tilde{x}_4}{dt} = (R)[(1/2)\tilde{x}_4 + (1/2)\tilde{x}_5] - (R + F)\tilde{x}_4 + F.Z_F + V[(1/2)\tilde{y}_3 + (1/2)\tilde{y}_4] - V\tilde{y}_4 \quad (4-12d)$$

Enriching Section Trays

$$M_L \frac{d\tilde{x}_5}{dt} = (R)[(5/8)\tilde{x}_5 + (5/8)\tilde{x}_6 + (-1/4)\tilde{x}_7] - (R)\tilde{x}_5 + V[(5/12)\tilde{y}_4 + (5/8)\tilde{y}_5 + (-1/24)\tilde{y}_6] - V\tilde{y}_5 \quad (4-12e)$$

$$M_L \frac{d\tilde{x}_6}{dt} = (R)[(-1/24)\tilde{x}_5 + (5/8)\tilde{x}_6 + (5/12)\tilde{x}_7] - (R)\tilde{x}_6 + V[(-1/4)\tilde{y}_4 + (5/8)\tilde{y}_5 + (5/8)\tilde{y}_6] - V\tilde{y}_6 \quad (4-12f)$$

Reflux Drum

$$M_{LD} \frac{d\tilde{x}_7}{dt} = -(R)\tilde{x}_7 + V[(1/2)\tilde{y}_6 + (1/2)\tilde{y}_7] - D\tilde{x}_7 \quad (4-12g)$$

where

- $i = 1, 2, \dots, 7$ represent the collocation points
- $\tilde{x}_i(t)$ = Liquid phase compositions at collocation point i ;
- $\tilde{y}_i(t)$ = Vapor phase compositions at collocation point i
- M_L = Tray inventories assumed constant for all trays
- M_{LB} = Inventory in bottoms sump
- M_{LD} = Reflux drum inventory
- R = Reflux flow rate
- D = Distillate flow rate
- B = Bottoms flow rate
- F = Feed flow rate
- Z_i = Feed composition

These are the model equations that were used in the optimizer after discretization.

4.4 Optimization Problem Formulation

The main aim of the study is to develop an optimization algorithm that will continuously receive inputs from the process, and optimize these inputs and steer the process to an economic optimum. The objective of this optimizer is thus to maximize the profit made by the distillation column, which is simply the difference between the value that the products give and the cost of the raw materials necessary for the separation. The optimization is subject to several constraints, which may be physical limitations of the column; design limitations; safety considerations; product quality constraints etc.

The specification of the objective function and the constraints constitutes the optimization problem. This is developed as follows –

Costs and Values

These costs and values for the column are summarized below:

Costs

For Feed

$$= (\text{Feed flow rate, lb/hr}) (\text{Feed cost, \$/lb}) = \mathbf{FC_F, \$ /hr}$$

For Reboiler steam

$$= (\text{Steam flow rate, lb/hr}) (\text{Steam cost, \$/lb}) = \mathbf{SC_S, \$ /hr}$$

Values

For Top product

$$= (\text{Top product price, lb/hr}) (\text{Top product cost, \$/lb}) (\text{Top Product Cost function})$$

$$= \mathbf{DV_D Z(x_D), \$ /hr}$$

For Bottoms product

= (Bottom product price, lb/hr) (Bottom product cost, \$/lb) (Bottom Product Cost function)

= $BV_B Z(x_B)$, \$/hr

where, $Z(x_i)$ is a cost function for the i th product, and X_i is the minimum purity for which the i th product has any value

Thus, the objective function becomes:

$$\text{Maximize } J = \Sigma[(DV_D Z(x_D) + BV_B Z(x_B)) - (FC_F + SC_S)] \Delta t \quad (4-13a)$$

The following simplifications can be made

- The cost function $Z(x_i, X_i)$, is a function which describes the cost decrease as a function of product purity. For purposes of this study, this will be approximated as a linear function of purity. Thus, $Z(X_D) = X_D$ and $Z(X_B) = X_B$
- The feed to the column is usually an unmeasured disturbance, and it is assumed to flow at no cost to the distillation column. Hence this can be removed from the optimization as it will not affect the optimization
- The steam flow rate is assumed to be related to the vapor boilup using:

$$S\lambda_S = V\lambda_V$$

where the λ represent the latent heat of vaporization of the respective streams.

Hence, in the objective function, SC_S is replaced by VC_V where

$$C_V = (\lambda_S/\lambda_V)C_S$$

- Although the reflux is not a product per se, increasing the reflux does cost us in the sense that the product withdrawn is reduced, and also pumping and other costs increase. This is reflected by including the reflux cost C_R in the objective function.

- Also, in conventional Optimizers, there is a rate of change constraint, which penalizes overly aggressive control action. In this study, these rate constraints for manipulated variable changes are not accounted for.

Based on the above simplifications, the objective function becomes:

$$\text{Maximize } J = \Sigma[(DV_D x_D + BV_B x_B - VC_V - RC_R)] \Delta t \quad (4-13b)$$

This is the objective function commonly used in online optimization studies such as those by Moore et. al (1991) and Pollard et al. (1970).

Depending on the rigorousness of the economics required, other costs such as pumping, cooling and even taxes payable can be included in the analysis. However, for the sake of simplicity, only the above costs are considered.

Constraints

The constraints for the distillation column are given below:

- | | |
|---------------------------------|--|
| • Design Pressure | $P \leq P_{\text{design}}$ |
| • Flooding limit for the column | $R \leq R_{\text{max}}$ |
| • Weeping limit for the column | $R \geq R_{\text{min}}$ |
| • Bottoms flow | $0 \leq B \leq F$ |
| • Reflux drum level | $h_{\text{acc,min}} \leq h_{\text{acc}} \leq h_{\text{acc,max}}$ |
| • Bottoms level | $h_{\text{bot,min}} \leq h_{\text{bot}} \leq h_{\text{bot,max}}$ |
| • Product quality | $x_D^L \leq x_D \leq x_D^U$
$x_B^L \leq x_B \leq x_B^U$ |
| • Equilibrium | $y_i = \alpha x_i / (1 + (1-\alpha)x_i)$ |
| • Model constraints | Eq. 4-12a-e |

Of these, the pressure constraint cannot be modeled easily. The constant pressure assumption makes this constraint irrelevant. The reflux drum and the column base are assumed to be perfectly level controlled. Hence, these constraints are also invalid. Also, using the collocation model,

$$x_b \equiv \tilde{x}_1 \text{ and } x_d \equiv \tilde{x}_7$$

Thus the optimization problem becomes

$$\text{Maximize } J = \Sigma(DV_D x_D + BV_B x_B - VC_V - RC_R)\Delta t$$

Subject to

$$C_1 \leq R \leq C_2 (B+C_3)-F$$

$$R \geq R_{min}$$

$$0 \leq B \leq F \quad (4-14)$$

$$x_D^L \leq x_D \leq x_D^U$$

$$x_B^L \leq x_B \leq x_B^U$$

$$y_i = \alpha x_i / (1 + (1-\alpha)x_i)$$

Model constraints Eq. 4-12a-e

This simplified objective function will be used for the distillation column to test the proposed control strategy.

This chapter discussed the optimization and the simulation of the distillation column. The “control aspects” will be discussed in the next chapter, where the proposed strategy will be compared with conventional PI control and online optimization.

CHAPTER 5

ALGORITHM DEVELOPMENT

Thus far, the basics for the development for a dynamic optimization algorithm, whose objective is to maximize profit over a time horizon, were discussed. With these basics, it is now possible to develop a strategy for implementation of this concept. First, the steps for the development of the algorithm for Control to Economic Optimum are described.

The performance of this strategy will be compared with conventional control schemes, a discussion on the development of the algorithms for conventional PI control and online optimization follows. A point worth noting in these comparison is that since this is a “first step” study which involves preliminary demonstration of a new concept, idealized models and simplifications have been made. Thus, a very simple PI control and supervisory steady state optimization scheme have been chosen for comparison. It must be emphasized that the performance differences between the new and conventional schemes would probably not be as great if more advanced conventional control strategies such as DMC are chosen. These studies must be carried out before this concept is ready for implementation.

5.1 Control to Economic Optimum

In Chapter 1, it was mentioned that any control strategy should specify

- A set of control objectives
- A set of measured variables
- A set of manipulated variables

- A structure interconnecting measured and manipulated variables

The concept of control to economic optimum will be analyzed with respect to the above control aspects:

- *Control Objectives –*

The objective for this approach, as discussed earlier is to maximize profit. However, since the process should also be kept under control, it is necessary that while maximizing profit, the process not violate any design, safety and environmental constraints. For the distillation column, the profit to be maximized is given by the objective function in Eq. 4-14.

- *Measured Variables –*

It is necessary to measure certain variables, so that, based on the values measured, the control system can take appropriate action to steer the process in such a way that the control objective mentioned above is maximized. For the distillation process, the performance of the process can be gauged by measuring the *compositions* and *temperatures* at each tray/section in the column, and the *flow rates* of all the streams entering and leaving the process. If the compositions and temperatures are within bounds and at the values dictated based on the control objective, the process is under control; on the other hand, the controller should take appropriate action. In the simplified model, which assumes equimolar overflow, the energy balance is not considered; hence, only the compositions and flow rates will be measured.

- *Manipulated Variables –*

If the measured variables are not at their respective optimal values, then the controller should manipulate certain variables to move the process in a direction that

would maximize the control objective. For the distillation column, the variables that can affect the control objective are the *top and bottom compositions; the distillate and bottoms flow rate; the feed flow rate; and the reflux and vapor boilup*. These are all decision variables for the controller in its quest to maximize the control objective. Since the distillation column has 2 degrees of freedom (Luyben 1992), in reality, only 2 of the above variables are “adjustable” by the optimizer, and the other variables are fixed if particular values for these are chosen by the optimizer. These manipulated variables for the distillation column are chosen to be the vapor boilup and the reflux flow rate (see Henry and Mujtaba 1998). However it must be emphasized that the controller chooses values for these variables only after due consideration to the constraints and economic values for the other variables.

- *Interconnecting the Variables –*

As mentioned before, the model fixes the relationship between the variables of the process. For the optimizer, the model chosen was the collocation model developed in Chapter 4. The reasons why this model was chosen were explained in Chapter 4. The model equations are added as equality constraints to the dynamic optimization problem.

Using the above control structure and the concepts of orthogonal collocation on finite elements discussed in Chapter 4, it is possible to develop a dynamic optimization algorithm for the distillation column.

5.1.1 The Optimization Problem – Applying Orthogonal Collocation

In Chapter 3, the method of orthogonal collocation on finite elements was discussed. The method involves discretizing both independent and dependent variable

profiles using polynomial approximations, and expressing the objective function and the inequality constraints in terms of these discretized variables. The model differential equations are expressed as residuals using the discretized variables. Also, time is discretized by partitioning finite elements and further into collocation elements within the finite elements. A simple example for applying orthogonal collocation to a system of differential equations is given in Appendix C. The steps for converting the distillation column optimization problem into a form suitable for applying orthogonal collocation follow very similar steps.

The optimization problem for the distillation column was developed in Chapter 4 and is shown below:

$$\text{Maximize } J = \Sigma(DV_D x_D + BV_B x_B - VC_V - RC_R)\Delta t$$

Subject to

$$C_1 \leq R \leq C_2(B+C_3)-F$$

$$R \geq R_{\min}$$

$$0 \leq B \leq F \quad (4-14)$$

$$x_D^L \leq x_D \leq x_D^U$$

$$x_B^L \leq x_B \leq x_B^U$$

$$y_i = \alpha x_i / (1 + (1-\alpha)x_i)$$

Model constraints Eq. 4-12a-e

The procedure to convert the above optimization problem for the distillation column follows:

Each of the state and control variables in the above equations must be discretized. The discretized equivalent of each control and state variable is given in Table 5-1:

Table 5-1: Discretization of Distillation Column Variables

Variable	Symbol	Discretized Equivalent
Bottoms flow rate	B	$\sum_{j=1}^{NCOL} B_{[ij]} \Psi_{[ij]}(t)$
Distillate flow rate	D	$\sum_{j=1}^{NCOL} D_{[ij]} \Psi_{[ij]}(t)$
Vapor boilup flow rate	V	$\sum_{j=1}^{NCOL} V_{[ij]} \Psi_{[ij]}(t)$
Reflux flow rate	R	$\sum_{j=1}^{NCOL} R_{[ij]} \Psi_{[ij]}(t)$
Distillate composition	$x_d \equiv \tilde{x}_7$	$\sum_{j=0}^{NCOL} \tilde{x}_{7[ij]} \Phi_{[ij]}(t)$
Bottoms composition	$x_b \equiv \tilde{x}_1$	$\sum_{j=0}^{NCOL} \tilde{x}_{1[ij]} \Phi_{[ij]}(t)$

Using the discretized equivalents of the variables, and the property that,

$$\Phi_{[ij]}(\tau) = \prod_{\substack{k=0 \\ k \neq j}}^{NCOL} \frac{(\tau - \tau_k)}{(\tau_j - \tau_k)} \Rightarrow \Phi_{[ij]}(\tau_j) = 1, \text{ where } j \text{ is an interior collocation point}$$

$$\Psi_{[ij]}(\tau) = \prod_{\substack{k=1 \\ k \neq j}}^{NCOL} \frac{(\tau - \tau_k)}{(\tau_j - \tau_k)} \Rightarrow \Psi_{[ij]}(\tau_j) = 1$$

the objective function can be rewritten in discretized form as:

Maximize

$$\sum_{i=1}^{NFE} \left[\sum_{j=1}^{NCOL} [D_{ij} \psi_{[ij]}(1)] \tilde{x}_{7ij} V_d + \sum_{j=1}^{NCOL} [B_{ij} \psi_{[ij]}(1)] (1 - \tilde{x}_{1ij}) V_b - \sum_{j=1}^{NCOL} [V_{ij} \psi_{[ij]}(1)] C_v - \sum_{j=1}^{NCOL} [R_{ij} \psi_{[ij]}(1)] C_R \right] \cdot (1 - \tau_{NCOL-1}) \Delta \alpha_i$$

< ----- objective function value at end of each finite element ----- >

$$+ \sum_{i=1}^{NFE} \left[\sum_{j=1}^{NCOL} [D_{ij} \tilde{x}_{7ij} V_d + B_{ij} (1 - \tilde{x}_{1ij}) V_b - V_{ij} C_v - R_{ij} C_R] \{ \tau_{j+1} - \tau_j \} \right] \Delta \alpha_i$$

< --- objective function value at interior collocation point ----- >

where the first $i = 1$ to NFE sum is **nothing but the objective function value at the end condition of each finite element; the second $i = 1$ to NFE sum represents the objective value at the interior collocation points.**

The constraints are also discretized using the above table and the final objective function and constraints are written in discretized form suitable for applying orthogonal collocation as shown in Appendix D. Appendix D lists the final objective function and constraints as used in the GAMS optimizer.

The equalities and inequalities given in Appendix D form the constraints to the dynamic optimizer – the optimal solution is one which maximizes the objective function in the above equation without violating constraints.

Some comments on the optimization are in order – these are covered in greater detail in Chapter 7:

The solution to the optimization problem above are the control profiles R and V which maximize the objective function. It is to be noted that, in the above optimization problem, the α_i are finite element lengths and *these are specified by the user*. This leads to several issues: In problems that are nonlinear in state variables, the optimal control profiles are difficult to obtain as these optimal profiles have bang-bang (up and down) and/or singular arc portions (Cuthrell and Biegler 1988). Thus, control profiles with discontinuities are very difficult to approximate. This is because the optimal profile is constrained to have the point of discontinuity at the end of each finite element, whose location is specified by the user.

Two different solutions have been proposed for this problem. Cuthrell and Biegler (1988) propose that the correct points of discontinuity can be found if the location of the finite element points are made decision variables in the optimization algorithm. In other words, we let the optimizer decide what the optimal length for each finite element is. Thus in the objective function, the $\Delta\alpha_i$'s are left as decision variables, further increasing the complexity and the nonlinearity of the problem.

Tanartkit and Biegler (1997 a/b) propose a second solution where a single optimization problem suggested by Cuthrell and Biegler is replaced by two nested problems. In this nested approach, the element placement problem of Cuthrell and Biegler is decoupled from the optimization of other decision variables. Briefly, the inner problem involves finding the optimal values of the parameters, state variables and control variables for a given set of finite elements; then the outer problem is used to update the element spacing according to the optimality and the stability of the overall problem (Tanartkit and Biegler 1997b). These issues will be discussed later.

The point is that both the above solutions were not included in the current study. There are several reasons for this, the principal reason being that the optimization in the demonstration version of GAMS used in the study could only support a certain number of nonlinear elements and decision variables. The reader is directed to Appendix-B for further discussion on the constraints due to the demonstration version.

The implementation of the control to economic optimum strategy follows.

5.1.2 Implementation

As mentioned briefly in Chapter 3, the operational objective of this unified optimizer-controller is to maximize the profit made by the process being controlled. Since the optimizer runs frequently (every three minutes in the study – see Chapter 6, Section 6.2), the optimization algorithm receives the most current operating points as input and provides the optimal values to the process. Hence, the optima are a better reflection of the current state of the plant. Further, a dynamic optimization algorithm also provides the most optimum path to the optimal conditions. This is the first step towards developing a maneuverable process that steers itself to the optimum conditions along an optimal control path.

Before the actual mechanism is discussed, the entities involved in the study are listed:

- *The Process* – As mentioned in the previous chapter, the process being chosen for the current study is a methanol-water distillation column simulation. The main reason for studying this process is its industrial relevance. Also, its multivariable and nonlinear nature provide just enough complexity. The *Process* model developed in

Section 3-2 is used. The current values of the independent and dependent variables of the process are the inputs to the subsequent optimization block.

- *The Optimization Algorithm* – This is a “black box” into which inputs from the process flow. The black box contains the optimization program – the NLP developed in the previous section. Usually, the optimization is carried out by dividing the physical space into different co-ordinates (one for each control and state variable) and moving in a stepwise manner along that direction which improves the performance criterion. The Optimizer achieves this by guessing a direction, calculating the performance criterion and if it is found to improve to advance in that direction, and if it does not to re-guess a new direction. Having guessed the optimal direction to take for each control variable, it thus provides a *trajectory* or *path* for the control variables to reach the final optimal point. These trajectories form the input to the process. In this study, the optimization algorithm chosen is a nonlinear local optimization engine called GAMS/CONOPT. The algorithms used in GAMS/CONOPT, its unique features and comparisons with other optimization packages in GAMS are given in Appendix-B.
- *Simulator* – The simulator is a test device (included solely for the purpose of analyzing the optima provided by the optimizer) which simulates the trajectories provided by the Optimizer *over the entire prediction horizon*. To understand the need for this simulator the actual mechanism of implementation described below must be understood.

Mechanism –

The following steps take place using the above entities –

1. Computation of Optimal Control Sequence - The Optimizer decides a sequence of control steps (as mentioned above, the *trajectory*) over a *prediction horizon*. This prediction horizon is chosen to be of the order of 2/3 of the process settling time.

2. Implementation on Process – The optimal control sequence determined by the Optimizer is an input to the *Process*. However, the entire optimal sequence is not implemented in the *Process*. *Only the first step of the control sequence is implemented*. The reasons for this is two-fold:
 - The Process may be subject to disturbances, which may cause it to behave in a manner different from that expected by the Optimizer when it computed the optimal sequence. Hence, the optimal values in the face of these disturbances are likely to be different
 - The Optimizer uses a model to determine optimal trajectories. However, no model is an adequate representation of reality. Thus, the DAEs, which are used in the model, cannot be considered as a perfect representative of the system. Therefore, operations using these optimal control profiles are no longer optimal (Mujtaba and Hussain 1998). So, the optimal paths determined by the Optimizer need to be updated as in model predictive control to reflect this Process-Model mismatch. Since we implement only the first step of the trajectory, it is impossible to know what would happen if the entire optimal trajectory were implemented assuming there are no disturbances. This is the reason why, for the sole purpose of “seeing” what the Optimizer “says,” a simulator is used to mimic process behavior for analysis.

3. Model Mismatch Update – Since it is impossible to determine whether a discrepancy between the process behavior and the behavior expected by the Optimizer based on

its model, is due to model mismatch or due to disturbances, it is assumed that any discrepancy is entirely due to model mismatch. Hence, to reflect this, we need to choose initial conditions for the Optimizer consistent with its model. This is done as follows:

We define a Process-Model Mismatch (PMM) term as follows:

$PMM = x_{process} - x_{predicted}$, where

$x_{process}$ = Actual measured value of state variable after implementing
the first control step in the optimal control trajectory (5-2)

$x_{predicted}$ = value of state variable predicted by the Optimizer
based on its model

The first time the Optimizer is run the Process-Model Mismatch (PMM) is assumed to be zero. However in subsequent runs, the PMM will be determined by the above equation. The way the PMM is incorporated in the optimization is by correcting the values of the state vector predicted by the Optimizer by summing the PMM term before evaluating the objective function as follows:

$$x_{corrected} = x_{predicted} + PMM \quad (5-3)$$

and using these $x_{corrected}$ values in the objective function.

Also, to provide initial conditions consistent with the Optimizer model, the initial conditions chosen are the $x_{predicted}$ values at the end of the control step implemented in the process.

Thus, this strategy is used to provide economic, optimal, nonlinear control to the process. This should steer the process in the direction of optimal economic operation.

The actual “numbers” used for the prediction horizon, the finite element lengths etc will be discussed in the next chapter.

5.2 PI Control

In the PI control strategy, a very simple scheme is chosen to provide a basis for comparison with the control to economic optimum strategy. Setpoints are chosen for x_d (x_{dset}) and x_b (x_{bset}) and these are kept fixed during the time for which the study is carried out, irrespective of disturbances. In other words, there is no optimization carried out, and the setpoints are kept fixed. The reflux rate R , and the vapor boilup V are chosen to be the manipulated variables to control x_d and x_b respectively. This means that R and V are continuously manipulated in accordance with the PI control laws to keep the compositions x_d and x_b at their respective setpoints as follows:

$$V_{new} = V_{old} + K_{cB} \left[e_b + \frac{\int e_b dt}{\tau_{IB}} \right] \quad (5-4)$$

$$R_{new} = R_{old} + K_{cD} \left[e_d + \frac{\int e_d dt}{\tau_{ID}} \right] \quad (5-5)$$

where,

the subscripts $_{new}$ and $_{old}$ represents the new value of the respective manipulated variable.

K_{cB} , τ_{IB} and K_{cD} , τ_{ID} represent the PI tuning parameters of the bottom and top composition controllers respectively

e_b and e_d are the bottom and top composition errors defined by:

$$\begin{aligned} e_d &= x_{dset} - x_d \\ e_b &= x_{bset} - x_b \end{aligned} \quad (5-6)$$

The tuning parameters chosen for the purposes of the study are based on open-loop tests, using Ziegler-Nichol's rules. The values are given in the next chapter. This control algorithm should regulate the process in such a way that the deviation from setpoint is dealt with by adjusting the manipulated variables in accordance with the PI control laws given above. Comparisons were made between PI control and control to economic optimum for feed composition and flow disturbances. The results are discussed in the next chapter.

5.3 Steady State Online Optimization

The main differences between the steady state optimization strategy and the control to economic strategies were outlined in Chapter 3. In the steady state optimization, a steady state model is used and set point updates are made on a fairly infrequent basis. The setpoint updates are assumed to change the x_{bset} and the x_{dset} in the PI control laws discussed in the PI control scheme above, based on a steady state economic optimization. Thus, a simple steady state supervisory optimization and an underlying PI regulatory control scheme are chosen to demonstrate the online optimization strategy and provide a comparison with the control to economic optimum scheme.

5.3.1 Developing the Steady State Model

The dynamic models developed in the previous chapter can be easily changed to steady state models by setting the derivatives to zero. These steady state equations form the equality constraints for the optimization problem discussed in the next section. In conventional online optimization studies on distillation columns, such as those by Moore and Corripio (1991), the steady state optimum is determined analytically by setting the derivative of the objective function with respect to a cost variable to zero, and

solving the resulting equations. These studies also assume a simple empirical yield model. The analytical equations developed are extremely complex and this is just for single-ended composition control, which guarantees purity on only one end of the column.

In this study, to avoid the complexity of the analytical solution and the dubitable empirical yield model, the optimum is determined as a solution to a steady state optimization problem where the model equations form equality constraints and design limits, product quality constraints etc constitute the inequality constraints. The steady state model uses the same assumptions as the Process model with the additional assumption of steady state, which makes all the derivatives vanish. These steady state equations as mentioned above form the equality constraints to the optimization problem.

The equations without their derivation are given below:

$Fx_f = Dx_D + Bx_B$	(Overall component material balance)
$V = D + R$	(Material balance in accumulator)
$Vy_{N_t} = (D + R)x_D$	(Component balance in accumulator)
$y_{N_t-1} = \frac{Vx_d + Rx_d/(\alpha - (\alpha - 1)x_d)}{V}$	(Component balance in top tray)
$y_{i-1} = \frac{Vy_i - Rx_{i+1} + Rx_i}{V}; i = N_t - 1 \text{ to } N_f + 1$	(Component balance on enriching trays)
$y_{i-1} = \frac{Vy_i - Rx_{i+1} + (R + F)x_i - FZ_f}{V}$	(Component balance on feed tray)

$$y_{i-1} = \frac{Vy_i - (R+F)x_{i+1} + (R+F)x_i}{V}; i = N_t - 1 \text{ to } 1$$

(Component balance on stripping trays)

$$B = R + F - V$$

(Material balance in reboiler)

$$x_b = \frac{L_1 x_1 - Vy_b}{B}$$

(Component balance in reboiler)

$$y_i = \frac{\alpha x_i}{(1 + (\alpha - 1)x_i)}$$

(Equilibrium)

(5-7)

5.3.2 Development of the Optimization Problem

In accordance with the definition of steady state (static) optimization, time is not considered in the optimization. The optimal values are based on values at the current time. With this, the optimization program can be written as follows, based on Eq. 4-14

$$\text{Maximize } J = \Sigma(DV_D x_D + BV_B x_B - VC_V - RC_R)$$

Subject to

$$C_1 \leq R \leq C_2 (B + C_3) - F$$

$$R \geq R_{\min}$$

$$0 \leq B \leq F$$

(5-8)

$$x_D^L \leq x_D \leq x_D^U$$

$$x_B^L \leq x_B \leq x_B^U$$

$$y_i = \alpha x_i / (1 + (1 - \alpha)x_i)$$

Model constraints Eq. 5-7

This optimization problem receives its initial inputs from the process, and is made to run at a frequency of once every 1 hour (see Section 6.2). Comparisons with control to economic optimum have been made for feed flow and composition disturbances. These will be discussed in the next chapter.

This chapter discussed the development of the control to economic optimum, PI Control, and simple steady state optimization with PI control algorithms. The results of implementing these algorithms on a distillation column simulation form the focus of the next chapter.

CHAPTER 6

RESULTS AND DISCUSSION

The algorithms for the three control schemes – Control to Economic Optimum (CEO); Steady State Online Optimization (OO) and PI Control (PI) – were discussed in the previous chapter. The results from these control schemes for various test data will be presented in this chapter. Comparisons of the results obtained from the three schemes will be made and the reasons for differences in the results will be analyzed. First however, the input data and preliminary calculations will be discussed.

6.1 Column Data

The process under consideration to demonstrate the performance of the control to economic optimum approach, is as mentioned earlier, a methanol-water distillation column. To run the simulation, as was mentioned in Chapter 4, the column design parameters must be specified. Also, consistent initial conditions must be specified. The design data is based on the binary distillation column simulation given in Luyben (1990). A McCabe-Thiele diagram for a methanol-water system was constructed (as the equimolal assumption is valid), for a top composition of 0.96, a bottom composition of 0.04 and a feed composition of 0.48. The hydraulic time constants, reboiler and reflux drum holdup were obtained from the simulation in Luyben (1990).

The design data for the column are given in Table 6-1 below:

Table 6-1: Design data for distillation column

Total number of trays, N_T	15
Feed tray, N_f	8
Feed composition, z_f	0.48 (mol fraction methanol)
Distillate composition (design), x_d	0.96 (mol fraction methanol)
Bottoms composition (design), x_b	0.04 (mol fraction methanol)
Relative volatility, α	2
Initial tray holdups, M_L	10 mol
Reflux drum hold-up, M_{LD}	100 mol
Bottom sump hold-up, M_{LB}	100 mol
Tray hydraulic time constant, β	0.1 s
Tray efficiency	100 %

Initial compositions given as input to the process are based on the design conditions from the McCabe-Thiele diagram. Initial convergence from these input conditions guarantees that these conditions are made consistent. The above data is provided to the simulation from input text files to the Visual Basic simulation, and at the end of each time step, the outputs are written to an appropriate file as follows –

- Data to be used for subsequent simulation get written to simple text files, which are used as input files in the future
- Data to be displayed – top and bottom compositions; reflux and vapor boilup flow rates – are written to the Excel worksheet in the simulation interface, which allows the user to follow the simulation "live"

- Data to be used by the Optimizer (for the CEO and OO schemes) are written to .GMS files, which are later compiled and executed by GAMS for optimization

6.2 *Open Loop Response Studies*

Open loop studies were carried out on the column from the initial conditions for step changes in specific process variables, while keeping others constant. The simulation is allowed to run for 2 hours and a step change in a variable (reflux for Fig 6-1a and vapor boilup for Fig 6-1b) and the appropriate controlled variable is monitored.

From the open loop studies, settling time and steady state gain data can be obtained, using which the tuning parameters for PI controllers as well as the prediction horizon for predictive control can be decided. Fig 6-1a shows the open loop response of the top composition to a step increase in reflux flow rate while keeping other variables constant. This is studied because the top composition (controlled variable) will be controlled by manipulating the reflux. The specific response shown is for a 5% increase in reflux flow rate. Similarly, Fig 6-1b shows the open loop response in bottom composition to a step decrease in vapor boilup, which is its manipulated variable.

It is worth comparing these open loop responses with the responses obtained when a controller takes compensating action. This ability to compensate for disturbances and still maintain process variables at desired points of operation is the purpose of a controller. These responses will be discussed for the three control schemes (PI, OO and CEO) in the following sections.

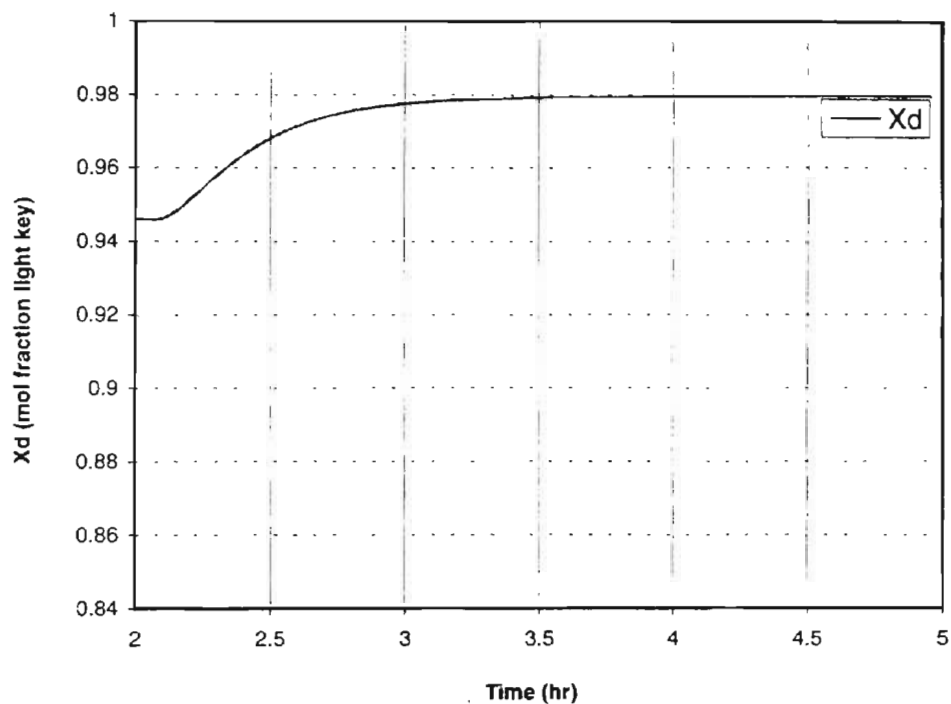


Fig 6-1a Open loop response to step increase in reflux at Time = 2.08 hr

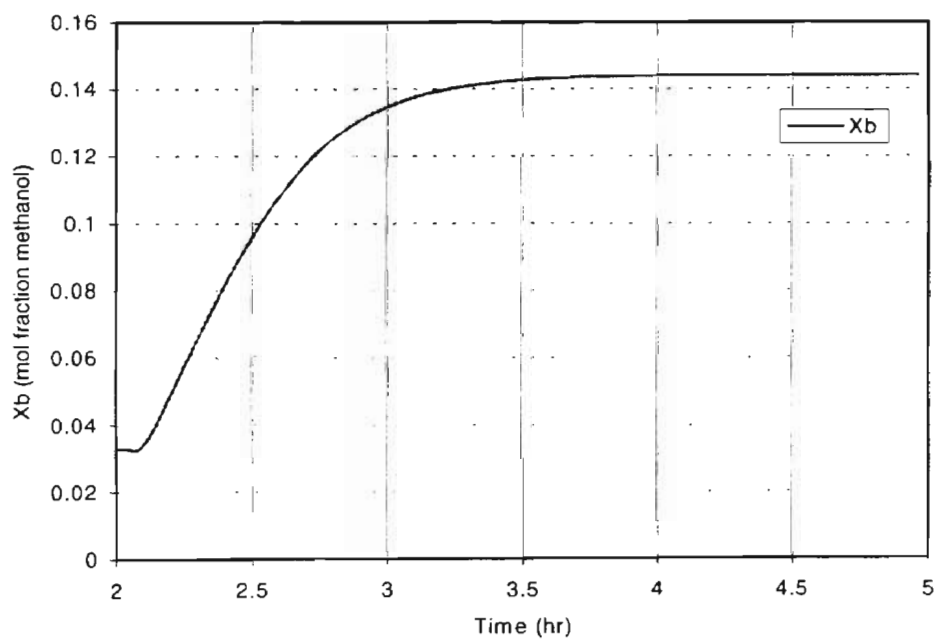


Fig 6-1b - Open Loop Response to Step Decrease in Vapor Boilup at Time = 2.08 hr

The process "reaction" curve in Fig 6-1a/b may be approximated as a first order system with time delay and approximate tuning rules for PI controllers such as Ziegler-Nichols or Cohen-Coon rules. The Ziegler-Nichols rules were chosen to estimate the tuning parameters for top and bottom composition controllers. These are listed in Table 6-4 in Section 6.3.

It is worth noting that the tuning rules are at best approximate. Hence, the comparisons provided below should not be taken as the final word on the performance of the control schemes. Better tuning rules are expected to give better control and possibly, more profitable performance. Also, distillation columns are multivariable in nature – as a result, a step change in a manipulated variable will produce changes in variables not controlled by this manipulated variable as well. For example, a change in the vapor boilup will cause a change in bottom composition, but it will also cause a less significant, but nevertheless, perceptible change in top composition. This can only be resolved using multivariable control techniques mentioned briefly in Chapter 2. Such control schemes will definitely give better control and performance and must also be studied in order to provide a fair comparison. This study, it must be stressed used simple models and control strategies to provide a first step in the direction of economic optimal control. These issues will be discussed further in Chapter 7.

From Fig 6-1 a/b, it is seen that the settling time for the process is found to be of the order of 1-1.2 hours. We define settling time as the time for the process variable to reach within 5% of its ultimate value for a step change in the input. As mentioned in the previous chapter, the prediction horizon for the predictive control in the CEO approach is about 2/3 of the settling time. Thus, for the distillation column under study, the prediction

horizon would be of the order of $2/3$ hours. This translates to the sum of finite element lengths to be $2/3$ hours for the dynamic optimization.

6.3 Optimization Parameters

Since this is a study on a fairly idealized, theoretical simulation of a distillation column, it is difficult to determine exact values of parameters, which play a very crucial role in determining the optimal operating point: these include cost coefficients and constraints on reflux and vapor boilup.

- Cost coefficients were chosen from crude market data available from Chemical magazines and online resources, and by no means is the accuracy of these values claimed. The numbers are chosen to reflect the relative order of magnitude of the values and costs of products and raw materials respectively. A preliminary sensitivity analysis to the values of these cost coefficients is carried out in the study (see Tables 6-5 and 6-7). The values listed below are those which were finally used to study effects of disturbances
- Constraints on reflux and vapor boilups were chosen to be equal to 20% higher than steady state design values for the base case and varied to study the effect of constraints. The optimal manipulated variable profiles are found sensitive to these constraints. This can be explained by the fact that the optimizer tends to push one of the degrees of freedom to its constraint and manipulate the other to keep the process variables within their constraints. Hence, if the constraints are changed, the optimal profile changes also. The values given in Table 6-2 for the reflux and vapor boilups are 120% of the steady state design values, which are respectively 125 mol/hr for reflux and 160 mol/hr for vapor boilups.

For the optimizations involved in the Control to Economic Optimum and Online Optimization strategies, the following parameters shown in Table 6-3 below:

Table 6-2 – Optimization Parameters: Base Case

Parameter	Value
<i>Cost coefficients</i>	
Distillate product value, V_D	6.12 \$/mol
Bottoms product value, V_B	0.95 \$/mol
Vapor boilup cost, C_V	0.002 \$/mol
Reflux cost, C_R	0.001 \$/mol
<i>Bounds</i>	
Lower bound for bottom composition, X_B^L	0.04 mol fraction methanol
Upper bound for bottom composition, X_B^U	0.08 mol fraction methanol
Lower bound for top composition, X_D^L	0.95 mol fraction methanol
Upper bound for top composition X_D^U	0.98 mol fraction methanol
Lower bound for reflux rate, R^L	100 mol/hr
Upper bound for reflux rate, R^U	150 mol/hr
Lower bound for vapor boilup, V^L	130 mol/hr
Upper bound for vapor boilup, V^U	190 mol/hr

6.3.1 Control to Economic Optimum Parameters

As mentioned in previous chapters, CEO is a horizon predictive strategy involving profit maximization over a prediction horizon. The profit objective requires appropriate cost functions to be included in the objective function. The parameters for the strategy are given in Table 6-3:

Table 6-3: Control to Economic Optimum — Dynamic Optimization Parameters

Parameter	Value
<i>Prediction horizon</i>	2/3 hr
<i>Number of finite elements, NFE</i>	2
<i>Number of collocation points, NCOL</i>	2
<i>Finite element lengths, α_1, α_2</i>	1/3 hr; 1/3 hr
<i>Reprediction frequency</i>	Once every 0.03 hr

The results using the above parameters are discussed in section 6-4. The finite elements are chosen to be of equal size, an important issue to be discussed later.

6.3.2 PI Control Parameters

As mentioned earlier in the chapter, PI tuning parameters were decided by simple Ziegler-Nichols rules based on a first order with time delay approximation of the open loop response. These are given in Table 6-4.

Table 6-4: PI tuning parameters using Ziegler-Nichols rules

Controller	Tuning Parameters
Top composition	$K_{cD} = 1186 \text{ mol/hr}$ $\tau_{iD} = 2.7 \text{ /hr}$
Bottom composition	$K_{cB} = 1127 \text{ mol/hr}$ $\tau_{iB} = 1.7 \text{ /hr}$
Setpoints	For $X_D = 0.96$
(mol. fraction methanol)	For $X_B = 0.04$

6.3.3 Online Optimization

The important parameter to be decided in online optimization is the time when the steady state optimizer is made to run and dictate setpoints. For purposes of this study, the time interval between the steady state optimizations will be chosen to be of the order of the settling time of the process or once every hour. This is based on industrial input (see Appendix E). The starting setpoints are chosen to be the same as in PI control.

With these parameters, the results for the three control schemes were obtained as discussed in the next section

6.4 ***Results and Comparison Between the Control Schemes***

The results for performance under a case when there are no disturbances for the CEO scheme are discussed below. In the presence of feed flow and composition disturbances, comparisons with the other two approaches are given. For performance under no disturbances, the column is allowed to start from sub-optimal conditions and after 2-3 minutes the controllers are allowed to take over. Sensitivity to parameters and constraints, and finite element size is analyzed under no disturbances for the CEO approach and these form the 5 preliminary case studies.

For performance under disturbances, the parameters in Table 6-3 are used. Feed flow disturbances studied include 5% step increase and decrease in flow. Composition disturbances include 10% increase and decrease in feed composition.

6.4.1 Preliminary Case Studies – Control to Economic Optimum

These case studies listed in Table 6-5 were carried out without introducing disturbances other than a starting vapor boilup of 177 kmol/hr and a reflux flow rate of 114 kmol/hr, the initial conditions under which the simulation is started.

Table 6-5: Case Studies Conducted

Case	Description
0. Base Case - Table 6-2 values	$R_{\max} = 150$, $V_{\max} = 190$, $R_{\min} = 100$, $V_{\min} = 130$; $V_D = 6.12$ \$/mol, $V_B = 0.95$ \$/mol, $C_v = 0.002$ \$/mol, $\alpha_1 = \alpha_2 = 1/3$
1. Effect of finite element length	
a) $\alpha_1 : \alpha_2 = 1:3$	$\alpha_1 = 2/12$; $\alpha_2 = 6/12$;
b) $\alpha_1 : \alpha_2 = 3:5$	$\alpha_1 = 3/12$; $\alpha_2 = 5/12$
c) $\alpha_1 : \alpha_2 = 5:3$	$\alpha_1 = 5/12$; $\alpha_2 = 3/12$
2. Effect of constraint limits	
a) 10% increase in reflux flow constraint	$R_{\max} = 162.5$; other parameters kept constant
b) 10% decrease in reflux flow constraint	$R_{\max} = 137.5$; other parameters kept constant
c) 10% increase in vapor boilup constraint	$V_{\max} = 208$; other parameters kept constant
d) 10% decrease in vapor boilup constraint	$V_{\max} = 176$; other parameters kept constant
3. Effect of cost coefficients	
a) 10% increase in methanol cost coefficient	$V_D = 6.732$ \$/mol; other parameters kept constant
b) 10% decrease in methanol cost coefficient	$V_D = 5.508$ \$/mol; other parameters kept constant

c) 10% increase in water cost coefficient	$V_B = 1.045$ \$/mol; other parameters kept constant
d) 10% decrease in water cost coefficient	$V_B = 0.855$ \$/mol; other parameters kept constant
e) 10% decrease in water cost coefficient	$C_V = 0.0022$ \$/mol; other parameters kept constant
f) 10% decrease in water cost coefficient	$C_V = 0.0018$ \$/mol; other parameters kept constant

These will be discussed case by case:

6.4.1.1 Case 0: Base Case

The optimal control profile is shown in Fig 6-2a (Case 0). As mentioned in Table 6-5, the base case uses reflux and vapor boilup constraints of 120% of the steady state design values. It is seen that the optimizer drives the vapor boilup to its constraint of 190 mol/hr, while the reflux reaches a final average value of 142 mol/hr. The comparison with other cases follows, which throws greater light on the significance of these numbers.

6.4.1.2 Case 1: Effect of Finite Element Length

In the CEO strategy, it was mentioned that the *finite element lengths were chosen to be of equal lengths*. This is an important assumption in that it influences the optimum profile obtained. As was briefly mentioned in Chapter 4, the step size plays a crucial role in optimal control profiles that have discontinuities in the boundaries between the finite elements. Before the problem is analyzed, the optimal control profiles for the control to economic optimum scheme for various finite element sizes (for R and V) are as shown in Fig 6-2a/b (Case 1a-1c) below.

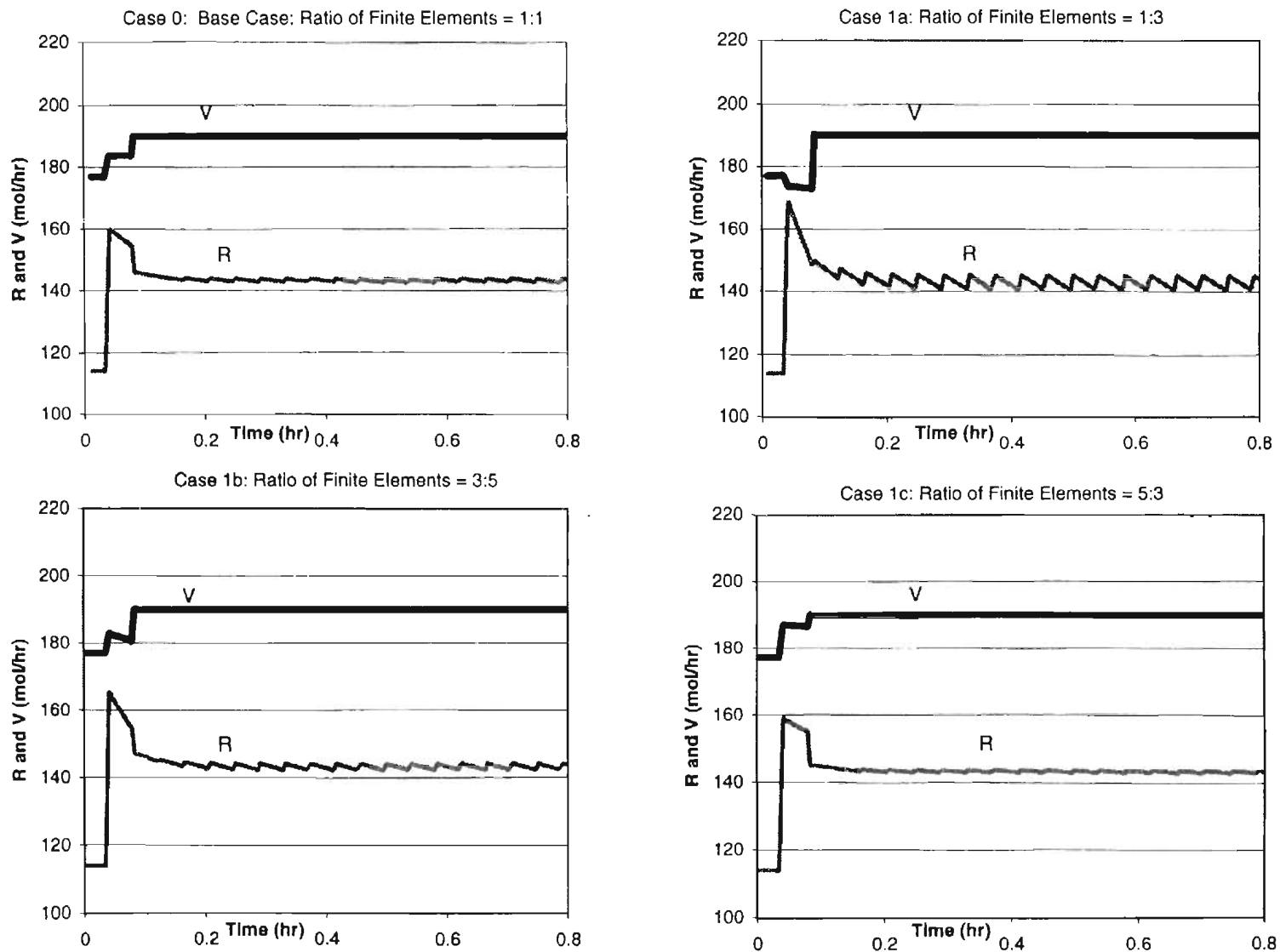


Fig 6-2a Optimal Control Profiles for R/V - Base Case and Case 1 (Effect of Finite Element Lengths)

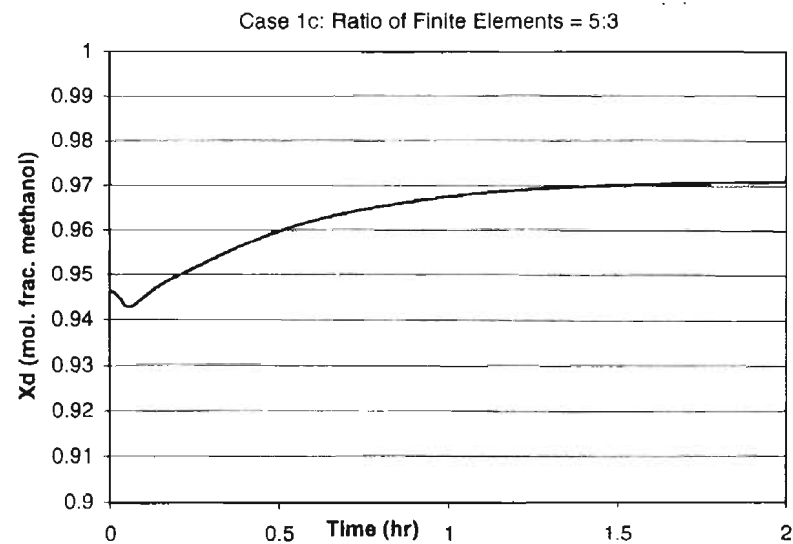
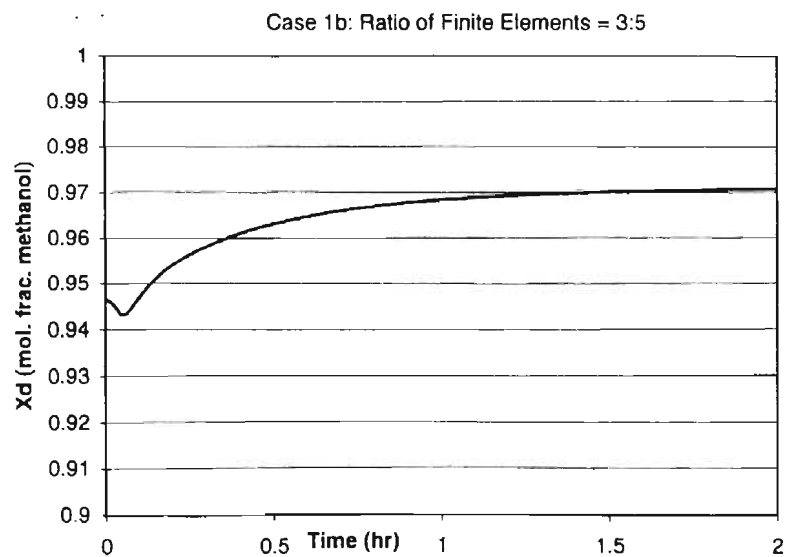
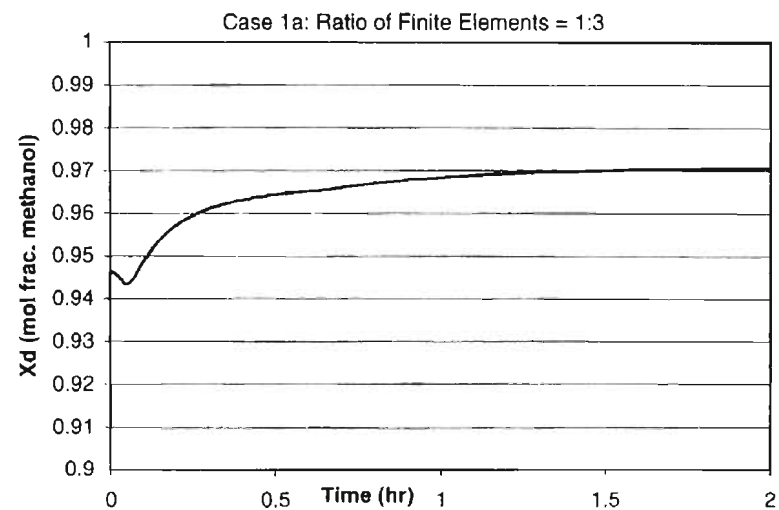
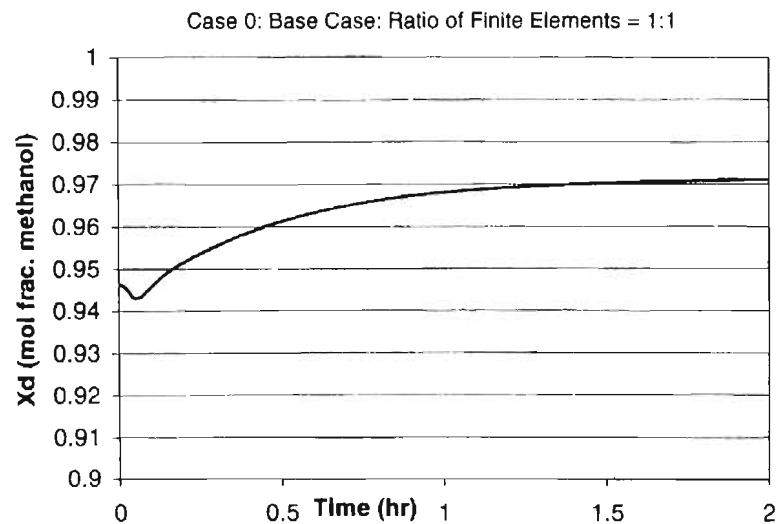


Fig 6-2b Optimal Control Profiles for R and V - Base Case and Case 1 (Effect of Finite Element Lengths)

As shown in Table 6-2, for the base case the finite elements are chosen to be of equal lengths. For cases 1a to 1c, finite element lengths are varied as mentioned in Table 6-5. It is seen that as step size changes the shape of the optimal control profile changes.

This may be because the optimal control profiles may have points of discontinuity in them. *This point of discontinuity is forced to be at the edge of a finite element boundary, when a finite element length is fixed.* In other words, fixing the finite element length fixes the point(s) of discontinuity at the boundary between the finite elements. Such a method does not guarantee that the "best" profile, with the point of discontinuity at its optimal point is found. Thus, there is no way of knowing whether a given profile is *the* optimal profile.

In this problem for the distillation column, *for the given set of parameters*, it is seen that there is a smoothing of the control profile when the first finite element length increases. This may suggest that when the first finite element is of the length of prediction horizon, there would be no ridges. This means that the optimal profile has no point of discontinuity. *However, it must be emphasized that this may merely be a coincidence.* There is no guarantee that with different parameters, the control profile may not have points of discontinuity. A general algorithm thus, should have the capability to fix the optimal point of discontinuity.

An excellent description of the problem is provided in Cuthrell and Biegler (1989), where a problem whose optimal control profile is a "bang-bang" profile is analyzed. The orthogonal collocation strategy uses discretized values of variables. Since this relies on numerical approximations in the discretization, the results obtained depends on the following:

- The number of finite elements, which must be sufficient to cover all points of discontinuity
- The length of the finite elements, which must be so chosen so that the finite element "knots" are at the points of discontinuity
- The degree of the polynomial approximation and interpolation

In the above paper, Cuthrell and Biegler develop a new set of elements known as superelements, which are chosen so as to determine the optimal locations of the points of discontinuity. However, this introduces unnecessary complexity. Cuthrell and Biegler (1989b) again develop another simpler strategy for this problem. The solution is the inclusion of the finite element lengths as decision variables in the optimization. If this is done, then the location of the finite element knots will represent optimal points of discontinuity. However, the nonlinearity of the process goes up by an order of magnitude inducing additional complexity.

Tanartkit and Biegler (1996/1997) develop another solution to the problem. Here they treat the knot placement problem as an outer problem. Thus in the outer problem the finite element lengths are adjusted, while the inner problem is the actual optimization problem. Tanartkit and Biegler also advocate the use of additional constraints called the error approximation constraints to control the discretization error and ensure the accuracy of the approximation, in the outer problem.

In our study, this aspect of the problem remains unsolved, the main reason being that the study is constrained by the limitations in the demonstration version of GAMS, which only allows a fixed number of nonlinear elements, variables etc (see Appendix B). Hence, in this study *equal finite element lengths are chosen to retain the generality of*

the method. Hence, it cannot be said that the points of discontinuity are at their optimal positions.

From 6-2b it is seen that the top composition trajectories have higher slopes when the first finite element length decreases. The bottom composition graphs have similar shapes and hence are not shown. The final top composition for all the cases is found to be 0.971 for the top composition and 0.046 for the bottoms. The saw-toothed may be attributed to the fact that the Optimizer takes more aggressive control actions when the time period available for action is made smaller, as is the case with smaller finite elements. This would explain the fact that the optimal profile has an up-and-down appearance. As the first finite element length increases it is seen that there is a smoother approach of the top composition to its steady state value. The profit for all cases is found to be \$ 668 at the end of 2 hours.

To conclude, finite element lengths should be left as decision variables in the Optimizer so that optimal points of discontinuity in control profiles can be found.

6.4.1.3 Effect of Constraints

This is an important aspect of the study as the freedom available with the manipulated variable constraints determines the final optimum. Hence, in theory, increasing the bounds on the vapor boilup and reflux should provide higher purities of the top and bottom products. The results for the effect of changing the constraints on the reflux and vapor boilup from their base case values are shown in Fig 6-2b. More results are given in Table 6-6.

Table 6-6: Effect of Constraints

Variable	Value
Steady state compositions (mol fraction methanol)	Base case $X_b = 0.047$ $X_d = 0.971$ Case 2a $X_b = 0.047$ $X_d = 0.971$ Case 2b $X_b = 0.047$ $X_d = 0.967$ Case 2c $X_b = 0.048$ $X_d = 0.976$ Case 2d $X_b = 0.049$ $X_d = 0.956$
Steady state values for manipulated variables (mol/hr)	Base case $V = 190$ $R = 150$ Case 2a $V = 190$ $R = 163$ Case 2b $V = 190$ $R = 138$ Case 2c $V = 198$ $R = 150$ Case 2d $V = 176$ $R = 150$
Cumulative Profit (\$)	Base case : 668 Case 2a : 668 Case 2b : 669 Case 2c : 672 Case 2d : 663

- When the reflux flow constraint is relaxed to its Case 2a value, it is seen that the optimum value does not change. This can be explained by the fact that since the vapor boilup has already reached its upper constraint; hence, the optimizer cannot increase the reflux in the hope of increasing the profit as the vapor boilup cannot be further increased
- Tightening the reflux constraint (Case 2b) brings the reflux to its upper constraint, and this forces the vapor boilup down from its upper constraint. Hence, the top product purity drops. However, since the reflux cost has been reduced, it just compensates for the loss of purity and a very slight increase in profit is obtained as shown

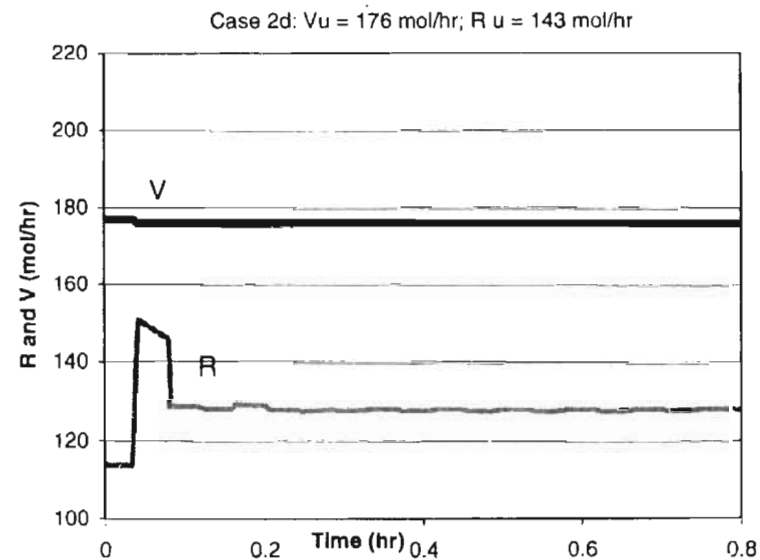
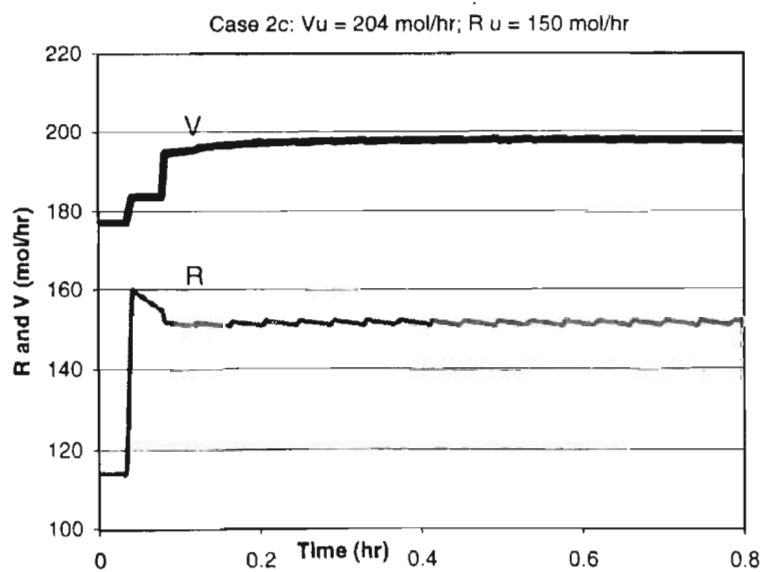
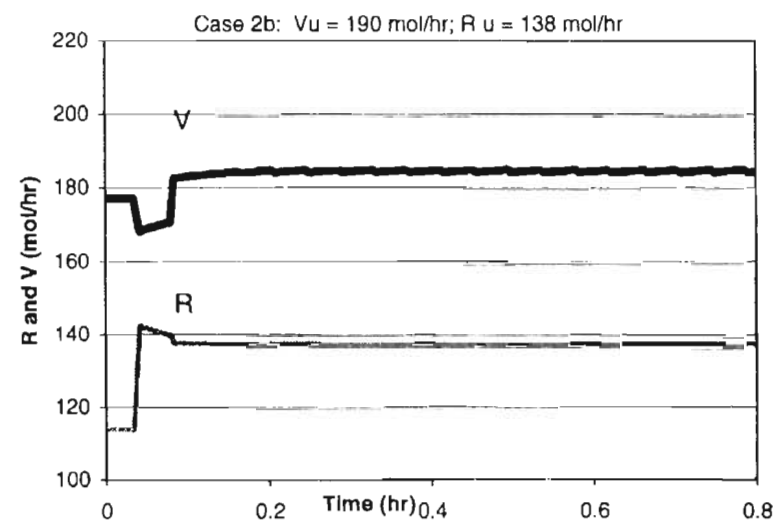
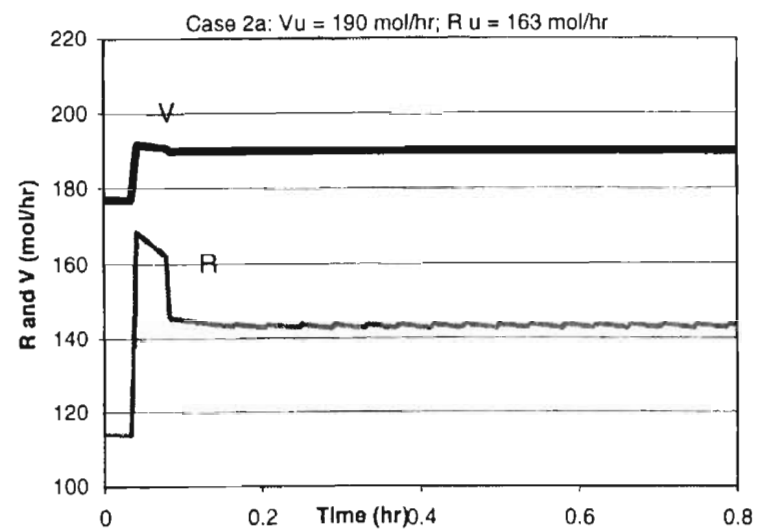


Fig 6-2c- Optimal Control Profiles for R/V. Case 2: Effect of Constraints

- Relaxing the vapor boilup constraint (Case 2c) has two effects. While the increase in vapor boilup increases bottom purity, relaxing this constraint allows the optimizer to increase the reflux to a value higher than Case 2a, resulting in higher purity. This increases the profit to a slightly higher value
- Tightening the vapor boilup constraint (Case 2d) forces the optimizer to drop the reflux and decreases the top composition. This causes the profit to drop slightly.

6.4.1.4 *Effect of Cost Coefficients*

The values of the top product is an order of magnitude higher than the bottom product, which is in turn higher than the costs of the reflux and vapor boilup. These cost coefficients as was emphasized in the previous section, are by no means accurate, and are chosen to be order-of-magnitude-representative values.

With this distribution of costs, it is expected that a change of 10% in the cost or value of any product or raw material would not force the optimizer to abandon its policy of maximizing top product quality and quantity. Tests with 10% changes in cost coefficients for methanol, water and the vapor boilup validate this point. *The optimal control trajectory is exactly the same for all the six cases.* The profit changes are only due to the change in the cost coefficients, and the compositions and control profiles remain unchanged (Table 6-7). In the study, one of the products has much higher value than the other. The optimum operating point is at the upper constraint of the vapor boilup, the nearest constraint. In fact, it is found that a change of 50% is needed in the methanol cost for the optimizer to "consider" a different profile. An order of magnitude change is needed in the bottoms value or the vapor boilup cost for the optimal profile to change. In this case, the products have similar value, and the minimum cost (or

maximum profit) will be achieved by minimizing utility consumption (Shinskey, 1992) and the Optimizer is found to bring both the products to their lower specification limits and minimize utility consumption.

Table 6-7 – Effect of Cost Coefficients

Case	Compositions (steady state)	R,V Profiles	Cumulative profit, \$
0 Base Case	$X_d = 0.971$, $X_b = 0.047$	Fig 6-2a (Case 0)	668
3a $V_D = \$ 6.732/\text{mol}$	Same as above	Same as above	725
3b $V_D = \$ 5.508/\text{mol}$	Same as above	Same as above	611
3c $V_B = \$ 1.045/\text{mol}$	Same as above	Same as above	678
3d $V_B = \$ 0.855/\text{mol}$	Same as above	Same as above	658
3e $C_v = \$ 0.0022 / \text{mol}$	Same as above	Same as above	668
3f $C_v = \$ 0.0018 / \text{mol}$	Same as above	Same as above	668

Hence, it is concluded that the optimal control profile is not very sensitive to the cost coefficients chosen for the given order of magnitude of the cost coefficients. These cost coefficients are one of the "business" aspects of the optimization problem formulation. The optimization problem can be formulated in such a way as to answer some of these business concerns. Accordingly, the Optimizer dictates the direction the process should take to optimize the particular performance criterion. These business aspects of optimization are detailed in Appendix H.

6.4.2 Base Case Comparison Between the Control Schemes

Using the base case values given in Table 6-2 for the CEO scheme, and the parameters for the PI and the OO schemes from Table 6-4 and Section 6.3.3, a base case comparison between the methods was made. The results are given in Fig 6-3a/b/c/d. It is thus seen that the three control schemes give about the same profit when there are no disturbances (Table 6-8). The CEO strategy gives about 3% more profit than the OO, which gives about 3% more profit than the PI scheme. The steady state Optimizer and the CEO Optimizer use the same optimization coefficients. Hence, it is expected that they must predict the same values of state and manipulated variables at steady state. Results for the base case support the above fact. It is seen that the two Optimizers reach the same steady state.

However, the most dramatic improvement of the CEO scheme is its early determination of the optimal conditions and its crisp determination of the path to the optimal conditions. This is to be expected as we treat time as an explicit entity in the optimization. From the reflux and vapor boilup curves (see Fig 6-3 c/d) it is seen that the control to economic optimum scheme reaches the optimum conditions in about 10 minutes. This brings the process to steady state faster. The PI control algorithm causes the oscillatory response in the other two control schemes which makes the process go up and down before it settles to a final steady state. The setpoints chosen for the PI control scheme were chosen from the steady state design values for the top and bottom composition, and hence they are quite close to the optimum when there are no disturbances. The steady state Optimizer is run every 1 hour and it is seen therefore that for the first one hour the profiles match that of the PI control strategy and after 1 hour, the Optimizer catches up with the CEO Optimizer.

Fig 6-3a: Top Composition curves - Base Case

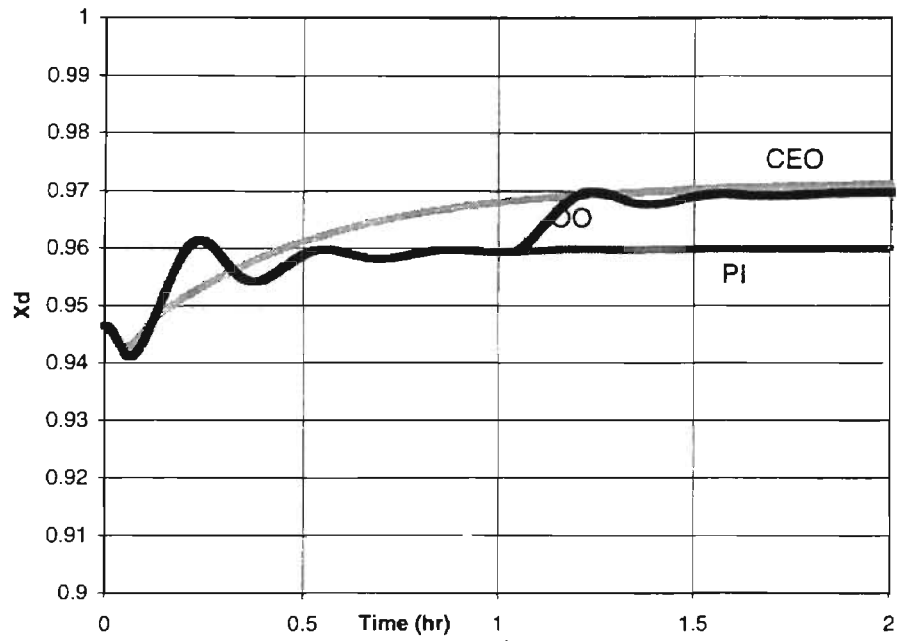


Fig 6-3b: Bottom Composition curves - Base Case

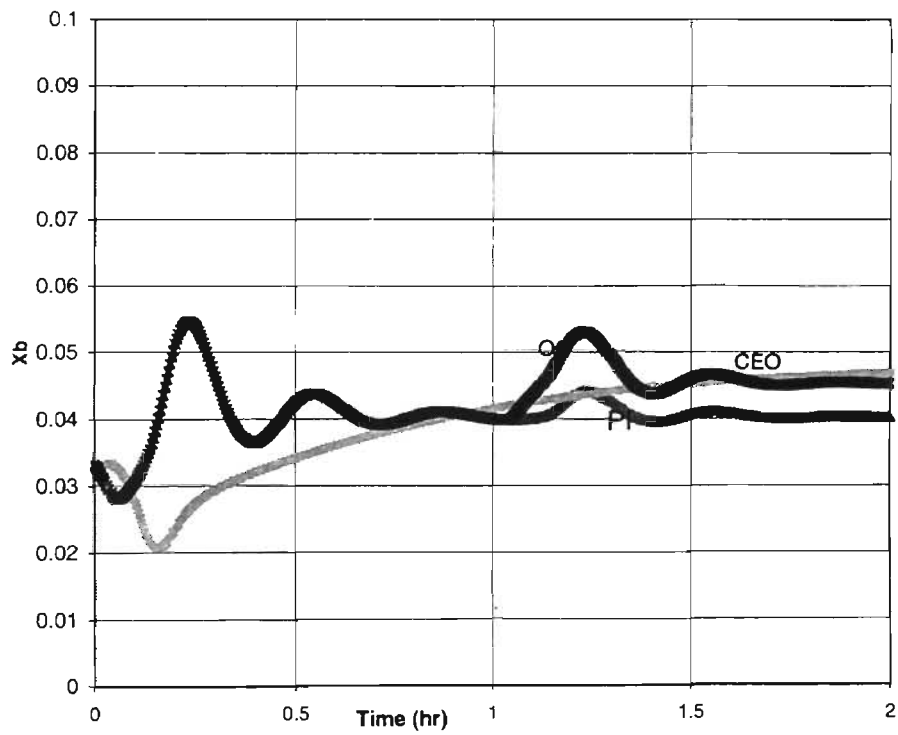


Fig 6-3c: Manipulated Variables (R)

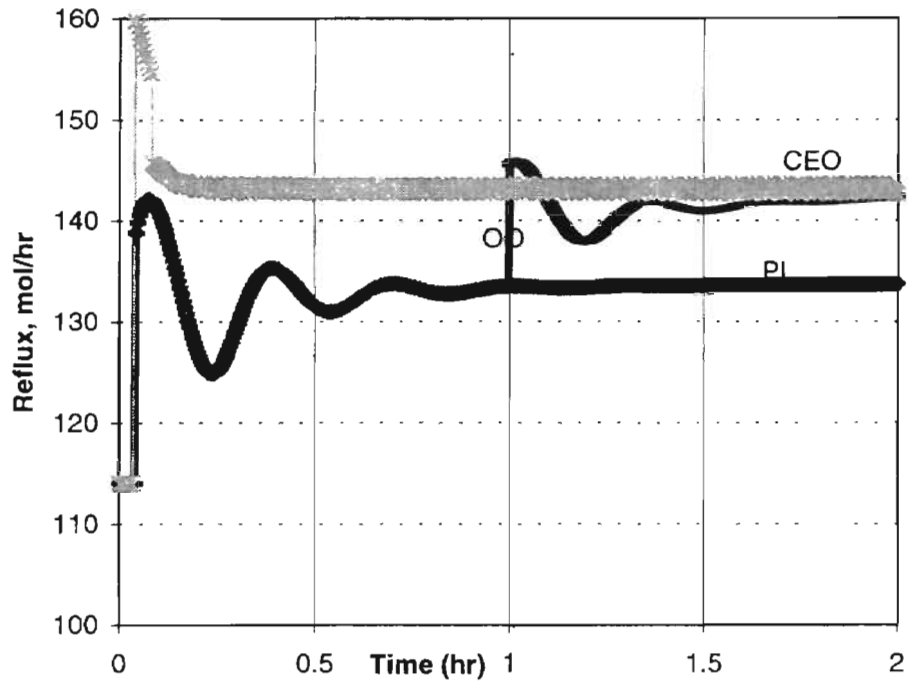
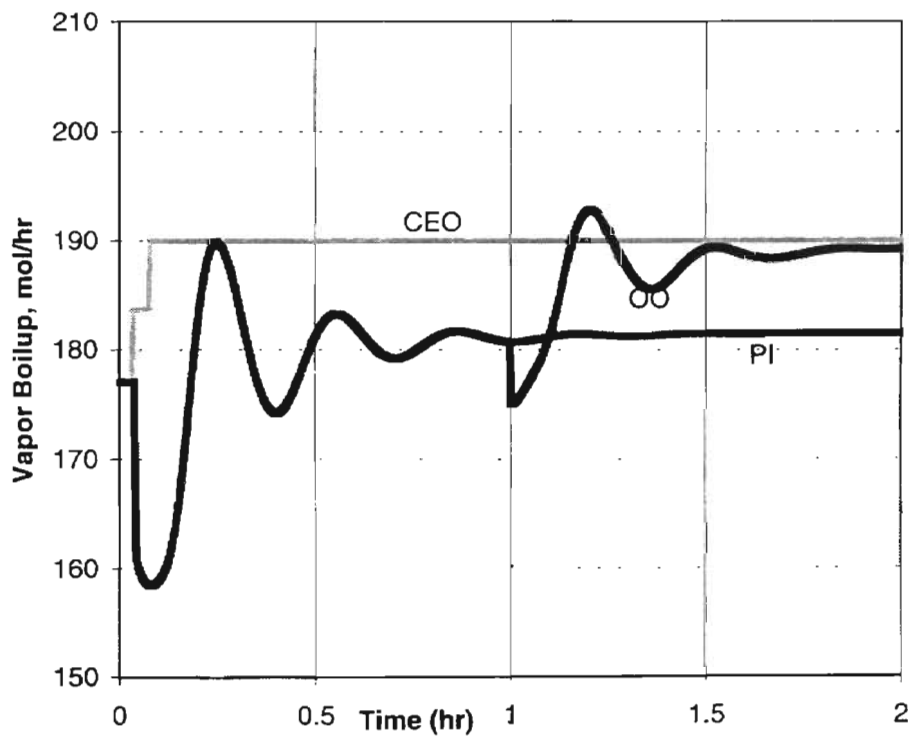


Fig 6-3d: Manipulated Variables (V)



6.4.3 Comparison under Feed Flow Rate Disturbances

Studies were made for the three control schemes under step changes in feed conditions. The step tests conducted include those for 5% feed flow rate increase and decrease. The disturbances are introduced into the process after 0.1 hr and the simulation is carried out for 2 hours. The results for the profits are summarized along with those for feed composition changes in Table 6-8.

It is seen that the control to economic optimum strategy (Fig 6-4 a/b) provides a much crisper and quicker approach to the optimal conditions. The final optimal control variable profile is found as quickly as 0.2 hr for feed flow disturbances. In contrast, it is seen that PI controller takes about 1 hr to reach the setpoint, which is anyway sub-optimal under the current process conditions. The steady state Optimizer is run only once an hour and hence the process operates sub-optimally for this period. After it runs on the process, the steady state Optimizer takes the process to its optimal value in the next settling time.

As with the base case, the final steady state values for the CEO and the OO Optimizers are the same. Since they use the same optimization parameters, they predict the same steady states. The CEO Optimizer determines the steady state early as it is run more often and it also looks at getting to the optimal conditions as fast as possible. Thus the approach to the final optimum is smooth. In contrast, the supervisory Optimizer is run once every hour and it has no "concern" for how to get to the optimum. This implies that the profit during the suboptimal path taken by the steady state Optimizer is not at its maximum, but only becomes maximum after the steady state is reached.

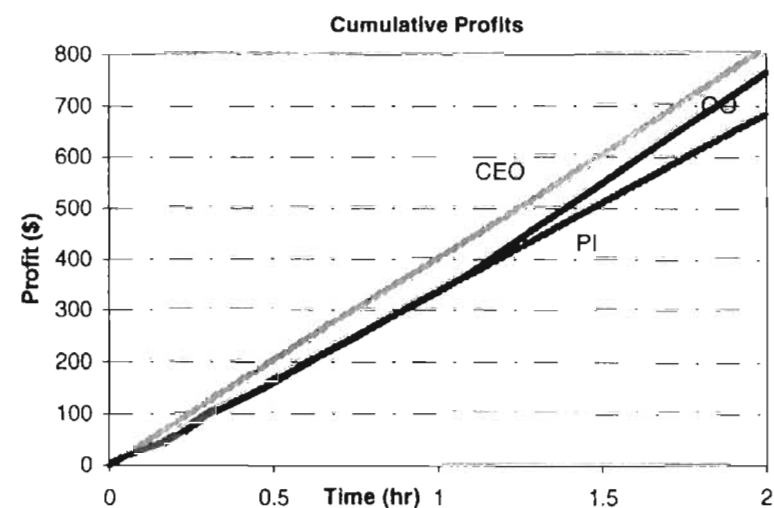
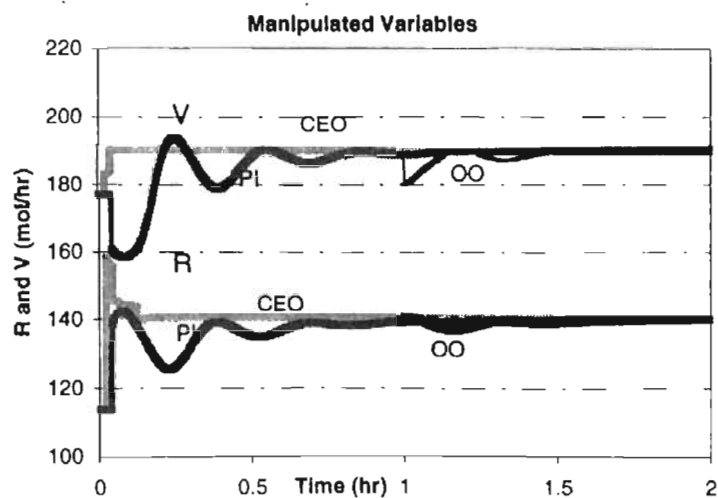
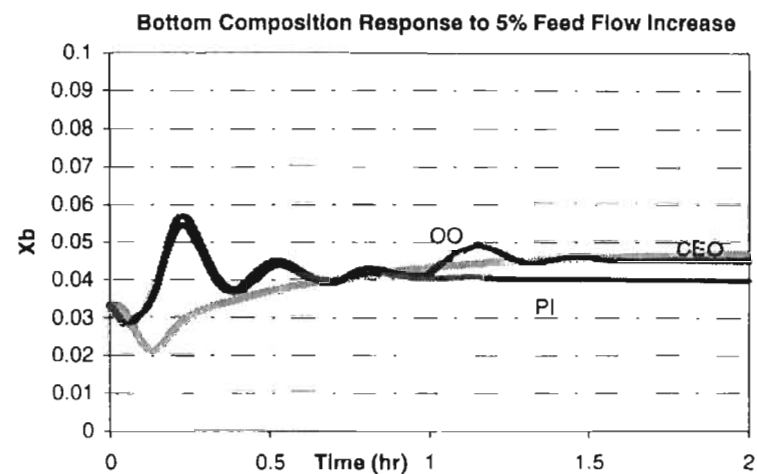
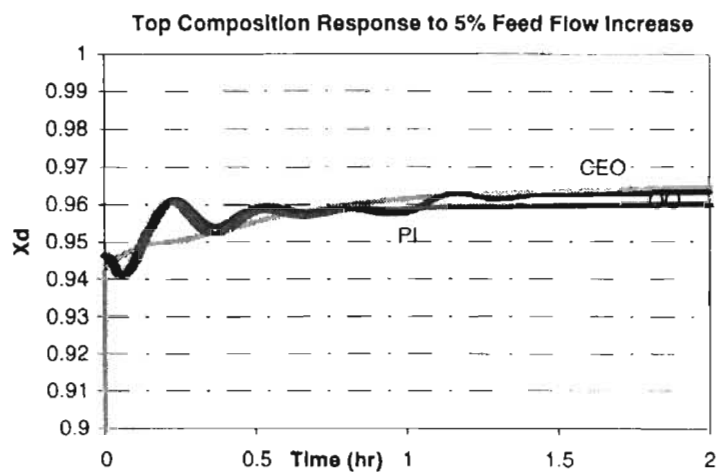


Fig 6-4a Response to 5% Increase in Feed Flow Rate

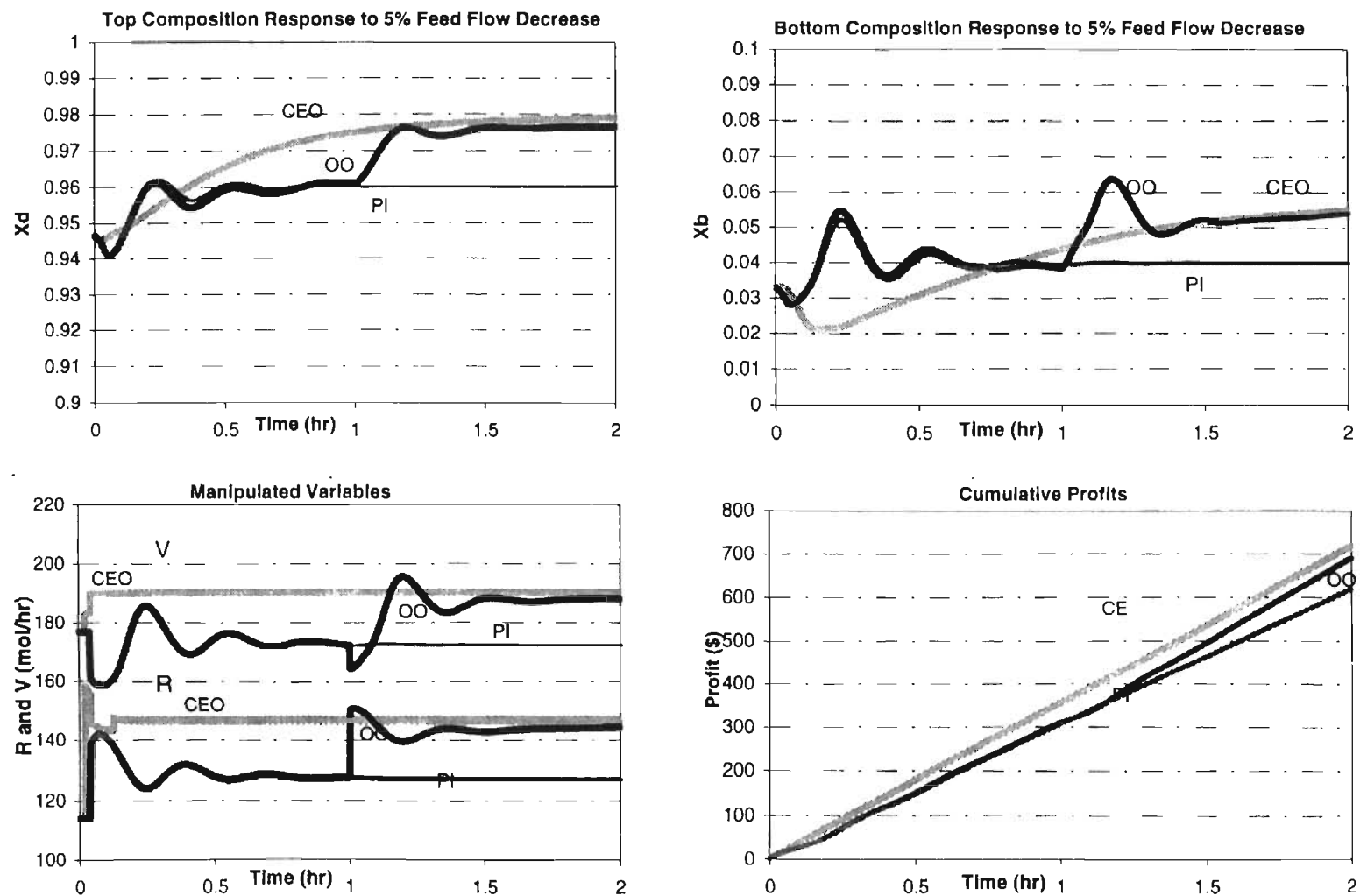


Fig 6-4b Response to 5% Decrease in Feed Flow Rate

Both the Optimizers reach to a steady state value of 190 mol/hr for the vapor boilup value and 140 mol/hr for the reflux value for a 5% feed increase disturbance. The compositions are as shown in Fig. 6-4a. For a 5% feed decrease disturbance, the Optimizers reach to a value of 190 mol/hr for the vapor boilup and 146 mol/hr for reflux at steady state. The PI controller sticks to its setpoint value of 0.96 even when there are disturbances, which leads to a suboptimal performance.

The CEO strategy "looks ahead" in time while making a decision on profitability. Thus it combines control objectives with economic objectives. Hence, it adds a level of intelligence to the steady state Optimizer, which is only concerned with optimizing current conditions, but has no idea of dynamics. Both Optimizers tend to push one of the variables to its constraint limit, and manipulate the other variable so as to maximize profit. This is in accordance with expectations as one of the products is of much higher economic value than the other and hence maximizing recovery of that product translates to maximizing profit.

A comparison of profits obtained is shown in Table 6-6 and Fig 6-3 a/b. It is seen that the OO and PI control strategies have the same profit during the first one hour. This is because the OO Optimizer runs only every hour. By this time, the PI controllers have taken enough action to bring the process back on track after the disturbance. After the first hour, the steady state Optimizer catches up to the CEO Optimizer and hence the profit using the steady state Optimizer starts catching up with that of the CEO approach. The profits obtained would be more in favor of the steady state Optimizer when it is run more frequently or when a disturbance appears not too long before it is run. With the CEO strategy, the process makes the maximum profit every step of the way; with the OO strategy, the profit is maximized only after reaching steady state. These studies are

not discussed here as the emphasis is on testing the performance of the new strategy. The CEO strategy gives about 5% more profit than the OO scheme, which gives 12% more than the PI scheme for a 5% feed increase. For 5% feed decrease, the CEO gives about 4% more profit than the OO, which gives about 11% more profit than the PI scheme.

Also, it is seen that the optimal profile for a 5% decrease in feed flow is slightly oscillatory. This could be because the equal finite element sizes used do not determine the optimal point of discontinuity as discussed in the previous section.

6.4.4 Comparison under Feed Composition Disturbances

The performance for the control schemes under larger (10%) composition disturbances is similar to those under feed flow disturbances. The CEO strategy again outperforms the other strategies in its early aggressiveness in determining the optimal control profile. The steady state Optimizer catches up to the CEO Optimizer when it is run at the end of 1 hour.

The approach to steady state is faster for the CEO strategy. The plots for the responses are shown in Fig 6-4 c/d and some of the results are summarized in Table 6-8. The dynamic Optimizer brings the process to a steady state top composition of 0.979 for a step decrease in composition and to a top composition of 0.968 for a step increase in feed composition. Bottom compositions are correspondingly higher. The steady state Optimizer reaches these values after it is run. Over the time horizon the CEO ensures that the process is optimal. As discussed in the case of feed flow disturbances, the steady state Optimizer only predicts the optimal steady state, but the path to the steady state is not economically optimal.

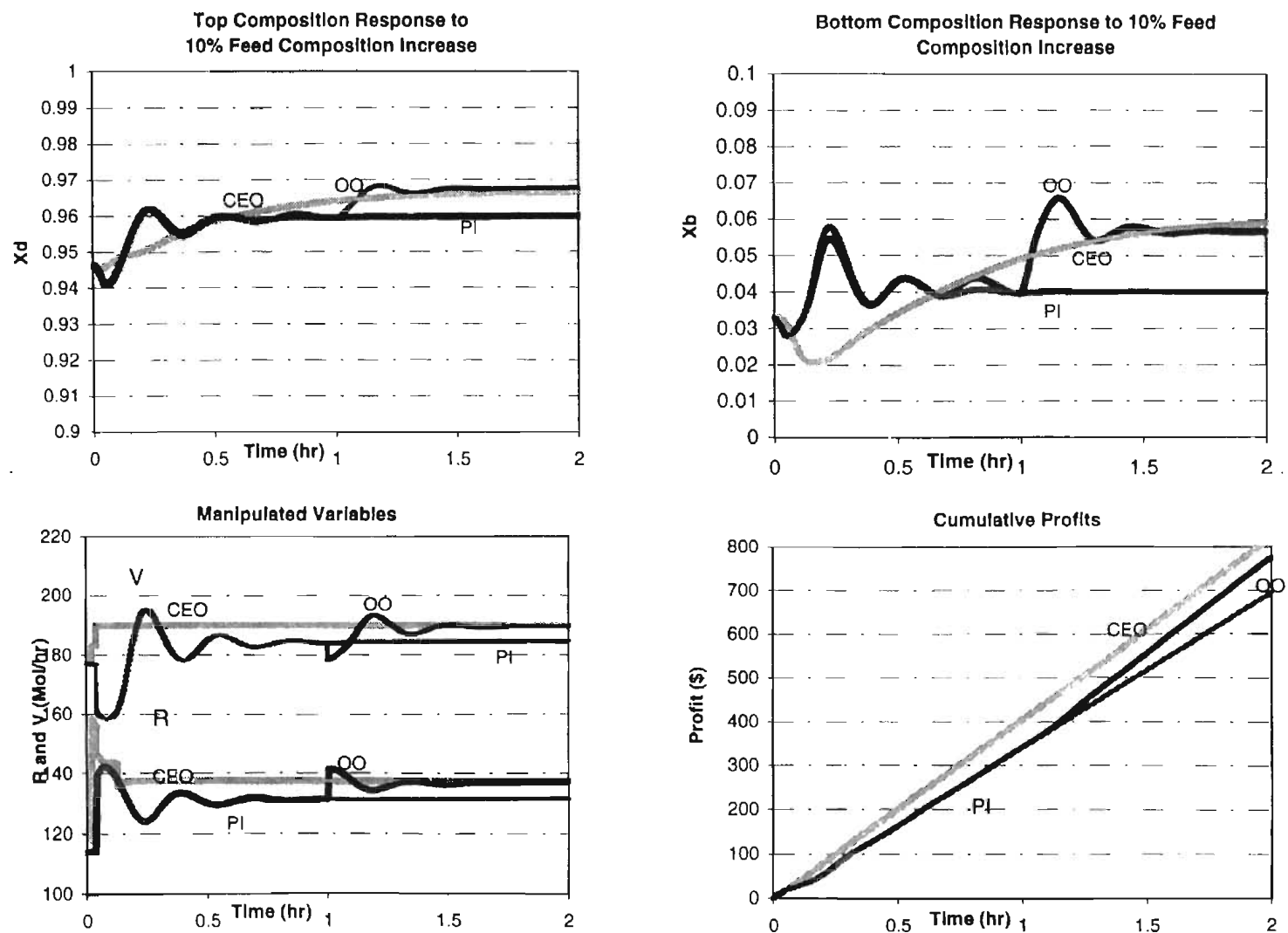
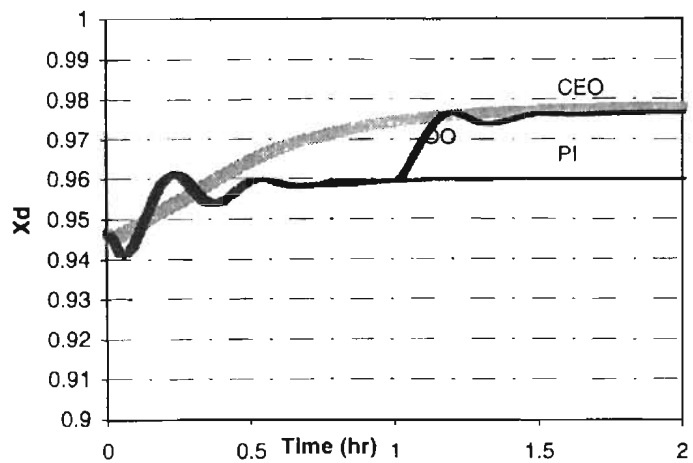
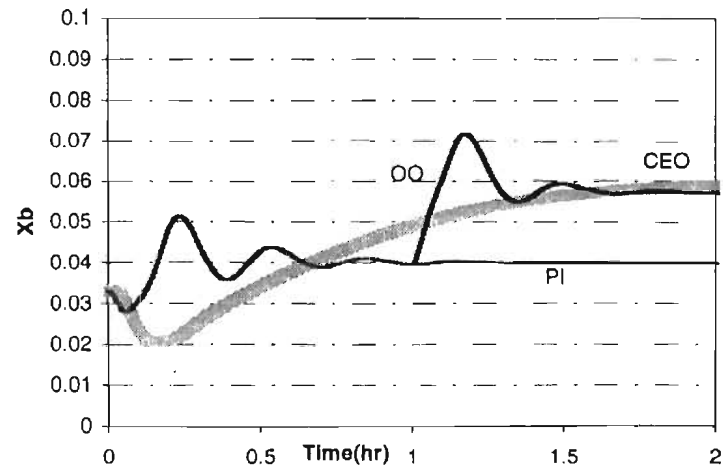


Fig 6-4c: Response to 10% Increase in Feed Composition

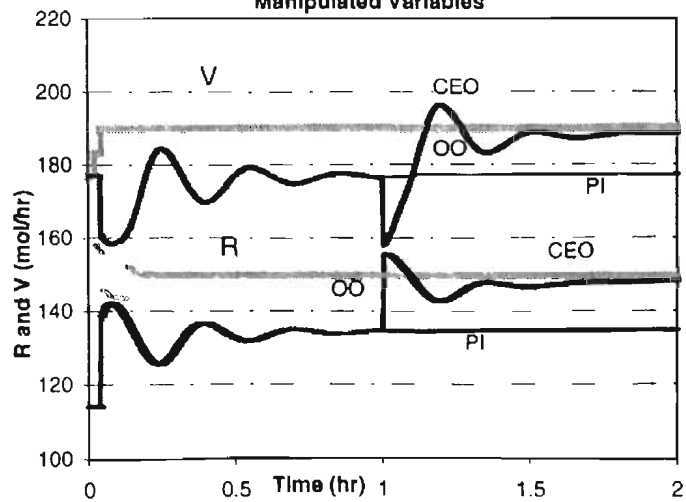
Top Composition Response to
10% Feed Composition Decrease



Bottom Composition Response to
10% Feed Composition Decrease



Manipulated Variables



Cumulative Profits

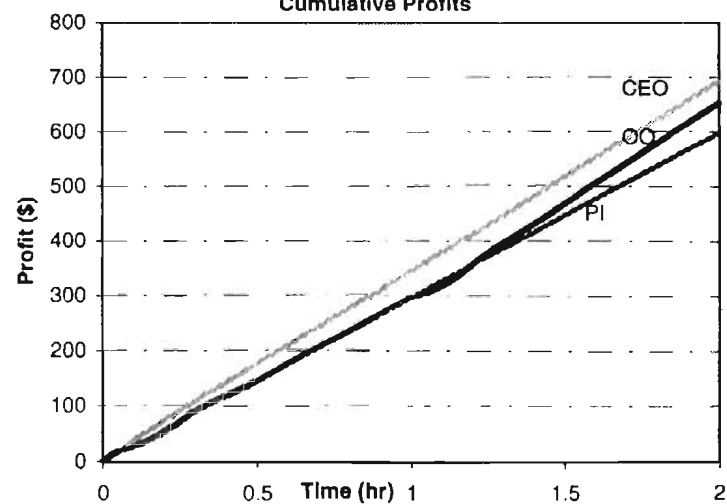


Fig 6-4d Response to 10% decrease in Feed Composition

The profit obtained is about 4% higher for a step increase in feed composition and about 6% higher than online optimization for step decrease. Table 6-8 summarizes the results for the profits obtained. Fig 6-4 a/bc/d show the responses for top and bottom compositions and the manipulated variable values. The cumulative profits are also compared as a function of time.

Table 6-8 Results for Feed Flow and Composition Disturbances

Parameter	Control to Economic Optimum	Online Optimization	PI Control
<i>Profit (Cumulative over 2 hours), \$</i>			
Base Case	668	648	631
5% step increase in feed flow	808	768	685
5% step decrease in feed flow	719	691	619
10% step decrease in feed composition	694	654	599
10% increase in feed composition	821	778	696

6.4.5 Computational Requirements

If implemented in industry, the CEO approach would require extremely advanced computer requirements as compared to the steady state Optimizer and the PI control

schemes. These are the GAMS Optimizer, and an interface, which displays the GAMS results. In this study, the GAMS Optimizer was linked to a Visual Basic interface and the results were displayed online on an Excel spreadsheet. Admittedly, this is an inefficient way of doing things, as this requires three packages viz., GAMS, Excel, and Visual Basic to be simultaneously active. The whole setup was run on a Pentium II, 400 MHz, Windows '98 Gateway computer. It was found that around 20% of the system resources were in use while the setup was running, and this caused frequent crashes of the machine. Also, the simulation could not be run for more than 2 hours of process time, after which the system became unstable and crashed. Hence, the possibility of using other software packages must be considered. These issues will be addressed in the next chapter. The steady state Online Optimizer computational requirements are also the GAMS Optimizer and the Excel interface to display the optimizer setpoints.

The optimization problem solved in the CEO approach is highly nonlinear and this nonlinearity is bound to increase if the approach is further refined by adding finite elements as decision variables and when more complex systems are considered. It is clear that the measure of merit as far as the computational requirements are concerned is the execution time for the Optimizer – the time it takes to converge to a final solution.

The GAMS Optimizer includes a feature, which enables the user to determine the compilation and execution times (through the listing file – see Appendix B), and these and compared below for the CEO and the OO approaches, for the worst case. (The worst case occurs either during initial convergence from inconsistent initial conditions or after a disturbance is introduced)

Table 6-9 - Worst Case Computational Requirements

Property	GAMS Optimizer (CEO)	GAMS Optimizer (OO)
Compilation time	0.120 s	0.100 s
Model generation time	0.080 s	0.080 s
Execution time	0.120 s	0.110 s
Iterations	36	14
Total CONOPT optimization time	0.281 s	0.223 s

Although the difference seems to be not so major, it must be kept in mind that the CEO Optimizer runs about 20-30 times more frequently than the OO Optimizer, as it runs every 2-3 minutes as compared to the steady state optimizer which runs every hour. This tremendously increases the computational time for the CEO approach.

The following points must also be emphasized when making a judgment on the relative performance of the control schemes:

- The optimal control relies on fast changes in a short time in order to aggressively track the optimum. In reality however, the sudden spurts in values of the variables also costs money. Hence if changes are penalized the control will not be as aggressive and hence profit differences not as large.
- Even with less aggressive control action, this strategy tends to be a still more aggressive than a steady state optimizer. To control the process from becoming unstable, there must be a *layer of regulatory control* which keeps the manipulated variables in their previous optimum values, when there is a loss of convergence in the optimizer or when excessive control action

threatens instability in the process. This layer of regulatory control is the backup for the process to go into when there is a failure in the optimizer. Thus, although this approach can help get rid of some of the setpoints for compositions and other controlled variables, the setpoints for the backup regulatory control layer must remain as a fall-back option.

- The optimal profile will change when the constraints on the manipulated variables are changed. The aggressiveness of control also depends on these bounds. For example, it was seen that when the bounds on the reflux were tightened, the vapor boilup could not be pushed to its constraint limit and hence changes were slower and less aggressive.
- The economic objective function is a linear function of the top and bottom composition. This means that the optimizer "thinks" that when the composition increases, the value of a product goes up and hence it is encouraged to keep increasing the composition even if it means increasing the cost variables. In reality however, the value of a product is not a linear function of cost. Hence, for instance, a 0.96 composition product would not be significantly more valuable than a 0.97 composition product predicted by the dynamic optimizer. This would play a crucial role in determining the economic optimum. This could be addressed by using a discontinuous cost function for product purity. The discontinuity in pricing could create problems in convergence during the repeated solution of the optimization problem.
- In industry, rate of change constraints are enforced on variables which force the optimizer not to abruptly change process variables in a short period of time, which may lead to instability. Such constraints would curtail the aggressiveness of the controller and hence the rapidity of the approach to the optimum.

- The single distillation column in isolation is not enough to really comment on the performance of the CEO strategy. There are not enough disturbances that radically affect the economics of an isolated column.
- Adding the aspects mentioned above into the formulation of the optimization problem is likely to increase the nonlinearity and hence the computational effort and time involved in the solution.
- CEO, if used for a plant in isolation, might suggest an optimal point of operation for that plant in response to a disturbance, but this may lead to sub-optimal performance in downstream processes. This may in fact lead to propagation of disturbances.

These considerations must be kept in mind when evaluating the performance differences between the control schemes. These form the basis for further improvement and fine-tuning of the strategy. In spite of these limitations, the comparisons provided above form an important first step for development of the dynamic optimization strategy. Hence, while it is safe to say that the strategy will address the issue of best economics at every step of its implementation, it must be emphasized that further testing on more complex models is required before the industry has enough confidence to implement it.

This chapter discussed the results for the three strategies with respect to performance under disturbances. However, these preliminary results though promising must not be taken as the last word on the subject. Several other issues must be kept in mind while considering the implications of the strategy. Some of the limitations of the strategy and the points to be kept in mind for future directions will be explored. The next chapter outlines future directions and summarizes the conclusions.

Chapter 7

Conclusions and Recommendations

7.1 Conclusions

In this study, a new strategy, which attempts to address the basic motive of industrial operations – maximizing profitability, and thus integrates both control and economic objectives, has been proposed. The strategy involves a dynamic optimizer providing optimal control profiles to the process by solving a dynamic optimization problem whose objective is to maximize profit. By maintaining the manipulated variables at the optimal values suggested by the Optimizer, it is then possible to maximize profit over a time horizon. This strategy has been tested on a binary distillation column simulation as a first step.

Simulations for the distillation column using simplifying assumptions were developed as part of the study. The objective function for the proposed strategy was developed for the distillation column. Various numerical methods were analyzed and orthogonal collocation was chosen for its generality and simplicity of implementation. A first principles model was developed and the model equations were embedded as equality constraints in the optimization problem. The results from the proposed strategy were compared with conventional schemes – steady state online optimization and PI control. The following conclusions were drawn from the comparisons:

The proposed control to economic optimum strategy provides aggressive control and fast approach to economic optimum. Typically, the dynamic optimizer finds the new economic optimum when disturbed from the optimum within 20-30% of the process settling time. The steady state Optimizer predicts the same optimal steady state as the

CEO Optimizer, but the path to the optimum is not optimal. The conventional approaches thus show a slow approach to the economic optimum. Tests were carried out for feed flow and feed composition disturbances and comparisons were made with conventional control schemes.

The tests on disturbances in feed flow and composition demonstrate that dynamic optimization provides on an average about 5% higher profits than the steady state Optimization scheme, which in turn yields about 10% more profit than regular PI control. The economic optimum strategy tends to "push the limits" much more than the conventional regulatory PI control. For instance, it is seen that the vapor boilup is at its constraint of 190 mol/hr in many of the cases discussed. Disturbances lead to large changes in manipulated variables due to the time-optimal search for the optimum.

Tests were also carried out to determine the *effect of parameter uncertainties* in the search for the optimum. These included tests for constraint limit sensitivities, cost coefficient sensitivities, etc. It is found that uncertainties in constraints play a major role in determining the final optimum. From the results, it is seen that relaxing or tightening a constraint causes changes in product compositions and optimal control profiles. For this strategy to be successful, these parameters must be updated regularly.

The CEO strategy also required higher computational requirements than the OO strategy. The execution time is about 0.01 s higher for every time the Optimizers run. This adds to a large difference over the entire duration of optimization.

This study used various simplified models and simple economics. These need to be improved and fine tuned before a fully functional strategy can be developed. These are discussed in the recommendations below.

7.2 *Recommendations*

Overall, the study demonstrated the efficacy of a dynamic optimization strategy. The results show a good improvement in profitability in comparison to conventional control methods. However, further testing and studies should be carried out before a functional algorithm can be developed. The initial focus of future directions should be to refine the existing strategy developed in the study. After this is done, this must be extended to more complex situations and tested. These aspects are given below:

- *Improving the current models –*

This study used simple models and very simple economics. The profitability objective implies that a *rigorous economic model* is necessary to ensure that the optimum dictated by the dynamic optimizer is indeed the correct one. Based on the simple economic function used, CEO would attempt to make unlimited amounts of the most valuable product. However, there might not be a market for such large volumes of this product, or there might be a reduced price after a particular amount of production. Similarly, a slightly purer product might not have a higher value. The economic model must take into account these issues and incorporate it in the objective function. Also, the model must be able to incorporate incremental costs of production increase versus costs incurred. Some of these business concerns are further discussed in Appendix-H.

This study was limited by the demonstration version of the GAMS optimizer available and hence, finite element lengths could not be included as decision variables in

the optimizer. The importance of *finite element lengths* was discussed and their role in discontinuous profiles was analyzed in the previous chapter. It is recommended that this is done to complete the strategy. Also, the use of several software for this strategy led to computer crashes. More user-friendly, less restrictive software such as MatLab, GenSym's G-2 etc may be explored for easier implementation.

For implementation on an actual plant, the optimizer must run on plant data, which may be unreliable due to random errors. Future work should focus on incorporating *data reconciliation and gross error detection algorithms*, which must be carried out before the data is processed by the optimizer.

Also, uncertainties in model parameters must also be analyzed for each process and robust *model parameter updating* algorithms must be incorporated specific to each process being investigated. These model parameter updating algorithms are optimization problems by themselves and these must be incorporated when necessary before performing the dynamic optimization.

Since this is a first-step study, the current study did not consider the cost of control action, which means that the optimizer does not penalize excessive control action. In addition, *rate of change constraints* were not included in the optimization problem. These issues should also be analyzed.

This study assumed that the feed to the process is fixed by an upstream unit. Future work must also consider using the feed as a decision variable in the optimization, so as to achieve *product maximization* (see Appendix E).

The study provided comparison with conventional PI control-based strategies. In industry, advanced control strategies such as MPC are available, which are also based on dynamic optimization. Such algorithms, if implemented properly would necessarily track setpoints better than PI strategies. Hence, for fairer comparisons should be made with *more rigorous control algorithms* such as model predictive control, which are in practice in industry today.

- *Extension to more complex processes –*

The current study demonstrated the working of the proposed strategy for a distillation column. Although this is a good starting step, distillation units do not exist in isolation and the economics must be considered in conjunction with other units. The real test for the strategy would be when used with a more complex process.

Future work on implementation of this strategy could be divided into two directions – *continuous* and *batch* processes:

- For studies on continuous processes, a *3-unit process* such as an FCC unit or the flotation plant in IMC Agrico may be chosen to implement the strategy. These are far more complex processes than the simple distillation process chosen in the study. These are also economically significant parts of the operating plant. Hence, the concept should be tested on these processes for its performance.
- Batch processes form another set of industrially important processes. Such processes may optimize on other objectives such as time for batch operation, conversion etc. These processes are well suited for implementation of the proposed strategy and this could be another possible future direction. Some aspects of use of the proposed strategy are given in Appendix-H.

Finally, this strategy should be studied during a *long-term period* of perhaps a year, including transient periods such as start-ups and shutdowns, so that its robustness can be verified. These transient periods are fraught with disturbances and upsets and optimal performance under such conditions would alone vindicate the use of this strategy for everyday industrial applications.

Once this concept is established for a complex three-unit process on a long-term basis, the final goal of plantwide optimization can be addressed, and hopefully, realized.

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APPENDICES

APPENDIX –A

DEVELOPMENT OF A REDUCED ORDER LUMPED MODEL FOR A DISTILLATION COLUMN

The following is an example for obtaining a reduced order model for a distillation column and has been directly taken from Poupadourakis and Rijndorp, 1992.

Consider a sequence of M stages used for any separation as follows:

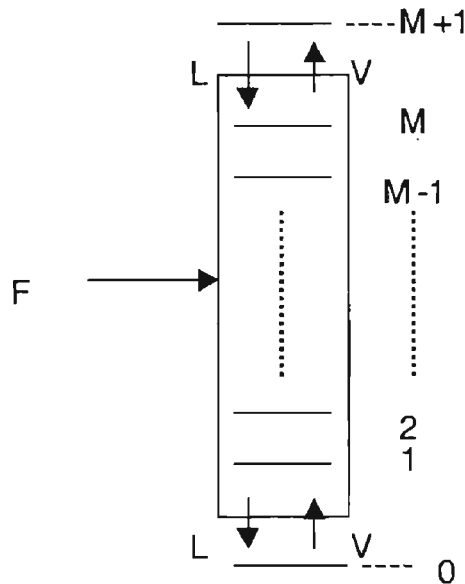


Fig 4-3: A sequence of M stages used for separation of a mixture

Assuming constant molar overflow, the dynamic component material balances on each tray s is given by:

$$M_L \frac{dx(s,t)}{dt} = L x(s+1,t) - L x(s,t) + V y(s-1,t) - V y(s,t); \quad s=1,\dots,M \quad (A-1)$$

The compositions in this module of trays can now be approximated by polynomials, using $n < M$ interior grid points plus two entry points $s_{n+1} = M + 1$ for the liquid and $S_0 = 0$ for the vapor. The corresponding equations of the collocation model for the module are given by:

$$M_L \frac{d\tilde{x}(s_j, t)}{dt} = L \tilde{x}(s_j + 1, t) - L \tilde{x}(s_j, t) + V \tilde{y}(s_j - 1, t) - V \tilde{y}(s_j, t); \quad j = 1, \dots, n \quad (\text{A-2})$$

where the tilde represents an approximate value

Thus the number of equations describing the component material balances for the module is reduced from M (number of stages in the module) to n (number of collocation points in the module). The location of these points, s_1, s_2, \dots, s_n are the zeros of what are called Hahn polynomials and they are given in Table A-1

Table A-1: Collocation Points for a Module Consisting of M Stages

Number of Collocation Points, n	Points s_j
1	$\frac{M+1}{2}$
2	$\frac{M+1}{2} \pm \sqrt{\frac{M^2-1}{12}}$
3	$\frac{M+1}{2}, \frac{M+1}{2} \pm \sqrt{\frac{3M^2-7}{20}}$

The compositions at each stage of the module are given by:

$$\begin{aligned} \tilde{x}(s, t) &= \sum_{j=1}^{N+1} \Phi_{jL}(s) \tilde{x}(s, t) \\ \tilde{y}(s, t) &= \sum_{j=0}^N \Phi_{jL}(s) \tilde{y}(s, t) \end{aligned} \quad (\text{A-3})$$

where the Φ functions are the Lagrange polynomials given by:

$$\Phi_{jL}(s) = \prod_{\substack{k=1 \\ k \neq j}}^{n+1} \frac{s - s_k}{s_j - s_k}; \quad j = 1, \dots, n+1$$

$$\Phi_{jV}(s) = \prod_{\substack{k=0 \\ k \neq j}}^n \frac{s - s_k}{s_j - s_k}; \quad j = 0, \dots, n$$
(A-4)

Thus for $M = 15$, the reduced order model is developed as follows:

Reboiler

Using the reboiler as one collocation point, for $M=1$, $n=1$, we get, from Table A-1 $s_1 = 1$

The equation for the reboiler is:

$$M_{LB} \frac{d\tilde{x}(s_1, t)}{dt} = (L + F) \tilde{x}(s_1 + 1, t) - B \tilde{x}(s_1, t) - V \tilde{y}(s_1, t)$$
(A-5)

Stripping Section

Assuming the stripping section can be described by only 2 collocation points, the mass balance equations become:

$$M_L \frac{d\tilde{x}(s_2, t)}{dt} = (L + F) \tilde{x}(s_2 + 1, t) - (L + F) \tilde{x}(s_2, t) + V \tilde{y}(s_2 - 1, t) - V \tilde{y}(s_2, t)$$

$$M_L \frac{d\tilde{x}(s_3, t)}{dt} = (L + F) \tilde{x}(s_3 + 1, t) - (L + F) \tilde{x}(s_3, t) + V \tilde{y}(s_3 - 1, t) - V \tilde{y}(s_3, t)$$
(A-6)

where s_2 and s_3 are the collocation points for the stripping section

The location of the collocation points for $M= 7$ (number of stripping trays) and $n = 2$ is found from Table A-1. For example, $s_2 = 2$ and $s_3 = 6$. Since there is one reboiler stage below, we have, $s_2 = 3$ and $s_3 = 7$.

Feed Tray

The mass balance for the feed tray is given by:

$$M_L \frac{d\tilde{x}(s_4, t)}{dt} = (L) \tilde{x}(s_4 + 1, t) - (L + F) \tilde{x}(s_4, t) + F.Z_1 + V \tilde{y}(s_4 - 1, t) - V \tilde{y}(s_4, t) \quad (A-7)$$

where s_4 is the collocation point corresponding to the feed tray

Again, using Table A-1, for $n=1$ and $M=1$, we get $s_4 = 1$. However, since there are 8 stages below this point (7 stripping trays + 1 reboiler), we have $s_4 = 9$

Enriching trays

Mass balance equations for the enriching trays assuming 2 collocation points is given by:

$$\begin{aligned} M_L \frac{d\tilde{x}(s_5, t)}{dt} &= (L) \tilde{x}(s_5 + 1, t) - (L) \tilde{x}(s_5, t) + V \tilde{y}(s_5 - 1, t) - V \tilde{y}(s_5, t) \\ M_L \frac{d\tilde{x}(s_6, t)}{dt} &= (L) \tilde{x}(s_6 + 1, t) - (L) \tilde{x}(s_6, t) + V \tilde{y}(s_6 - 1, t) - V \tilde{y}(s_6, t) \end{aligned} \quad (A-8)$$

The location of the collocation points s_5 and s_6 can be found from Table A-1, for $M=7$ (7 enriching trays) and $n=2$. Using this table, we get $s_5 = 2$, $s_6 = 6$; since there are 9 trays below these points, we have $s_5 = 11$ and $s_6 = 15$

Reflux drum

The mass balance for the reflux drum takes the form:

$$M_{LD} \frac{d\tilde{x}(s_7, t)}{dt} = - (L) \tilde{x}(s_7, t) - D \tilde{x}(s_7, t) - V \tilde{y}(s_7 - 1, t) \quad (A-9)$$

Using Table A-1, we get $s_7 = 17$

In the above equations, the vapor compositions can be found using:

$$\tilde{y}(s_i, t) = \frac{\alpha \tilde{x}(s_i, t)}{1 + (\alpha - 1) \tilde{x}(s_i, t)} \quad (A-10)$$

The remaining variables in the preceding equations are functions of the liquid and vapor compositions in the previous equations. For example,

$$x(s_3 - 1, t) = x(6, t) = \sum_{j=2}^4 \phi_{jL}(6) \tilde{x}(s_j, t) \text{ where} \quad (A-11)$$

$$\phi_{jL}(6) = \prod_{\substack{k=2 \\ k \neq j}}^4 \frac{6 - s_k}{s_j - s_k}; \quad j = 2, \dots, 4$$

APPENDIX – B

GAMS OPTIMIZER FEATURES

GAMS (General Algebraic modeling System) was developed to solve general optimization problems with the following aspects in the mind:

- Providing a high-level language for the compact representation of large and complex models.
- Allowing changes to be made in model specifications simply and safely
- Allowing ambiguous statements of algebraic relationship
- Permitting model descriptions that are independent of solution algorithms

The features of GAMS and an overview of the GAMS program structure are discussed below, followed by a discussion of the nonlinear solvers available, and applications in dynamic optimization.

B.1 GAMS Features

The design of GAMS has incorporated ideas drawn from relational database theory. It offers the following features [1]:

- Use of existing algorithmic methods and development of new methods without changing model representation. Linear, nonlinear, mixed integer, mixed integer nonlinear optimization and complementarity problems can currently be accommodated
- Optimization independent of the data used
- Ease and flexibility for construction of large and complex models

- Concise representation of the mathematical description of the system to be optimized
- Documentation embedded within program
- Portability on various computers

B.2 STRUCTURE OF GAMS PROGRAMS

A GAMS model is a collection of statements in the GAMS language. The only rule governing the ordering of statements is that an entity of the model cannot be referenced before it is declared to exist. The creation of GAMS entities involves two steps: a declaration and an assignment or definition. ‘Declaration’ means declaring the existence of something and giving it a name. ‘Assignment’ or ‘Definition’ means giving something a specific value of form [1].

The entities in GAMS program are as follows:-

SETS - Sets are building blocks of a GAMS model, corresponding exactly to the indices in the algebraic representation of models. Three fundamentally different formats are allowable for entering data. The three formats are

- Lists
- Tables
- Direct assignments

VARIABLES - The decision variables (or endogenous variable) of a GAMS-expressed model must be declared with the Variables statement. Each variable is given a name, a domain, if appropriate, and (optionally) documentary text [1].

EQUATIONS - Equations must be declared in separate statement after the keyword "Equations." The entities included under this key word include both equality and inequality relationships between variables and parameters [1].

OBJECTIVE FUNCTION - GAMS has no explicit entity called the 'objective functions.' To specify the function to be optimized, you must create a variable, which is free (unconstrained in sign) and scalar-valued (has no domain) and which appears in an equation definition that equates it to the objective function [1].

MODEL - A specified collection of equations constitutes a model. Like other GAMS entries, it must be given a name in a declaration. Once the model has been declared, we are ready to call the solver. This is done with a solve statement as follows [1]:

```
SOLVE <model name> USING lp/nlp/minlp/mip MINIMIZING/MAXIMIZING  
<objective function variable>
```

B.3 INPUT/ OUTPUT IN GAMS

To solve a problem, we must create the model using the entities discussed above and key it in a file with a .gms extension. This is the *Input File*

GAMS solves the problem and displays output in <filename>.lst. This is the *Output* or *Listing* file. GAMS provides extremely detailed output which help in quick debugging and analysis.

The output consists of

- Echo prints – A copy of the input file
- Error messages – if any

- Reference maps – a list of all entities and the lines where they are referenced
- Equation listing – lists the equations with current values of sets and parameters plugged into the general algebraic models
- Model statistics – statistics on model size
- Status report – summary of solution
- Solution reports – details of solution

After the solver runs and executes the program, the user can examine the listing file and read the solution.

B.4 NONLINEAR PROGRAMMING IN GAMS

Nonlinear models created with GAMS must be solved with a nonlinear programming algorithm. Currently there are two standard NLP algorithms available, MINOS and CONOPT, which is available in two versions, CONOPT and CONOPT2. *All algorithms attempt to find the local optimum.* The algorithms in CONOPT and MINOS are based on fairly different mathematical algorithms and behave differently on most models. This means that while MINOS is superior in some models, CONOPT is superior in others [2].

GAMS/CONOPT is suited for problems with very nonlinear constraints. If it is seen that MINOS has problems maintaining stability during optimization, CONOPT may be tried. On the other hand, for models with few nonlinearities outside the objective function, MINOS would be better. CONOPT has a fast method for finding the first feasible solution that is particularly suited for models with few degrees of freedom. If the model has roughly the same number of constraints as variables, CONOPT may be more suitable. If the number of variables is much larger than the number of constraints, then

MINOS would work better [2]. For this study, GAMS/CONOPT is used as the NLP solver.

B.5 Limitations in the GAMS demonstration version

Because the version of GAMS available is only a demonstration version, the following restrictions apply:

Total nonzero elements	1000
Nonlinear nonzero elements	200
Discrete variables	20

Due to these restrictions the following limitations were encountered:

- Number of finite elements could not be increased more than 2, as then the nonlinear nonzero element limit was crossed
- Number of collocation point could not be increased beyond 2
- Finite element lengths could not be used as decision variables in the optimizer

A simple example from [3] follows:

Example B-1:

Minimize

$$Z = x_1^2 + x_2^2 + x_3^2$$

subject to

$$x_2 - x_3 \geq 0$$

$$x_1 - x_3 \geq 0$$

$$x_1 - x_2^2 + x_2 x_3 - 4 = 0$$

$$0 \leq x_1 \leq 5; 0 \leq x_2 \leq 3; 0 \leq x_3 \leq 3$$

The program for solving this problem with GAMS with comments is given below

(Comments are those lines which have an asterisk (*) as the first character):

```
* Declare the title for the problem
$ TITLE TEST PROBLEM

* Declare variables using the VARIABLES statement
VARIABLES X1, X2, X3, Z;

* Declare domain for variables
POSITIVE VARIABLES X1, X2, X3;

* Declare equations using EQUATIONS statement
EQUATIONS CON1, CON2, CON3, OBJ;

* Define equations from constraints
CON1.. X2-X3 =G= 0;
CON2.. X1-X3 =G= 0;
CON3.. X1 -X2**2 + X1*X2 -4 =E= 0;

* Objective function is also treated as an equation
OBJ.. Z =E= SQR(X1) + SQR(X2) + SQR(X3);

* Declare Bounds- Lower bound is not declared since the variable is already declared positive
X1.UP = 5;
X2.UP = 3;
X3.UP = 3;

* Declare initial point
X1.L = 4;
X2.L = 2;
X3.L = 2;

* Declare MODEL statement and specify equations to be included in the model. /ALL/ means that all equations are included

MODEL TEST / ALL / ;

* Declare SOLVE statement and specify direction and variable of optimization
SOLVE TEST USING NLP MINIMIZING Z;
```

This is a valid GAMS program which solves the above optimization problem.

This can be executed by typing

GAMS <filename.GMS> at the MSDOS prompt

Outputs can be viewed by typing

EDIT <filename.LST> at the MSDOS prompt

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APPENDIX – C

APPLICATION OF ORTHOGONAL COLLOCATION FOR DAE SYSTEMS- A SIMPLE EXAMPLE

The following example from [1] illustrates the method of discretizing DAE systems using orthogonal collocation.

Example

The system is that of a car starting and ending at rest, and covering a fixed distance (300 meters) in a minimum amount of time. The problem involves finding the optimum acceleration profile, which minimizes the time taken to cover the 300 meters. The performance is controlled by the acceleration, which is to be kept between the limits of -1m/s^2 and 2 m/s^2 . It is of interest to determine the optimum acceleration profile over time, which minimizes the time taken, t_f , to cover the distance of 300 meters.

The mathematical definition for this optimization problem is:

Minimize t_f

$$\frac{dx^1}{dt} = x^2 \quad (\text{C - 1})$$

$$\frac{dx^2}{dt} = u \quad (\text{C - 2})$$

$$x^1(0) = 0 \quad (\text{C - 3})$$

$$x^2(0) = 0 \quad (\text{C - 4})$$

$$x^1(t_f) = 300 \quad (\text{C - 5})$$

$$x^2(t_f) = 0 \quad (\text{C - 6})$$

$$-2 \leq u(t) \leq 1 \quad (\text{C - 7})$$

where x^1 is the distance and x^2 is velocity.

and $u(t)$ is the acceleration at time t

DISCRETIZATION

Time is discretized using orthogonal collocation as follows

$$t_f = \sum_{l=1}^{NFE} \Delta \alpha_l$$

where the α_l represent finite elements of time

The differential equations are discretized using the principles mentioned in Chapter 3. The first step is to discretize the differential equations (C-1) and (C-2).

For example, considering equation (C-1):

$$\frac{dx^1}{dt} = x^2$$

This contains two state variables x^1 and x^2

Using Lagrange polynomials, these continuous state variables are discretized as in Eq. (3-7):

$$x_i^s(t) = \sum_{j=0}^{NCOL} x_{[ij]} \Phi_{[ij]}(t), \text{ where the } i\text{'s represent finite elements } j \text{ represent state}$$

variables and the superscript s represents the s 'th state variable

Thus, for example x^1 is discretized in the i th finite element as:

$$x_i^1(t) = \sum_{j=0}^{NCOL} x_{[ij]} \Phi_{[ij]}(t)$$

The residual of this equation can be written as [2]:

$$R(t) = \sum_{j=0}^{NCOL} x_{[ij]}^1 \dot{\Phi}_{[ij]}(t) - \sum_{j=0}^{NCOL} x_{[ij]}^2 \Phi_{[ij]}(t) \quad (C-8)$$

Using the Villadsen and Michelson method of weighted residuals, this residual has the property that [2]:

$$\int_0^1 R(t) \delta(t - t_i) dt = 0; \quad i = 1, \dots, k$$

This integral can simply be written as:

$$R(t_i) = 0 \quad (C-9)$$

Applying eq. (C-9) in (C-8),

$$R(t_i) = \sum_{j=0}^{NCOL} x_{[ij]}^1 \dot{\Phi}_{[ij]}(t_i) - \sum_{j=0}^{NCOL} x_{[ij]}^2 \Phi_{[ij]}(t_i) = 0 \quad (C-10)$$

Since, $\Phi_{[ij]}^i(t_i) = 1$ (which is the reason why Lagrange polynomials are chosen),

(C-10) can be written simply as:

$$\sum_{j=0}^{NCOL} x_{[ij]}^1 \dot{\Phi}_{[ij]}(t_i) - x_{[ij]}^2 = 0 \quad (C-11)$$

Using $\dot{\Phi}_{[ij]}(t_i) = \frac{\Phi_{[ij]}(t_i)}{\Delta\alpha_i}$, the above equation may be written as:

$$\sum_{n=0}^{NCOL} x_{in}^1 \frac{\Phi_{ij}(t_{[ij]})}{\Delta\alpha_i} = x_{[ij]}^2$$

which reduces to :

$$\sum_{n=0}^{NCOL} x_{in}^1 \varphi_n(\tau_j) - \Delta\alpha_i (x_{ij}^2) = 0$$

Here NCOL is the number of collocation points, n is a collocation point within the ith finite element.

In a similar manner, other equations can be discretized. The only other addition is that of the continuity equations, which are added to enforce continuity at the finite

element boundaries as was discussed in Chapter 3. Thus the DAE system can be converted into a discrete algebraic system and the optimization problem can be re-written as:

$$\text{Min} \sum_{i=1}^{NFE} \Delta \alpha_i$$

$$\sum_{j=0}^{NCOL} x_{[ij]}^1 \phi_{[ij]}(t_j) - \Delta \alpha_i (x_{[ij]}^2) = 0 \quad (\text{C - 1a})$$

$$\sum_{j=0}^{NCOL} x_{[ij]}^2 \phi_{[ij]}(t_j) - \Delta \alpha_i (u_{[ij]}) = 0 \quad (\text{C - 2a})$$

$$i = 1, NFE, j = 1, NCOL$$

$$x_{i0}^1 = \sum_{j=0}^{NCOL} x_{[ij]}^1 \phi_{[ij]}(t = 1) \quad (\text{Continuity equation 1})$$

$$x_{i0}^2 = \sum_{n=0}^{NCOL} x_{[in]}^2 \phi_{[in]}(t = 1) \quad (\text{Continuity equation 2})$$

$$x_{i0}^1 = 0, \quad (\text{C - 3a})$$

$$x_{i0}^2 = 0 \quad (\text{C - 4a})$$

$$\sum_{i=0}^{NCOL} x_{[NFE,j]}^1 \phi_n(\tau = 1) = 0 \quad (\text{C - 5a})$$

$$\sum_{n=0}^{NCOL} x_{[NFE,j]}^2 \phi_n(\tau = 1) = 300 \quad (\text{C - 6a})$$

$$\Delta \alpha_i \geq 0$$

$$-\alpha \leq u_{[ij]} \leq 1 \quad (\text{C - 7a})$$

This can now be solved as an NLP using a normal NLP engine.

References

1. Morari, M., Grossmann, I.E., "CACHE – Process Design Case Studies: Chemical Engineering Optimization Models with GAMS", Vol. 6., 1991
2. Cuthrell, J.E., Biegler, L.T., "On the Optimization of Differential-Algebraic Process Systems," *AIChE Journal*, 1987

APPENDIX – D

FINAL OBJECTIVE FUNCTION AND CONSTRAINTS IN DISCRETIZED FORM USING ORTHOGONAL COLLOCATION METHOD

Using the method of discretization outlined in Chapter 3 and Appendix C, and the collocation model developed in Chapter 4, it is possible to develop an NLP for the dynamic optimization of the distillation column. This will form the optimization algorithm in GAMS. The final objective function and constraints are given below:

Maximize:

$$\sum_{i=1}^{NFE} \left[\sum_{j=1}^{NCOL} [D_{ij} \Psi_{[ij]}(1)] \tilde{x}_{7ij} V_d + \sum_{j=1}^{NCOL} [B_{ij} \Psi_{[ij]}(1)] (1 - \tilde{x}_{1ij}) V_b - \sum_{j=1}^{NCOL} [V_{ij} \Psi_{[ij]}(1)] C_v - \sum_{j=1}^{NCOL} [R_{ij} \Psi_{[ij]}(1)] C_R \right] \cdot (1 - \tau_{NCOL-1}) \Delta \alpha_i$$

<----- objective function value at end of each finite element ----->

$$+ \sum_{i=1}^{NFE} \left[\sum_{j=1}^{NCOL} [D_{ij} \tilde{x}_{7ij} V_d + B_{ij} (1 - \tilde{x}_{1ij}) V_b - V_{ij} C_v - R_{ij} C_R] (\tau_{j+1} - \tau_j) \right] \Delta \alpha_i$$

<--- objective function value at interior collocation point ----->

subject to

$$C_1 \leq R_{[ij]} \leq C_2 (B_{[ij]} + C_3) - F \quad \text{(flooding limit)}$$

$$R_{[ij]} \geq R_{\min} \quad \text{(weeping limit)}$$

$$0 \leq B_{[ij]} \leq F \quad \text{(bottoms flow rate constraint)}$$

$$\tilde{x}_{7[ij]}^L \leq \tilde{x}_7 \leq \tilde{x}_{7[ij]}^U \quad \text{(top composition bounds)}$$

$$\tilde{x}_{1[ij]}^L \leq \tilde{x}_1 \leq \tilde{x}_{1[ij]}^U \quad \text{(bottom composition bounds)}$$

$$\tilde{y}_{k[ij]} = \alpha \tilde{x}_{k[ij]} / (1 + (\alpha - 1) \cdot \tilde{x}_{k[ij]}) \quad \text{(equilibrium)}$$

(model constraints)

$$B_{[ij]} = F + R_{[ij]} - V_{[ij]} \quad \text{(Reboiler total material balance)}$$

$$M_{LB} \sum_{j=0}^{N_{COL}} \tilde{x}_{1[ij]} \frac{\varphi_{[ij]}(\tau_j)}{\Delta\alpha_i} - (R_{[ij]} + F) \left[(1/2)\tilde{x}_{1[ij]} + (1/2)\tilde{x}_{2[ij]} \right] + B_{[ij]} \tilde{x}_{1[ij]} + V_{[ij]} \tilde{y}_{1[ij]} = 0$$

(Reboiler component balance)

$$M_L \sum_{j=0}^{N_{COL}} \tilde{x}_{2[ij]} \frac{\varphi_{[ij]}(\tau_j)}{\Delta\alpha_i} - (R_{[ij]} + F) \left[(5/8)\tilde{x}_{2[ij]} + (5/8)\tilde{x}_{3[ij]} + (-1/4)\tilde{x}_{4[ij]} \right] + (R_{[ij]} + F) \cdot \tilde{x}_{2[ij]} \\ - V_{[ij]} \cdot \left[(5/12)\tilde{y}_{1[ij]} + (5/8)\tilde{y}_{2[ij]} + (-1/24)\tilde{y}_{3[ij]} \right] + V_{[ij]} \tilde{y}_{2[ij]} = 0$$

(Component balance for collocation point 1
in stripping section)

$$M_L \sum_{j=0}^{N_{COL}} \tilde{x}_{3[ij]} \frac{\varphi_{[ij]}(\tau_j)}{\Delta\alpha_i} - (R_{[ij]} + F) \left[(-1/24)\tilde{x}_{2[ij]} + (5/8)\tilde{x}_{3[ij]} + (5/12)\tilde{x}_{4[ij]} \right] + (R_{[ij]} + F) \cdot \tilde{x}_{3[ij]} \\ - V_{[ij]} \cdot \left[(-1/4)\tilde{y}_{1[ij]} + (5/8)\tilde{y}_{2[ij]} + (5/8)\tilde{y}_{3[ij]} \right] + V_{[ij]} \tilde{y}_{3[ij]} = 0$$

(Component balance for collocation point 2
in stripping section)

$$M_L \sum_{j=0}^{N_{COL}} \tilde{x}_{4[ij]} \frac{\varphi_{[ij]}(\tau_j)}{\Delta\alpha_i} - (R_{[ij]} + F) \left[(1/2)\tilde{x}_{4[ij]} + (1/2)\tilde{x}_{5[ij]} \right] + (R_{[ij]} + F) \cdot \tilde{x}_{4[ij]} - F \cdot Z_F \\ - V_{[ij]} \cdot \left[(1/2)\tilde{y}_{3[ij]} + (1/2)\tilde{y}_{4[ij]} \right] + V_{[ij]} \tilde{y}_{4[ij]} = 0$$

(Component balance for the
Feed Tray collocation point)

$$M_L \sum_{j=0}^{N_{COL}} \tilde{x}_{5[ij]} \frac{\varphi_{[ij]}(\tau_j)}{\Delta\alpha_i} - (R_{[ij]}) \left[(5/8)\tilde{x}_{5[ij]} + (5/8)\tilde{x}_{6[ij]} + (-1/4)\tilde{x}_{7[ij]} \right] + (R_{[ij]}) \cdot \tilde{x}_{5[ij]} \\ - V_{[ij]} \cdot \left[(5/12)\tilde{y}_{4[ij]} + (5/8)\tilde{y}_{5[ij]} + (-1/24)\tilde{y}_{6[ij]} \right] + V_{[ij]} \tilde{y}_{5[ij]} = 0$$

(Component balance for collocation point 1
in enriching section)

$$M_L \sum_{i=0}^{N_{COL}} \tilde{x}_{6[i]} \frac{\Phi_{[i]}(\tau_i)}{\Delta\alpha_i} - (R_{[i]}) \left[(-1/24)\tilde{x}_{5[i]} + (5/8)\tilde{x}_{6[i]} + (5/12)\tilde{x}_{7[i]} \right] + (R_{[i]}) \cdot \tilde{x}_{6[i]} \\ - V_{[i]} \cdot \left[(-1/4)\tilde{y}_{4[i]} + (5/8)\tilde{y}_{5[i]} + (5/8)\tilde{y}_{6[i]} \right] + V_{[i]} \tilde{y}_{6[i]} = 0$$

(Component balance for collocation point 2
in enriching section)

$$M_{LD} \sum_{j=0}^{N_{COL}} \tilde{x}_{7[j]} \frac{\Phi_{[j]}(\tau_j)}{\Delta\alpha_j} - (V_{[j]}) \left[(1/2)\tilde{y}_{6[j]} + (1/2)\tilde{y}_{7[j]} \right] + R_{[j]} \tilde{x}_{7[j]} + D_{[j]} \tilde{x}_{7[j]} = 0$$

(Component balance for accumulator)

$$D_{[i]} = V_{[i]} - R_{[i]}$$

(Total material balance for accumulator)

$$\tilde{x}_{x[0]} = \sum_{j=0}^{N_{COL}} \tilde{x}_{[1-\tau_j]} \Phi_{[j]}(\tau = 1)$$

(state profile continuity equations)

The objective function, with the above constraints, forms the NLP whose solution is the optimal control profiles that will be implemented in the process.

APPENDIX – E

CEO Tutorial

As mentioned in Chapters 3 and 5, the CEO strategy involves a dynamic Optimizer dictating optimal control profiles to the Process. The implementation of these entities is described below.

PROCESS

A screenshot of the Process interface is shown in Fig F-1 below:

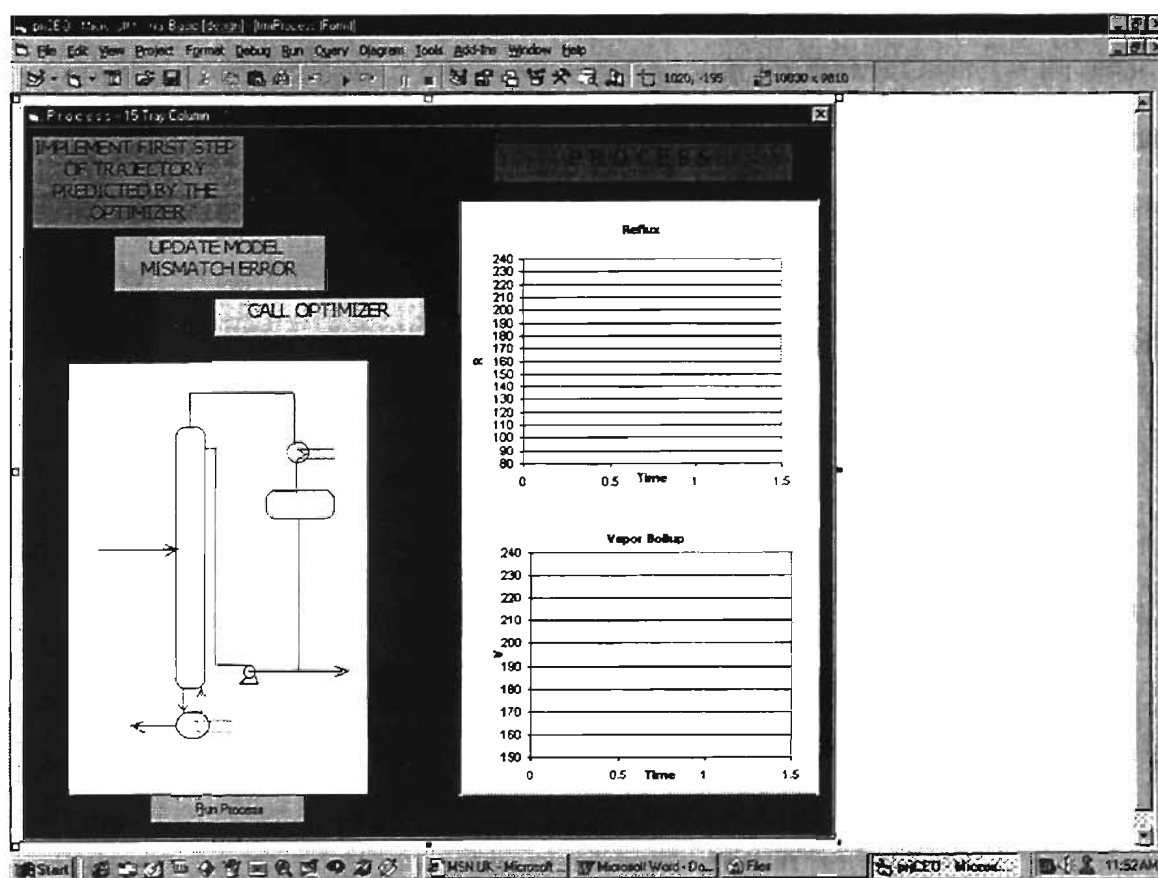


Fig F-1: Process VB Interface

The above interface comes up when the CEO program is invoked in Visual Basic. When the "Run Process" command button in the above interface is clicked, the simulation "officially" begins. The simulation is run for a few minutes (determined by the user) so as to converge the initial conditions to bona fide conditions. The progress of the simulation can be tracked on the Excel chart on the interface. Then, the GAMS Optimizer is called by the Process itself. For purposes of the study, the Process is kept "on hold" while the Optimizer is running.

VB GAMS Interface

For the Visual Basic Process simulation to "call" the GAMS Optimizer (in other words, to link Visual Basic and GAMS), a plug-in is necessary. This plug-in is available at www.gams.com, the official GAMS web site. For linking the two software, the forms for the plug-in named frmGAMS must be included as part of the current Visual Basic project. The particular lines of code that must be included to run VB GAMS is as follows:

frmGams.Show

CALL frmGams.cmdRunGams_Click

During runtime when the VB compiler encounters this piece of code, it will run the VB GAMS code, and call up the interface shown in Fig F-2. This interface can be kept normal (as shown in Fig F-2), minimized, or completely hidden. The second line of code causes the GAMS to get activated and compile and execute the GAMS file mentioned in the textbox of the interface in Fig. F-2. Then, the GAMS file is executed and the Optimizer builds an output file which dictates the optimal profile to the Process.

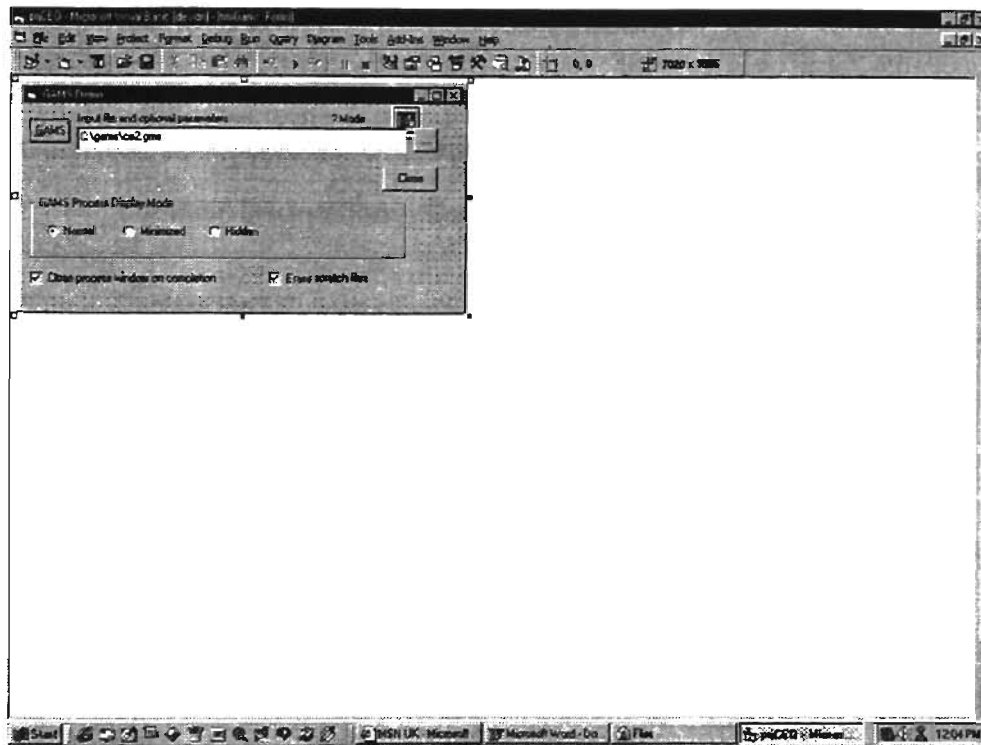


Fig F-2: VB GAMS Interface Form

After writing the output file, the VB GAMS is made to recall the Process interface and run the simulation with the optimal profile dictated by the Optimizer.

The above setup then loops over till the end of the specified process time (2 hr in the study).

APPENDIX – F

CODE FOR THE THREE CONTROL SCHEMES

CONTROL TO ECONOMIC OPTIMUM

" Common Declarations - Common to All Modules

" Declare the following variables (arrays as appropriate)

i	Tray number
Nt	Number of trays
Nf	Feed tray location
X (i)	Liquid phase compositions on a given tray
X0(i)	Initial liquid phase compositions on a given tray
Y(i)	Vapor phase compositions on a given tray
L(i)	Liquid flow rate leaving a given tray
Lo(i)	Initial liquid phase inventories on a given tray
Mdot(i)	Material balance derivatives on a given tray
Mxdot(i)	Component balance derivative on a given tray
M(i)	Inventory on a given tray
M0	Initial inventory on a given tray
Mb0	Bottom sump inventory
Md0	Reflux drum inventory
Zf	Feed composition
F	Feed flow rate
Yb, Yd	Bottoms and distillate vapor composition
Xb, Xd	Bottoms and distillate liquid composition
Beta	Tray hydraulic time constant
Alpha	Relative volatility
B	Bottoms flow rate
V	Vapor flow rate
R	Reflux flow rate
D	Distillate flow rate
delta	Integration step size
Tim	Process Time
Upd	Dummy variable to keep track of real time
Tprint	Time step for printing results
Iteration	Overall iteration number
objExcel	Excel spreadsheet object for graphical display

Dim X(1 To 20) As Single, Y(1 To 20) As Single, L(1 To 20) As Single, L0(1 To 20) As Single, M(1 To 20) As Single

Dim MX(1 To 50) As Single, Mdot(1 To 50) As Single, Mxdot(1 To 50) As Single, Yb As Single, Yd As Single

Dim M0 As Single, Mb0 As Single, Md0 As Single, Tdum(1 To 2) As Single, Zf As Single

Dim Nt As Integer, Nf As Integer, F As Single, Beta As Single

Dim Tprint As Single, delta As Single, Xb As Single, Xd As Single

Dim Alpha As Single, B As Single, V As Single, R As Single, D As Single

Dim Str1 As String, Str2 As String, objExcel2 As Object

Dim X0(1 To 20) As Single, Xd0 As Single, Xb0 As Single, Bop As Single

Dim Iter As Single, Upd As Single

```

' MODULE A - PROCESS SIMULATION MODULE

Public Sub cmdRun_click()
'   LOCAL VARIABLE DECLARATION
'   objExcel      Excel object for graphical display of results
'   Xp(i)         Liquid phase composition based on Optimizer collocation model
'   PMM(i)        Process Model Mismatch in the ith tray
'   t1 - t7       Time periods whose lengths match the finite element
'                 lengths in the Optimizer
'   R1-R7         Reflux flow rates dictated by the Optimizer for above time periods
'   V1-V7         Vapor Boilup flow rates dictated by Optimizer for above time periods

'   Create the Excel Spreadsheet object for the graphical display of data
Set objExcel = ole1.object
Rem The Model is described below:
Rem Assumptions:
Rem - Constant relative volatility
' - Equimolal overflow
' - Theoretical trays
' - Simple tray hydraulics
' Initial Conditions - Open Input file and receive inlet conditions

Open App.Path & "/input1a.txt" For Input As #1
Input #1, Nt, Nf, Md0, Mb0, M0, R0, V0, Beta, Alpha
Close #1
Open App.Path & "/input2a.txt" For Input As #2
Input #2, tim
Input #2, Xb
For I = 1 To Nt
Input #2, X(I)
Next I
Input #2, Xd
Input #2, lter
Close #2
Tprint = tim
Upd = tim

'   Reset time to its appropriate value as given by Upd
If Upd > 0 Then lter = lter - 1
'   Receive Feed conditions
Open App.Path & "/input5a.txt" For Input As #6
Input #6, F, Zf
Close #6
'   Optional disturbance (could be feed flow rate or composition)
If tim > 1.2 Then F = 95
If tim = 0 Then      ' Initialize conditions on trays
For I = 1 To Nt
M(I) = M0
MX(I) = M(I) * X(I)
L0(I) = R0 + F
If (I > Nf) Then
L0(I) = R0
End If
Next I
Else
Open App.Path & "/liqflow.txt" For Input As #10      'Else proceed from previous values

```

```

For I = 1 To Nt
    M(I) = M0
    MX(I) = M(I) * X(I)
    Input #10, L0(I)
Next I
Close #10
End If
' Obtain optimal control trajectory and predicted compositions from the Optimizer: if time
= 0, then just read initial conditions
Open "C:/gams/opt.gms" For Input As #10
Input #10, t1, V1, R1
Input #10, t2, V2, R2
Input #10, t3, V3, R3
If tim > 0 Then
    Input #10, t4, V4, R4
    Input #10, t5, v5, R5
    Input #10, t6, V6, R6
    Input #10, t7, V7, R7
    Input #10, t8, V8, R8
    For I = 1 To 7
        Input #10, Xp(I)
    Next I
End If
Close #10

' Tray hydraulics and VLE
10 For I = 1 To Nt
    L(I) = L0(I) + (M(I) - M0) / Beta           ' EQUATION (4-10)
    Y(I) = alpha * X(I) / (1 + X(I))           ' EQUATION (4-11) FOR EACH TRAY
Next I
Yb = alpha * Xb / (1 + Xb)                     ' EQUATION (4-11) FOR BOTTOMS
Yd = alpha * Xd / (1 + Xd)                     ' EQUATION (4-11) FOR DISTILLATE

' Recreate optimal profile based on the Lagrange Polynomial basis approximation
for the first step

If tim >= t1 + Upd And tim <= t3 + Upd + 0.5 Then
    V = V2 * (tim - Upd - t3) / (t2 - t3) + V3 * (tim - Upd - t2) / (t3 - t2)
    R = R2 * (tim - Upd - t3) / (t2 - t3) + R3 * (tim - Upd - t2) / (t3 - t2)
End If

' Assuming perfect level controllers in column base and reflux drum
D = V - R           ' EQUATION (4-4) WITH ACCUMULATION TERM = 0
B = L(1) - V        ' EQUATION (4-7) WITH ACCUMULATION TERM = 0

' Check for validity of R and V
If ((R < 0) Or (V < 0) Or (D < 0) Or (B < 0)) Then
    GoTo 100
End If

' Evaluate Derivatives and Tray Temperatures
' Step 1: for Bottoms
Xbdot = (L(1) * X(1) - V * Yb - B * Xb) / Mb0 ' EQUATION (4-8)
' Step 2a: for first tray
Mdot(1) = L(2) - L(1) ' EQUATION (4-1) FOR TRAY 1 WITH
F(1) = 0

```

```

Mxdot(1) = V * (Yb - Y(1)) + L(2) * X(2) - L(1) * X(1) ' EQUATION (4-2) FOR TRAY 1 WITH
F(1) = 0
' Step 2b: Stripping section trays
For I = 2 To Nf - 1
Mdot(I) = L(I + 1) - L(I) ' EQUATION (4-1) FOR TRAYS 2-7 WITH F(I) = 0
Mxdot(I) = V * (Y(I - 1) - Y(I)) + L(I + 1) * X(I + 1) - L(I) * X(I)
' EQUATION (4-2) FOR TRAY 2-7 WITH F(I) = 0
Next I
' Step 2c: Feed Tray
Mdot(Nf) = L(Nf + 1) - L(Nf) + F
' EQUATION (4-1) FOR TRAY Nf
Mxdot(Nf) = V * (Y(Nf - 1) - Y(Nf)) + L(Nf + 1) * X(Nf + 1) - L(Nf) * X(Nf) + F * Zf
' EQUATION (4-2) FOR TRAY Nf
' Step 2d: Enriching section trays
For I = Nf + 1 To Nt - 1
Mdot(I) = L(I + 1) - L(I) ' EQUATION (4-1) FOR TRAY 9-14 WITH F(i) = 0
Mxdot(I) = V * (Y(I - 1) - Y(I)) + L(I + 1) * X(I + 1) - L(I) * X(I)
' EQUATION (4-2) FOR TRAY 9-14 WITH F(i) = 0
Next I
' Step 2e: Top Tray
Mdot(Nt) = R - L(Nt)
' EQUATION (4-1) FOR TRAY Nt WITH F(i) = 0
Mxdot(Nt) = V * (Y(Nt - 1) - Y(Nt)) + R * Xd - L(Nt) * X(Nt)
' EQUATION (4-2) FOR TRAY Nt WITH F(i) = 0

' Step 3: Reflux Drum
Xddot = V * (Y(Nt) - Xd) / Md0 ' EQUATION (4-5)

' Print current conditions in the Excel Spreadsheet object
If tim < Tprint Then GoTo 20
ole1.Action = 7
objExcel.worksheets("Process Values").Cells(Iter + 2, 1).Value = tim / 12 'output Time
objExcel.worksheets("Process Values").Cells(Iter + 2, 2).Value = Xd ' Distillate compositions
objExcel.worksheets("Process Values").Cells(Iter + 2, 3).Value = Xb ' Bottom compositions
objExcel.worksheets("Process Values").Cells(Iter + 2, 4).Value = R ' Reflux flow rates
objExcel.worksheets("Process Values").Cells(Iter + 2, 5).Value = V ' Vapor boilups
objExcel.worksheets("Process Values").Cells(Iter + 2, 6).Value = (6.12 * (V - R) * Xd + 0.95 * (F +
R - V) * (1 - Xb) - 0.002 * V - 0.001 * R) ' output Current Profit
Print #4, tim; Tab(10); Xb; Tab(20); X(10); Tab(30); Xd; Tab(40); R; Tab(50); V
Iter = Iter + 1 ' Update iteration number
Tprint = Tprint + 0.05 ' Update print time

' Euler Integration
20 tim = tim + delta ' Step forward in time
tim = Round(tim, 3)
Xb = Xb + delta * Xbdot ' Integrate the Bottoms Component Material Balance

For I = 1 To Nt
M(I) = M(I) + Mdot(I) * delta ' Integrate the Total Material Balance Equation for each
tray
MX(I) = MX(I) + Mxdot(I) * delta ' Integrate the Component Material Balance for each tray
X(I) = MX(I) / M(I) ' Update tray liquid compositions

If X(I) < 0 Or X(I) > 1 Then
GoTo 100
End If

```

Next I

$X_d = X_d + X_{ddot} * \Delta t$ ' Integrate reflux drum Component Material Balance

If tim > Upd + 0.5 Then GoTo 110 Else GoTo 10

100 message = MsgBox("Level too low or composition unreal!", vbOKCancel, Alert)

Provide alert in case of inconsistent conditions

110 Close #4

' **Update conditions in appropriate input/output files**

' **Update input compositions for next iteration**

Open App.Path & "/input2a.txt" For Output As #2

Write #2, Round(tim - 0.01, 2)

Write #2, Xb

For I = 1 To Nt

Write #2, X(I)

Next I

Write #2, Xd

Write #2, Iter

Close #2

'OLE1.Action = 9

' **Update Process Model Mismatch for next iteration**

PMM(1) = Xb - Xp(1)

PMM(2) = X(2) - Xp(2)

PMM(3) = X(6) - Xp(3)

PMM(4) = X(8) - Xp(4)

' EQUATION (5-3)

PMM(5) = X(10) - Xp(5)

PMM(6) = X(14) - Xp(6)

PMM(7) = Xd - Xp(7)

' **If time = 0, initialize Process Model Mismatch**

If Upd = 0 Then

Xp(1) = Xb

Xp(2) = X(2)

Xp(3) = X(6)

Xp(4) = X(8)

Xp(5) = X(10)

Xp(6) = X(14)

Xp(7) = Xd

For I = 1 To 7

PMM(I) = 0

Next I

End If

If tim < 24 Then

Open App.Path & "/liqflow.txt" For Output As #10

For I = 1 To Nt

Print #10, L(I)

' Update Liquid flow rates

Next I

Close #10

Call frmCEO.cmdOpt_Click(F, Zf, X(), V, R, L(), M0, Mb0, Md0, Xd, Xb, B, D, Upd, PMM(), Xp())

' Call GAMS optimizer

frmProcess.Hide

' "Hide" Process form

End If

' **At the end of simulation, update all input files for future simulations**

frmProcess.Show

' **Update liquid compositions**

Open App.Path & "/input2a.txt" For Output As #2

Print #2, "0"

Print #2, "0.03307186"

Print #2, " 0.05707043"

Print #2, "0.09118611"

Print #2, "0.1371004"

Print #2, "0.194544"

Print #2, "0.2601927"

Print #2, "0.3278891"

Print #2, "0.3906865"

Print #2, "0.4434727"

Print #2, "0.4876422"

Print #2, "0.5445065"

Print #2, "0.6129248"

Print #2, "0.6888504"

Print #2, "0.7659057"

Print #2, "0.8373332"

Print #2, "0.8981946"

Print #2, "0.9464403"

Print #2, "0"

' **Update initial flow rates**

Open "C:/gams/opt.gms" For Output As #10

Print #10, "0, 177, 114"

Print #10, "0.5, 177, 114"

Print #10, "1, 177, 114"

Close #10

End Sub

' **MODULE - B FOR CONSTRUCTING THE INPUT FILE TO THE OPTIMIZER**

Rem This subroutine "creates" a GAMS program by writing the text following the PRINT statements below to the file "C:/gams/ce2.gms." The Code for the PRINT statements is not shown below. Instead the GAMS file itself is provided.

Rem The documentation for the statements below are provided in the GAMS file

' **Call the subroutine that executes GAMS**

Call frmGams.cmdRunGams_Click

Iter = 1

End Sub

CEO GAMS PROGRAM

*** GAMS OPTIMIZER THAT DICTATES OPTIMAL PROFILES FOR R AND V FOR THE PROCESS**

*** DECLARE TITLE**

\$TITLE Control to Economic Optimum

*** MAKE GAMS CASE-INSENSITIVE**

\$OFFUPPER

*** SET OTHER PROGRAM OPTIONS**

\$OFFSYMXREF OFFSYMLIST

\$OFFDIGIT

*** (SEE APPENDIX B FOR DEFINITION OF KEYWORDS)**

*** DECLARE SETS**

SETS K equation # (max 10) /K1*K7/
I finite elements # (max 20) /I1*I20/
J collocation coeff. # /J1*J6/
COL # possible coll pt (max 4) /C1*C4/
ALIAS (K,KP)
(J,JP,JJ,JS) ;

*** DECLARE SCALARS AND SET FLAG OPTIONS**

SCALARS NK actual # of equations /7/
NFE actual # of FE used /2/
NCOL actual # coll. pt used /2/ ;
SCALAR NCOF equal to ncol+1 ;
NCOF = ncol+1 ;
SCALAR NCOT equal to ncol+2

*** SEE APPENDIX A FOR COLLOCATION MODEL DEVELOPMENT**

F FEED FLOW RATE

ML MATERIAL ON TRAY

MLB MATERIAL IN BOTTOMS

MLD MATERIAL IN DRUM

RELVOL RELATIVE VOLATILITY

PMM1 process model mismatch between process and collocation model for variable x(s1,t)

PMM2 process model mismatch between process and collocation model for variable x(s2,t)

PMM3 process model mismatch between process and collocation model for variable x(s3,t)

PMM4 process model mismatch between process and collocation model for variable x(s4,t)

PMM5 process model mismatch between process and collocation model for variable x(s5,t)

PMM6 process model mismatch between process and collocation model for variable x(s6,t)

PMM7 process model mismatch between process and collocation model for variable x(s7,t)

xf feed composition;

relvol = 2.0;

*** ASSIGN CURRENT PROCESS VALUES AND VALUES FOR PROCESS MODEL MISMATCH**

F = 100 ;
XF = 0.48 ;
ML = 10 ;
MLB = 100 ;
MLD = 100 ;
PMM1 = 0 ;
PMM2 = 0 ;
PMM3 = 0 ;
PMM4 = 0 ;
PMM5 = 0 ;
PMM6 = 0 ;
PMM7 = 0 ;
NCOT = ncol+2 ;

=====

*** DEFINE DIMENSIONS FOR COLLOCATION COEFFICIENTS, CONTROL VARIABLES, LAGRANGE POLYNOMIAL BASIS FUNCTION PHI, ITS DERIVATIVE PHIPR, ERROR APPROXIMATION EQUATIONS, FINITE ELEMENT LENGTH EQUATIONS, CONTROL PROFILES, END CONDITION EQUATIONS**

=====

SET SXCOL(k,i,jp) actual dim of coll. coeff. (XCOL) ;
 SXCOL(k,i,jp) = YES \$ ((ORD(k) LE nk) \$ (ORD(i) LE nfe) \$ (ORD(jp) LE ncof)) ;

SET SU(i,j) actual dim of control variable ;
 SU(i,j) = YES \$ ((ORD(i) LE nfe) \$ (ORD(j) GT 1) \$ (ORD(j) LE ncof)) ;

SET SPHIPR(j,jp) actual dim of PHIPR ;
 SPHIPR(j,jp) = YES \$ ((ORD(j) GT 1) \$ (ORD(j) LE ncot) \$ (ORD(jp) LE ncof)) ;

SET SDPHI(jp) actual dim of dominator of PHI ;
 SDPHI(jp) = YES \$ ((ORD(jp) LE ncof)) ;

SET SRES(i,j) actual dim of residual eq ;
 SRES(i,j) = YES \$ ((ORD(i) LE nfe) \$ (ORD(j) GT 1) \$ (ORD(j) LE ncof)) ;

SET SERR(i,j) actual dim of error eq ;
 SERR(i,j) = YES \$ ((ORD(i) LE nfe) \$ (ORD(j) EQ ncot)) ;

SET SALF(i) actual dim of alpha ;
 SALF(i) = YES \$ (ORD(i) LE nfe) ;

SET SUPRO(i) dim of control profile ;
 SUPRO(i) = YES \$ (ORD(i) LE nfe) ;

SET SXEND(k,i) end condition for state variables ;
 SXEND(k,i) = YES \$ ((ORD(k) LE nk) \$ (ORD(i) EQ nfe)) ;

SET SCONT(k,i) actual dim of continuity eq ;
 SCONT(k,i) = YES \$ ((ORD(k) LE nk) \$ (ORD(i) GT 1) \$ (ORD(i) LE nfe)) ;

=====

*** DECLARE PARAMETERS**

=====

PARAMETERS TAU(jp) tau at specified ncol SEE EQUATION (3-6)
 PHIPR(j,jp) 1-st deriv of phi
 alpha(i) finite element length
 DPHI(jp) dominator of phi ;

* SET AT ALPHA('I1') = ALPHA('I2') = 4 SEE DISCUSSION IN SECTION 6.4.1.2
 alpha('i1') = 4 ;
 alpha('i2') = 4 ;

=====

*** SET THE ROOTS OF THE LAGRANGE POLYNOMIALS:**

=====

TABLE GENTAU(col,jp) the roots of Lagrange polyn.

	J2	J3
C1	.5	1.
C2	.211324865405187	.788675134594813
C3	.1127016653792585	.5
C4	.0694318442	.3300094783
+	J4	J5
C2	1.	
C3	.8872983346207415	1.
C4	.6699905218	.9305681558
+	J6	
C4	1. ;	

```

=====
* * Assign tau according to the specified NCOL
TAU(jp) $ ( ORD(jp) LE ncol) = gentau('C1',jp) $(ncol EQ 1) + gentau('C2',jp) $(ncol EQ 2) +
gentau('C3',jp) $(ncol EQ 3) + gentau('C4',jp) $(ncol EQ 4) ;

* Calculate DPHI (needed for calculating PHIPR)
DPHI(JP) $ SDPHI(JP) = PROD(J $ ( (ORD(J) LE ncol) $ (ORD(J) NE ORD(JP)) ), (TAU(JP) -
TAU(J)) ) ;

* Calculate PHIPR (1-st derivative of PHI)
PHIPR(J,JP) $ SPHIPR(J,JP) = SUM (JS $ ( (ORD(JS) LE ncol) $ (ORD(JS) NE ORD(JP)) ),
PROD(JJ $ ( (ORD(JJ) LE ncol) $ (ORD(JJ) NE ORD(JP)) $ (ORD(JJ) NE ORD(JS)) ), (TAU(J) -
TAU(JJ)) ) ) / DPHI(JP) ;
=====
* DECLARE VARIABLES
=====
VARIABLES XCOL(k,i,jp) collocation coefficients
          XEND(k,i)   state variable at the end condition
          L(I,J)      REFLUX FLOW
          V(I,J)      VAPOR FLOW RATES
          OBJ          objective function ;
=====
* DECLARE EQUATIONS
=====
EQUATIONS ERES1(i,j) residual equations from EQUATION 4-12a & r(t[i,j]) in
EQUATIONS 3-9
          ERES2(i,j) residual equations from EQUATION 4-12b & r(t[i,j]) in EQUATIONS 3-9
          ERES3(i,j) residual equations from EQUATION 4-12c & r(t[i,j]) in EQUATIONS 3-9
          ERES4(i,j) residual equations from EQUATION 4-12d & r(t[i,j]) in EQUATIONS 3-9
          ERES5(i,j) residual equations from EQUATION 4-12e & r(t[i,j]) in EQUATIONS 3-9
          ERES6(i,j) residual equations from EQUATION 4-12f & r(t[i,j]) in EQUATIONS 3-9
          ERES7(i,j) residual equations from EQUATION 4-12g & r(t[i,j]) in EQUATIONS 3-9
          ECONT(k,i) continuity equations from EQUATION (3-8)
          Ello(i)    Lower limit for Reflux Control Profile from Table 6-2 for RL
          Elup(i)    Upper limit for Reflux Control Profile from Table 6-2 for RU
          Evlo(i)    Lower limit for Vapor Boilup Control Profile from Table 6-2 for VL
          Evup(i)    Upper limit for Vapor Boilup Control Profile from Table 6-2 for VU
          XEND(k,i) end conditions
          EOBJ          objective function ;
=====
* SEE APPENDIX D FOR FOR FURTHER EXPLANATION OF EACH EQUATION
=====
* residual equations from EQUATION 4-12a & r(t[i,j]) in EQUATIONS 3-9
* Component balance Equation for Reboiler Collocation Point

ERES1(i,j) $ SRES(i,j) ..
MLB*SUM(jp $ (ORD(jp) LE ncol), XCOL('K1',i,jp)*PHIPR(j,jp) ) - ALPHA(i) *
((L(I,J)+F)*((1/2)*XCOL('K1',i,J)+(1/2)*XCOL('K2',i,J))-(L(I,J)+F-V(I,J))*XCOL('K1',i,J)-
V(I,J)*(RELVOL*XCOL('K1',i,J)/(1+(RELVOL-1)*XCOL('K1',i,J)))) =E= 0 ;
=====
* residual equations from EQUATION 4-12b & r(t[i,j]) in EQUATIONS 3-9
* Component balance Equation for Collocation Point 1 in Stripping Section

```

ERES2(i,j) \$ SRES(i,j) ..
 ML*SUM(jp \$ (ORD(jp) LE ncof), XCOL('K2',i,jp)*PHIPR(j,jp)) - ALPHA(i) *
 ((L(I,J)+F)*((5/8)*XCOL('K2',I,J)+(5/8)*XCOL('K3',I,J)+(-1/4)*XCOL('K4',I,J))-
 (F+L(I,J))*XCOL('K2',I,J)-V(I,J)*(RELVOL*XCOL('K2',I,J)/(1+(RELVOL-
 1)*XCOL('K2',I,J)))+V(I,J)*((5/12)*(RELVOL*XCOL('K1',I,J)/(1+(RELVOL-
 1)*XCOL('K1',I,J)))+(5/8)*(RELVOL*XCOL('K2',I,J)/(1+(RELVOL-1)*XCOL('K2',I,J)))+(-
 1/24)*(RELVOL*XCOL('K3',I,J)/(1+(RELVOL-1)*XCOL('K3',I,J))))) =E= 0 ;

*** residual equations from EQUATION 4-12c & r(t[i,j]) in EQUATIONS 3-9**

*** Component balance Equation for Collocation Point 2 in Stripping Section**

ERES3(i,j) \$ SRES(i,j) ..
 ML*SUM(jp \$ (ORD(jp) LE ncof), XCOL('K3',i,jp)*PHIPR(j,jp)) - ALPHA(i) *((L(I,J)+F)*((-
 1/24)*XCOL('K2',I,J)+(5/8)*XCOL('K3',I,J)+(5/12)*XCOL('K4',I,J))-(F+L(I,J))*XCOL('K3',I,J)-
 V(I,J)*(RELVOL*XCOL('K3',I,J)/(1+(RELVOL-1)*XCOL('K3',I,J)))+V(I,J)*((-
 1/4)*(RELVOL*XCOL('K1',I,J)/(1+(RELVOL-
 1)*XCOL('K1',I,J)))+(5/8)*(RELVOL*XCOL('K2',I,J)/(1+(RELVOL-
 1)*XCOL('K2',I,J)))+(5/8)*(RELVOL*XCOL('K3',I,J)/(1+(RELVOL-1)*XCOL('K3',I,J))))) =E= 0 ;

*** residual equations from EQUATION 4-12d & r(t[i,j]) in EQUATIONS 3-9**

*** Component balance Equation for Feed Tray Collocation Point**

ERES4(i,j) \$ SRES(i,j) ..
 ML*SUM(jp \$ (ORD(jp) LE ncof), XCOL('K4',i,jp)*PHIPR(j,jp)) - ALPHA(i) *
 ((L(I,J))*((1/2)*XCOL('K4',I,J)+(1/2)*XCOL('K5',I,J))-(F+L(I,J))*XCOL('K4',I,J)+F*XF-
 V(I,J)*(RELVOL*XCOL('K4',I,J)/(1+(RELVOL-
 1)*XCOL('K4',I,J)))+V(I,J)*((1/2)*(RELVOL*XCOL('K3',I,J)/(1+(RELVOL-
 1)*XCOL('K3',I,J)))+(1/2)*(RELVOL*XCOL('K4',I,J)/(1+(RELVOL-1)*XCOL('K4',I,J))))) =E= 0 ;

*** residual equations from EQUATION 4-12e & r(t[i,j]) in EQUATIONS 3-9**

*** Component balance Equation for Collocation Point 1 in Enriching Section**

ERES5(i,j) \$ SRES(i,j) ..
 ML*SUM(jp \$ (ORD(jp) LE ncof), XCOL('K5',i,jp)*PHIPR(j,jp)) - ALPHA(i) *
 ((L(I,J))*((5/8)*XCOL('K5',I,J)+(5/8)*XCOL('K6',I,J)+(-1/4)*XCOL('K7',I,J))-L(I,J)*XCOL('K5',I,J)-
 V(I,J)*(RELVOL*XCOL('K5',I,J)/(1+(RELVOL-
 1)*XCOL('K5',I,J)))+V(I,J)*((5/12)*(RELVOL*XCOL('K4',I,J)/(1+(RELVOL-
 1)*XCOL('K4',I,J)))+(5/8)*(RELVOL*XCOL('K5',I,J)/(1+(RELVOL-1)*XCOL('K5',I,J)))+(-
 1/24)*(RELVOL*XCOL('K6',I,J)/(1+(RELVOL-1)*XCOL('K6',I,J))))) =E= 0 ;

*** residual equations from EQUATION 4-12f & r(t[i,j]) in EQUATIONS 3-9**

*** Component balance Equation for Collocation Point 2 in Enriching Section**

ERES6(i,j) \$ SRES(i,j) ..
 ML*SUM(jp \$ (ORD(jp) LE ncof), XCOL('K6',i,jp)*PHIPR(j,jp)) - ALPHA(i) * ((L(I,J))*((-
 1/24)*XCOL('K5',I,J)+(5/8)*XCOL('K6',I,J)+(5/12)*XCOL('K7',I,J))-L(I,J)*XCOL('K6',I,J)-
 V(I,J)*(RELVOL*XCOL('K6',I,J)/(1+(RELVOL-1)*XCOL('K6',I,J)))+V(I,J)*((-
 1/4)*(RELVOL*XCOL('K4',I,J)/(1+(RELVOL-
 1)*XCOL('K4',I,J)))+(5/8)*(RELVOL*XCOL('K5',I,J)/(1+(RELVOL-
 1)*XCOL('K5',I,J)))+(5/8)*(RELVOL*XCOL('K6',I,J)/(1+(RELVOL-1)*XCOL('K6',I,J))))) =E= 0 ;

*** residual equations from EQUATION 4-12g & r(t[i,j]) in EQUATIONS 3-9**

*** Component balance Equation for Accumulator Collocation Point**

ERES7(i,j) \$ SRES(i,j) ..
 MLD*SUM(jp \$ (ORD(jp) LE ncof), XCOL('K7',i,jp)*PHIPR(j,jp)) - ALPHA(i) * (-
 L(I,J)*XCOL('K7',I,J)-(V(I,J)-
 L(I,J))*XCOL('K7',I,J)+V(I,J))*((1/2)*(RELVOL*XCOL('K6',I,J)/(1+(RELVOL-
 1)*XCOL('K6',I,J)))+(1/2)*(RELVOL*XCOL('K7',I,J)/(1+(RELVOL-1)*XCOL('K7',I,J)))) =E= 0 ;

*** Continuity Equation from Equation 3-8**

ECONT(k,i) \$ SCONT(k,i) ..
 XCOL(k,i,'J1') =E= SUM(j \$ (ORD(j) LE ncof), XCOL(k,i-1,j)*PROD(jp \$ (ORD(jp) NE ORD(j) AND
 ORD(jp) LE ncof), ((1.0 - tau(jp))/(tau(j) - tau(jp))))) ;

*** Lower limit for Reflux Control Profile from Table 6-2 for RL**

EVLO(i) \$ SUPRO(i) ..
 SUM(jp \$ (ORD(jp) GT 1 AND ORD(jp) LE ncof), V(i,jp)* PROD(js \$ (ORD(js) NE ORD(jp) AND
 ORD(js) GT 1 AND ORD(js) LE ncof), ((0 - tau(js))/(tau(jp) - tau(js))))) =G= 130 ;

*** Upper limit for Reflux Control Profile from Table 6-2 for RU**

EVUP(i) \$ SUPRO(i) ..
 SUM(jp \$ (ORD(jp) GT 1 AND ORD(jp) LE ncof), V(i,jp)* PROD(js \$ (ORD(js) NE ORD(jp) AND
 ORD(js) GT 1 AND ORD(js) LE ncof), ((1.0 - tau(js))/(tau(jp) - tau(js))))) =L= 190 ;

*** Lower limit for Vapor Boilup Control Profile from Table 6-2 for VL**

ELLO(i) \$ SUPRO(i) ..
 SUM(jp \$ (ORD(jp) GT 1 AND ORD(jp) LE ncof), L(i,jp)* PROD(js \$ (ORD(js) NE ORD(jp) AND
 ORD(js) GT 1 AND ORD(js) LE ncof), ((0 - tau(js))/(tau(jp) - tau(js))))) =G= 100 ;

*** Lower limit for Vapor Boilup Control Profile from Table 6-2 for VL**

ELUP(i) \$ SUPRO(i) ..
 SUM(jp \$ (ORD(jp) GT 1 AND ORD(jp) LE ncof), L(i,jp)* PROD(js \$ (ORD(js) NE ORD(jp) AND
 ORD(js) GT 1 AND ORD(js) LE ncof), ((1.0 - tau(js))/(tau(jp) - tau(js))))) =L= 150 ;

*** end condition equations**

EXEND(k,i) \$ SXEND(k,i) ..
 XCOL(k,i+1,'J1') =E= SUM(j \$ (ORD(j) LE ncof), XCOL(k,i,j)* PROD(jp \$ (ORD(jp) NE ORD(j)
 AND ORD(jp) LE ncof), ((1.0 - tau(jp))/(tau(j) - tau(jp))))) ;

*** the objective function - See Appendix -D**

EOBJ ..
 OBJ =E= SUM(I \$(ORD(I) LE NFE), ((6.12*(V(I,'J2')-
 L(I,'J2'))*(XCOL('K7',I,'J2')+PMM7)+0.95*(L(I,'J2')+F-V(I,'J2'))*(1-(XCOL('K1',I,'J2')-PMM1))-
 0.002*V(I,'J2')-0.001*L(I,'J2'))*(0.211*ALPHA(I))+
 (6.12*(V(I,'J3')-L(I,'J3'))*(XCOL('K7',I,'J3')+PMM7)+0.95*(L(I,'J3')+F-
 V(I,'J3'))*(1-(XCOL('K1',I,'J3')-PMM1))-0.002*V(I,'J3')-0.001*L(I,'J3'))*(0.679*ALPHA(I)))+
 (6.12*(EVUP.L('I1')-
 ELUP.L('I1'))*(XCOL('K7',I2,'J1')+PMM7)+0.95*(ELUP.L('I1')+F-EVUP.L('I1'))*(1-(XCOL('K1',I2',
 'J1')-PMM1))-0.002*EVUP.L('I1')-0.001*ELUP.L('I1'))*(0.211*alpha('i1'))+
 (6.12*(EVUP.L('I2')-
 ELUP.L('I2'))*(XCOL('K7',I3,'J1')+PMM7)+0.95*(ELUP.L('I2')+F-EVUP.L('I2'))*(1-
 (XCOL('K1',I3,'J1')-PMM1))-0.002*EVUP.L('I2')-0.001*ELUP.L('I2'))*(0.211*alpha('i2')));

*** SET BOUNDS FOR ALL COLLOCATION COEFFICIENTS AND CONTROL VARIABLES**

XCOL.LO('K1',I,JP)\$ SXCOL('k1',i,jp) = 0.04;
 XCOL.UP('K1',I,JP)\$ SXCOL('k1',i,jp) = 0.09;
 XCOL.LO('K2',I,JP)\$ SXCOL('k2',i,jp) = 0.09;
 XCOL.UP('K2',I,JP)\$ SXCOL('k2',i,jp) = 0.22;
 XCOL.LO('K3',I,JP)\$ SXCOL('k3',i,jp) = 0.20;
 XCOL.UP('K3',I,JP)\$ SXCOL('k3',i,jp) = 0.40;
 XCOL.LO('K4',I,JP)\$ SXCOL('k4',i,jp) = 0.35;
 XCOL.UP('K4',I,JP)\$ SXCOL('k4',i,jp) = 0.52;
 XCOL.LO('K5',I,JP)\$ SXCOL('k5',i,jp) = 0.5;
 XCOL.UP('K5',I,JP)\$ SXCOL('k5',i,jp) = 0.75;
 XCOL.LO('K6',I,JP)\$ SXCOL('k6',i,jp) = 0.7;
 XCOL.UP('K6',I,JP)\$ SXCOL('k6',i,jp) = 0.935;
 XCOL.LO('K7',I,JP)\$ SXCOL('k7',i,jp) = 0.95 ;
 XCOL.UP('K7',I,JP)\$ SXCOL('k7',i,jp) = 0.98 ;
 L.LO(i,j)\$SU(I,J) = 100.0 ;
 L.UP(i,j)\$SU(I,J) = 150;
 V.LO(I,J)\$SU(I,J) = 130.0 ;
 V.UP(I,J)\$SU(I,J) = 190.0 ;

*** starting guesses for collocation coefficients**

XCOL.L('K1',I,JP)\$ SXCOL('k1',i,jp) = .06;
 XCOL.L('K2',I,JP)\$ SXCOL('k2',i,jp) = .18 ;
 XCOL.L('K3',I,JP)\$ SXCOL('k3',i,jp) = .40 ;
 XCOL.L('K4',I,JP)\$ SXCOL('k4',i,jp) = .60 ;
 XCOL.L('K5',I,JP)\$ SXCOL('k5',i,jp) = .70;
 XCOL.L('K6',I,JP)\$ SXCOL('k6',i,jp) = .8 ;
 XCOL.L('K7',I,JP)\$ SXCOL('k7',i,jp) = .95 ;

*** initial conditions from Process Measurements**

XCOL.FX('K1','I1','J1') = 3.331115E-02 ;
 XCOL.FX('K2','I1','J1') = 9.222243E-02 ;
 XCOL.FX('K3','I1','J1') = 0.3287193 ;
 XCOL.FX('K4','I1','J1') = 0.4418286 ;
 XCOL.FX('K5','I1','J1') = 0.5336051 ;
 XCOL.FX('K6','I1','J1') = 0.8142292 ;
 XCOL.FX('K7','I1','J1') = 0.9434926 ;
 XCOL.lo('K7','I3','J1') = 0.95;
 XCOL.up('K7','I3','J1') = 0.98;
 XCOL.lo('K1','I3','J1') = 0.04;
 XCOL.up('K1','I3','J1') = 0.09;
 ELLO.L('i1') = 114 ;
 EVLO.L('I1') = 177 ;
 ELUP.L('i1') = 114 ;
 EVUP.L('I1') = 177 ;

*** Initial value of Objective function from Process**

Obj.I = (6.12*(EVLO.L('I1')-ELLO.L('i1'))*(XCOL.I('K7','I1','J1')+PMM7)+0.95*(ELLO.L('I1')+F-
 EVLO.L('I1'))*(1-(XCOL.I('K1','I1','J1')-PMM1))-0.002*EVLO.L('I1')-
 0.01*ELLO.L('I1'))*(alpha('i1')+alpha('i2'));

```
MODEL PROBLEM2/ALL/ ;
SOLVE PROBLEM2 USING NLP MAXIMIZING OBJ ;
```

```
*=====
* Open Output File and Display Optimum Values
*=====
```

```
file TRAJ /opt.gms/ ;
Put TRAJ ;
Traj.nd = 4;
Put @1, '0', 'EVLO.I('I1')', 'ELLO.I('I1')/';
Put @1, (alpha('I1')*0.211)', 'V.I('I1', 'J2')', 'L.I('I1', 'J2') /';
Put @1, (alpha('I1')*0.789)', 'V.I('I1', 'J3')', 'L.I('I1', 'J3') /';
Put @1, ALPHA('I1')', 'EVUP.I('I1')', 'ELUP.I('I1')/';
Put @1, (ALPHA('I1')+0.01)', 'EVLO.I('I2')', 'ELLO.I('I2')/';
Put @1, (alpha('I1')+0.211*ALPHA('I2'))', 'V.I('I2', 'J2')', 'L.I('I2', 'J2') /';
Put @1, (alpha('I1')+0.789*(alpha('I2')))', 'V.I('I2', 'J3')', 'L.I('I2', 'J3') /';
Put @1, (alpha('I1')+ALPHA('I2'))', 'EVUP.I('I2')', 'ELUP.I('I2')/';
Put @1, XCOL.I('K1', 'I1',
'J2')', XCOL.I('K2', 'I1', 'J2')', XCOL.I('K3', 'I1', 'J2')', XCOL.I('K4', 'I1', 'J2')', XCOL.I('K5', 'I1', 'J2')', X
COL.I('K6', 'I1', 'J2')', XCOL.I('K7', 'I1', 'J2')/';
*
```

```
*=====
```

PI CONTROL

```

"      Declare the following variables (arrays as appropriate)

'      i          Tray number
'      Nt         Number of trays
'      Nf         Feed tray location
'      X (i)      Liquid phase compositions on a given tray
'      X0(i)      Initial liquid phase compositions on a given tray
'      Y(i)       Vapor phase compositions on a given tray
'      L(i)       Liquid flow rate leaving a given tray
'      Lo(i)      Initial liquid phase inventories on a given tray
'      Mdot(i)    Material balance derivatives on a given tray
'      Mxdot(i)   Component balance derivative on a given tray
'      M(i)       Inventory on a given tray
'      M0         Initial inventory on a given tray
'      Mb0        Bottom sump inventory
'      Md0        Reflux drum inventory
'      Zf         Feed composition
'      F          Feed flow rate
'      Yb, Yd     Bottoms and distillate vapor composition
'      Xb, Xd     Bottoms and distillate liquid composition
'      Beta       Tray hydraulic time constant
'      Alpha      Relative volatility
'      B          Bottoms flow rate
'      V          Vapor flow rate
'      R          Reflux flow rate
'      D          Distillate flow rate
'      delta      Integration step size
'      Tim        Process Time
'      Upd        Dummy variable to keep track of real time
'      KcD, TauD  Distillate Composition Controller Tuning parameters
'      KcB, TauB  Bottom Composition Controller Tuning parameters
'      Tprint     Time step for printing results
'      Iteration  Overall iteration number
'      objExcel   Excel spreadsheet object for graphical display

```

```

Private Sub cmdPIControl_Click()
Set objExcel = OLE1.Object
Errintb = 0
Errintd = 0
iter = 0

```

Rem The Model is described below:

Rem Assumptions:

Rem - Constant relative volatility

' - Equimolal overflow

' - Theoretical trays

' - Simple tray hydraulics

' Initial Conditions - Open Input file and receive inlet conditions

```

Open App.Path & "/inputPI1.txt" For Input As #1
Input #1, Nt, Nf, Md0, Mb0, M0, R0, V0, Beta, Alpha
Close #1

```

```

F = 100
Xbset = 0.04
Xdset = 0.96
tim = 0
'Tprint = 0

Open App.Path & "/inputPI2.txt" For Input As #2
Input #2, Xb
For i = 1 To Nt
Input #2, X(i)
Next i
Input #2, Xd
Close #2

Open App.Path & "/inputPI3.txt" For Input As #3
Input #3, Kcd, Kcb, TauD, TauB, delta
Close #3
Tprint = 0
delta = 0.01

ZF = 0.48

' Initial Conditions
For i = 1 To Nt
M(i) = M0
MX(i) = M(i) * X(i)
L0(i) = R0 + F
If (i > Nf) Then
    L0(i) = R0
End If
Next i

' Display Conditions in Interface
picR.Cls
picR.Print R0
picFeed.Cls
picFeed.Print F
PicFeedComp.Cls
PicFeedComp.Print ZF
picB.Cls
picB.Print L(1) - V0
picD.Cls
picD.Print V0 - R0
picS.Cls
picS.Print V0

' Tray hydraulics and VLE

10 For I = 1 To Nt
L(I) = L0(I) + (M(I) - M0) / Beta
Y(I) = alpha * X(I) / (1 + X(I))
Next I

Yb = alpha * Xb / (1 + Xb)
Yd = alpha * Xd / (1 + Xd)

```

EQUATION (4-10)
 EQUATION (4-11) FOR EACH TRAY

 EQUATION (4-11) FOR BOTTOMS
 EQUATION (4-11) FOR DISTILLATE

' Two feedback controllers

ErrB = Xbset - Xb

ErrD = Xdset - Xd

If tim ≤ 0.5 Then

V = V0

R = R0

Else

V = V0 - Kcb * (ErrB + Errintb / TauB)

' PI CONTROL ALGORITHM

R = R0 + Kcd * (ErrD + Errintd / TauD)

' PI CONTROL ALGORITHM

End If

' Assuming perfect level controllers in column base and reflux drum

D = V - R ' EQUATION (4-4) WITH ACCUMULATION TERM = 0

B = L(1) - V ' EQUATION (4-7) WITH ACCUMULATION TERM = 0

' Check for validity of R and V

If ((R < 0) Or (V < 0) Or (D < 0) Or (B < 0)) Then

GoTo 100

End If

' Evaluate Derivatives and Tray Temperatures

' Step 1: for Bottoms

Xbdot = (L(1) * X(1) - V * Yb - B * Xb) / Mb0 ' EQUATION (4-8)

' Step 2a: for first tray

Mdot(1) = L(2) - L(1) ' EQUATION (4-1) FOR TRAY 1 WITH

F(1) = 0

Mxdot(1) = V * (Yb - Y(1)) + L(2) * X(2) - L(1) * X(1) ' EQUATION (4-2) FOR TRAY 1 WITH

F(1) = 0

' Step 2b: Stripping section trays

For I = 2 To Nf - 1

Mdot(I) = L(I + 1) - L(I) ' EQUATION (4-1) FOR TRAYS 2-7 WITH F(I) = 0

Mxdot(I) = V * (Y(I - 1) - Y(I)) + L(I + 1) * X(I + 1) - L(I) * X(I) ' EQUATION (4-2) FOR TRAY 2-7 WITH F(I) = 0

Next I

' Step 2c: Feed Tray

Mdot(Nf) = L(Nf + 1) - L(Nf) + F

' EQUATION (4-1) FOR TRAY Nf

Mxdot(Nf) = V * (Y(Nf - 1) - Y(Nf)) + L(Nf + 1) * X(Nf + 1) - L(Nf) * X(Nf) + F * Zi ' EQUATION (4-2) FOR TRAY Nf

' Step 2d: Enriching section trays

For I = Nf + 1 To Nt - 1

Mdot(I) = L(I + 1) - L(I) ' EQUATION (4-1) FOR TRAY 9-14 WITH F(i) = 0

Mxdot(I) = V * (Y(I - 1) - Y(I)) + L(I + 1) * X(I + 1) - L(I) * X(I) ' EQUATION (4-2) FOR TRAY 9-14 WITH F(i) = 0

Next I

' **Step 2e: Top Tray**

$$\dot{M}(N_t) = R - L(N_t)$$

EQUATION (4-1) FOR TRAY N_t WITH $F(i) = 0$

$$\dot{M}x(N_t) = V * (Y(N_t - 1) - Y(N_t)) + R * X_d - L(N_t) * X(N_t)$$

EQUATION (4-2) FOR TRAY N_t WITH $F(i) = 0$

' **Step 3: Reflux Drum**

$$\dot{X}_d = V * (Y(N_t) - X_d) / M_d$$

EQUATION (4-5)

' **Print current conditions in the Excel Spreadsheet object**

If tim < Tprint Then GoTo 20

ole1.Action = 7

objExcel.worksheets("Process Values").Cells(Iter + 2, 1).Value = tim / 12 'output Time

objExcel.worksheets("Process Values").Cells(Iter + 2, 2).Value = X_d ' Distillate compositions

objExcel.worksheets("Process Values").Cells(Iter + 2, 3).Value = X_b ' Bottom compositions

objExcel.worksheets("Process Values").Cells(Iter + 2, 4).Value = R ' Reflux flow rates

objExcel.worksheets("Process Values").Cells(Iter + 2, 5).Value = V ' Vapor boilups

objExcel.worksheets("Process Values").Cells(Iter + 2, 6).Value = $(6.12 * (V - R) * X_d + 0.95 * (F + R - V) * (1 - X_b) - 0.002 * V - 0.001 * R)$ ' output Current Profit

Print #4, tim; Tab(10); X_b ; Tab(20); $X(10)$; Tab(30); X_d ; Tab(40); R ; Tab(50); V

Iter = Iter + 1

' Update iteration number

Tprint = Tprint + 0.05

' Update print time

' **Update Results**

picR.Cls

picR.Print R

picFeed.Cls

picFeed.Print F

PicFeedComp.Cls

PicFeedComp.Print ZF

picB.Cls

picB.Print B

picD.Cls

picD.Print D

picS.Cls

picS.Print V

Tprint = Tprint + 0.05

' **Euler Integration**

20 tim = tim + delta

' Step forward in time

tim = Round(tim, 3)

$X_b = X_b + \text{delta} * \dot{X}_b$

' Integrate the Bottoms Component Material Balance

For I = 1 To N_t

$M(I) = M(I) + \dot{M}(I) * \text{delta}$

' Integrate the Total Material Balance Equation for each

tray

$MX(I) = MX(I) + \dot{M}x(I) * \text{delta}$

' Integrate the Component Material Balance for each tray

$X(I) = MX(I) / M(I)$

' Update tray liquid compositions

If $X(I) < 0$ Or $X(I) > 1$ Then

GoTo 100

End If

Next I

```
Xd = Xd + Xddot * delta      ' Integrate reflux drum Component Material Balance
Errintd = Errintd + ErrD * delta  ' Integrate Error
Errintb = Errintb + ErrB * delta
```

```
100 message = MsgBox("Level too low or composition unreal", vbOKCancel, Alert)
                        ' Provide alert in case of inconsistent conditions
```

```
picStatus.Cls
picStatus.Print tim
'If ((tim > 1#) And (tim < 1.00012)) Then
'  picFeed.Print Zf
'  Zf = Zf + 0.1 * Zf
'  PicFeedComp.Print Zf
'  n = MsgBox("Feed Composition change", vbOKOnly, "Alert!")
'End If
```

```
If (tim < 40) Then GoTo 10 Else GoTo 30
```

```
100 picStatus.Print "Level too low or composition unreal"
```

```
Close #4
```

```
30 End Sub
```

ONLINE OPTIMIZATION – VB CODE

```
'      REM: THE CODE FOR ONLINE OPTIMIZATION IS THE SAME AS FOR PI CONTROL  
'      REM: THE ONLY EXTRA CODE IS TO CALL THE OPTIMIZER AS GIVEN BELOW  
,
```

```
If tim / 12 = Int(tim / 12) Then          ' IF IT IS TIME TO RUN OPTIMIZER THEN (1 HR)
```

```
'      CALL VBGAMS OPTIMIZER  
      Call Optimize_conditions  
      Open "C:\Gams\onli.gms" For Input As #8  
      Input #8, Ropt, Vopt, Xbsetopt, Xdsetopt  
      Close #8
```

```
'      UPDATE SETPOINTS FOR XB AND XD
```

```
      Xdset = Xdsetopt  
      Xbset = Xbsetopt
```

```
'      LOOP BACK TO PI CONTROL LOOP  
      GoTo 25  
End If
```

ONLINE OPTIMIZATION – GAMS PROGRAM

```
* =====
*   DECLARE TITLE - ONLINE OPTIMIZATION
* =====
$ TITLE ONLINEOPT

* =====
*   DECLARE SETS
* =====

SETS
  I   TRAY NUMBER / 1 * 15 /
  TOP(I) Top TRAY
  ENR(I) ENRICHING SECTION TRAYS
  FEED(I) FEED TRAYS
  STR(I) STRIPPING SECTION TRAYS
  BOT(I) COLUMN BOTTOMS;
  TOP(I) = YES $(ORD(I) EQ 15);
  ENR(I) = YES $((ORD(I) LE 14)$(ORD(I) GE 9));
  FEED(I) = YES $(ORD(I) EQ 8);
  STR(I) = YES $((ORD(I) LE 7)$(ORD(I) GE 2));
  BOT(I) = YES $(ORD(I) EQ 1);

* =====
*   DECLARE SCALARS
* =====

SCALARS
  Alpha RELATIVE VOLATILITY
  F FEED
  ZF FEED COMPOSITION;
  ALPHA = 2 ;
  F = 100 ;
  ZF = 0.456 ;

* =====
*   DECLARE VARIABLES
* =====

VARIABLES
  Xd Top COMPOSITION
  Xb BOTTOM COMPOSITION
  Y(I) VAPOR COMPOSITIONS
  Yb REBOLIER VAPOR COMPOSITION
  V VAPOR BOILUP
  R REFLUX
  PROF PROFIT ;

* =====
*   DECLARE EQUATIONS
* =====

EQUATIONS
  OMB OVERALL MATERIAL BALANCE
  CMBACCU(I) OVERALL MATERIAL BALANCE IN THE ACCUMULATOR
  CMBTOP(I) COMP. BALANCE IN TOP TRAY
  CMBEN(I) COMP. BALANCE IN ENRICHING SECTION
  CMBF(I) COMP. BALANCE IN FEED TRAY
  CMBST(I) COMP. BALANCE IN STRIPPING SECTION
  CMBBOT COMP. BALANCE IN BOTTOMS
  OBJ OBJECTIVE FUNCTION;
```

REBEQ

EQUILIBRIUM IN REBOILER

```
* =====
* DEFINE EQUATIONS -- EQUATIONS (5-7) PAGE 70
* =====
```

```
CMBACCU(I)$STOP(I)..
XD =E= Y(I);
OMB..
F*ZF =E= (V-R)*XD + (R+F-V)*XB;
CMBTOP(I-1)$STOP(I)..
Y(I-1) =E= (V * Xd - R * Xd + R *(Xd / (Alpha - (Alpha - 1) *Xd)) ) / V;
CMBEN(I-1)$ENR(I)..
Y(i-1) =E= (V * Y(i) - R *(Y(i+1) / (Alpha - (Alpha - 1) * Y(i+1))) + R * (Y(i) / (Alpha - (Alpha - 1) *
Y(i)))) / V;
CMBF(I-1)$FEED(I)..
Y(I-1) =E= (V * Y(I) - R * (Y(I+1) / (Alpha - (Alpha - 1) * Y(I+1))) + (R + F) * (Y(I) / (Alpha - (Alpha
- 1) * Y(I))) - F * Zf) / V;
CMBST(I-1)$STR(I)..
Y(i-1) =E= (V * Y(i) - (R + F) * (Y(i+1) / (Alpha - (Alpha - 1) * Y(i+1))) + (R + F) * (Y(i) / (Alpha -
(Alpha - 1) * Y(i)))) / V;
CMBBOT..
Xb =E= ((R+F)*(Y('2'))/(ALPHA-(ALPHA-1)*Y('2')))-V*Y('1'))/(R+F-V) ;
REBEQ..
Yb = Xb*Alpha/(1+(Alpha-1)*Xb)
```

```
* =====
* DEFINE OBJECTIVE FUNCTION
* =====
```

```
OBJ..
PROF =E= 6.12*(V-R)*XD+0.95*(R+F-V)*(1-XB)-0.002*V-0.001*R;
```

```
* =====
* DECLARE BOUNDS
* =====
```

```
XB.LO = 0.04;
XB.UP = 0.08;
XD.LO = 0.95;
XD.UP = 0.98;
R.LO = 110;
R.UP = 150;
V.LO = 160;
V.UP = 190;
Y.UP('15')= 0.98;
R.L = 134.26 ;
V.L = 178.7489 ;
XD.L = 0.9593144 ;
XB.L = 3.980564E-02 ;
```

```
* =====
MODEL ONLINEOPT /ALL;
SOLVE ONLINEOPT USING NLP MAXIMIZING PROF;
```

```
* =====
* OUTPUT RESULTS
* =====
```

```
file onli /onli.gms/ ;  
Put onli ;  
onli.nd = 4;  
Put @1, R.L/;  
Put @1, V.L/;  
Put @1, Xb.L/;  
Put @1, Xd.L/;
```

APPENDIX – G

SUMMARY OF TECHNICAL INPUT FROM INDUSTRY

To better understand the requirements of industry, and to appreciate the practice of control in industry, it was decided to seek help from people working in industries that are part of the Measurement, Control and Engineering Center, the symposium which is the project sponsor. The following questions mainly aimed at understanding the method of online optimization in practice in the industry were asked.

- 1) Does your company do any kind of optimization?
- 2) If no, on what basis are the setpoints changed and at what frequency?
- 3) If yes, how frequently do you update setpoints?
- 4) Is the optimizer "on" all the time or are there times when it is turned "off"?
- 5) Is the optimizer kept "on" even during start-up and pre-shutdown periods?
- 6) What algorithms/software do you use for optimization?
- 7) What algorithms/software do you use for model parameter updating and data reconciliation?
- 8) Is the optimization on a plantwide basis or on a process-to-process basis?

These questions were asked of several MCEC members and the responses were surveyed for deciding future directions. The answers from the majority of industrialists were as follows:

- 1) Yes, on selected applications
- 2) For applications not on optimizers, the setpoints are changed on the basis of
 - Product specifications requirements
 - Disturbances

- Feedstock changes

The frequency of updates varies from once to twice daily to once weekly

- 3) For applications on optimizers, setpoints are changed on a more frequent basis, depending on the process response time. Setpoints may be changed every few hours by running the supervisory optimizer
- 4) There is usually a provision to turn the optimizer "off." This usually happens during transient periods or at the discretion of the operators. Sometimes, the optimizers may be taken offline when analyzers are taken out for maintenance
- 5) Optimizers are rarely kept on during transient periods such as start-up and shutdown
- 6) The popular software in use include
 - RT OPT (AspenTech)
 - Profit Max (Honeywell)
 - ROMEO (Simsci)
- 7) Software used for model parameter updating are
 - RT OPT (AspenTech)
 - LSGREG
 - MS Excel
- 8) Optimization is carried out using steady state models on both a process-wide and plantwide basis

OTHER INPUT FROM MCEC MEETINGS

The original intention of this project was to develop a control optimization scheme, which would completely eliminate the need for setpoints. This was to be accomplished

by making the Optimizer directly "write" its optima to valves, which would necessitate that valve position models be encoded as part of the Optimizer.

Input from industry regarding this was that such an Optimizer would have problems of maintaining stability, unwarranted complexity, and difficulty in convergence. The general consensus was that an optimizer determining economic optimal profiles for manipulated variables and dictating these profiles as setpoints to regulatory controllers would be more suitable for industrial application. Hence, this was the preferred direction of approach.

Further, in this study, it was assumed that the feed to the process is fixed by an upstream unit. Industrial concern regarding this was that companies are always interested in product maximization, by corresponding feed optimization. This means that the optimal feed flow should also be a decision to be made by the Optimizer. This is also an issue that must be included in future studies.

Other input for future directions include application of CEO principles to batch processes. Input from industry on this issue was that batch problems would be of smaller size and easier to accomplish in the short run. Some aspects of application of CEO principles in batch optimization are given in Appendix-H.

We acknowledge all the MCEC members whose valuable suggestions have given impetus and direction to this project.

APPENDIX – H

APPLICATION OF CEO PRINCIPLES TO BATCH REACTOR OPTIMIZATION

The determination of optimal feed rate profiles for batch reactors is an important control problem, especially in biochemical industries. Some complications are slow rates of production, low yield of high-value product, nonlinear models, and discontinuous (bang-bang type) control profiles. Additionally, there could be constraints on both control (manipulated) and state variables (Cuthrell and Biegler 1989). Some objectives that can be handled in an optimal control problem are to optimize the time for which the batch is treated by determining the optimal feed rate policy; to maximize the conversion (yield) of a particular product; or, in the case of competing reactions, to maximize the rate of a particular reaction.

Such problems are generally amenable to the dynamic optimization solution approaches discussed in Chapter 3, specifically the orthogonal collocation approach used in the CEO strategy and the control vector parameterization approach. This is because the mathematical equations describing the system behavior contain DAEs. For the orthogonal collocation approach, (Cuthrell and Biegler 1989, 1987), both control and state profiles can be discretized. By leaving the finite element lengths as decision variables in the Optimizer, it is possible to determine the optimal control profiles, even in the presence of discontinuities. Other studies (Vassiliadis et al 1994a/b) solve the optimization problem using the control vector parameterization approach. Here, only the control variables are discretized and the optimal profile is obtained by checking for feasibility in a separate integration stage.

To implement the CEO strategy on a batch process, the same steps as were used in the study can be used. These include developing a first principles process simulation and the optimization tools. Then, the optimal profiles can be obtained either online or off-line and implemented on the simulation. Systematic reoptimization can be carried out to compensate for process-model mismatch and disturbances (Iyer et al 1999). Parameter adjustment algorithms should also be included to dynamically update process model parameters (Dhir et al. 2000, Iyer et al 1999)

To summarize, the DAEs in the batch optimization problem can be handled in the same way as in the CEO approach. Either orthogonal collocation on finite elements or control vector parameterization can be used to solve the problem.

References

1. Cuthrell, J. E., and L. T. Biegler, "Simultaneous Optimization and Solution Methods for Batch Reactor Control Profiles" *Computers Chem. Engng.*, Vol. 13 No. 1/2, pp. 49-62, 1989
2. Dhir, S., K.J. Morrow, Jr. , R.R. Rhinehart, T. F. Wiesner, "Dynamic Optimization of Hybridoma Growth in a Fed-Batch Bioreactor," *Biotechnology and Bioengineering*, Vol. 67, No.2, pp. 198-205, 2000
3. Iyer, M.S., T.F. Wiesner, R.R. Rhinehart, " Dynamic Reoptimization of a Fed-Batch Fermentor," *Biotechnology and Bioengineering*, Vol. 63, No.1, pp. 10-21
4. Vassiliadis, V.S., R.W.H. Sargent, and C.C. Pantelides, "Solution of a Class of Multistage Dynamic Optimization Problems. 1. Problems without Path Constraints," *Ind. Eng. Chem. Res.*, 33, pp. 2111-2122, 1994
5. Vassiliadis, V.S., R.W.H. Sargent, and C.C. Pantelides, "Solution of a Class of Multistage Dynamic Optimization Problems. 2. Problems with path constraints," *Ind. Eng. Chem. Res.*, 33, pp. 2123-2133, 1994

APPENDIX – I

BUSINESS CONSIDERATIONS IN THE CEO STRATEGY

The production goals of a company are grouped under several levels. Ogunnaike and Ray (1994) discuss the activities and objectives of these levels as shown in Fig I –1:

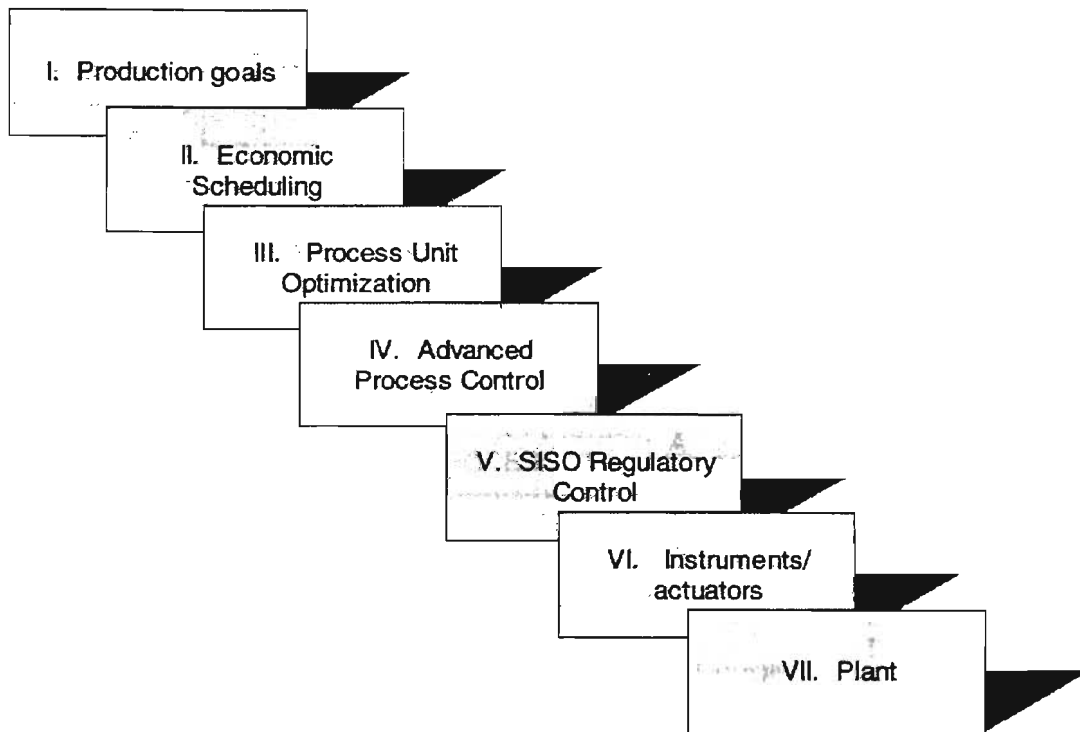
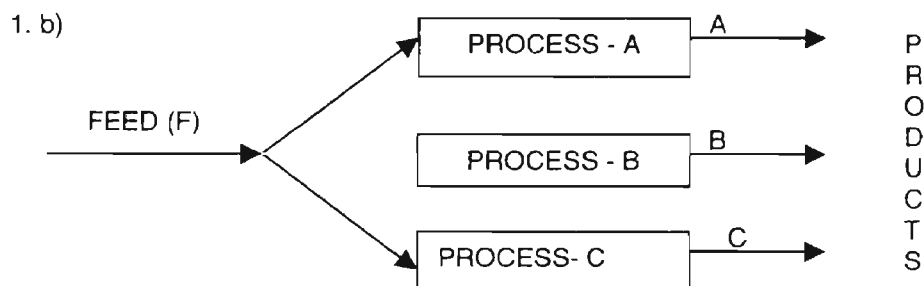
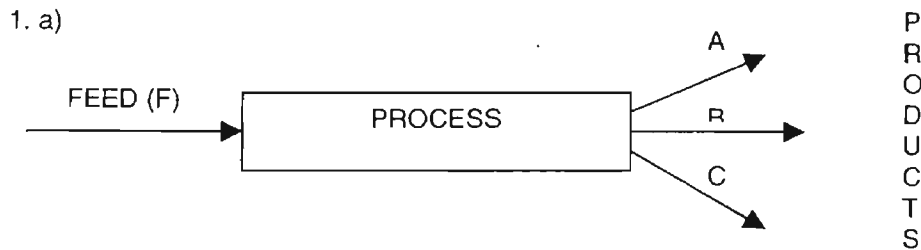


Fig I-1: Hierarchy of Process Operations

In the CEO strategy, the Optimizer is mainly concerned with Levels III, IV and V. The reason for this is that in the time-scale in which the Optimizer is run, the parameters in the higher "business" level do not change and it may be unnecessary to include these in the "control" level optimization. However, these business objectives may be included in the CEO optimization problem and a higher level optimization carried out on this larger time scale, whenever the business parameters (market prices, demand for particular products, costs of raw materials etc) change. This can be done by including/neglecting

appropriate terms in the CEO objective function and adding/deleting constraints on specific variables in the optimization as the situation demands. Some of these scenarios are given below:

Case 1. Consider the following two cases given below.



The business objectives behind each of these scenarios is different:

In scenario 1a), one has to decide how much of A, B and C to produce and the optimum F. Here, changes in any of A, B or C affect the production and quality of the other two products. An example of such a case is a multi-component distillation column in a refinery.

On the other hand, in scenario 1b), one has to decide how to "route" the feed in the processes A, B and C, given F and individual process constraints. Here, once the

individual feed flowrates are decided, changes in any of A, B or C do not have any effects on the other two. The objective function for maximizing profit would be:

$$\text{Max Profit} = AP_A + BP_B + CP_C - FP_F - \text{Capital costs} - \text{Running costs}$$

Subject to:

FOR CASE 1a) Overall process model constraints

FOR CASE 1b) Process A model constraints,

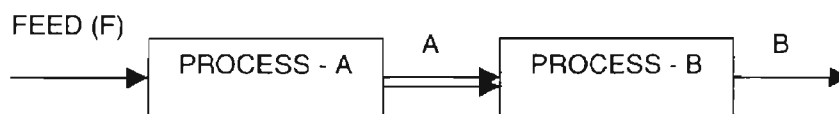
Process B model constraints

Process C model constraints and individual equipment constraints

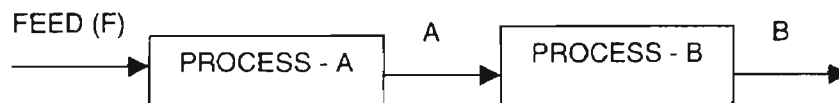
Where, the P's are the values (\$/mol), and A, B, C and F are flowrates (mol/hr).

Thus by formulating the problem in different ways, different concerns can be addressed.

Case 2. Consider the two cases given below.



2. a) Intermediate product A can vary between certain limits



2. b) Intermediate product A is fixed

In scenario 2a), one can choose to vary the amount and quality of A produced (between certain limits) and decide the rate at which A & B are produced, given F, to maximize the

profit. So, here optimization of the overall process is the key issue. On the other hand in scenario 2b), the amount of A is fixed by an upstream process-A and one has to decide how much of B to produce, given A, to maximize the profit. So, here process B gives the degree of freedom for optimization.

The CEO approach is thus amenable to inclusion of higher business objectives in the lower levels of control. By changing the way the objective function and constraints are written, the optimization problem can address different economic objectives.

VITA

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