NONLINEAR MODEL PREDICTIVE CONTROL OF A DISTILLATION COLUMN USING HAMMERSTEIN MODEL AND NONLINEAR AUTOREGRESSIVE MODEL WITH EXOGENOUS INPUT

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TABLE OF CONTENTS

APPENDICES

LIST OF TABLES

LIST OF FIGURES

LIST OF PLATES

LIST OF ABBREVIATIONS

ADMC	Adaptive dynamic matrix control
AIC	Akaike information criterion
ANN	Artificial neural network
ARMA	Autoregressive moving average
ARMAX	Auto-regressive moving average model with exogenous inputs
ASME	American society of mechanical engineers
AT	Assay transmitter
BFGS	Broyden-Fletcher-Goldfarb-Shanno
BIBO	Bounded input-bounded output
BIC	Bayesian information criterion
CPI	Chemical process industries
CPU	Central processing unit
CSTR	Continuous stirred-tank reactor
DMC	Dynamic matrix control
EKF	Extended Kalman filter
FCC	Fluid catalytic cracking
FIR	Finite impulse response
FPE	Final prediction error
GRV	Gaussian random variables
GWN	Gaussian white noise
HJB	Hamilton-Jacobi-Bellman
IAE	Integral of absolute value of error
IDCOM	Identification and command

IMC	Internal model control
IWMPC	Inverse Wiener model predictive control
LC	Level controller
LED	Light emitting diode
LI	Level indicator
LILC	Law of iterated logarithms criterion
LMPC	Linear model predictive control
LP	Linear programming
MAP	Method of approximate programming
MATLAB	Matrix laboratory
MCB	Miniature circuit breakers
MFNN	Multilayer feed forward neural network
MIMO	Multiple-input multiple output
MISO	Multiple-input-single-output
MPC	Model predictive control
MSE	Mean square error
MVC	Multivariable control
NAMPC	Nonlinear analytical model predictive control
NARMAX	Nonlinear auto-regressive moving average model with exogenous inputs
NARX	Nonlinear auto-regressive with exogenous inputs
NC	Number of components
NEQ	Non-equilibrium stage
NGA	Narendra Gallman algorithm
NLP	Nonlinear program
NMPC	Nonlinear model predictive control

NT	Number of trays
ODE	Ordinary differential equation
OE	Output Error
PEM	Prediction error method
PID	Proportional-integral-derivative
PRBS	Pseudo random binary signal
PT	Pressure transmitter
PV	Process value
PWMPC	Polytopic Wiener model predictive control
QDMC	Quadratic dynamic matrix control
QP	Quadratic program
RDNN	Recurrent dynamic neuron network
RI	Refractive index
RMSE	Relative mean square error
RPEM	Recursive prediction error method
SISO	Single-input single-output
SLP	Successive linear programming
SQP	Sequential quadratic programming
SVD	Singular value decomposition
TEMA	Tubular exchanger manufacturers association
UKF	Unscented Kalman filter
UNIFAC	UNIQUAC functional group activity coefficients
VLE	Vapor liquid equilibrium

LIST OF SYMBOLS

a_{mn}	Group interaction parameter (K)
a_n	Output coefficients vector in sigmoidnet function
Apc	Amplitude ratio
a_{sk}	Scaling coefficients
a_{wk}	Wavelet coefficients
B	Bottom product flow rate (l/min)
b_n	Dilation matrix in sigmoidnet function
b_{sk}	Scaling dilation coefficients
b_{wk}	Wavelet dilation coefficients
C	Third virial coefficient
c_n	Translation vector in sigmoidnet function
c_{sk}	Scaling translation coefficients
c_{wk}	Wavelet translation coefficients
d	Output offset scalar in sigmoidnet function
	Output offset scalar in wavenet function
D	Distillate flow rate (l/min)
$e(k)$	Model prediction error
F	Feed flow rate (l/min)
$f(u)$	Scaling function
$F(x)$	Nonlinear regression function
F_L	Liquid flow rate over weir (m^3/s)
g	Gauge pressure (bar)
$g(u)$	Wavelet function
h	Liquid height (m)
$H(z)$	Linear dynamic element in Hammerstein model
h_D	Enthalpy of distillate (J/kmol)
h_F	Enthalpy liquid in feed (J/kmol)
h_N	Enthalpy of liquid in N^{th} tray (J/kmol)
H_N	N^{th} tray vapor enthalpy (J/kmol)
h_{NF}	Feed stage liquid enthalpy (J/kmol)
H_{NF}	Feed tray vapor enthalpy (J/kmol)
H_{ow}	Height over outlet weir (m)

i	Time instant
k	Current sampling instant
l	Dummy indices
L	Linear coefficients vector in sigmoidnet function
	Linear term coefficients in wavenet function
	Reflux flow rate (l/min)
L_N	N^{th} tray liquid flow rate (l/min)
L_{NF}	Feed tray liquid flow rate (l/min)
l_w	Weir length (m)
M	Control horizon.
M_B	Liquid holdup in reboiler (l)
M_C	Liquid holdup in condenser (l)
M_{NF}	Feed tray liquid holdup (l)
N	Tray number
$N(\cdot)$	Nonlinear static element in Hammerstein model
na	Number of past output terms
nb	Number of past input terms
ne	Delay from input
P	Nonlinear subspace matrix in sigmoidnet function
	Nonlinear subspace parameters in wavenet function
	Prediction horizon
p	Integer order parameter
P_c	Critical pressure (bar)
P_r	Reduced pressure
Q	Linear subspace matrix in sigmoidnet function
	Linear subspace parameters in wavenet function
	Positive-definite weighing matrix
q	Fraction of liquid in feed
Q_B	Reboiler heat load(kW)
Q_C	Heat removed in condenser (kW)
q_i	Relative molecular surface area
R	Positive-definite weighing matrix
r	Regressor mean vector in sigmoidnet function
	Regressor means in wavenet function

r_i	Relative molecular volume
S	Positive-definite weighing matrix
T	Temperature (K)
t	time (min)
T_c	Critical temperature (K)
t_f	Final time (min)
$\mathrm{T_r}$	Reduced temperature
u	Manipulated input
$u(k)$	Scalar input (manipulated variable)
$U(k)$	Vector of manipulated input variables
u_1	First manipulated input (Reflux flow rate)
$u_1(k)$	Input to the first nonlinear static block of the Hammerstein model
$u_1(k\text{-}1)$, $u_2(k\text{-}1)$	Past input regressors
$u_{1\max}$	Maximum value of the reflux flow rate
$u_{1\min}$	Minimum value of the reflux flow rate
u_2	Second manipulated input (Reboiler heat load)
$u_2(k)$	Input to the second nonlinear static block of the Hammerstein model
$u_{2\max}$	Maximum value of the reboiler heat load
$u_{2\min}$	Minimum value of the reboiler heat load
u_s	Steady-state input
$\Delta u_{1\max}$	Maximum value of rate of change of reflux flow rate
$\Delta u_{1\min}$	Minimum value of rate of change of reflux flow rate
$\Delta u_{2\max}$	Maximum value of rate of change of reboiler heat load
$\Delta u_{2\min}$	Minimum value of rate of change of reboiler heat load
V_c	Critical molar volume (cm^3/mol)
V_N	N^{th} tray vapor flow rate (l/min)
V_{NF}	Feed tray vapor flow rate (l/min)
$x(k)$	Output of the nonlinear static block
$X(k)$	Vector of state variables
$x_1(k)$	Output of the first nonlinear static block of the Hammerstein model

$x_2(k)$	Output of the second nonlinear static block of the Hammerstein model
x_B	Bottom product composition
X_{Bj}	Liquid mole fraction of j^{th} component in bottom product
x_D	Top product composition
x_{Dj}	Liquid mole fraction of j^{th} component in distillate
x_{ij}	Liquid mole fraction of j^{th} component in i^{th} stage
X_m	Mole fraction of group *m* in the mixture
$\hat{y}$	Predicted output
$y(k)$	Output of the linear dynamic block
$y(k)$	Scalar output (response variable)
$Y(k)$	Vector of controlled output variables
$y_1(k\text{-}1)$, $y_2(k\text{-}1)$	Past output regressors
$y_1\mathrm{max}$	Maximum value of the top product composition
$y_{1\mathrm{min}}$	Minimum value of the top product composition
$y_{2\mathrm{min}}$	Minimum value of the bottom product composition
$y_{2\mathrm{max}}$	Maximum value of the bottom product composition
y_{ij}	Vapor mole fraction of j^{th} component in i^{th} stage
ys	Steady-state response
Z_c	Critical compressibility factor
Z_F	Feed composition
$\mathrm{z}_{\mathrm{F,j}}$	Mole fraction of j^{th} component in feed

Greek letters

θ_m	Area fraction of group *m*
Ψ_{mn}	Group interaction parameter
φ	Fugacity coefficient
γ	Activity coefficient
$\mathrm{\omega}$	Acentric factor
Ω_T	Ellipsoidal or polytopic set
ω_{gc}	Gain crossover frequency
ω_{pc}	Phase crossover frequency

KAWALAN RAMALAN MODEL TAK LELURUS BAGI TURUS PENYULINGAN MENGGUNAKAN MODEL HAMMERSTEIN DAN MODEL AUTO MUNDUR TAK LELURUS DENGAN MASUKAN LUAR KAWALAN

ABSTRAK

Turus penyulingan adalah unit proses penting dalam industri penapisan petroleum dan kimia. Ia perlu dikawal hampir dengan keadaan-keadaan pengendalian yang optima demi insentif-insentif ekonomi. Kebanyakan turus penyulingan industri pada masa kini dikawal oleh pengawal berbilang gelung yang berasaskan model-model lelurus yang mengakibatkan beberapa kekurangan. Skim kawalan berasaskan model tak lelurus merupakan salah satu pilihan terbaik untuk diselidiki bagi mencapai pengawalan turus penyulingan yang baik. Dalam kerja ini, dua skim model ramalan kawalan tak lelurus (NMPC) yang menggunakan model Hammerstein dan model NARX telah dibina untuk mengawal turus penyulingan. Turus penyulingan perduaan untuk pemisahan metanol-air telah digunakan untuk mengesahkan prestasi skim-skim kawalan yang dibangunkan.

Turus penyulingan loji pandu yang bergaris pusat 10.2cm dan 15 dulang-dulang ayak telah direkabentuk, difabrikasi dan digunakan dalam kajian ini. Model matematik berasaskan jumlah imbangan jisim, imbangan komponen dan imbangan entalpi telah dibangunkan berasaskan prinsip-prinsip pertama. Pengiraan kegiatan dan fugasiti telah dimasukkan dalam model tersebut untuk mengambil kira ketakunggulan sistem tersebut. Satu algoritma yang sesuai telah dibina untuk menyelesaikan persamaan-persamaan model dalam persekitaran MATLAB. Eksperimen-eksperimen telah dijalankan dengan menggunakan turus penyulingan

loji pandu pada keadaan-keadaan mantap dan dinamik untuk mengesahkan model prinsip pertama yang dibina. Nilai-nilai kecekapan dulang telah ditala dengan menggunakan hasil-hasil eksperimen pada keadaan mantap. Hasil-hasil model menunjukkan tahap konsistensi yang tinggi dengan hasil-hasil eksperimen. Model prinsip pertama yang telah disahkan digunakan sebagai proses model dalam pengenalpastian sistem tak lelurus dan kajian-kajian kawalan.

Pengenalpastian tak lelurus bagi turus penyulingan telah dibuat dengan menggunakan dua model tak lelurus iaitu model *Hammerstein* berasaskan *wavenet* dan model auto mundur tak lelurus dengan model input-input luar kawalan (NARX) berasaskan *sigmoidnet*. Parameter untuk kedua-dua model tersebut dianggarkan dengan menggunakan kaedah peminimuman ramalan-ralat berlelar. Penganggaran parameter, pengesahan model dan analisis model telah dijalankan dengan menggunakan kotak perkakas bagi sistem pengenalpastian dalam MATLAB dan keupayaan model-model untuk mewakili dinamik model tak lelurus untuk turus penyulingan telah disahkan.

Dua jenis teknik NMPC iaitu NMPC model Hammerstein dan NMPC model NARX telah dibangunkan. Masalah NMPC telah dirumuskan dengan menimbangkan fungsi objektif, kekangan dikenakan oleh model tak lelurus dan juga pembolehubah-pembolehubah masukan dan keluaran. Turas *Unscented Kalman* (UKF) telah digunakan untuk menganggar pembolehubah keadaan dan permasalahan NLP telah diselesaikan dengan menggunakan kaedah program kuadratik berjujukan (SQP) dalam kedua-dua teknik NMPC. Kajian-kajian kawalan gelung tertutup telah dikendalikan dalam persekitaran MATLAB untuk mengesahkan prestasi teknik-

teknik NMPC dalam penolakan gangguan-gangguan dan penjejakan titik set. Kajian-kajian kawalan gelung tertutup ini menunjukkan bahawa prestasi Hammerstein NMPC adalah lebih baik daripada NARX NMPC dalam pengawalan turus penyulingan.

NONLINEAR MODEL PREDICTIVE CONTROL OF A DISTILLATION COLUMN USING HAMMERSTEIN MODEL AND NONLINEAR AUTOREGRESSIVE MODEL WITH EXOGENOUS INPUT

ABSTRACT

Distillation column is an important processing unit in petroleum refining and chemical industries, and needs to be controlled close to the optimum operating conditions because of economic incentives. Most of the industrial distillation columns are currently controlled by multiloop controllers based on linear models which are penalized by several shortcomings. Nonlinear model based control scheme is one of the best options to be explored for proper control of distillation columns. In the present work, two nonlinear model predictive control (NMPC) schemes using Hammerstein model and nonlinear autoregressive model with exogenous input (NARX) were developed to control distillation column. The binary distillation column separating methanol-water was used to verify the developed control schemes performance.

The pilot plant distillation column of 10.2 cm diameter with 15 sieve trays was designed, fabricated and used in this work. A mathematical model based on total mass balance, component balance and enthalpy balance was developed based on first principles. The activity and fugacity calculations were included in the model in order to account for the non-ideality of the system. A suitable algorithm was developed to solve the model equations in MATLAB environment. The experiments were carried out in pilot plant distillation column under steady-state and dynamic conditions to validate the first principle model. The tray efficiency values used in the first principle model were tuned using the steady state experimental results. The model results

showed a high level of consistency with the experimental results. The validated first principle model was used as a process model in nonlinear system identification and control studies.

The nonlinear identification of distillation column was done using two nonlinear models namely wavenet based Hammerstein model and sigmoidnet based NARX model. The parameters of both the models were estimated using an iterative prediction-error minimization method. The parameters estimation, model validation and model analysis were carried out using system identification toolbox in MATLAB and the capability of the models to capture the nonlinear dynamics of the distillation column was verified.

Two types of NMPC techniques namely Hammerstein model NMPC and NARX model NMPC were developed. The NMPC problem was formulated by considering the objective function, constraints imposed by nonlinear model as well as input and output variables. The Unscented Kalman Filter (UKF) was used to estimate the state variables and the nonlinear programming problem was solved using sequential quadratic programming (SQP) method in both the NMPC techniques. The closed loop control studies were conducted in MATLAB environment to verify the performance of the NMPC techniques in disturbances rejection and set-point tracking. The closed loop control studies indicated that the performance of Hammerstein NMPC was superior than NARX NMPC in controlling the distillation column.

CHAPTER 1

INTRODUCTION

1.1 Distillation

Distillation is one of the most important unit operations in chemical engineering. The aim of a distillation column is to separate a mixture of components into two or more products of different compositions. The physical principle of separation in distillation is the difference in the volatility of the components. The separation takes place in a vertical column where heat is added to a reboiler at the bottom and removed from condenser at the top. A stream of vapor produced in the reboiler rises through the column and is forced into contact with a liquid stream from the condenser flowing downwards in the column. The volatile (light) components are enriched in the vapor phase and the less volatile (heavy) components are enriched in the liquid phase. A product stream taken from the top of the column therefore mainly contains light components, while a stream taken from the bottom contains heavy components.

1.2 Distillation equipment

A simple continuous binary tray distillation column for separating a feed stream into two fractions, an overhead distillate product and a bottoms product is shown in Figure 1.1. The column is normally provided inside with horizontal plates or trays.The liquid mixture to be separated is introduced more or less centrally into a vertical cascade of trays. A reboiler is provided at the bottom of the column to supply

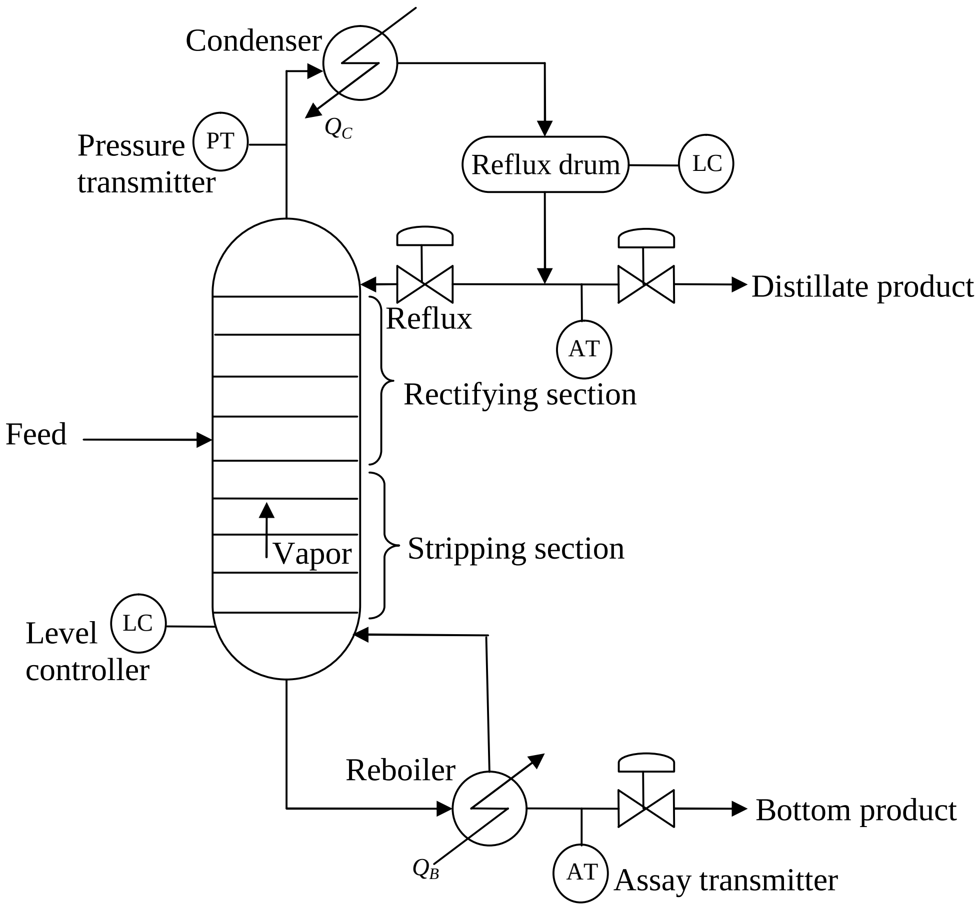

Figure 1.1: Schematic of continuous binary tray distillation column

the heat required for the vaporization involved in distillation and also to compensate for heat loss. A water-cooled or air-cooled condenser is provided at the top of the column to condense and cool the overhead stream. The purity of the top product can be improved by recycling some of the externally condensed top product liquid as reflux from the upper part of the column. The more reflux that is provided, the better is the column separation of the lower boiling from the higher boiling components of the feed. The feed tray divides column into two parts namely rectifying section and stripping section. In rectifying section, the vapor rising is rectified with liquid flowing down from top to remove less volatile component and in stripping section the liquid is stripped of volatile components by vapor produced at bottom by partial vaporization of bottom liquid in reboiler. The condensed liquid that is removed from reflux drum is known as distillate or top product and the liquid removed from reboiler is known as bottom product.

1.3 Need for distillation control

Distillation is used in many chemical processes for separating feed streams and for purification of final and intermediate product streams. There are many reasons for the interest in distillation control. From an academic point of view distillation control is an interesting multivariable problem, and from an industrial point of view improved distillation control has a potential to substantially increase the profit. Distillation accounts for approximately 95% of the separation systems used for refining and chemical industries (Humphrey *et al.*, 1991). It has a major impact upon the product quality, energy usage, and plant throughput of these industries. It consumes enormous amounts of energy, both in terms of cooling and heating requirements. It can contribute to more than 50% of plant operating costs. The energy requirement may be reduced significantly through improved operations. This is achieved not only through optimal column design, but requires, in addition, a control system which is able to maintain the optimal conditions.

Distillation control is a challenging endeavor due to (1) the inherent nonlinearity of distillation, (2) multivariable interaction, (3) the non-stationary behavior and, (4) the severity of disturbances (Shinskey, 1984). Tighter control of distillation columns is consequently important for energy savings, and will also yield increased profit through improved product recovery. The major benefits of improved distillation control are reduced energy consumption, increased yield and higher throughput.

1.4 Distillation control techniques

Distillation columns provide a very challenging example within the field of process dynamics and process control. Traditionally PID controllers were used in the process industries for control of the distillation column. The main drawback of the conventional feedback PID control is that corrective action for disturbances does not begin until the controlled variable deviates from the set point (Skogestad, 1997b). In industry, most of the columns are operated by single-input single-output (SISO) controllers and usually only one composition is automatically controlled (one point control). This leads to waste of valuable products and excessive energy. However, automatic control of both compositions may be very difficult to obtain due to strong interaction between top and bottom product compositions (Shinskey, 1984). Skogestad *et al.*(1988) have reported that high purity columns, i.e. columns where both top and bottom compositions are very pure; suffer from strong interaction which makes the system very sensitive to small changes in the manipulated variables (input uncertainty). Without a rigorous method for dealing with uncertainty it may be practically impossible to tune a two point controller for a system with strong interaction. This may in fact be one of the reasons to why one point control is so commonly used. Another disadvantage with such a decentralized (multiloop) control is that the control performance may seriously deteriorate if the system hit some constraints. For example, if a stabilizing loop saturates, the system goes unstable. To avoid this, the plant has to be operated sufficiently far away from the constraints, or facilities for reconfiguration have to be installed ‘on-top’ of the SISO controllers (Lundstrom and Skogestad, 1995).

Configuration selection is an important aspect in the case of multiloop controller design. Control configuration for a distillation column can be selected from the knowledge of the thermodynamic parameters, reflux ratio, vapor boil-up rate and distillate to bottoms ratio for binary and multicomponent distillation (Stilchmar, 1995). Improper choice of manipulated/controlled variable pairings can result in poor control performance. Decouplers are introduced into the multiloop configuration to compensate for the process interactions and reduce the control loop interactions. Hurowitz *et al*.(2003) have used decouplers to control the top product composition using reflux flow rate, and bottom product composition using vapor boil-up rate for the xylene/toluene column and the depropanizer. In both cases, the decouplers resulted in improved control performance compared to the feedback controllers without a decoupler.

The insufficient performance of SISO controllers leads to the development of specialized single loop control strategies such as feedforward control (Broll *et al.*, 1995), inferential control (Zhang and Agustriyanto, 2001), cascade control (Kano *et al.*, 2000), adaptive control (Natarajan *et al.*, 2006) etc. The abilities of the specialized single-loop control strategies and multiloop controllers were not satisfactory for increasingly stringent performance requirements of the chemical processes which led to the development of multivariable control techniques.

1.4.1 Multivariable controllers

Processes which are multivariable in nature, i.e. processes where the variables to control and the variables available to manipulate cannot be separated into independent loops where one input only would affect one output, constitute a major source of difficulty in process control. These processes show a certain degree of interaction, i.e. one control loop affects other loops in some way. The complexity of the control problem raises as this interaction increases (Luyben, 1992). Multivariable processes in industrial and other applications are often of higher order, where there are many, possibly tens or hundreds, of control loops interacting (Skogestad and Postlethwaite, 1996).

The term multivariable control refers to the class of control strategies in which each manipulated variable is adjusted on the basis of errors in all of the controlled variables, rather than the error in the single controlled variable, as in the case of multiloop control. Multivariable control is particularly well-suited for controlling processes with several interacting controls which need to be simultaneously decoupled (Liptak, 2007).

An adequate model is generally considered as a prerequisite for multivariable controller design. The model is used to predict the behavior of the controlled variables with respect to changes in the input variables (Sagfors and Waller, 1998). Established multivariable control techniques rely on the availability of the linear system models. This is to ensure that the resulting control scheme is closely matched to the dynamics of the process. The multivariable system must therefore first be modeled either analytically using set of differential equations to describe the system behavior or empirically by fitting experimental obtained data to an assumed structure of the process i.e. black-box modeling. Obviously, how well the resulting control strategy performs depends on the accuracy of the model. In applications where the physical and/or chemical characteristics of the system are well known, usually the former approach is adopted. In the process industries, where the higher degree of uncertainty about the process behavior emprical modeling approach is often employed. However for control system design purposes, the input-output (transfer function) model obtained using later approach is generally adequate (Boling *et al.*, 2004). Multivariable controls strategies can also be developed that include integral, derivative and feedforward control action. Among the multivariable controllers, Model Predictive Control (MPC) is an important advanced control technique which can be used for difficult multivariable control problems (Goodwin *et al.*, 2001).

1.4.2 Model Predictive Control

The term MPC describes a class of computer control algorithms that control the future behavior of the plant through the use of an explicit process model. At each control interval the MPC algorithm computes an open-loop sequence of manipulated variable adjustments in order to optimize future plant behavior. The first input in the optimal sequence is injected into the plant, and the entire optimization is repeated at subsequent control intervals (Henson, 1998). MPC technology was originally developed for power plants and petroleum refinery applications. However, at present MPC is used in wide variety of manufacturing environments including chemicals, food processing, automotive, aerospace, metallurgy, and pulp and paper (Qin and Badgewell, 1998).

The success of MPC technology as a process control paradigm can be attributed to three important factors. First and foremost is the incorporation of an explicit process model into the control calculation. This allows the controller, in principle, to deal directly with all significant features of the process dynamics. Secondly the MPC algorithm considers plant behavior over a future horizon in time. This means that the effects of feedforward and feedback disturbances can be anticipated and removed, allowing the controller to drive the plant more closely along a desired future trajectory. Finally the MPC controller considers process input, state and output constraints directly in the control calculation. This means that constraint violations are far less likely, resulting in tighter control at the optimal constrained steady-state for the process. It is the inclusion of constraints that most clearly distinguishes MPC from other process control techniques (Qin and Badgwell, 2003).

It is interesting to note that in the early usage of MPC technology, the nonlinear process behavior was addressed using a linear dynamic model in the control algorithm. Richalet *et al*. (1978) have described how nonlinear behavior due to load changes in a steam power plant application was handled by executing their Identification and Command (IDCOM) algorithm at a variable frequency. Prett and Gillette (1980) have applied a Dynamic Matrix Control (DMC) algorithm to control a fluid catalytic cracking unit and model gains were obtained at each control iteration by perturbing a detailed nonlinear steady-state model.

The original IDCOM and DMC algorithms provided excellent control of unconstrained multivariable processes. However, constrained handling was not planned in those two algorithms. Engineers at Shell Oil addressed this weakness by posing the DMC algorithm as Quadratic Program (QP) in which the input and output constraints appear explicitly and is known as Quadratic Dynamic Matrix control (QDMC). Its key features include linear step response model for the plant, quadratic performance over a finite prediction horizon and future plant output behavior specified by trying to follow the set point as closely as possible subject to a move suppression term (Cutler *et al.*, 1983). Even though MPC is having many advantages, many processes are sufficiently nonlinear to preclude the successful application of MPC technology. This has led to the development of nonlinear model based controllers such as nonlinear model predictive control (NMPC) in which more accurate nonlinear model is used for process prediction and optimization.

1.4.3 Nonlinear Model Predictive Control

NMPC can be applicable to the areas where process nonlinearities are strong and market demands require frequent changes in operating conditions. There are cases where nonlinear effects are significant enough to justify the use of NMPC technology. These include regulator control problems where the process is highly nonlinear and subject to large frequent disturbances (example: pH control); and servo control problems where the operating points change frequently (example: Polymer manufacturing and distillation column) and span a sufficiently wide range of nonlinear process dynamics (Qin and Badgewell, 1998). The overall basic structure of NMPC control loop is depicted in Fig. 1. The NMPC algorithm (Findeisen *et al.*, 2000) can be summarized as follows.

The nonlinear dynamic model of the process is used to predict the future values of the output from the current measurements. Then the appropriate changes in the input values can be calculated based on both predictions and current measurements. Based on the predicted values and constraints the optimal control problem is solved online in the dynamic optimizer. Set of control moves will be calculated and the first part of the optimal input signal will be implemented until new measurements or estimates of the state are available. The above procedure will be repeated for next time instant.

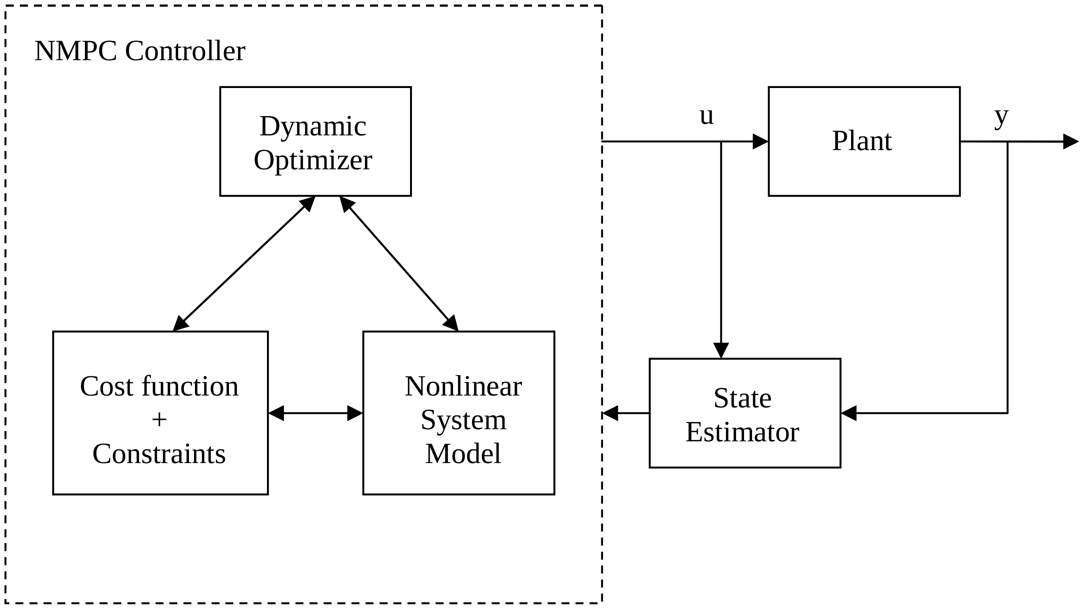

Figure 1.2: Basic NMPC control loop

The key characteristics of NMPC are as follows.

i. It allows the use of nonlinear model for prediction
ii. It allows an explicit consideration of state and input constraints
iii. A specified performance criteria is minimized online
iv. In general, the predicted behavior is different from the closed loop behavior
v. The online solution of an open-loop optimal control problem is necessary
vi. The system states must be measured or estimated to perform the prediction

The major steps in implementation of NMPC includes development of a suitable nonlinear process model to be used with NMPC, formulating NMPC problems with inherently better computational characteristics and finding out an efficient and reliable solution methods for the nonlinear programming problem with better computational efficiency.

In their survey of industrial applications of NMPC, Qin and Badgwell (1998) listed nonlinear model development as one of the three most significant obstacles to NMPC application, by noting that there is no systematic approach for building nonlinear dynamic models for NMPC. Lee (1998) drawn the same conclusion by arguing that the inability to construct, a nonlinear model on a reliable and consistent basis is the most important reason that nonlinear MPC has less influence on industrial control practice than linear MPC. He also has a view that nonlinear dynamics are significant in industrial manufacturing processes.

The nonlinearity of the process should be measured in order to select suitable nonlinear model structure for the process to be used with NMPC. The information about the nonlinearity of the process will be helpful to make a decision as to whether it would be worthwhile attempting to identify a nonlinear model of the process and also to select the model structure. In this context, Pearson (1995) classified processes using a degree of nonlinearity, i.e. mild, intermediate, or strongly nonlinear based on the qualitative nature of process nonlinear behavior such as asymmetric response to symmetric changes in input, input multiplicities i.e., the same output could be generated by different input magnitudes, output multiplicative behavior, chaotic dynamics etc. There are three types of nonlinear models available namely fundamental models, empirical models and hybrid models.

Fundamental model are derived by applying transient mass, energy and momentum balances to the process. In the absence of spatial variations, the resulting models have the general form

$$\dot{x} = f(x,u) \tag{1.1}$$

$$0 = g(x,u) \tag{1.2}$$

$$y = h(x,u) \tag{1.3}$$

where x is a n-dimensional vector of state variables, u is a m-dimensional vector of manipulated input variables and y is a p-dimensional vector of controlled output variables. The ordinary differential equations (1.1) and algebraic equations (1.2) are derived from conservation laws and various constitutive relations, while the output equations (1.3) are chosen by the control system designer (Pearson, 2003). Since NMPC is most naturally formulated in discrete time, it is necessary to discretize the continuous time differential equations. This is usually achieved by orthogonal collocation or finite elements.

Fundamental models for processes of realistic complexity tend to involve on the order of 10^2 - 10^3 nonlinear differential equations and a comparable number of algebraic relations (Michelsen and Foss, 1996). Further, in many cases it is not realistic to simplify these models by excluding subtle details. Gross *et al*.(1998) made this point strongly, by noting that even construction details of particular equipment sometimes can have a profound influence on process dynamics. Another drawback of fundamental model is that the lack of process knowledge often leads to disappointing results, since it is hard to capture all relevant phenomena in the model.

In many cases, the fundamental models are too complex to be used for control purposes. Empirical models, also called black-box models are useful in this scenario (Sjoberg *et al.*, 1995). In empirical modeling, a model structure is first selected and the model identification problem involves determining the model parameters that best fit the input-output data. The development of empirical nonlinear models from plant data is known as nonlinear system identification. In contrast to linear models, the identification problem is considerably more complex for nonlinear systems. To begin with, nonlinear models exhibit a diverse range of nonlinear behavior, and unlike linear models, nonlinear model structures are generally not equivalent. Because of this diversity, selection of an appropriate model structure becomes critical. Also, selection of an appropriate input is also considerably more challenging for nonlinear models than their linear counterparts. As an example, the PRBS sequence that is widely used for linear model identification is inadequate for identification of a broad class of the block-oriented models (Doyle III *et al.*, 2002). The input should also possess enough energy to exercise the full range of process nonlinear behavior, and this persistence of excitation condition, well established for linear systems, and does not have a well-defined nonlinear equivalent.

The types of discrete time nonlinear models utilized for NMPC in the recent literature includes Hammerstein models (Jurado, 2006; Harnischmacher and Marquardt, 2007; Huo *et al.*, 2008), wiener models (Lazar *et al.*, 2007; Shafiee *et al.*, 2008), NARX model (Lee and Lee, 2005), Nonlinear auto-regressive moving average model with exogenous inputs (NARMAX) (Zeybek *et al*., 2006), Volterra models (Wang and Zhu, 2008), neural network models (Nagy, 2007; Al Seyab and Cao, 2008a; Al Seyab and Cao, 2008b) and fuzzy models (Cetinkaya *et al.*, 2006; Prakash and Senthil, 2008).

Hybrid models are developed by combining the fundamental and empirical modeling approaches. This is the case when some physical insight is available, but several parameters remain to be determined from observed data. It is useful to consider two sub cases in this hybrid models namely physical modeling and semi-physical modeling. In physical modeling, a model structure can be built on physical grounds, which has a certain number of parameters to be estimated from data. In semi-physical modeling, physical insight is used to suggest certain nonlinear combinations of measured data signal. These new signals are then subjected to model structures of emprical character (Sjoberg *et al.*, 1995).

After suitable nonlinear model is developed for the process, the NMPC problem is formulated by considering the constraints on input and output variables, as well as constraints imposed by the nonlinear model equations. One of the key obstacles for a successful application of NMPC in practice is that most existing NMPC schemes require the explicit state information for the prediction. Since in practice not all states are available by measurements, a suitable observer for the estimation of the system states must be used (Findeisen *et al*., 2003).

NMPC requires the repeated on-line solution of a nonlinear optimal control problem. In the case of linear MPC the solution of the optimal control problem can be cast as the solution of a (convex) quadratic program and can be solved efficiently even on-line. This can be seen as one of the reasons why linear MPC is widely used in industry. For the NMPC problem the solution involves the solution of a nonlinear program. In general the solution of a nonlinear (non-convex) optimization problem can be computational expensive. One could address the solution of nonlinear programming problem for the purpose of model predictive through successive linearization of model equations, sequential model solution and simultaneous model solution.

1.5 Problem statement

NMPC has been around for many years and has been scientifically discussed extensively, but several issues that affect the industrial practice of NMPC are yet to be resolved. The NMPC approach assumes availability a suitable nonlinear dynamic model of the controlled process. In most application studies of NMPC, the nonlinear model is readily obtained due to the simplicity of the process considered. The nonlinear modeling problem is significantly more challenging for large scale complex processes. Consequently, the development of nonlinear model is of highest importance to the continued advancement of NMPC. Foss *et al*. (1998), in their case study on process modeling in Germany and Norway concluded that despite the commercially available modeling tools, the effort spent for all kinds of modeling activities is the most time consuming step in an industrial project where model based process engineering techniques are applied.

Many researchers (Eskiant *et al*., 1991; Sriniwas *et al*., 1995; Fruzzetti *et al*., 1997) already proved that the performance of linear models is insufficient in capturing the dynamics of the distillation column due to its nonlinear nature. Henson (1998) also has drawn the same conclusion by arguing that many nonlinear processes including distillation column are sufficiently nonlinear to preclude the successful application of linear models. Hence the development of nonlinear process models is tremendously essential due to the unavoidable nonlinearity of the process and complexity of nonlinear system.

The practical difficulty of nonlinear dynamic model development arises from several sources, of which the following two are fundamental. First is the fact that model utility can be measured in several, generally conflicting ways. Second, the class of nonlinear models does not exhibit the unity that the class of linear models does. The four extremely important measures of model utility are approximation accuracy, physical interpretation, suitability for control and ease of development.

Fundamental model is generally far superior to empirical moel and hybrid model with respect to the first two of these criteria, but they also suffer badly with respect to the last two. On the other hand, the empirical model does not require the detailed process understanding for model development and also, complexity of the model can be avoided. The main drawback of empirical model is that the nonlinear model identification problem is very tedious. In the case of hybrid models, it is very difficult to distinguish the particular part of the process to be modeled using fundamental model or empirical model.

The NMPC problem formulation involves online computation of a sequence of manipulated inputs which optimize an objective function and satisfy process constraints. The development of NMPC techniques for large scale systems may require problem formulations which exploit the specific structure of the nonlinear model. Finally, NMPC requires online solution of a nonlinear program (NLP) at each iteration. The solution of such NLP problems can be very time consuming, especially for large scale systems. An additional complication is that the optimization problem generally is nonconvex because the nonlinear model equations are posed as constraints (Cannon, 2004). Consequently, NLP solvers designed for convex problems may converge to local minima or even diverge. So it is necessary to find out an improved solution algorithm for nonconvex NLP problems. The vital parts of the present research are to develop suitable nonlinear models for distillation column, formulate NMPC problem and to identify an efficient optimization algorithm to be used with NMPC.

1.6 Research objectives

The objectives of this study are

1. To design a pilot plant distillation column, condenser and reboiler, and to fabricate the experimental set up based on design specifications.
2. To identify a suitable first principle model to be used as process model in nonlinear model identification and in NMPC, and to develop an algorithm to solve the model equations in MATLAB environment.
3. To validate a first principle model through experimentation using pilot plant distillation column, and to conduct open loop simulation studies under steady- and unsteady-state conditions.
4. To develop suitable nonlinear emprical models and to identify an efficient optimization algorithm to be used with NMPC.
5. To design and to evaluate the performance of NMPC for different changes in disturbances and set-points using closed loop simulation studies.

1.7 Scope of work

The main focus of the present work is to develop suitable nonlinear models and to identify an efficient optimization algorithm to be used with NMPC to control a distillation column.

The detailed design of binary sieve tray distillation column is carried out based on the VLE data of methanol-water system. Based on the tray spacing and the plate hydraulics, the design details of the tray such as tray thickness, weir length, weir height, hole size, hole pitch, number of holes etc. are calculated. A reboiler and a total condenser are designed based on the condenser duty and heat duty for the system. A detailed process design and mechanical design of plates are also carried out. Stainless steel is the material of construction for the column, condenser, reboiler and column internals, and rock wool with aluminum foil is used as insulation material. Provisions are provided to take the sample and to measure the temperature in each tray. Horizontal in-shell TEMA E-type condenser with vertical baffle cuts is used and water is used as a cooling medium in the condenser. A kettle type reboiler with resistance type electrical heaters is used. The column is commissioned and the required instruments like flow meters, temperature measuring devices, pressure measuring device, level measuring devices, and transmitters are installed. A few test runs are made to calibrate the instruments and also to check the proper functioning of the various signal processing units.

A mathematical model based on total mass balance, component balance and enthalpy balance is developed based on first principles. The activity and fugacity calculations are included in the model in order to account for the non-ideality of the system. A suitable algorithm is developed to solve the model equations using MATLAB. Simulation studies are carried out in the MATLAB environment for steady-state and unsteady-state conditions.

The experiments are carried out to study the steady-state and dynamic characteristics of the column. The steady-state experimental data is used to fix optimum operating conditions. Then dynamic studies involving changes in feed flow rate, feed composition and reflux flow rate are carried out and from those results the dynamic behavior of the system is obtained. The result of simulation studies are compared with experimental data. The tray efficiencies used in the simulation studies are calibrated to match the first principle model results with experimental results and the developed first principle model is validated.

Suitable nonlinear empirical models are developed and used with NMPC. The main factor considered for nonlinear model development is that the model developed for binary distillation column should have the flexibility to extend to the multicomponent distillation column. Two nonlinear models namely wavenet based Hammerstein model and sigmoidnet based NARX mode are found to be good in capturing the nonlinear dynamics of the distillation column and also they can be easily modified for multicomponent distillation column. The data required for nonlinear model parameter estimation and validation are generated from experimentally validated first principle model. Two types of NMPC techniques namely Hammerstein model NMPC and NARX model NMPC are developed. The NMPC problem is formulated by considering the constraints imposed by nonlinear model, input and output variables. The sequential quadratic programming (SQP) method is used in both the NMPC techniques to solve the NMPC problem.

The control problem is solved in MATLAB environment. The top and bottom product compositions are the controlled variables in distillation column. The reflux flow rate and reboiler vapor boil up rate are used as manipulated variables, whereas feed flow rate and feed composition are considered as disturbances. The closed loop simulation studies are carried out in MATLAB environment to verify the performance of both NMPC techniques for different disturbances, changes in set points and simultaneous changes in disturbances and set points.

1.8 Organization of thesis

This thesis consists of five chapters. Chapter 1 provides a brief description of distillation process, distillation equipment, need for distillation control, and distillation control techniques including the advanced control strategies like MPC and NMPC. This chapter also includes the problem statement that provides foundation to identify research directions and objectives. The objectives and scope of study are then elucidated followed by the organization of the thesis.

Chapter 2 summarizes the past research works in the field of nonlinear modeling of distillation column including nonlinear characteristics, fundamental models, empirical models and hybrid models. The NMPC problem formulation and various optimization algorithms used with NMPC were discussed. Finally, current applications of NMPC technology were discussed along with the advantages and drawbacks. This chapter serves as the background information about the specific problems that have to be addressed in this research work.

Chapter 3 presents the details of the materials, chemicals and research methodology used in the present study. The design specifications of pilot plant distillation column are explained and the experimental set up is elaborated along with the specifications of other instruments. The development of first principle model for distillation which is used as a platform in this research work is described along with solution algorithm. Finally, the methodology for the development of NMPC and closed loop control studies are presented.

Chapter 4 is the main part of the thesis in which all important findings and results of this research work are discussed. This chapter includes experimental validation of fist principle model, steady-state and unsteady-state simulation results using first principle model, nonlinear identification of Hammerstein model and NARX model, NMPC control problem formulation, sequential quadratic programming (SQP) optimization algorithm as well as results of closed loop simulation studies to validate NMPC controller performance.

Chapter 5 summarizes the results reported in the previous chapters and also some concluding remarks are made based on those results. The conclusions are obtained from each individual study carried out in the present research work. This chapter also suggests the ways to improve the present work and recommend the possible future studies in this field. These recommendations and suggestions are given after taking into consideration of significant findings, limitations, the conclusions obtained as well as difficulties encountered in this study.

CHAPTER 2

LITERATURE REVIEW

2.1 Importance of distillation control

Malaysia is a significant Southeast Asian producer of oil and natural gas. According to *Oil & Gas Journal* (*OGJ*), Malaysia held proven oil reserves of 3.0 billion barrels and 75 trillion cubic feet (Tcf) of proven natural gas as of January 2007 (Country analysis brief: Malaysia, 2007). Most of the separation processes employed in petroleum refineries and other chemical processing industries (CPI) are distillation columns for separating feed streams, and for purification of final and intermediate product streams. The separation needs relatively large amount of energy. Close control of distillation column improves the product quality, minimizes energy usage and maximizes the plant throughput and its economy (Hurowitz *et al.*, 2003). Also producing products with low variability is many times crucial for the success of CPI (Downs and Doss, 1991). For most high-value added products, low variability is a primary customer concern and can determine the market demand of a product. The reduction in the variation in the products can also be used to increase production rates or decrease utility usage (Riggs, 2001). Clearly, reduced variability is economically important to the CPI and can be achieved by proper control of unit operation in the plant, especially the distillation column. Hence, the development of nonlinear model based control system for distillation column would be beneficial for CPI.

2.2 Major disturbance in distillation control

The type and magnitude of disturbances affecting a distillation column have a direct effect on the resulting product variability. An analysis of the major types of disturbances encountered in distillation column are mentioned in the following sections.

2.2.1 Feed composition upsets

Changes in the feed composition represent the most significant upsets with which a distillation control system must deal on a continuous basis. Most industrial columns do not have a feed composition analyzer; therefore, feed composition upsets usually appear as unmeasured disturbances. When a feed composition analyzer is available, a feed forward controller can be applied using the on-line measurements of the feed composition (Stichlmair, 1995). Feed composition changes represent a major disturbance for distillation control, thus the sensitivity of potential control configurations to feed composition upsets is a major issue for configuration selection. Luyben (2005) has studied the effect of feed composition on the selection of control structures for high purity binary distillation column using methanol-water system. He concluded that feed composition changes largely affect the product purities compare to other disturbances. Zhang *et al*. (2006) noted that a feed composition change shifts the composition profile through the column resulting in a large upset in the product compositions.