A SIMPLIFIED WIENER BASED MODEL PREDICTIVE CONTROL FOR DISTILLATION COLUMN

by

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

AE	Algebraic equation
ARMAX	Autoregressive moving average with exogenous input
ARX	Autoregressive with exogenous input
CSTR	Continuous stirred tank reactor
CV	Controlled variable
CV1	1st controlled variable (tray 23 temperature)
CV2	2nd controlled variable (tray 7 temperature)
DAE	Differential algebraic equation
DMC	Dynamic matrix control
FFNN	Feed forward neural network
FIR	Finite impulse response
GMC	General model control
GMN	Generalized multiple level noise
GRG	Generalized reduced gradient
IAE	Integral absolute error
IDCOM	Identification and command
IMC	Internal model control
ISE	Integral squared error
ITAE	Integral time absolute error
LMPC	Linear model predictive control
LP	Linear programming
LSE	Least square estimate
MHE	Moving horizon estimation

MIMO	Multi input multi output
MISO	Multi input single output
MPC	Model predictive control
MV	Manipulated variable
MV1	1st manipulated variable (reflux flowrate)
MV2	2nd manipulated variable (reboiler duty)
NARX	Nonlinear autoregressive with exogenous input
NLP	Nonlinear programming
NMPC	Nonlinear based model predictive control
ODE	Ordinary differential equation
PID	Proportional integral derivative controller
PRBS	Pseudo random binary signal
PWL	Piecewise linear
QDMC	Quadratic dynamic matrix control
QP	Quadratic programming
RDNN	Recurrent dynamic neural network
RPEM	Recursive predictive error method
RSQP	Reduced sequential quadratic programming
SISO	Single input single output
SLP	Successive linear programming
SO	Simple optimization algorithm
SQP	Sequential quadratic programming algorithm
SVD	Singular value decomposition
SWLC	Simplified Wiener based linear control scheme
T7	Temperature tray number 7

T23	Temperature tray number 23
WLC	Wiener based linear control scheme
WPID	Wiener based PID control scheme

LIST OF SYMBOLS

a	Laguerre filter pole parameter
A	State-space parameters
B	State-space parameters
c	Laguerre filter model parameter
C	State-space parameters
d	Disturbance
D	State-space parameters
$\mathbb{D}$	Decoupling transfer function model
d_i	i-th disturbance
e	error
e_{ML}	Murphree tray efficiency for liquid phase
e_{MV}	Murphree tray efficiency for vapor phase
f	Quadratic programming problem constant vector
F	Decoupled process transfer function model
G	Process transfer function model
G_s	Gain matrix of process transfer function model
H	Quadratic programming problem constant symmetric matrix
J	Objective function
K_c	PID controller proportional gain
$\mathcal{L}$	Laguerre filter
M	Control horizon
m	Order of polynomial model

N	Order of Laguerre filter model
N_{PID}	PID controller derivative filter constant
$\mathbb{O}$	Zero matrix
P	Predictive horizon
p_i	Parameter of i-th order polynomial model
q	Error penalty
Q	Diagonal matrix of error penalty
q_i	Penalty of i-th output error
r	Input move suppression
R	Diagonal matrix of input move suppression
R^2	R-squared value
r_i	Suppression for i-th input move
s	Laplace transform domain
t	Time (hour)
t_0	Simulation starting time (hour)
T_c	System time constant (hour)
t_{end}	Simulation ending time (hour)
T_s	Sampling time (hour)
T_{sett}	Process settling time (hour)
T_{sw}	Switching time (hour)
u	Input
U	Input vector
U_F	Future input vector
U_{iK}	K number of i-th input data

U_K	K number of input data
U_{Ks}	K number of steady-state input data
U_{svd}	Resulting left singular vector in SVD
v	Intermediate variable
V	Intermediate vector
v^{sp}	Intermediate set-point
V^{sp}	Intermediate set-point vector
v_a	Output of the first nonlinear block in Hammerstein-Wiener model
v_b	Output of linear block in Hammerstein-Wiener model
V_{iK}	K number of i-th intermediate data
V_K	K number of intermediate data
$\hat{v}$	Intermediate variable from model
$\hat{V}$	Vector of intermediate variable from the model
$\hat{V}_{iK}$	K number of i-th intermediate data from model
$\hat{V}_K$	K number of intermediate data from model
$\hat{V}_{Ks}$	K number of steady-state intermediate data from model
$\bar{V}_F^{sp}$	Modified future intermediate set-point vector
V_F^{sp*}	Corrected modified future intermediate set-point vector
w	Input of decoupled process transfer function model
x	State variable
X	State vector
x_n^{tray*}	Component molar fraction at equilibrium in liquid phase on tray n
x_n^{tray}	Component molar fraction in liquid phase on tray n
x_i	i-th state variable

x_{QP}	Quadratic programming problem varying variables
y	Output
y^{sp}	Output set-point
y_n^{tray*}	Component molar fraction at equilibrium in vapor phase on tray n
y_n^{tray}	Component molar fraction in vapor phase on tray n
Y_{iK}	K number of i-th output data
Y_K	K number of output data
Y_{Ks}	K number of steady-state output data
$\hat{y}$	Output from model
z	Backward shift operator

Greek letters

α	Simultaneous approach regressor vector
β	Simultaneous approach parameter vector
δ_F	Constant matrix for future input vector in calculating the future input change
δ_U	Constant matrix for input vector in calculating the future input change
Δu	Input change
ΔU	Input change vector
$\mathcal{D}$	Disturbance vector
γ_F	Constant matrix for future input vector in calculating the future intermediate variable
γ_U	Constant matrix for input vector in calculating the future

intermediate variable

γ_X Constant matrix for state vector in calculating the future intermediate variable

Λ_K K number of simultaneous approach regressor vector

ϕ Laguerre filter model parameter vector

ψ Laguerre filter model regressor vector

Ψ_K K number of Laguerre filter model regressor

θ Polynomial model parameter vector

τ_d PID controller derivative gain

τ_i PID controller integral gain

ξ Polynomial model regressor vector

Ξ_K K number of polynomial model regressor

Kawalan Model Ramalan Berasaskan Wiener Dipermudah bagi Turus Penyulingan

ABSTRAK

Proses turus penyulingan memerlukan sejumlah tenaga yang besar, oleh itu mengawal turus ini dengan cekap boleh meminimumkan kos operasi. Kawalan model ramalan tak lelurus (NMPC) merupakan salah satu strategi kawalan terbaik sedia ada untuk mengawal turus tersebut. Dalam pelaksanaan NMPC, teknik pelelurusan kerap digunakan untuk menjamin penyelesaian optimum sejagat dan untuk mengurangkan beban pengiraan. Salah satu skim kawalan yang menggunakan teknik pelelurusan adalah skim kawalan lelurus berasaskan Wiener (WLC) yang menggunakan songsang blok tak lelurus, dan ia tidak memerlukan hasil bezaan model. Walau bagaimanapun, skim WLC memerlukan sama ada blok tak lelurus atau blok songsang untuk disongsangkan, sehingga menghadkan jenis model yang boleh digunakan untuk mewakili kedua-dua blok.

Dalam kerja ini, sebuah skim kawalan berasaskan Wiener yang tidak memerlukan blok-blok boleh songsang telah dibangunkan. Skim kawalan ini, yang dinamakan sebagai skim kawalan lelurus berasaskan Wiener yang dipermudah (SWLC), hanya menggunakan blok lurus dan blok songsang. Skim SWLC dengan algoritma pengoptimuman mudah (SO) yang telah diterbitkan dari penyelesaian tak terkekang bagi masalah pengoptimuman kawalan model ramalan, telah dilaksanakan dalam turus penyulingan. Turus ini, yang diselakukan dalam perisian Aspen Dynamics dan MATLAB simulink, mempunyai 33 dulang dan mengandungi sebuah campuran n-butana, n-pentana, n-heksana, dan n-oktana. Hasil pengesahan

menunjukkan bahawa hasil penyelakuan adalah setara dengan literatur pada ralat purata 0.63% (Errico et al., 2009).

Tiga pendekatan pengenalpastian Wiener iaitu pendekatan N-L, L-N, dan serentak, telah dibandingkan dalam pengenalpastian blok lelurus dan blok songsang. Pembandingan ini telah dilakukan untuk sistem satu masukan satu keluaran (SISO), dan hasil-hasil menunjukkan bahwa pendekatan L-N merupakan pedekatan pengenalpastian terbaik. Algoritma pengenalpastian untuk sistem berbilang masukan berbilang keluaran (MIMO) kemudian dibangunkan berasaskan pendekatan L-N. Blok linear dan blok songsang yang telah dikenalpasti digunakan untuk membangunkan pengawal MPC berasaskan skim SWLC. Pengawal MPC yang dihasilkan dan algoritma SO dibandingkan dengan pengawal MPC berasaskan skim WLC dan algoritma pengoptimuman pengaturcaraan kuadratik (QP). Pengawal berkadaran-kamiran-bezaan (PID) juga telah digunakan untuk pembandingan prestasi.

Hasil-hasil bagi kes SISO menunjukkan bahwa prestasi PID dan semua MPC dalam menjejaki titik set adalah setara. Walau bagaimanapun, prestasi PID merosot bila kawasan kendali mendekati kekangan. Sebaliknya, PID lebih baik sedikit dalam menolak gangguan, sementara MPC lebih kukuh bila ketidaktentuan parameter berlaku. Untuk kes MIMO, pengawal-pengawal MPC menghasilkan prestasi lebih baik daripada PID dalam menjejaki titik-titik set. MPC juga lebih kukuh daripada PID bila ketakpadanan model wujud. Sementara itu, pengawal MPC dan PID menunjukkan prestasi yang setara dalam menolak gangguan. Di antara semua pengawal MPC dicadangkan, SWLC-SO menghasilkan prestasi yang serupa dengan MPC yang lain tetapi dapat memendekkan masa pengiraan dengan ketara.

A Simplified Wiener Based Model Predictive Control for Distillation Column

ABSTRACT

The distillation column process requires a large amount of energy, thus efficiently controlling the column can significantly minimize the operational costs. Nonlinear model predictive control (NMPC) is one of the best control strategies available to control such a column. In the NMPC implementation, the linearization technique is often used to guarantee the global optimum solution and to reduce the computational burden. One of the promising control schemes that uses the linearization technique is the Wiener based Linear Control (WLC) scheme which uses the inverse of the nonlinear block, and does not require the derivative of the model. However, the WLC scheme requires either the nonlinear block or the inverse block to be inverted thus limiting the type of model that can be used to represent both blocks.

In this work, a Wiener based control scheme which does not require invertible blocks was developed. The developed control scheme, which was called the simplified Wiener based linear control (SWLC) scheme, only used the linear block and the inverse block. The SWLC scheme with simple optimization (SO) algorithm that was derived from the unconstrained solution of the model predictive control (MPC) optimization problem was implemented in the distillation column control. The column, which was simulated using Aspen Dynamics and MATLAB simulink software, had 33 trays and contained a mixture of n-butane, n-pentane, n-hexane, and n-octane. The validation results showed that the simulation produced a

comparable result with the literature with the average error of 0.63% (Errico et al., 2009).

Three Wiener identification approaches i.e. N-L approach, L-N approach, and simultaneous approach were compared in the identification of the linear and inverse blocks. The comparison was performed for the single input single output (SISO) system, and the results indicated that the L-N approach was the best identification approach. The identification algorithm for the multi input multi output (MIMO) system was then developed based on the L-N approach. The identified linear and inverse blocks were used to develop the MPC controller based on the SWLC scheme. The resulting MPC controller and SO algorithm were compared with the MPC controller based on the WLC scheme and the quadratic programming (QP) optimization algorithm. Proportional integral derivative (PID) controller was also implemented for performance comparison.

The results for the SISO case show that the performance of the PID and all MPCs are comparable in set-point tracking. However, the PID performance deteriorated when the operating region is near constraint. On the other hand, the PID is slightly better in rejecting disturbance while the MPC is more robust when parameter uncertainty occurs. In the MIMO case, the MPC controllers produce better performance than the PID in tracking the set-points. The MPC is also more robust than the PID when model mismatch exists. Meanwhile, the MPC and the PID controller show comparable performance in rejecting the disturbance. Among all the MPC controllers proposed, the SWLC-SO produces a similar performance with other MPCs but significantly shortens the calculation time.

CHAPTER 1: INTRODUCTION

1.1 Distillation column

Distillation is a separation technique based on different boiling points of the components in a mixture. In the distillation process, components with lower boiling points are vaporized by introducing heat to the mixture while majority of the components with higher boiling points remain as liquids. The vaporized components are then condensed by removing the heat. A Distillation column is a column where the distillation process takes place. The simple distillation column contains a column, a reboiler where the heat is added, and a condenser where the heat is removed. The column is the place where heat is added to the liquid and removed from the vapor simultaneously. Mass transfer inside the column is done by contacting the vapor phase and liquid phase. Depending on the contents of the column, the contact can occur in either the tray or bed of pack. If a reaction occurs simultaneously with the distillation process, then this is called reactive distillation.

1.2 Distillation column control

The distillation column process is the most common separation technique which involves a large amount of heat addition and removal. A distillation column can consume up to 50% of the total plant operational costs (Cheremisinoff, 2000). Improper control of the distillation column can waste high amounts of heat (energy) and increases unnecessary heat consumption which leads to plant profit reduction. The distillation column is usually located at the end of the process sequence which determines the final product quality specification. To cope with market demand, the distillation column control should easily shift the distillation product from one product specification to another in order to maximize profits. An effective control should be able to perform the specification shifting at minimum energy costs, even in the presence of other regulations such as environmental and safety regulations.

In the direct control of the product specification, the composition measurement device must be available. Often, the composition measurement rate of such a device is very slow which leads to the slow response rate of the controller. If disturbances occur when the composition is still being measured, then the controller cannot take any action since the new measurement is not available. A slower controller will result in an off-spec product which is unwanted from the economic point of view. To provide a more feasible controller, it is common to indirectly control the product specification by controlling the tray temperature since the composition can thermodynamically relate to the temperature.

In the traditional way, a distillation column is controlled by a proportional-integral-derivative (PID) controller. However, the PID controller, which is a single input and single output (SISO) controller, performs very poorly, when constraint is involved. In a multi input multi output (MIMO) case, it is also difficult to directly use two PID controllers when two variables need to be controlled, for example the top and bottom product specifications, due to the interaction between the manipulated variables. Skogestad et al. (1988) found that for distillation columns with a high purity of top and bottom compositions, the interaction was so high until it was nearly impossible to implement two SISO PID controllers. When the operation reached constraint, the PID controllers might suffer integral wind-up i.e. a condition where the integral action of the PID controller keeps integrating and increasing the control value even though it is already at its saturation. This condition causes the poor performance of the PID controller since the manipulated variable cannot move from the saturation irrespective of the type of signal given by the PID controller.

Decoupling is one technique developed to overcome the limitation of the PID controller which can be employed to reduce the interaction between the variables before implementing the PID controller. However, decoupling a high sensitive column is not feasible (Weischedel & McAvoy, 1980). An anti wind-up algorithm can be applied to the PID controller to improve its performance when the operating region is close to the saturation.

The most promising approach to control a distillation column is by implementing model based advanced control strategies such as internal model control (IMC) (Wassick & Tummala, 1989), model predictive control (MPC) (Norquay, Palazoglu, & Romagnoli, 1999) and general model control (GMC) (Karacan, Hapoglu, & Alpbaz, 2007). Among those advanced control strategies, MPC is the only advanced controller that explicitly incorporates constraint handling inside its algorithm. In the MPC, variable interaction is also taken into account without requiring the decoupling technique. However, the majority of industrial MPCs are a linear model based MPCs (LMPC) which only gives a satisfactory performance on the linear to mildly nonlinear process and processes with narrow operating regions where the linear model is acceptable. Due to this reason, the development of a nonlinear model based MPC (NMPC) that can handle moderate to highly nonlinear processes and a wider operating condition has been intensively studied.

1.2.1 Nonlinear model based MPC

There are three general nonlinear models that can be used within a NMPC. These nonlinear models are the white-box model, the grey-box model and the black-box model. The in-depth review about the applications of those models in the NMPC for the distillation column control is provided in the next chapter. Concisely, the nonlinear white-box or grey-box model based NMPC for a distillation column is heavily computational demanding due to the large number of ordinary differential equations (ODE) and differential algebraic equations (DAE). The white-box model or first-principle model for the distillation column is derived from the energy balance, equilibrium relationship and mass balance for each component and tray which results in a large number of ODEs and DAEs. The simplifications and assumptions in the grey-box model usually reduce the number of ODEs but increase the number of the DAEs. As an example, Zongzhou et al. (2010) used a grey-box model which reduced the number of ODEs in the white-box model of a distillation column from 180 ODEs to 10 ODEs. However, the number of DAEs increased from 137 to 299. Due to this reason, the nonlinear the black-box model can be used to overcome this problem. The significantly simpler structure of black-box model, even for a complex process such as a distillation process, leads to a faster NMPC controller. Even though the black-box model successfully reduces the calculation complexity and computational burden, it still possesses the same non-convex optimization problem as in the white-box and grey-box models.

1.2.2 Linearization strategy in NMPC

Without any treatment, all nonlinear model based MPCs naturally, have a non-convex optimization problem which exhibits the possibility of the local optimum solution besides the global optimum solution. The presence of the local optimum solution can deceive the optimization algorithm from the global optimum solution. To tackle such a problem, a linearization technique can be applied to the nonlinear model. The linearization technique is commonly applied by means of the first order of the Taylor series expansion. Several examples of this technique in the NMPC for a distillation column can be seen in Ławryńczuk (2011b) and Shaw and Doyle (1997). One class of black-box model offers the possibility to perform the linearization technique without requiring the first order nonlinear model derivative. This class of the black-box model, which is called the block-oriented model, embeds the nonlinear characteristic to a linear dynamic model by either transforming the input, or the output, or the input and output using a static nonlinear function. Therefore, the nonlinearity of the block-oriented model can be removed easily by the inverse of the static nonlinear function (inverse block). Fruzzetti et al. (1997) used the polynomial model as the static nonlinear model and used its root as the inverse block to cancel the nonlinearity. Among the sub-classes of block-oriented models (Wiener and the Hammerstein model), the Wiener model has a structural advantage in the modeling nonlinear behavior over the Hammerstein model (Pearson & Pottmann, 2000). The unique and relatively simpler way to transform the nonlinear control problem into a linear control problem in a block-oriented model based controller offers an interesting option to realize effective control in a distillation column.

1.3 Problem statement

The linearization of the Wiener model via the inverse block (function) is called the Wiener based Linear Control (WLC) scheme. Until now, the application of the WLC scheme requires an invertible nonlinear block. Bloemen et al. (2001) and Norquay et al. (1999) used the polynomial model as the nonlinear block which can be inverted by its root. Such a requirement limits the number of models that can be used in the block-oriented model. It also prevents the application of models that are known to have good flexibility and accuracy but difficult to be inverted directly such as the neural network model. Therefore, it is very important to develop a strategy to remove the limitation which exists in the block-oriented model.

The linearization technique also successfully reduces the optimization difficulty. When no linearization technique is applied to the model, the sequential quadratic programming (SQP) is often used to solve the nonlinear optimization algorithm (nonlinear programming). If the nonlinear model is linearized, solving the optimization problem only requires a quadratic programming (QP) algorithm. However, even though the QP is simpler than the SQP, its algorithms are still iterative algorithms. Calculating the optimum solution without considering the constraints considerably reduces the computational time especially in the QP optimization problem whose unconstrained solution can be calculated using a non iterative Least Square Estimate (LSE) algorithm. The constrained solution is usually better than the unconstrained solution.

The aim of this study is to develop a simple and fast Wiener based MPC for the distillation column. The proposed NMPC strategy includes the Simplified version of the WLC (SWLC) scheme which is a Wiener based linearization technique without requiring an invertible nonlinear block and a suitable unconstrained optimization algorithm that can increase the calculation speed, which is called the Simple Optimization (SO) algorithm. The controller is implemented on the petroleum distillation column which has been known involves multiple component in its feed.

1.4 Research objectives

The objectives of this study are:

1. To compare several Wiener model based identification approaches in terms of model accuracy, data requirement, and calculation time.

2. To develop and validate Aspen dynamic model for the distillation column case study.
3. To develop a Wiener based MPC controller with SWLC scheme and SO algorithm (SWLC-SO) for the distillation block column.
4. To compare and evaluate the performance of the SWLC-SO controller with the Wiener based MPC using a SWLC scheme and a QP algorithm (SWLC-QP), the Wiener based MPC using a WLC scheme and a QP algorithm (WLC-QP), and the PID controller in controlling the distillation column.

1.5 Scope of work

This study focuses on the development of a simplified Wiener based MPC strategy (SWLC-SO) for a multicomponent distillation column. The SWLC-SO control strategy consists of a SWLC scheme and a SO algorithm. The application of the SWLC scheme will linearize the Wiener model without inverting the nonlinear block or the inverse block.

The white-box model of the continuous multi-component (four components) distillation column with trays as the contact medium is used as the nonlinear process throughout the study. The Aspen dynamic software is used to solve and simulate the white-box model which is rigorously developed using the Aspen plus software. The Aspen dynamic software is then connected with the MATLAB simulink environment for data generation and close loop performance evaluation. The result of the Aspen dynamic simulation is then compared with data available in the literature.

The identification algorithm and the process to obtain the block parameters of the Wiener model which are required for the development of the proposed control strategy are performed in the MATLAB environment. The blocks of the Wiener model are identified from the data which is generated from the open-loop simulation of the distillation process. The input and output of the model are the manipulated and controlled variables respectively.

The fast, unconstrained SO algorithm is also developed using MATLAB software, which is also used to solve the constrained optimization problem. Only the manipulated variable constraint is considered in this study since it is the constraint that exists naturally in the control problem. The objective function of the optimization problem is formulated by the sum of the quadratic error between the controlled variables and their set-point along the prediction horizon plus the sum of quadrate of the controlled variable changes along the controlled horizon. The NMPC controller is used to control the top and bottom tray temperature of the distillation column by manipulating the reboiler duty and the reflux mass flowrate. The pair of controlled variable and manipulated variable is determined using the singular value decomposition (SVD) analysis. All the control simulations are performed using a personal computer with 2.00 GHz dual core CPU speed and 3.00 GB RAM. To evaluate the control performance, set-point tracking and disturbance rejection with feed mass flowrate as the disturbance variable are conducted. An additional robustness test is also carried out by reducing the tray efficiency in the column.

1.6 Organization of the thesis

This thesis is divided into five chapters. Chapter 1 provides a brief introduction on the distillation process, the need to control the distillation column effectively and the available controllers to perform effective control on distillation column. The problem statement of this study is also provided. Then, the objectives and the scope of this study are highlighted. Finally, the organization of this thesis is given at the end of the chapter.

Chapter 2 consists of the literature review related to this study. In this chapter, the details of the MPC are explained. Various types of nonlinear models that can be embedded in the MPC with their respective advantages and disadvantages are explained. Then, various control schemes based on the Wiener model that are available in the literature are reviewed. In the last part of the chapter, the summary of the Wiener model identification available in the literature is given.

Chapter 3 explains the methodology adopted in this study. At the beginning of Chapter 3, the multicomponent distillation process under consideration and the approach to simulate the column are explained. Steps taken in the development of a SWLC-SO control strategy are then explained. Next, the procedures to tune the PID controller and to develop the NMPC with a WLC scheme are provided. The MPC tuning procedure is then explained. Finally, the control performance studies, the robustness tests and the criteria to measure the performance of the controller used are explained.

Chapter 4 consists of the results and discussion of this study. The first part of this chapter reports and discusses the simulation results from the Aspen dynamic software. The second part provides the results of the tray selection test. The effects of reflux mass flowrate, reboiler duty, and feed mass flowrate on the control variables are discussed in the third part of this chapter. Then, the identification and validation results of the linear block, the inverse of the nonlinear block and the linear dynamic model is provided. Next, the performance of the SWLC-SO and other controllers used for the SISO and MIMO are evaluated. Finally, the robustness evaluation of all the controllers is provided.

Chapter 5 summarizes all the important findings in the work. Some suggested future studies are also proposed.

CHAPTER 2: LITERATURE REVIEW

2.1 Model predictive control

The model predictive control is a model based controller that utilizes a process model to predict the future output of the process. It also utilizes an optimization algorithm to find the future process input that minimizes a specified objective function which normally relates the predicted process output and the set-point. The MPC is the most applied advanced controller in industry and its application has increased in the recent decade (Tatjewski, 2007). The application of the MPC started over 30 years ago when the first Identification and Command (IDCOM) and Dynamic Matrix Control (DMC) appeared. The MPC was originally applied in the refining and petrochemical industry before its application expanded into a significantly broader range of industries (Qin & Badgwell, 2003).

Figure 2.1 illustrates the general MPC procedures as explained below:

1. Select a set of future control trajectory over a control horizon $(u_{|k}, u_{|k+1}, \dots, u_{|k+M-1})$.
2. Calculate the quadratic error along prediction horizon P between the future set-point $\left(y^{sp}_{|k+1}, y^{sp}_{|k+2}, \dots, y^{sp}_{|k+P}\right)$ and the predicted future output $(\hat{y}_{|k+1}, \hat{y}_{|k+2}, \dots, \hat{y}_{|k+P})$, and the quadratic of the future input changes $(\Delta u_{|k+1}, \Delta u_{|k+2}, \dots, \Delta u_{|k+M})$ from the selected future control trajectory to obtain the value of the MPC objective function. The calculation is performed using the available measurements until the current sampling point.
3. Update the set of future control trajectory using the MPC optimization algorithm and repeat steps 1 and 2 until the future control trajectory that produces the optimum value of the MPC objective function is obtained.

4. Implement the first part of the future control trajectory to the process.

5. Move to the next sampling point and repeat all the steps beginning with step 1.

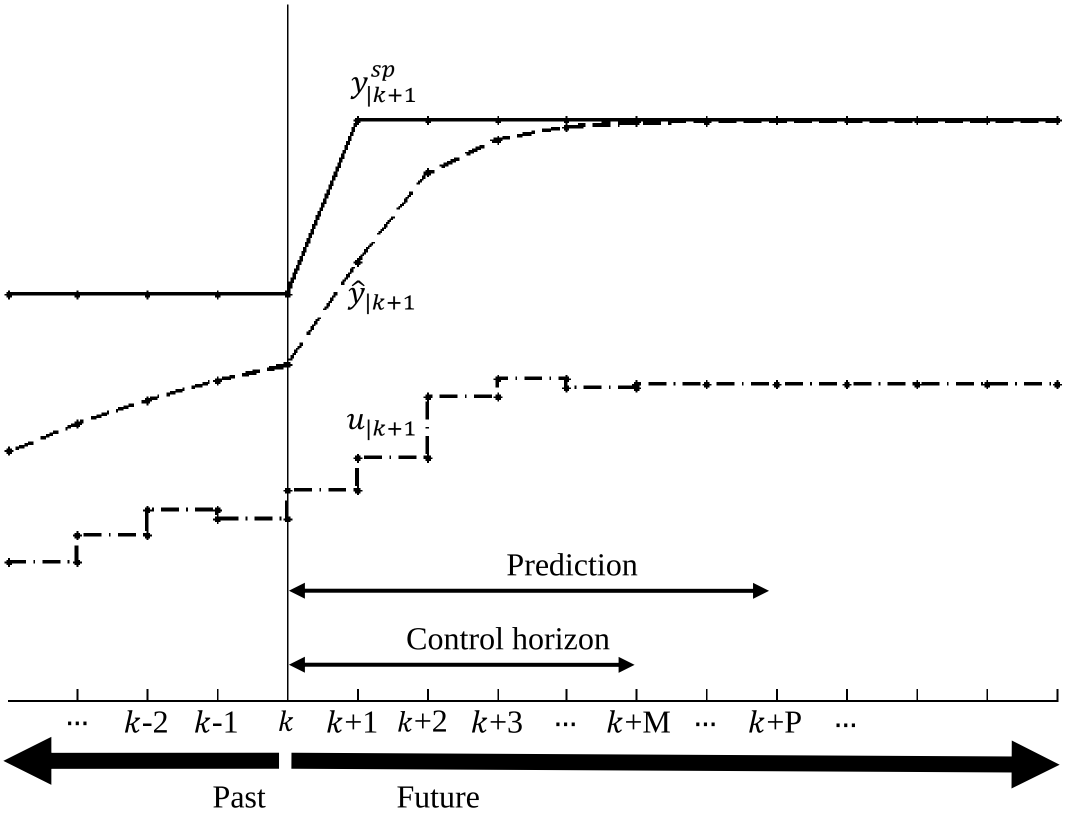

Figure 2.1: General MPC procedures (Seborg, Edgar, & Mellichamp, 2011)

Based on the general procedures explained, it can be concluded that there are two core components of the MPC controller, i.e. the model of the process to predict the future output of the process and the optimization algorithm to find the optimum control trajectory.

In the MPC controller, the model should be able to approximate the process with adequate accuracy and should also have the simplest structure possible. Most of the optimization algorithms are iterative algorithms that involve repetitive calculations of the model equation thus, the computational effort of the MPC controller will increase as the complexity of the model increases. On the other hand, models with poor accuracy will lead to the wrong optimum solution of the process. Processes are naturally nonlinear but some processes have low degrees of nonlinearity thus, the linear model is enough to approximate such processes. However, when the process nonlinearity is high, a nonlinear model is required to get a good approximation of the process. A MPC with a linear model is known as a linear MPC and a MPC with a nonlinear model is known as a nonlinear MPC.

In the MPC, the optimization algorithm should have a reasonable computational demand that can provide the optimum solution during the sampling interval. Based on the objective function and the constraint addressed, two general optimization algorithms are available i.e. the linear optimization algorithm or linear programming (LP) and the nonlinear optimization algorithm or nonlinear programming (NLP). The optimization problem in the MPC is a nonlinear optimization problem since the MPC objective function is usually represented in quadratic form even though the constraints are usually linear. Therefore, the optimization algorithm in the MPC is a NLP algorithm.

The following paragraphs are the brief explanations about NLPs (Edgar, Himmelblau, & Lasdon, 2001).

1) Quadratic programming.

Quadratic programming solves a specific form of objective function subject to several linear constraints thus, its algorithm is specific and simple. The objective function J of QP problem is:

$$J = f^T x_{QP} + 0.5 x^T H x_{QP} \tag{2.1}$$

where f and H is a vector and a symmetric matrix with a constant coefficient. The objective function is convex if H is positive semidefinite and since the constraint is linear, the overall NLP problem is convex. Therefore, the local optimum solution does not exist and the solution of the NLP problem is the global optimum solution when matrix H is positive semidefinite. The gradient of the QP objective function is linear and since the gradient at the optimum solution is zero, solving the first order derivative of the QP problem to find the optimum solution can be done using an LP algorithm. Solving the QP problem with n variables and m constraints requires almost the same computational burden when solving the LP with $(n + m)$ number of rows. For the unconstrained case, the QP problem is solved by calculating the solution of the objective function which is a linear equation. The optimization problem in the LMPC is naturally posed as the QP problem. On the other hand, if the future output is predicted using a nonlinear model, the resulting objective function cannot be arranged as the QP objective function hence an optimization algorithm that can handle more general optimization problems must be used.

2) Penalty and barrier method.

These two methods are among the NLPs that can handle more general optimization problems. The penalty and barrier methods transform the constrained problem into an easier, unconstrained problem by reformulating the objective function. In the penalty method, the new objective is defined as the sum of the original objective function, the quadratic equality constraint and the maximum function of the inequality constraint. Each constraint in the new objective function is multiplied by a positive penalty factor which penalizes the violation of the constraint. However, the quadratic form of the equality constraint in the new objective function is not effective since it makes the effect of small violations smaller. Thus, the absolute form of the equality constraint can be used to replace the quadratic form. In the barrier method, the inequality constraint is included in its logarithmic form which creates a barrier effect when it approaches zero. The logarithmic inequality constraint is also multiplied by a positive parameter which is called the barrier parameter. In contrast with the penalty parameter, the solution of the barrier method converges into its true value as the barrier parameter reaches zero. However, the equality constraint cannot be applied directly in the barrier method. The barrier method must be combined with the penalty method for the equality constraint handling. These methods are not quite popular because the absolute of the equality constraint and the maximum function of the inequality constraint produce discontinuity on the gradient of the objective function which cannot be solved by the gradient based optimization algorithm. Moreover, the distance between the calculated optimum solution and its true value depends on the barrier and penalty method parameters, which affect the degree of optimization difficulty significantly.

3) Successive linear programming (SLP).

The SLP method is based on the successive linearization of the objective function and constraints using the first term of Taylor expansion. The resulting linearized optimization problem is then solved using linear programming. Since the first term of the Taylor expansion is only accurate for the neighborhood of the initial point, additional step constraint must be supplied. SLP is very efficient when the optimum solution is located on the constraint vertex since the LP algorithm searches for the optimum solution on the vertices of the optimization region. When the optimum solution is not located in the vertex, the rate of SLP convergence is significantly low. Besides, the solution for the sub LP problem oscillates around the optimum solution and will never convergence if the step constraint is not reduced.

4) Successive quadratic programming

Successive quadratic programming searches for the optimum solution of an optimization problem by sequentially solving a QP problem. In SQP, at each iteration the gradient and the hessian of the objective function at the current point are calculated to form the QP problem. The resulted QP problem is then solved to obtain the direction to the next point. The optimum step size to the calculated search direction is then obtained using line search algorithm or trust region algorithm. The next point can be calculated from the optimum step size and the search direction. These steps are repeated for other points. The SQP algorithm usually reaches the optimum solution in smaller amounts of iteration than the SLP but the time spent at each iteration is longer since solving the QP problem is usually slower than solving the LP problem.

5) *Generalized reduced gradient (GRG).*

GRG is the extended version of the basic descent algorithm for the constrained problem. The steps of the general descent algorithm are generally similar with the steps of SQP except the search direction is calculated from the gradient of the objective function at each point as well as from the previous point. The equality constraint is handled by substituting it into the objective function before calculating the gradient, which is called the reduced gradient. Meanwhile, the inequality constraint is handled by introducing slack variables to convert it into the equality constraint. In comparison with the SLP and the SQP algorithm, the number of iteration in the GRG is usually larger than the number of iterations in SLP or SQP. The equality constraint must also be fulfilled when solving the optimization problem using the GRG. However, the requirement to fulfill the equality constraint makes the GRG more robust than SLP and SQP. The SLP and SQP could produce negative values while violating the equality constraint which cannot be evaluated when a log function is involved. Both SLP and SQP will also produce the imaginary value when the fractional power function is involved.

2.2 Nonlinear model based MPC application in distillation column

The nonlinear models that ae used in the NMPC algorithm can be generally divided into three groups based on its complexity and the prior knowledge used to develop those models. These three groups are known as the white-box model, the grey-box model and the black-box model.

2.2.1 White-box model

The white-box model, which is also called the first principle model or fundamental model, is built entirely from the prior knowledge of the process. The equation of the white-box model is derived from the mass balance, energy balance, equilibrium relationship, etc. Therefore, the white-box model has a very high accuracy and is valid in almost all ranges of operating conditions. However, the white-box model is very complex and large if it is used to approximate complicated processes.

The white-box model of the distillation column consists of a large amount of DAEs and ODEs, since the mass balance, energy balance, and vapor-liquid equilibrium equations are derived for each tray, reboiler and condenser in the distillation column. The number of equations also increases as the number of components involved in the process increases.

Two strategies can be applied in the optimization of an objective function with the DAE and the ODE equation (Kawathekar & Riggs, 2007).

1) *Sequential solution and optimization algorithm.*

In this strategy, optimization is carried out in two steps. First, the differential equation is solved for a given future control trajectory in order to obtain the future output profile and to calculate the objective function. Secondly, the optimization algorithm is employed to update the control trajectory. Both steps are repeated until the optimum control trajectory is achieved. This is a relatively simple strategy but the time required to solve the optimization problem is very large since all the differential equations are integrated at every iteration. About 85% of the total calculation time is used only for integrating the model equations (Jones & Finch, 1984).

2) *Simultaneous solution and optimization algorithm.*

This strategy fuses the solution of the differential equations of the model inside the optimization algorithm by applying it as the equality constraint. Thus, the model equation and the optimization algorithm can be solved simultaneously. However, the complexity of the optimization algorithm is significantly increased. For a small model with a short prediction horizon, the sequential solution and optimization algorithm is faster while for a large scale model, the simultaneous solution and the optimization algorithm is more feasible (Meadows & Rawlings, 1997).

Since the number of DAEs and ODEs for the white-box distillation column model is large, the simultaneous approach is preferred. The following literature is related to the application of a white-box based MPC in the distillation column.

Diehl et al. (2002) implemented a simultaneous solution and optimization approach by using a direct multiple-shooting algorithm to solve the DAE and ODE equations of a binary distillation process. For real-time implementation, the SQP was used with the model states and parameters in order to provide a fast feedback response. The proposed control strategy was successfully implemented to control the top and bottom tray temperatures by manipulating the reflux flowrate and the reboiler duty.

Kawathekar and Riggs (2007) developed a first principle model of a reactive tray distillation column to produce methyl acetate and water from acetic acid and ethanol. The resulting model was implemented in the NMPC framework using the simultaneous solution and optimization algorithm strategy. SNOPT software was used to solve the nonlinear optimization problem and the simulation results showed that the proposed NMPC controller performed better than the PI controller.

K Nagy et al. (2007) reported the successful application of a NMPC using a simultaneous solution and optimization algorithm to control a reactive distillation column with four components mixture. The multiple-shooting algorithm was used to solve the white-box model, and the resulting nonlinear optimization problem was solved using OptCon optimization software. The proposed control strategy was compared with a coupled PID controller and an LMPC controller. Their results showed that the proposed NMPC outperformed the other controllers.

Schäfer et al. (2007) improved the real-time algorithm proposed by Diehl et al. (2002) by applying the modified SQP algorithm which was called Reduced SQP (RSQP). The proposed control strategy was tested by using a fundamental model of a ternary distillation column which was developed by Lang (1991). The results showed that the application of the RSQP algorithm successfully reduced the time needed to complete the optimization.

Kühl et al. (2011) extended the application of the real-time optimization algorithm proposed by Diehl et al. (2002) to the state and parameter estimation in the moving horizon estimation (MHE) problem. The real-time optimization algorithm was used together with the numerically efficient algorithm to update the arrival cost. The proposed state-estimation strategy was compared with the extended kalman filter algorithm and was applied in a distillation column for the separation of methanol,

ethanol and 1-propanol, and the Tennessee Eastman process. The simulation results showed that the proposed strategy was capable of delivering better estimates either at the same or shorter calculation time than an extended kalman filter.

The white-box model of a distillation process is computationally demanding and the optimization algorithm is usually involves an iterative algorithm which increases the calculation burden. As a result, earlier works which implemented the white-box model of the distillation column in their NMPCs are mainly focused on the modification of the optimization algorithm that can reduce the calculation burden. Even though the modification on the optimization method and the strategy successfully reduced the computational burden, the application of the white-box model in the NMPC is still impractical due to following reasons:

1. The White-box model is difficult to develop for most industrial cases (Sivakumar, Manic, Nerthiga, Akila, & Balu, 2010). Most industrial multicomponent distillation columns separate mixtures which often contain components with no thermodynamic, vapor liquid equilibrium, physical property and other essential data for the development of the White-box model (Ravi Sriniwas, Arkun, Chien, & Ogunnaike, 1995).
2. The White-box model usually consists of large amounts of ODEs and DAEs which are not only computationally demanding but also lead to numerical problems (Ławryńczuk, 2009).

2.2.2 Grey-box model

For practical implementation, the complexity and the number of equations of the white-box model can be reduced by replacing some equations using empirical relationships or assumptions. The model which combines prior knowledge as in the white-box model with empirical relationships is classified as the grey-box model or the hybrid model. The application of empirical relationship in the grey-box model reduces the accuracy of the white-box model but at the same time it reduces its complexity thus reducing computational burden and becomes more practical. The following are some literature that implemented the hybrid model as the process predictor in the NMPC optimization algorithm.

Maiti et al. (1995) combined the steady-state part of the fundamental model with a first order dynamic model for each controlled variable to form an overall dynamic nonlinear model. The proposed hybrid-model was used in the NMPC to control the top and bottom product composition in a pilot plant of an ethanol-water distillation column. However, the details of the optimization aspect were not reported.

Due to the memory limitations in practical implementation, Patwardhan and Edgar (1993) simplified the white-box model of a packed distillation column by replacing the energy balances around the sump and reboiler with vapor-liquid equilibrium relationship. The simplified model was then used to formulate the NMPC objective function with only one control horizon. The NMPC optimization problem was also combined with the state and parameter estimation problem which was then solved using GRG2 software which was based on the GRG algorithm. The proposed model and the NMPC control strategy were implemented successfully in a packed distillation column to separate cyclohexane and n-heptane.

Zhongzhou et al. (2010) developed a NMPC based on a hybrid model for a distillation column. The hybrid model, which was known as the compartmental model, was derived by dividing the distillation column into several subsections called compartments. The dynamics of each compartment was developed by combining the balances for each stage inside the compartment with the overall balances of the compartment. The dynamics of the compartment was significantly slower than the dynamics of the individual stages within the compartment if the number of stage inside the compartment was large and the liquid holdup was similar. Therefore, the ODEs for each stage within the compartment can be reduced into Algebraic Equations (AE) while the dynamics of the compartment was represented by one of the stages whose liquid hold up was equal to the total liquid hold up in the compartment. Even though the number of AEs was increased, this approach has successfully reduced the ODEs which is more preferable in the NMPC application. The simultaneous solution and the optimization strategy were used to solve the resulting compartmental model based MPC which was performed using the AMPL software.

Although the grey-box model successfully reduced the complexity of the white-box model, the complexity of the optimization algorithm remained the same. The ODEs still have to be solved at each optimization which led to high computational burden and calculation time.

2.2.3 Black-box model

Another way to model the nonlinear process is by directly approximating the relation between the output variables and the input variables with nonlinear empirical relationships. The parameters of the nonlinear empirical relationships are obtained from the process data through model identification. In comparison with the white-box and grey-box models, this model which is known as the black-box model has a simpler structure with less accuracy. However, in most cases the accuracy of the black-box model is sufficient to produce excellent control performance (Fruzzetti, et al., 1997; Ravi Sriniwas, et al., 1995). This fact stimulates the development of the NMPC based on the black-box model in the distillation process.

One type of black-box model is called the neural network model which is known as the universal approximator (Hornik, Stinchcombe, & White, 1989). The neural network model can provide high accuracy if it is trained with sufficient amounts of good identification data and time. Shaw and Doyle (1997) applied the Recurrent Dynamic Neural Network (RDNN) model to approximate the ethanol-methanol distillation process with reflux ratio and boil-up rate as the input while the overhead and the bottom methanol purity were the output. Two RDNN based NMPC strategies were proposed i.e. linear and nonlinear strategies. In the linear strategy, the RDNN model was linearized at every sampling time to obtain the Finite Impulse Response (FIR) model coefficient. The optimum control trajectory in the first strategy was calculated using the Quadratic Dynamic Matrix Control (QDMC) method where the FIR model was used to formulate the objective function in QP form. The unconstrained solution of the QP problem was then calculated using the least-square method. In the nonlinear strategy, the RDNN model was used directly to calculate the objective function. The resulting optimization problem was then solved using the SQP algorithm. It was found that the nonlinear strategy was better than the linear strategy.

Jazayeri-Rad (2004) proposed the multiple Multi Input Single Output (MISO) neural network model to approximate a MIMO system nonlinear process with time delays. The multiple-MISO neural model developed was then incorporated inside the MPC algorithm to control a ternary distillation column. The controlled variables chosen were the top and bottom tray temperature and the manipulated variables were the percentage of the reflux flow valve and the steam flow valve. However, no constraint was considered when minimizing the nonlinear objective function. The steepest-descent method was used to solve the unconstrained multivariable nonlinear optimization problem.

Chu et al. (2004) included the disturbance effect inside the neural network model to develop a feedforward NMPC controller. The advantages of the feedforward NMPC controller were analyzed by comparing it with the common feedback NMPC controller. Both controllers were implemented in the pH process and the bench-scale ethanol-water distillation column. The results showed that the feedforward neural network based MPC controller performed better than the feedback MPC.

Ławryńczuk (2011a) evaluated the performance of full nonlinear optimization and the suboptimal optimization in a neural network based MPC. Both optimization techniques were compared by controlling two nonlinear cases i.e. the polymerization reactor and the distillation column. The simulation result showed that the suboptimal strategy managed to produce very close close-loop performance with the nonlinear optimization strategy. The reduction of the nonlinear optimization problem into the linear optimization problem also guaranteed the existence of the global optimum solution and decreased the computational effort. However, the suboptimal strategy of the neural network based NMPC was relatively complex since the linearization was calculated by performing the Taylor series expansion on the neural network model. The optimization problem in the neural network based MPC with and without the linearization strategy was solved using the QP and SQP routine, respectively.

Later, Ławryńczuk (2011b) improved his work by changing the 1st step of the proposed suboptimal neural based NMPC optimization strategy. Instead of