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APPLICATION OF DATA RECONCILIATION FOR STEEL PICKLING PROCESS

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การควบคุมและการศึกษาพฤติกรรมของกระบวนการในโรงงานอุตสาหกรรมเคมีนั้นต้องอาศัยเครื่องมือวัดเพื่อให้ได้มาซึ่งข้อมูลของระบบที่ต้องการ แต่เนื่องจากข้อจำกัดในด้านเทคนิคหรือต้นทุนข้อมูลของระบบโดยทั่วไปไม่สามารถวัดหรือทราบค่าที่แน่นอนได้ อีกทั้งความผิดพลาดของเครื่องมือวัดก็เป็นอีกปัจจัยหนึ่งที่ทำให้ข้อมูลวัดของระบบไม่ถูกต้อง ดังนั้นการปรับให้สอดคล้องของข้อมูลจึงเป็นขั้นตอนที่สำคัญมากขั้นตอนหนึ่ง ก่อนที่ข้อมูลวัดจะถูกนำไปใช้ในการควบคุมหรือทำนายพฤติกรรมของระบบ

งานวิจัยนี้มุ่งเน้นให้เห็นถึงประโยชน์ของการประยุกต์ใช้ตัวควบคุมแบบเจเนอริกโมเดล (GMC) ร่วมกับการปรับให้สอดคล้องของข้อมูลแบบพลวัต (DDR) เพื่อควบคุมตัวแปรสเตทของกระบวนการกำจัดสนิมเหล็กและถังปฏิกรณ์คายความร้อนแบบกะให้มีค่าที่ต้องการ ซึ่งวิธีควบคุมดังกล่าวถูกทดสอบความทนทานทั้งในกรณีของแบบจำลองและตัวแปรผิดพลาด และในกรณีที่ระบบถูกรบกวนด้วยตัวแปรรบกวน ผลการทดสอบทั้งในกรณีการควบคุมตัวแปรสเตทให้เข้าสู่ค่าเป้าหมาย (Set point regulation) และการเปลี่ยนแปลงค่าเป้าหมาย (Set point tracking) แสดงให้เห็นถึงประสิทธิภาพของการปรับให้สอดคล้องของข้อมูลในการกำจัดความผิดพลาดจากการวัด และในการประมาณค่าตัวแปรระบบที่ไม่ทราบค่า ดังนั้นจึงอาจกล่าวได้ว่าขั้นตอนการปรับให้สอดคล้องของข้อมูล (DDR approach) เป็นขั้นตอนหนึ่งที่สำคัญในกระบวนการควบคุมชั้นสูง

ภาควิชาวิศวกรรมเคมี	ลายมือชื่อนิสิต..
สาขาวิชาวิศวกรรมเคมี	ลายมือชื่ออาจารย์ที่ปรึกษา......................................
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4270447721 : MAJOR CHEMICAL ENGINEERING
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Process measurements are taken in chemical plants for the purpose of evaluating process control or process performance. However, not all variables needed are generally measured due to technical infeasibility or cost. Furthermore, the measurements are often contaminated in the sense that random noise may be present due to result of miscalibration or failure of the measuring instruments. Thus, data reconciliation is frequently required before the data can be used for evaluating process control or process performance.

In this research, the benefits of combining linear dynamic data reconciliation (DDR) with Generic Model Control (GMC) are demonstrated on two example problems, a steel pickling process and an exothermic batch reactor. The robustness of the proposed control strategy is investigated with respect to changes in process condition, modeling error and disturbance variable for both set point regulation and set point tracking. The results show that a rudimentary treatment of measurement errors and an estimation of unknown quantities have proved extremely effective. Therefore, DDR approach is an important adjunct to advanced control.

Department Chemical Engineering Student’s signature..
Field of study Chemical Engineering Advisor’s signature..
Academic year 2002

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Pornsiri Kaewpradit

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NOMENCLATURES

CHAPTER III

Process flow and inventory data

a = a vector of adjustment
A = an incidence matrix with respect to x
L = Lagragian matrix
Q = a covariance matrix of measurement errors
x = a vector of state variables

Generalized linear data reconciliation

A = an incidence matrix with respect to x
B = an incidence matrix with respect to u
c = a vector of constant values
P = a Projection matrix
Q = a covariance matrix of measurement errors
u = a vector of unavailable parameters
x = a vector of state variables

Bilinear data reconciliation

a_{cj} = adjustment of stream j for the measured flow rate of component c which total flow rate and concentration are measurable
A = an incidence matrix of a process
A_1 = column 1 of matrix A correspond to the component in category 1
A_2 = column 2 of matrix A correspond to the component in category 2
B = an incidence matrix with respect to u
c = a vector of constant values
c_{cj} = concentration of component c in stream j
d = a vector of available concentration in category 2
D = a matrix as shown in equation (3.25)
F_j = Total flow rate of stream j
H = a matrix as shown in equation (3.33)
n = a vector of unknown total flow rates in category 2
N = a diagonal matrix of unknown flow rate in category 2

NOMENCLATURES (Continued)

P_1 = a Projection matrix corresponding to a matrix B
P_2 = a Projection matrix corresponding to a matrix D
Q_1 = a covariance matrix corresponding to a matrix x
Q_2 = a covariance matrix corresponding to a matrix ($N\delta$)
u = a vector of unknown variables including variables in category 3
x = a vector of measured component flow rate in category 1

Generalized linear dynamic data reconciliation

f = a vector of flow measurement error
F = a vector of flow
h = a vector of volume measurement error
H = a vector of volume
m_{ij} = an element (i,j) of an incidence matrix M
M = an incidence matrix of a process
Q_H = a known covariance matrix corresponding to H
Q_F = a known covariance matrix corresponding to F

DDR application to this work

A = a Jacobian matrix with respect to $X^{(k)}$
B = a Jacobian matrix with respect to $U^{(k)}$
D = a Jacobian matrix with respect to θ
E = a Jacobian matrix with respect to $X^{(k+1)}$
P = a Projection matrix corresponding to a matrix B
U = a vector of unknown variables
X = a vector of measured variables

Generic Model Control (GMC)

dt = sampling time
u = a manipulated variable
x = a state variable
Y = an output of the process
K_1, K_2 = tuning parameters

NOMENCLATURES (Continued)

CHAPTER IV

Steel pickling process

A = tank area (m^2)

C_i = concentration of i^{th} tank (mole/lit) , $i = 1,..6$

F_i = stream i^{th} flow rate (lit/min), $i = 1,..11$

h_i = level of i^{th} tank (m) , $i = 1,..6$

k = reaction rate constant

K_1, K_2 = tuning parameters

q = a amount of drag in-out (lit/min)

r = reaction rate

V = volume of tank (m^3)

Exothermic batch reactor

A = area (m^2)

C_p = heat capacity (kJ/kmol.°C)

F = flow rate (m^3/min)

k = reaction rate constant

M = molar mass (kmole)

MW = molecular weight (kg/kmol)

r = radius (m)

R = reaction rate

U = heat transfer coefficient (kJ/min.m^2.°C)

V = volume (m^3)

Q = Heat released

T = temperature (Celcious)

ΔH = heat (kJ/kmol)

Pervaporative membrane reactor

A = area (cm^2)

C_i = concentration of component i (mole/lit)

C_p = heat capacity (J/mol.K)

J_i = permeation flux of component i

NOMENCLATURES (Continued)

M = molar mass
q = flow rate (lit/hr)
S = membrane area for permeation (cm^2)
U = heat transfer coefficient ($J/hr.m^2.K$)
V = volume of reaction mixtures (ml)
Q = Heat released
T = temperature (Kelvin)
ΔH = heat (kJ/kmol)

GREEK LETTERS

λ = Lagrange Multipliers
δ_{cf} = adjustment of stream f for the unknown total flow rate of component c which total flow rate is unknown but concentration is measurable
ε = a vector of random measurement error
Φ^k = a matrix as shown in equation (3.45)
φ^k = the k^{th} block of row of matrix Φ^k
Σ = a matrix as shown in equation (3.48a,b), (3.52a)
Ω = a matrix as shown in equation (3.48c), (3.52b)
θ = a vector of unknown parameter
ρ = density

SUPERSCRIPT

j/(k) = at time instant j based on knowledge of measurement up to time (k)
j/(k+1) = at time instant j based on knowledge of measurement up to time (k+1)
k = at time instant k
k+1 = at time instant (k+1)
sp = set point
0 = initial
$'$ = adjusted

NOMENCLATURES (Continued)

~ = measured

SUBSCRIPT

A,B,C,D,E = component
cat = catalyst
j = jacket
r = reactor
sp = set point
w = water
est = estimated
20 = 20% HCl

CHAPTER I

INTRODUCTION

The desire to maximize products using minimum raw materials and energy is often presented as the primary motivation for process control. The need for control of many chemical processes is even more fundamental, because the successful manufacture of the products can be dependent on maintaining process conditions within certain boundaries. Indeed, for some chemical systems, such as exothermic batch reactor, the nature of the reaction mixture demand safe operation, and in such cases the control of process temperature within heat-up limit is clearly essential. For waste water treatment, the pH of effluent streams must be regulated to protect aquatic and human welfare, and to comply with limits imposed by legislation (HMG Control of Pollution Act, 1974).

In recent decades, several control strategies have been developed to improve system performance by including a model of the system within the control structure (model based control strategies: MBC). Of cause, the use of a non-linear model is not restricted to incorporation in a MBC structure as GMC. The usage of the nonlinear state-space model requires the measurement of all state-variable of process parameter. Clearly, reliable process data are the key to efficient operation of chemical process control.

Process measurements are taken in chemical plants for the purpose of evaluating process control or process performance. However, not all variables needed are generally measured, because of technical infeasibility or cost. Furthermore, the measurements often contain random and possibly gross errors as a result of miscalibration or failure of the measuring instruments. Also, the data do not generally satisfy the process constraints. Thus, many process control activities are based on small improvements in process performances ; error in process data or unreliable methods of dealing with these errors can easily exceed or mask actual changes in process performance. It should be common practice to adjust raw measurements taken from a process so that known errors and measurement noise are eliminated. This procedure is called data reconciliation.

Data reconciliation is of fundamental importance in plant operation due to inaccuracies and uncertainties in the measurements. In the data reconciliation process, data are adjusted to satisfy the process constraints while minimizing the error in the least square sense and the unmeasured variables are estimated whenever possible. Most previous works have been limited to the steady state systems involving unknown parameters (Hlavacek, 1977; Mah, 1981; Tamhane and Mah, 1985; Mah, 1987). In many practical situations, however, the process conditions are continuously undergoing changes and the steady state never truly reached. Later, Darouach and Zasadzinski (1991) presented dynamic data reconciliation (DDR) for generalized linear dynamic systems. This algorithm is based on the method developed in the steady state case and leads to a recursive scheme, which is very useful in real time processing. In addition, it reduces the computational problem such as singularities and round-off errors that many occur in complex systems.

As the previous discussion, parameter estimation is also important step in the verification and subsequent use of the mathematical model of the chemical process. It is well known that none of the methods can be relied upon to extract accurate parameter estimates from data that contains a relatively high level of measurement error (Nell L.Ricker, 1984). Then, there are many efforts to extend data reconciliation techniques to estimate process parameters. The attractive procedure proposed by MacDonald & Howat (1988) is a coupled procedure that simultaneously reconciles the data to satisfy the constraints and estimate the process parameters.

In this work, an application of Generic Model Control (GMC) coupled with DDR to continuous and batch system was investigated. Here, DDR was defined as the adjustment of measured state variables to reduce measurement error and the estimation of unavailable process parameter such as drag in-out content and heat transfer coefficient.

1.1 Research Objectives

The overall objectives of this research are:

1. To develop valid modeling of a pilot plant for continuous steel pickling process according to experimental data for designing control configuration.
2. To implement Generic Model Control (GMC) integrated with dynamic data reconciliation (DDR) for control purpose to continuous and batch system such as continuous steel pickling process and exothermic batch reactor, respectively.
3. To design and develop computer software as case study for illustrating an application of data reconciliation.

1.2 Scope of Research

1. A pilot plant, a model of steel pickling process, was designed and devised at process control laboratory, Chemical Engineering, Chulalongkorn University. The pilot plant consists of three pickling; 5%, 10% and 15% HCl respectively, and three rinsing baths connected in series.
2. Generic Model Control (GMC) coupled with dynamic data reconciliation (DDR) was implemented to control concentrations of the individual tanks of the continuous steel pickling process at desired values by simulation.
3. An application of Generic Model Control (GMC) with dynamic data reconciliation (DDR) for an exothermic batch reactor with irreversible reaction was also investigated.
4. Steady state data reconciliation was applied to a generalized flow process. In developed computer software, user can define a number of tanks not exceeding seven baths and a number of input-output flow streams not exceeding five streams in each case.
5. The computer software was developed based on Borland Delphi.

1.3 Contribution of Research

1. A pilot plant for steel pickling process has been devised to study behavior of the process.
2. A modeling of the pilot plant for the continuous steel pickling process has been developed based upon conservation laws and experimental data.

3. Unmeasured variables and uncertain parameters of an exothermic reactor and a continuous steel pickling process have been estimated.
4. The developed computer software has been used to study an application of steady state and dynamic data reconciliation.

1.4 Activity Plan

1. Relevant information regarding steel pickling process and data reconciliation is reviewed.
2. A pilot plant for the steel pickling process is devised to study control behavior of the process.
3. Mathematical modeling is developed to represent the pilot plant for the continuous steel pickling process.
4. Control configuration is designed and developed to control concentrations or pH values of the steel pickling process.
5. Dynamic data reconciliation (DDR) is applied to the steel pickling process for estimating unmeasured reaction rates, and uncertain drag in-out content.
6. Control configuration of an exothermic reactor is developed to control the reactor temperature at desired value.
7. DDR is applied to the exothermic reactor for estimating unmeasured heat released by the reaction, and uncertain heat transfer coefficient.
8. Computer software is designed and developed via Borland Delphi program.
9. The computer software is tested and compared the results with Matlab.
10. All simulation results are collected and summarized.

This thesis is divided into five chapters.

Chapter I is an introduction to this research. This chapter consists of research objective, scope of research, contribution of research and activity plan.

Chapter II reviews the work carried out on steady and dynamic data reconciliation (DDR), an application of the data reconciliation to chemical process and Generic Model Control (GMC).

Chapter III covers some background information of the steady and dynamic data reconciliation (DDR), Generic Model Control (GMC) and introduces DDR algorithm employed in this work.

Chapter IV describes process design and a modeling of a pilot plant for steel pickling process. Control simulation results are obtained by simulating the process under the proposed strategy. In addition, control results of an exothermic batch reactor are implemented via using GMC integrated with DDR.

For both example problems, the process simulations are demonstrated in the presence of measurement noise in cases of set point regulation and set point tracking.

Chapter V presents the conclusions of this research and makes the recommendations for the future work.

This is followed by:

References

Appendix A: Tuning of GMC controller for steel pickling process control,
Appendix B: Laboratory process,
Appendix C: Computer source code,
Appendix D: Data reconciliation program manual.

CHAPTER II

LITERATURE REVIEW

2.1. Data reconciliation

For more than twenty years, reconciliation problem has received consideration in the literature. Kuehn and Davidson (1961) used Lagrange multipliers to solve for optimal adjustments to measurements for the case when either all or none of component flow rates are measured. Much more work has subsequently been done by Mah et al. (1976), Romagnoli and Stephanopoulos (1981) and Mah and Tamhane (1982). Britt and Leucke (1973) and Knepper and Gorman (1980) provided an algorithm that can be used to adjust plant data to meet the constraints. In the last ten years, Hlavacek (1977) and Mah (1981) developed procedures to handle very large flowsheets.

In order to reduce the number of balance equations to a minimum number, Vaclavek et al. (1976) proposed a two-step reduction. Later, Stanley and Mah (1981a) developed the concepts of global and local observability of state variables, given a set of measurements and constraints, for the nonlinear problem. They also (1981b) applied graph theory to mass-energy flow networks to classify unmeasured variables as globally (or locally) observable or unobservable. Crowe et al. (1983) used a matrix projection method to decompose the problem so that the measured and unmeasured variables can be evaluated sequentially. The essence is to construct a matrix, which is orthogonal to the matrix in balance equations, which corresponds to unmeasured quantities. The problem can then be divided into a minimization problem to reconcile redundant measurements and then equation solution for the unmeasured variables. In 1986, Crowe extended this method for problems with bilinear constraints. The unknown component flow rates and extents of reaction are deleted, as in linear case, by the constant projection matrix. Then, the unknown total flow rates are deleted via a second projection matrix, which is stochastic because of the definition in terms of measured concentrations. The adjustments to component flow rates are iterative determined, starting with guessed values of unmeasured total flow rates.

Gertler and Almasy (1973) treated the linear dynamic data reconciliation. They showed that the dynamic material balance model could be represented by continuous-state space equations or after discretization by a sampled input-output representation. For this representation, Gertler (1979) showed that solving this problem in an optimal way is too complicated to allow a general closed-form solution and a sub-optimal approach was presented.

Narasimhan and Mah (1988) have extended the formulation of the hypothesis of Generalized Likelihood Ratio (GLR) method proposed by Willsky and Jones (1974) for gross error identification in closed-loop dynamic processes described by a stochastic linear discrete model. For estimating the time of occurrence of the gross error, a simple chi-square test on the innovations (measurement residuals) is used, which is computationally more efficient than the method used by Willsky and Jones. Through simulation studies of a level control process the appropriate selection of parameters of the GLR method is investigated. A new method for incorporating of data reconciliation and gross error detection was proposed by Narasimhan and Harikumar (1993). In Part I, the reconciliation problem that includes bounds on the process variables has been solved using a Quadratic Programming (QP) algorithm. More importantly, a method to obtain the statistical distributions of measurement residuals and constraint residuals has been developed which is useful for gross error detection. Gross error detection methods based on this approach are described in Par II. Simulation results show that compared to currently available methods, the proposed methods give better gross error detection performance and more accurate estimates which always satisfy the bounds especially when tight bounds are specified.

Almasy (1990) has presented a method for dynamic data reconciliation in state space model form, in which the environmental effects (EE) are described by a random walk process. The method is based upon using linear conservation equations to reconcile measured states. In this approach only balance equations are utilized. Other modeling equations are neglected due to claims that dynamic filtering can not be performed sufficiently quickly unless the model is linear. The data reconciliation in this case is reduced to a discrete Kalman Filter as in the quasi-steady state problem. After that, Darouach and Zasadzinski present a new on-line estimation algorithm for the systems of dynamic material balance equations in 1991. In this work, the generalized linear dynamic model or singular model, for which the standard state space representation and the Kalman filtering can not be applied, is used to develop a new algorithm to solve the linear dynamic material balance problem. This algorithm is based on the method developed in the steady-state case and leads to a recursive scheme, which is very useful in real-time processing. It reduces the computational problem such as singularities and round-off errors that may occur in complex systems. Convergence conditions are given and verified for the dynamic material balance case.

The data reconciliation procedures can be extended to analyze unit operations to obtain performance parameter estimates, for example, tray efficiencies for distillation, heat transfer coefficients (Stephenson and Shewchuk, 1986) and reaction rate constants. Hlavacek (1977) suggested that parameter estimation could be done sequentially after reconciliation or simultaneously with it. MacDonald and Howat (1988) combined data reconciliation with process parameter estimation in an application involving a single stage flash and flash efficiency. The data reconciliation techniques are successfully extended to estimate flash efficiency. Two developments are presented. The first is a sequential, decoupled procedure that reconciles the data to satisfy the material and energy balances, and then estimates the process parameters using maximum-likelihood estimation. The second is a coupled procedure that simultaneously reconciles the data to satisfy the constraints and estimate the process parameters. The former is computationally faster and is more easily adapted to the existing reconciliation algorithms, but is not statistically rigorous. The later is statistically rigorous.

Weiss et al. (1996) successfully applied data reconciliation to an industrial pyrolysis reactor. Both linear and non-linear methods were used to solve the data reconciliation problem. The linear methods, which included successive linearization, yielded results very similar to those from the non-linear method. The large computational time required by the non-linear method could not be justified, and the majority of the study used only the successive linearization method. The approach was tested using plant data collected at regular intervals over a full operational cycle of the reactor. The overall heat transfer coefficient, one of the operating parameters of the pyrolysis reactor, calculated using reconciled data showed a trend consistent with plant experience and could be used to determine better regeneration cycle time of the reactor.

2.2.Generic Model Control (GMC)

Generic Model Control (GMC) is a control algorithm capable of using non-linear process model directly. In GMC scheme, first-principles models derived from dynamic mass, energy and momentum balances are mostly used. The direct implement of the nonlinear process model into the GMC controller without resorting to linearization was first suggested by Lee and Sullivan (1988). They generalized relatively easy GMC framework that relied upon the process model to approximate plant behavior. In 1989, Lee et al. extended the application of the model based GMC controller to a forced circulation single-stage evaporator. The control structure was first presented in general form and then specifically applied to this process. Since the control in the face of process constraints is of great practical importance in the processing industries. Later, Lee et al. (1991) examined the use of GMC for controlling the level in a surge tank. The effect of certain user-selectable parameters on the controlled response to changes in the inlet flow rate and model inaccuracies are considered. The overall algorithm was shown to be significantly lower in computational requirements than previously proposed algorithms for surge tank control. Implementation was straightforward and was suitable for even small-scale process control computing systems.

Cott and Macchietto (1989) proposed a new model-based controller for the initial heat-up and subsequent temperature maintenance of exothermic batch reactor. The new controller was developed based upon the GMC framework of Lee and Sullivan (1988) incorporating with the nonlinear energy balance model of the reactor and the heat exchange apparatus. A deterministic on-line estimator was used to determine the unavailable amount and rate of heat released by the reaction. The control performance of the new GMC model-based controller was compared to that of the commonly used dual-mode controller. The simulation results showed the new controller to be as good as the dual mode controller for a nominal case for which both controllers were well tuned. However, the new controller was shown to be much more robust with respect to changes in process parameters and to model mismatch. In 1994, Kershenbaum and Kittisupakorn studied the temperature control of the same process as Cott and Macchietto (1989) via using GMC controller. But in this work, an extended Kalman Filter (EKF) was incorporated into the control algorithm to estimate the amount of heat released by the reaction. The results had shown that the EKF gave an accurate estimate of the amount of heat released and together with the GMC controller gave reliable robust control. Recently, neural network technique was also used as the on-line estimator for evaluating the heat released content within the GMC algorithm (Aziz et. al., 2000). The control strategy was compared with PI and PID to track the optimal reactor temperature profiles using the complex reaction scheme in the batch reactor. It is found that the GMC coupled with the neural network provided more effective and robust than the PI and PID controllers in delivering the reactor temperature toward its desired target.

The model-based controller, GMC has been applied to handle the reactor temperature continuously. In the previous work, an idealized single-input single-output (SISO) continuous stirred tank reactor (CSTR) and SISO heat exchanger were discussed by Riggs and Rhinehart (1990). The comparison of control performance between nonlinear internal model control (IMC) and GMC was presented. It points out that GMC and nonlinear IMC gave nearly the same performance throughout a wide range of process non-linearity and process gain. Nussara (1999) presented the application of GMC to control the temperature of a batch polyvinyl chloride polymerization reactor. In this work, the GMC integrated with on-line heat released estimator gave better control performance and more robust than the PID controller. Orladda (2002) recently implemented GMC coupled with extended Kalmen Filter (EKF) for a pervaporative membrane reactor that esterification of acetic acid and butanol was considered. Both optimal temperature set point and optimal temperature profile obtained in the off-line optimization were tracked in this research.

Farrell and Tsai (1995) implemented GMC algorithm for batch crystallization process. The resulting algorithm which was called batch GMC (BGMC) algorithm utilized a time variant reduced order input-output model derived by correlating historical data of solubility vs. weight mean size. Control of the weight mean size trajectory in response to seed disturbances was demonstrated in this paper. Vega et al. (1995) used a dynamic model of the evolution of the temperature of a batch cooling crystallizer for the development of a GMC system for the crystallizer. This servo-control system had been found experimentally to work adequately. The crystallizer had also been controlled with a conventional PI controller, and the process had been simulated with the model. The methodology described could be adapted to the study of other systems or control algorithms.

Barolo et al. (1993) presented a new on-line GMC algorithm for improving the automatic startup of a binary distillation column. The series of test had been performed on an industrial-scale distillation column. The implementation of the proposed algorithm was simple and could be accomplished with standard industrial instrumentation. And in 1994, Douglas studied the problem of dual product composition control of a high purity distillation column, a deisohexanizer (DIH). The different controllers based upon GMC framework incorporating different process models were implemented and compared. When a process model differed from the true process, the closed-loop qualities of a model-based control algorithm such as GMC are in doubt. The conditions under which stability of the closed loop GMC system was guaranteed (robust stability). And the performance of the closed loop system was guaranteed to meet predetermined performance objectives (robust performance) were given for the first time in terms of the model and its uncertainty description (Signal and Lee, 1993). The GMC parameters, which gave the best performance, could be determined through a simple optimization procedure. The analytical techniques were illustrated through a simple example. In the recent work, two adaptive GMC (AGMC) schemes were developed by Xie et al. (1999) that relied upon the theory of strong tracking filter (STF). The laboratory experimental results on the three tanks system demonstrated the effectiveness of the proposed AGMC approach. Furthermore, GMC with internal controlled variable was successfully applied for the concentration control of continuous stirred tank reactor with first-order exothermic reaction, which was the process of relative degree two (Pijak, 2002).

CHAPTER III

THEORY

The aim of this research is to apply data reconciliation to chemical plant control. Since major roles of data reconciliation are reconciliation of measured process data to satisfy defined constraints and estimation of uncertainty parameter. Thus, data reconciliation is applied here as estimator incorporating with advanced controller, Generic Model Control (GMC), to control performance of continuous and batch systems as desired trajectory.

In this chapter, some background information of data reconciliation and GMC controller is outlined in generalized form. Since data reconciliation is the most interested here then it is mentioned in the first section of this chapter in both cases of steady state and dynamic conditions. After that, configuration of the proposed control strategy, GMC integrated with data reconciliation is discussed in the next section.

3.1 Data Reconciliation

3.1.1 Introduction

Since the measurement obtained with imperfect instruments, measured process data inherently contain inaccurate and inconsistent information. When this information is used in process control, state of the system can be misrepresented resulting poor control performance. Therefore, data reconciliation is an imperative procedure in control strategy to estimate measured process data in order to force these data to agree in some sense with the model. The data provided via data reconciliation are defined as the optimal solution to a constrained least square and maximum likelihood objective function. The optimal estimates of physical properties such as concentration and temperature are employed in control strategy to reduce level of process data corruption and improve process performance, leading to better quality control. First of all, it is important to understand key features that cause errors in the process data. The key features of the process data problems are summarized briefly here (Mah, 1990).

1. All measurements are subject to errors.

   These errors result from the faulty instruments and individual measurements. They cause the measured values to be inconsistent in the sense of discrepancies in energy and material balance. They fall into two categories: random errors and gross errors.
2. Not all process variables are measured.

   Due to the reasons of cost, inconvenience or technical infeasibility, not all variables needed are generally measured.
3. Measurements are spatially redundant.

   There is a data redundancy in the sense that there are more measurements (or data) available than needed if the measurements are not subject to errors. In the other hand, there are more than enough data to completely define the process model at any instant in time, i.e. the system is over-determined.
4. Measurements are temporally redundant.

   With the data sampling and recording techniques now available, it is uncommon to find process data being sampled continually and regularly at great frequencies.

The process data are improved using the redundancies in the process model, the dynamic models that composed of algebraic and differential equations provide both spatial and temporal redundancy. Frequently, some variables are unmeasured and must be estimated (Man, 1976) based on measured data. Then the measurement error in the measured variables is the big feature of the process data problem. Measurements can contain any of several types of error (Liebman, 1992).

1 Random errors.

Random errors are typically assumed to be zero-mean and normally distributed (Gaussian). This type of error is usually attributed to the irreproducibility of the measurement device (Mah, 1990).

2 Systematic biases.

Systematic biases occur when measurement devices provide consistently erroneous values, either high or low. In this case, the expected value of measurement error is not zero. Bias may arise from sources such as incorrect installation or calibration of the measurement device.

3 Gross errors.

Gross error is usually caused by nonrandom events. In this case, the measurement value bears little or no relation to the true value of the desired property. Gross error can be subdivided into measurement-related errors such as malfunctioning sensors and process-related errors such as process leaks.

In this research the measurable variables are assumed to be measured directly then the relationship between the measurement of variable and its true value can be postulated in the absence of gross errors by:

$$\tilde{x} = x + \varepsilon \tag{3.1}$$

where

$\tilde{x}$ = a (s × 1) vector of measured variables.
x = a (s × 1) vector of true variables (state variables).
ε = a (s × 1) vector of random measurement errors.

A simplified view of measurement data improvement techniques (Edgar et.al, 1988) can be divided into three basic steps as shown in figure 3.1. The first step, variable classification provides types of variables, which ones are determinable and undeterminable. Several authors have published algorithms for this procedure (Crowe, 1986; Stanley and Mah, 1981; Mah, 1990). The undeterminable variables are not available for improvement. The variable classification technique proposed by Crowe et.al has been implemented in this work.

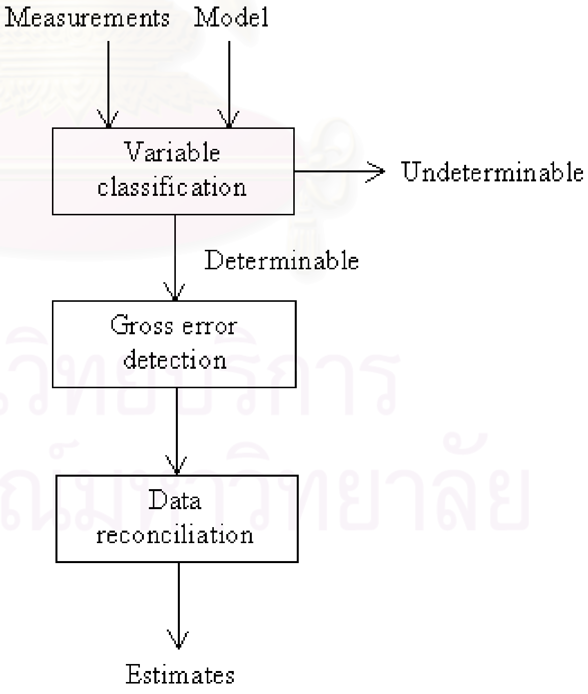

Figure 3.1 – Steps for data improvement.

Next, all gross errors are identified and removed. Several methods that are proposed for gross error detection have been evaluated by Mah (1990), Rollins et.al (1996) and Tong and Crowe (1997). For this step, it is regardless here. Lastly, data reconciliation concentrates on removing the remaining random measurement errors from the data. In this section, treatment of data reconciliation problem has been addressed through two distinct avenues, in case of process operating under steady state (Kuehn and Davidson, 1961) and dynamic (Gelb, 1974) conditions. Both techniques are developed for linear systems and weighted least squares objective function.

3.1.2 Steady-state data reconciliation

Linear reconciliation problem in steady state condition has been divided into three subsections. Firstly, the simplest situation is briefly outlined, which in this case all variables are measured (Mah et al, 1976). Secondly, the problem with unmeasured variables is discussed (Crowe et.al, 1983). And the linear data reconciliation technique is extended further to bilinear case (Crowe, 1986).

3.1.2.1 Process flow and inventory data

Let begin with the simplest situation: a process operating under steady state condition with all measured flow rates. Due to measurement error, material balances are not generally obeyed by the measured values. These values have to be adjusted or reconciled to obtain more accurate estimates of flow rates, which are, at the same time, consistent with the material balances. The reconciled or adjusted value, x', is related to the measured value, $\tilde{x}$, by the adjustment a :

$$x' = \tilde{x} + a \tag{3.2}$$

The data reconciliation problem may be formulated as the following constrained weighted least-squares estimation problem:

$$\mathrm{Min}[(\tilde{x} - x)^T Q^{-1} (\tilde{x} - x) = a^T Q^{-1} a] \tag{3.3}$$

subject to the conservation constraints

$$Ax = 0 \tag{3.4}$$

where A = an $(n \times s)$ incidence matrix of a process
Q = a $(s \times s)$ covariance matrix of measurement errors

In this case the constraints are linear and homogeneous [equation (3.4)], but in general, $A\tilde{x} \neq 0$. However, the reconciled values x' satisfy the constraints. From the objective function [equation (3.3)] which subject to the linear constraints [equation (3.4)], this problem is carried out using Lagrange multiplier method (Hildebrand, 1964). The solution is given by

$$x' = \tilde{x} - QA^{T}(AQA^{T})^{-1}A\tilde{x} \tag{3.5}$$

Since the constrained least-squares estimation is encountered many times in this section, it is worthwhile to take a little time going through the derivation. The Lagrangian for this estimation problem is

$$L = a^{T}Q^{-1}a + \lambda^{T}(A\tilde{x} + Aa) \tag{3.6}$$

Since Q is positive definite and the constraints are linear, the necessary and sufficient conditions for minimization are

$$\frac{\partial L}{\partial \lambda} = 0 \tag{3.7}$$

and
$$\frac{\partial L}{\partial a} = 0 \tag{3.8}$$

The differentiation is readily carried out if the product $\tilde{x}^{T}Ax$ is a scalar. The differentiation of a product obeys the usual product rule,

$$\frac{\partial \tilde{x}^{T}Ax}{\partial x} = \frac{\partial \tilde{x}^{T}}{\partial x}Ax + \frac{\partial x^{T}}{\partial x}A^{T}\tilde{x} \tag{3.9}$$

In the special case for which A is symmetric and $\tilde{x} = x$,

$$\frac{\partial x^{T}Ax}{\partial x} = 2Ax \tag{3.10}$$

Applying these relations to equations (3.7) and (3.8) we obtain

$$Aa = -A\tilde{x} \tag{3.11}$$

and
$$a = -\frac{1}{2}QA^{T}\lambda \tag{3.12}$$

Substituting equation (3.12) in equation (3.11),

$$\lambda = 2[\,AQA^{T}\,]^{-1}\,A\tilde{x} \tag{3.13}$$

Finally, the substitution of equation (3.13) in (3.12) yields the solution in equation (3.5). In the above treatment a weighted least-squares objective function is used. However, the data reconciliation using a linear objective function has also been reported (Smith, et. al., 1969; Mathiesen, 1974).

In the next subsection, the formulation is generalized to cover all data reconciliation problem involving linear model and constraints with unmeasured process data. It can be seen that the process flow and inventory data reconciliation problem considered above is a special case of the following reconciliation problem.

3.1.2.2 Generalized linear data reconciliation

Frequently, some variables are not measured so that two other classes of state variables or parameters are introduced here. Then the generalized constraints can be stated as:

$$Ax + Bu = c \tag{3.14}$$

where A = an $(n \times s)$ incidence matrix with respect to x
B = an $(n \times m)$ incidence matrix with respect to u
u = a $(m \times 1)$ vector of parameters which are not directly related to the measurements through equation (3.1)
c = a $(n \times 1)$ vector of constant values

The general linear reconciliation problem is the least-squares estimation of x and u subject to the constraints [equation (3.14)]. The flow and inventory data reconciliation is clearly a special case of the above formulation.

To improve this problem, the unmeasured variables need to be eliminated via using a projection matrix (Crowe et.al, 1983) which is defined shortly in this subsection. In the other words, this reconciliation problem can be reduced to the problem involving no unmeasured variables. Afterward the all measured reconciliation problem can be applied. The unmeasured variables may be calculated from the estimates of the measured variables in a subsequent step.

Let P be a (t × n) matrix such that it is defined as this following,

$$PB = 0 \tag{3.15}$$

From the definition of the projection matrix above, the constraints in equation (3.14) are henceforth considered in sense of all associated measured variables as seen in equation (3.17) where $\bar{A} = PA$ and $\bar{c} = Pc$.

$$PAx + PBu = Pc \tag{3.16}$$

$$\bar{A}x = \bar{c} \tag{3.17}$$

Now the solution of the weighted least squares estimation problem [equation (3.3)] subject to the constraints [equation (3.17)] may be obtained using the Lagrange multipliers in a manner entirely analogous to the derivation of equation (3.5) in the previous subsection (Mah and Tamhane, 1982). The solution becomes

$$x' = \tilde{x} + Q\bar{A}^T\,[\,\bar{A}Q\bar{A}^T\,]^{-1}\,(\,\bar{c} - \bar{A}\tilde{x}\,) \tag{3.18}$$

The solution in equation (3.18) can be reduced to equation (3.5) in flow reconciliation with $\bar{c} = 0$ and $\bar{A} = A$.

From equation (3.14) the estimates of the unmeasured variables can be provided as this following equation,

$$Bu' = c - Ax' \tag{3.19}$$

The covariance matrix Q may not be given. The matrix Q may be estimated from process data. If the process is in a steady state, the separated estimates of Q computed for successive time periods may be cumulatively pooled. The matrix Q may also be estimated from balance residuals (Almasy and Mah, 1984).

Now the linear data reconciliation technique for the linear constraints (material balances) is implemented. Next, case of bilinear constraints (component balances) is discussed based on previous knowledge.

3.1.2.3 Bilinear data reconciliation

As a result, the component balance equation generally contains products of pairs of variables then it is considered as bilinear. In this subsection, the linear data reconciliation technique, which presented in two previous subsections is extended to this case. The theoretical basis of the bilinear problem is developed and discussed by Vaclavek et al. (1976a,b). They assumed that either all or none of the concentrations in a stream are measured. Thus the stream can be portioned into four categories, namely:

Category	Total Flow	Concentrations
1	M	M
2	U	M
3	M	U
4	U	U

where M = measured, U = unmeasured.

However, with an arbitrary distribution of measurements, the classification must refer to components in streams, in which case categories 3 and 4 can be combined. Thus, there will be three categories of variables:

1. Total Flow rate and concentration measured and adjustable.
2. Concentration measured and adjustable.
3. Total flow rates unknown or measured; component flow rates unmeasured.

In order to reduce the number of balance equations to a minimum number, the two successive projection matrixes are constructed (Crowe, 1986). The first one is used to eliminate the entire unmeasured component flow rates and concentrations (category 3 and other unmeasured variables). And then the second eliminates the total flow rates corresponding to variables of category 2 from the balance equations. Thus the problem is divided into three sequentially solved sub-problems.

First of all, the constraints of this problem must be defined corresponding to the entire categories of variables above. The columns of the matrix A in equation (3.14) are partitioned so that

$$A \rightarrow \lfloor A_1 \mid A_2 \rfloor$$

where A_i = columns of matrix A correspond to the components in categories 1 and 2 respectively (i = 1,2)

The flow of component in category 1 is defined by

$$x_{cj} = F_j c_{cj} \tag{3.20}$$

where F_j = total flow rate of stream j

c_{cj} = concentration of component c in stream j

The reconciled value is related to the measured value as in equation (3.2). Thus, the reconciled values of the component flow in category 1 and concentration in category 2 are defined as following:

$$x'_{cj} = \tilde{x}_{cj} + a_{cj} \tag{3.21}$$

$$d'_{cf} = \tilde{d}_{cf} + \delta_{cf} \tag{3.22}$$

where a_{cj} = the adjustment in stream j for the measured flow rate of component c in category 1

δ_{cf} = the adjustment in stream f for the unknown total flow rate of component c in category 2

Equation (3.14) is represented, then the constraints must be obeyed by the estimated values, so that

$$A_1 (\tilde{x} + a) + A_2 N(\tilde{d} + \delta) + Bu = c \tag{3.23}$$

where N = the diagonal matrix of unknown flow rates in category 2

u = a vector of unknown variables including variables in category 3

c = a constant vector of exactly known variables

Now, the reconciliation problem can then be defined. As seen in equation (3.23) there are two unknown variables, N and u. Thus there are several steps that can be taken to simplify this problem. The first step of the reduction in the number of equations is to eliminate all unknown variables, u via the first projection matrix, $P_1^T B = 0$.

$$P_1^T\,[\,A_1\,(\,\tilde{x} + a\,) + A_2 N(\,\tilde{d} + \delta)] = P_1^T c \tag{3.24}$$

The second step of simplification involves defining the second projection matrix, P_2 that is a basis for the null space of

$$D^T \cong [\,A_{21}\,\tilde{d}_1 \mid A_{22}\,\tilde{d}_2 \mid \dots \mid A_{2\,f}\,\tilde{d}_f \mid \dots]^{\,T}\,P_1 \tag{3.25}$$

where $A_{2\,f}$ = the set of columns of A_2 corresponding to stream f
$\tilde{d}_f$ = the vector of measured concentrations in stream f

Then,

$$P_2^T D \cong 0 \tag{3.26}$$

so that equation (3.24) can be simplified to

$$P_2^T P_1^T\,[\,A_1\,(\,\tilde{x} + a\,) + A_2 N\delta\,] = P_2^T P_1^T c \tag{3.27}$$

Now, $(a, N\delta\,)$ be the solution to the following least-squares estimation problem:

$$\underset{x,(N\delta)}{\mathrm{Min}}\;a^{\,T} Q_1^{-1} a + (\,N\delta)^{\,T}\,Q_2^{-1}\,(\,N\delta) \tag{3.28}$$

subject to equation (3.27).

There are several advantages to defining P_1 and P_2 separately. First, the separate computations of projection matrix are more efficient than that of a larger combined matrix. Secondly, separate conditions are obtained for unmeasured variables in categories 3 and 2. Thirdly, P_1 is a constant matrix so that P_2 contains all of the statistical variability due to that of $\tilde{d}$.

The solution of this problem may be obtained by using the Lagrange multipliers. Then the Lagragian is defined by

$$L = a^{T} Q_1^{-1} a + (N\delta)^{T} Q_2^{T} (N\delta) + \lambda^{T} \{P_2^{T} P_1^{T} [A_1 (\tilde{x} + a) + A_2 (N\delta) - c]\} \qquad (3.29)$$

Then derivatives are taken with respect to a and $(N\delta)$, after that set equal to zero, giving respectively,

$$a = -\frac{1}{2} Q_1 A_1^{T} P_1 P_2 \lambda \qquad (3.30)$$

and

$$(N\delta) = -\frac{1}{2} Q_2 A_2^{T} P_1 P_2 \lambda \qquad (3.31)$$

which

$$\lambda = 2[(P_2^{T} H P_2)^{-1} P_2^{T} P_1^{T} (A_1 \tilde{x} - c)] \qquad (3.32)$$

and

$$H = P_1^{T} (A_1 Q_1 A_1^{T} + A_2 Q_2 A_2^{T}) P_1 \qquad (3.33)$$

From the solutions of the problem [equations (3.30) and (3.31)], equation (3.24) with equation (3.25) is rewritten to determine the vector of distinct unknown total flow rates in category 2, as

$$Dn = -P_1^{T} [A_1 (\tilde{x} + a) + A_2 (N\delta) - c] \qquad (3.34)$$

where n = the vector of unknown total flow rates in category 2

From equation (3.34), all unknown variables can be determined by rearranging equation (3.23) as this follow

$$Bu = -[A_1 (\tilde{x} + a) + A_2 N(\tilde{d} + \delta) - c] \qquad (3.35)$$

The previous subsections have been limited to the steady-state systems described by linear and bilinear constraints involving unknown parameters (Hlavacek, 1977; Mah, 1981; Tamhane and Mah, 1985; Mah, 1987). However, the actual process conditions change continuously so that the steady state is never truly reached. Thus, the on-line estimation algorithm for the system of dynamic material balance equations is considered in next section in case of all measured variables (Darouach and Zasadzinski, 1991). This algorithm is extended further to the system with unmeasured variables and uncertainty parameter.

3.1.3 Generalized linear dynamic data reconciliation (DDR)

Darouach and Zasadzinski (1991) have proposed estimation algorithm derived from dynamic material balance with all variables measured (inputs, outputs and states). The material balance equations can be written in the following discrete form:

$$H^{k+1} = H^{k} + MF^{k} \tag{3.36}$$

where F^{k} = a vector of the flows at time constant k

H^{k} = a vector of the volumes at time constant k

M = an incidence matrix of the process

Let m_{ij} is the element of the incident matrix M which $m_{ij} = 1$ if stream j is an input to node i and $m_{ij} = -1$ if stream j is an output to node i.

For simplicity, the balance equations are assumed to obtain only measured variables. The measurements are given by [as in equation (3.1)]

$$\tilde{H} = H + h \tag{3.37}$$

and

$$\tilde{F} = F + f \tag{3.38}$$

where h = a vector of volume measurement error with known covariance matrix $Q_H > 0$.

f = a vector of flow measurement error with known covariance matrix $Q_F > 0$.

Equation (3.36) can be written as

$$-Ex^{k+1} + Bx^{k} = 0 \tag{3.39}$$

where $x^{k} = \begin{bmatrix} H^{k} \\ F^{k} \end{bmatrix}$, $E = \begin{bmatrix} I \\ 0 \end{bmatrix}$ and $B = \begin{bmatrix} I \\ M \end{bmatrix}$

Also equations (3.37) and (3.38) become

$$\tilde{x} = x + \varepsilon \tag{3.40}$$

where $\tilde{x} = \begin{bmatrix} \tilde{H} \\ \tilde{F} \end{bmatrix}$ and $\varepsilon = \begin{bmatrix} h \\ f \end{bmatrix}$

with ε = a vector of measurement error with known covariance matrix.

$$Q = \begin{bmatrix} Q_H & 0 \\ 0 & Q_F \end{bmatrix} \tag{3.41}$$

Next, the problem of estimating the vector x^k at time instant k is considered. From Equations (3.39) and (3.40), the (k+1) measurements and the k constraints are collected as follows:

$$\tilde{x} = x + \varepsilon \tag{3.42a}$$

$$\Phi^k x = 0 \tag{3.42b}$$

and

$$\Phi^k = \begin{bmatrix} B & -E & 0 & . & . & . & 0 \\ 0 & B & -E & 0 & . & . & 0 \\ . & . & . & . & . & . & . \\ 0 & . & . & . & 0 & B & -E \end{bmatrix} = \begin{bmatrix} \varphi^1 \\ \varphi^2 \\ . \\ \varphi^k \end{bmatrix}$$

Now with these notations, dynamic data reconciliation (DDR) problem can be formulated as in the steady state case, that is, the minimization of

$$\mathrm{Min}(x - \tilde{x})^T Q^{-1} (x - \tilde{x}) \tag{3.43}$$

subject to the constraint, equation (3.42b).

Since, this problem is represented in the steady state case so that the solution of the process flow and inventory in subsection 3.1.2.1 [equation (3.5)] can be applied. Then the solution of this problem is given by

$$x' = \tilde{x} - Q(\Phi^k)^T \left[(\Phi^k) Q (\Phi^k)^T\right]^{-1} \Phi^k \tilde{x} \tag{3.44}$$

From equation (3.44) the computational volume increases with a number of observation, which leads to several numerical problems such as round-off errors and singularities. To avoid these, Darouach and Zasadzinski have presented a recursive solution based on the sequential method developed for the steady state case (Darouach et at., 1988b). Then matrix Φ^k is partitioned as follows:

$$\Phi^k = \begin{bmatrix} \Phi^{k-1} \\ \varphi^k \end{bmatrix} \tag{3.45}$$

where φ^k = the kth block of rows of matrix Φ^k given by

$$\varphi^k = [0 \quad 0 \quad . \quad . \quad . \quad 0 \quad B \quad -E] \tag{3.46}$$

From the steady state sequential method obtained by additional linear constraints (Darouach et.al., 1988b), it is proved that the new estimate $x'^{(k+1)}$ and its variance $\Sigma^{(k+1)}$ can be established in term of the additional constraint $\varphi^k x'^{(k+1)} = 0$, and the following results are obtained:

$$x'^{(k+1)} = P^{(k+1)} x'^k \tag{3.47}$$

$$\Sigma^{(k+1)} = P^{(k+1)} \Sigma^k \tag{3.48}$$

with $$P^{(k+1)} = I - \Sigma^k (\varphi^k)^T \Omega^k \varphi^k \tag{3.49}$$

and $$\Omega^k = [\varphi^k \Sigma^k (\varphi^k)^T]^{-1} \tag{3.50}$$

The covariance matrix Σ^k can be written as:

$$\Sigma^k = \begin{pmatrix} \Sigma_{11}^k & .. & \Sigma_{1k}^k & 0 \\ .. & .. & .. & .. \\ \Sigma_{k1}^k & .. & \Sigma_{kk}^k & 0 \\ 0 & .. & 0 & Q \end{pmatrix} \tag{3.51}$$

where Σ_{ij}^k is the element in the (i,j) block. After some manipulations, using equation (3.46) to (3.50), one obtains

$$\Omega^k = (B\Sigma^{kk} B^T + EQE^T)^{-1} \tag{3.52}$$

and $$P^{(k+1)} = \begin{pmatrix} I & 0 & . & 0 & -\Sigma_{1k}^k B^T \Omega^k B & \Sigma_{1k}^k B^T \Omega^k E \\ . & . & . & . & . & . \\ 0 & . & 0 & I & -\Sigma_{(k-1)k}^k B^T \Omega^k B & \Sigma_{(k-1)k}^k B^T \Omega^k E \\ 0 & . & . & 0 & I - \Sigma_{kk}^k B^T \Omega^k B & \Sigma_{kk}^k B^T \Omega^k E \\ 0 & . & . & 0 & QE^T \Omega^k B & I - QE^T \Omega^k E \end{pmatrix} \tag{3.53}$$

Equation (3.53) requires only the kth block column of the matrix Σ^k. From equation (3.53), the (k+1)th block column of covariance matrix $\Sigma^{(k+1)}$ is given by:

$$\begin{pmatrix} \Sigma^{(k+1)}_{1(k+1)} \\ . \\ \Sigma^{(k+1)}_{k(k+1)} \\ \Sigma^{(k+1)}_{(k+1)(k+1)} \end{pmatrix} = \begin{pmatrix} \Sigma^k_{1k} B^T \Omega^k EQ \\ . \\ \Sigma^k_{kk} B^T \Omega^k EQ \\ Q - QE^T \Omega^k EQ \end{pmatrix} \tag{3.54}$$

The estimate $x'^{(k+1)}$ is given in term of x'^k by:

$$x'^{(k+1)} = \begin{pmatrix} x'^{1/(k+1)} \\ . \\ x'^{k/(k+1)} \\ x'^{(k+1)/(k+1)} \end{pmatrix}$$

$$= P^{(k+1)} \begin{pmatrix} x'^k \\ \tilde{x}^{(k+1)} \end{pmatrix}$$

$$= P^{(k+1)} \begin{pmatrix} x'^{1/k} \\ . \\ x'^{k/k} \\ \tilde{x}^{(k+1)} \end{pmatrix} \tag{3.55}$$

which can be written as:

$$\begin{pmatrix} x'^{1/(k+1)} \\ . \\ x'^{k/(k+1)} \\ x'^{(k+1)/(k+1)} \end{pmatrix} = \begin{pmatrix} x'^{1/k} - \Sigma^k_{1k} B^T \Omega^k (Bx'^{k/k} - E\tilde{X}^{(k+1)} \\ . \\ x'^{k/k} - \Sigma^k_{kk} B^T \Omega^k (Bx'^{k/k} - E\tilde{X}^{(k+1)} \\ \tilde{x}^{(k+1)} + QE^T \Omega^k (Bx'^{k/k} - E\tilde{X}^{(k+1)} \end{pmatrix} \tag{3.56}$$

As seen in equation (3.56), the estimation $x'^{j/(k+1)}$ of the vector x^j at time instant j based on the knowledge of measurements up to time k+1 (j < k+1) is given by

$$x'^{j/(k+1)} = x'^{j/k} + \Sigma^k_{jk} B^T \Omega^k (E\tilde{x}^{(k+1)} - Bx'^{k/k}) \qquad \text{for } j < k+1 \tag{3.57a}$$

$$x'^{(k+1)/(k+1)} = QE^T \Omega^k Bx'^{k/k} + (I - QE^T \Omega^k E)\,\tilde{x}^{(k+1)} \tag{3.57b}$$

and its covariance matrixes are

$$\Sigma^{jk+1)}_{j(k+1)} = \Sigma^{k}_{jk} B^{T} \Omega^{k} EQ \qquad \text{for } j < k+1 \qquad (3.58a)$$

$$\Sigma^{(k+1)}_{(k+1)(k+1)} = Q - QE^{T} \Omega^{k} EQ \qquad (3.58b)$$

and $$\Omega^{k} = (B\Sigma^{k}_{kk} B^{T} + EQE^{T})^{-1} \qquad (3.58c)$$

with the initial conditions $x'^{1/1} = \tilde{x}^{1}$ and $\Sigma^{1}_{11} = Q > 0$.

The recursive expressions of equations (3.57) and (3.58) constitute a generalized algorithm of the Kalman filter in the absence of process noise and represent a systematic approach to real-time linear filtering (equation 3.57b) and smoothing (3.57a) with a well established optimality criterion. Standard Kalman filter can be obtained from equations (3.57) and (3.58) with $E = I$.

3.1.4. DDR application to this work

The dynamic data reconciliation (DDR) strategy presented above (Darouach and Zasadzinski, 1991) is used to estimate the current measured variable x^{k} based on [equation (3.57a)] the collecting measured variable at time instant x^{i}, i = 1,.., (k-1). In addition, the estimated values at current time k, is employed to foretell the measured variables at time (k+1). In this work, this strategy is applied by just considering the k and (k+1) measured variables, and the unmeasured variable is additionally considered. In that manner the discrete measurements and constraints as equations (3.42) are rewritten as follows:

$$\tilde{x}^{(k+1)} = X^{(k+1)} + \varepsilon \qquad (3.59a)$$

$$EX^{(k+1)} = AX^{(k)} + BU^{(k)} + c \qquad (3.59b)$$

where $U^{(k)}$ = a vector of unknown variables

E, A, B = a Jacobean matrix with respect to $X^{(k+1)}, X^{(k)}$ and $U^{(k)}$, respectively

c = a vector of constant values

Base on knowledge above, firstly, the number of equations is reduced by the projection matrix, P, to eliminate the vector of unknown variables, $U^{(k)}$ (C.M. Crowe, 1986). Therefore, equation (3.59b) is rewritten as follow:

$$\bar{E}X^{(k+1)} = \bar{A}X^{(k)} + \bar{c} \qquad (3.60)$$

where $\bar{E} = P^T E$, $\bar{A} = P^T A$, $\bar{c} = P^T c$ and $P^T B = 0$

The dynamic data reconciliation (DDR) problem can be formulated with these notations, that is, the minimization of

$$\mathrm{Min}(x - \tilde{x})^T Q^{-1} (x - \tilde{x})$$

Then, the DDR algorithm is shown as these follows;

$$x'^{(k)} = x'^{(k)} + \Sigma^k \bar{A}^T \Omega^k (\bar{E}\tilde{x}^{(k+1)} - \bar{A}x'^{(k)} - \bar{c}) \qquad (3.61a)$$

$$x'^{(k+1)} = \tilde{x}^{(k+1)} - Q\bar{E}^T \Omega^k (\bar{E}\tilde{x}^{(k+1)} - \bar{A}x'^{(k)} - \bar{c}) \qquad (3.61b)$$

and covariance matrix of estimation error is

$$\Sigma^{(k+1)} = Q - Q\bar{E}^T \Omega^k \bar{E} Q \qquad (3.62a)$$

where $\Omega^k = (\bar{A}\Sigma^k \bar{A}^T + \bar{E}Q\bar{E}^T)^{-1}$ (3.62b)

The proposed strategy is subjected to the constraint equation (3.60).

Next, the estimated variables, $X'^{(k)}, X'^{(k+1)}$ from equations.(3.61) are used to evaluate the unknown variables, $U^{(k)}$ from equation.(3.59b).

$$U'^{(k)} = (B.B^T)^{-1} B.[E.X'^{(k+1)} - A.X'^{(k)} - c] \qquad (3.63)$$

Since, the more general problem is one where a number of parameters, θ, are actually part of the constraint equations, that is, find the best estimates X' and θ' simultaneously (MacDonald and Howat, 1988). Then, the estimation of the uncertainty parameter is also presented here by using the algorithm proposed by Britt and Leucke (1973). In their algorithm, following additional equation is used for calculate θ' simultaneously with adjustment of the measured variables.

$$\theta'^{(k+1)} = \theta'^{(k)} + (\bar{D}^T \Omega^k . \bar{D})^{-1} \bar{D}^T \Omega^k .[\bar{E}\tilde{x}^{(k+1)} - \bar{A}X'^{(k)} - \bar{c}] \qquad (3.64)$$

where $\overline{D} = P^{T} D$ and D is the Jacobean matrix with respect to θ.

However, it is worthwhile to take a little time going through the derivation. The data reconciliation problem can be formulated as the following constrained weighted least-squares estimation problem:

$$\text{Min}(x - \tilde{x})^{T} Q^{-1} (x - \tilde{x})$$

subject to the conservation constraints

$$EX^{(k+1)} = AX^{(k)} + BU^{(k)} + D\theta^{(k)} + c \tag{3.65}$$

To eliminate the unknown variables, the projection method is applied to equation (3.66).

$$\overline{E}X^{(k+1)} = \overline{A}X^{(k)} + \overline{D}\theta^{(k)} + \overline{c} \tag{3.66}$$

From maximum likelihood, equations (3.61) and (3.64) are the solutions to the least-squares estimation problem which subject to equation (3.65). The unknown variables can be further determined by equation (3.63).

3.2 Control Configuration

A conventional controller, PI is generally used in pH control. But it is well known that PI controller can not handle a complicated and high nonlinear system as good enough. Then, the advanced controller is required in which GMC one of the advanced controllers is applied in this work. The GMC controller incorporates a nonlinear state-space model of the process directly within the control algorithm. Therefore, it has advantages over other model-based controllers in:

- Models derived from dynamic mass, energy and momentum balances can be directly used in the controller.
- Nonlinear, multivariable, time-dependent models comprise the dominant structure of the controller.
- Controller tuning is straightforward and easy to understand.
- The control is satisfactory, even in the presence of mild process/model mismatch and the techniques for the analysis of the stability of controllers are available.

In the following section GMC control algorithm is discussed. In addition, GMC integrated with dynamic data reconciliation (DDR) is outlined to control the process including with unknown parameter at desired set point.

3.2.1 Generic Model Control (GMC)

Lee and Sullivan (1988) have generalized many of the model-based techniques into a generic structure called Generic Model Control (GMC), which allows the incorporation of nonlinear process models directly in the control algorithm. Consider the process described by state space models:

$$\frac{dx}{dt} = F(x, u, t) \tag{3.67}$$

$$Y = H(x) \tag{3.68}$$

where x = a state variable
u = a manipulated variable
Y = an output of the process

Generally, F and H are nonlinear functions, they can be rewritten in derivative terms as following.

$$\frac{dY}{dt} = \frac{\partial H(x)}{\partial x} \cdot \frac{\partial x}{\partial t} \tag{3.69}$$

Substituting equation (3.67) into (3.69) to obtain,

$$\frac{dY}{dt} = \frac{\partial H(x)}{\partial x} . F(x, u, t) \tag{3.70}$$

Good control performance will be given by combination of the proportional and derivative term of error as,

$$\frac{dy}{dt} = K_1 (Y^{sp} - Y) + K_2 \int (Y^{sp} - Y)\, dt \tag{3.71}$$

where K_1, K_2 = tuning parameters of the controller.

From equation (3.71), the first term is used to control the process output to the desired target, Y^{sp} and the second provides zero offset response.

From equation (3.70) and (3.71) the control algorithm is restated as following:

$$K_1 (Y^{sp} - Y) + K_2 \int (Y^{sp} - Y)\, dt = \frac{\partial H(x)}{\partial x} . F(x, u, t) \tag{3.72}$$

For nonlinear system the process model is rewritten to obtain the linearized math model.

$$F(x, u, t) = F'(x) + G(x) . u \tag{3.73}$$

Finally the GMC control algorithm obtains,

$$K_1 (Y^{sp} - Y) + K_2 \int (Y^{sp} - Y)\, dt = \left[F'(x) + G(x) . u\right] \tag{3.74}$$

The process control performance is specified by choosing the different values of K_1 and K_2, with the appropriate values of these parameters the process response provides the reasonable desired trajectory. These values are related to the natural dynamic response of the process. By taking Laplace transform of the equation (3.71), transfer function becomes,

$$\frac{y}{y^{sp}} = \frac{2\tau\xi s + 1}{\tau^2 s^2 + 2\tau\xi s + 1} \tag{3.75}$$

where

$$\tau = \frac{1}{\sqrt{K_2}} \quad \text{and} \quad \xi = \frac{K_1}{2\sqrt{K_2}}$$

The design procedure can be specified as follows:

1. Choose ξ from figure 3.2 to obtain desired trajectory.
2. Choose τ from figure 3.2 to obtain appropriate time.
3. Calculate K_1 and K_2 using these following equations:

$$K_1 = \frac{2\xi}{\tau} \tag{3.76}$$

$$K_2 = \frac{1}{\tau^2} \tag{3.77}$$

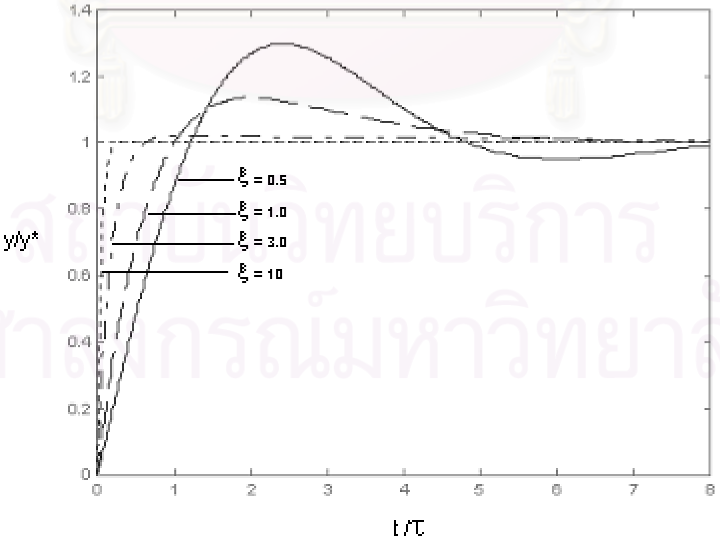

Figure 3.2 - Generalized GMC profile specification

Since GMC is the advanced controller based on mathematical modeling of the process so that the unavailability and uncertainty of the process parameter or variable causes the poor control performance. Thus, with these conditions the estimator is imperative procedure in control strategy to evaluate these values.

3.2.2 GMC coupled with data reconciliation

Due to unavailability of process parameters or variables resulting by cost, inconvenience or technical unfeasibility, it easily exceeds process control performance. Hence, the estimation of these data is a key feature to efficient control operation of chemical plants. The data reconciliation is then incorporated with GMC controller to estimate unknown parameter and variable.

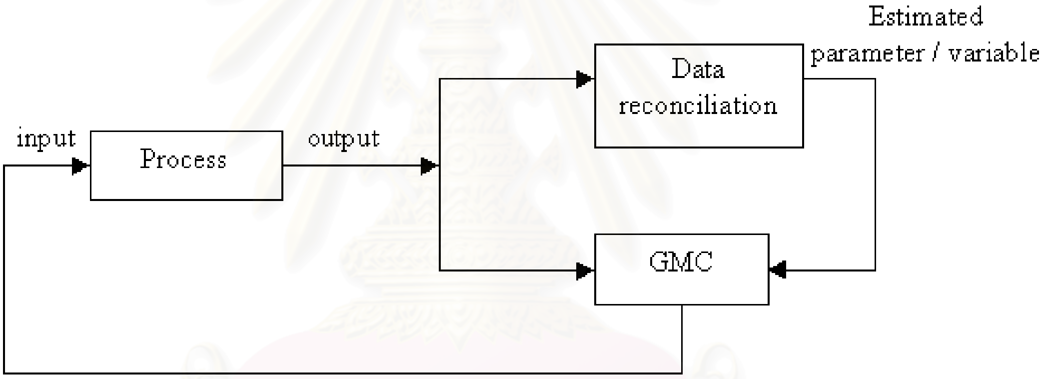

Figure 3.3 – GMC integrated with data reconciliation

As seen in figure 3.3, the unknown parameter and variable are estimated based on the reconciled estimates of measurements by data reconciliation algorithm. The GMC controller further calculates the control action relied upon these estimates. Thus data reconciliation is an imperative adjunct in control strategy. If the estimated quantities and the reconciled estimates are close to the actual values, the controller will give good control performance with less offset or none.

CHAPTER IV

APPLICATION OF DATA RECONCILIATION

This chapter demonstrates the feasibility of dynamic data reconciliation (DDR) to reconcile and estimate measured state and unmeasured process variables, respectively. The chosen system is a simulated continuous steel pickling process, which strongly nonlinear as described in the next section. Furthermore, it is also important to extend an application of DDR to an exothermic batch reactor, since the dynamic of the exothermic batch reactor is more complex than the continuous pickling process.

4.1 Continuous Steel Pickling Process

One of the country’s fundamental industries is the steel-processing industry, which has long existed and served the country’s steel demand. Though this industry is rather unique in the production point of view, the environmental standards used to control its effluent/emission in Thailand are the same as those specified for other industrial sectors. However, it is known that the part of this industry, which acts as the main waste generator is pickling activity. Hence, the need for control of steel pickling process is even more fundamental, because the pH of effluent streams must be regulated to protect aquatic and human welfare, and to comply with limits imposed by legislation. It is important to appreciate the diverse nature of the pH control application because it varies greatly in its degree of difficulty. For instance, pH control for some industrial processes can present a very difficult control problem, and indeed can be uncontrollable if the plant is inadequately designed. As stated earlier, the continuous steel pickling process presents the most challenging control problem due to highly nonlinear characteristics. Then, the pickling process design and construction is implemented, process modeling and control is further interpreted as referring to the continuous steel pickling process.

4.1.1 Process description

This section describes the production process for steel pickling process. Particular interest is on pickling stage, which consists of two major steps: pickling and rinsing. The former step is where the pickling effect takes place. Rust on the metal surface reacts with pickling acid, leaving the steel with clean surface. Then, drag-out pickling solution is removed from the metal surface using rinsing water in the rinsing step before the steel is sent to subsequent processes.

Pickling agents for iron and steel are mainly hydrochloric and sulfuric acids. There are pros and cons in using these acids, i.e. hydrochloric acid usually gives a better pickling activity, but they also can be vaporized more easily than sulfuric acid. However, hydrochloric acid (HCl) is more favorable for most of the factories in Thailand. Irreversible reaction between iron oxide and the acid is as follow:

$$FeO + 2\,HCl \rightarrow FeCl_2 + H_2O \qquad (4.1)$$

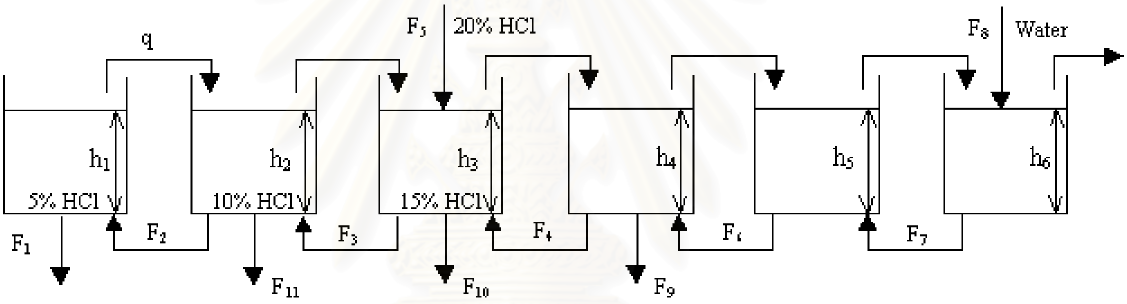

Figure 4.1 - Pickling process flow sheet.

Figure 4.1 is a process flow sheet of the pickling stage in the steel pickling process. The raw materials will be processed through pickling and rinsing step, respectively. In the pickling step, workpieces are immersed in the three pickling baths connected in series from low to high acid concentrations: 5%, 10% and 15% HCl, respectively. As the acid concentrations in the baths decrease, the spent acid in the pickling baths with the lowest concentration is discharged while the acid in the bath with higher concentration is pumped into the adjacent bath with lower acid concentration as shown in the figure 4.1. Fresh acid with 20% HCl is added directly into 15% HCl pickling bath to remain the concentration. In the rinsing step, a multistage counter-current rinse system is implemented; the moving direction of the workpieces is opposite to the rinse water flow as shown in process flow sheet.

Technically, the use of multiple cascade rinse tanks is very effective in reducing the volume of rinse water used. According to the study by Dahab et.al. (1994), the use of two counter-current rinsing baths could reduce the water consumption by approximately 83% comparing to single-stage rinse system. Furthermore, the use of three stage rinsing gains approximately 6.6% further reduction in water consumption from the system having two rinsing stages (Bureau of Industrial Environmental Technology, 1999).

Another way to diminish wastewater is return of rinsing concentrate into the pickling bath. This technique is beneficial in two ways: (1) the volume of wastewater from the rinsing step can be reduced in equivalent amount of the water used in the pickling bath, and (2) some of the acid drag-out is returned for being re-used in the pickling baths. Due to the difference in the rate of water consumption between the pickling and rinsing processes, a hold-up tank may be generally required to store the rinse water before being returned to the pickling bath. This rinse water is then mixed with fresh acid solution upon adding to the pickling bath. However, in the continuous control system, the rinse water can be returned directly to the pickling bath.

4.1.2 Mathematical modeling

Several key assumptions are made for the purposes of this study:

- The system is supposed to be perfectly mixed.
- All state variables are measured directly.
- Density is supposed to be constant.
- No the deterioration of pickling efficiency resulting by iron concentration exists in the reaction rate.
- The amount of drag in-out is assumed to be equal.

Mathematical modeling of continuous steel pickling process as presented in figure 4.1 can be derived under the assumptions above as follows:

Pickling step

$$A\frac{dh_1}{dt} = F_2 - F_1 - q \tag{4.2a}$$

$$A\frac{dh_2}{dt} = F_3 - F_2 - F_{11} \tag{4.2b}$$

$$A\frac{dh_3}{dt} = F_4 + F_5 - F_3 - F_{10} \tag{4.2c}$$

$$V_1 \frac{dC_1}{dt} = F_2 C_2 - C_1 (F_1 + q) - V_1 r_1 \tag{4.3a}$$

$$V_2 \frac{dC_2}{dt} = qC_1 + F_3 C_3 - C_2 (F_2 + F_{11} + q) - V_2 r_2 \tag{4.3b}$$

$$V_3 \frac{dC_3}{dt} = qC_2 + F_5 C_{20} + F_4 C_4 - C_3 (F_3 + F_{10} + q) - V_3 r_3 \tag{4.3c}$$

Rinsing step

$$A\frac{dh_4}{dt} = F_6 - F_4 - F_9 \tag{4.4a}$$

$$A\frac{dh_5}{dt} = F_7 - F_6 \tag{4.4b}$$

$$A\frac{dh_6}{dt} = F_8 - F_7 \tag{4.4c}$$

$$V_4 \frac{dC_4}{dt} = qC_3 + F_6 C_5 - C_4 (F_4 + F_9 + q) \tag{4.5a}$$

$$V_5 \frac{dC_5}{dt} = qC_4 + F_7 C_6 - C_5 (F_6 + q) \tag{4.5b}$$

$$V_6 \frac{dC_6}{dt} = qC_5 + F_8 C_w - C_6 (F_7 + q) \tag{4.5c}$$

To specify the absolutely mathematical modeling of this continuous process, the equation of the reaction rate in the pickling baths need to be imposed. As is illustrated in equation (4.1), the reaction is assumed to be first order regardless liquid diffusion and the deterioration of pickling efficiency resulted by excessive iron concentration. Therefore, the equation of the reaction rate studied here solely depends upon acid concentration in which it can be formulated as this following:

$$r = kC \tag{4.6}$$

Substituting the above equation into equation (4.3) by replacing r and C with the reaction rate and concentration of each bath.

It is important to show that the model can provide an accurate representation of the continuous steel pickling process before the project progresses to the control simulation. The reliability of the defined process model can be significantly enhanced if the model and pilot plant data provide the same manner. Laboratory process is described in Appendix B. The comparison of the actual and simulated performance operating under the same conditions are shown in figures 4.2 to 4.4. It is found that the first principle model of the pickling process provides closer responses to the experimental data in the pickling step than in the rinsing step. Note that in the last two rinsing tanks, the experimental and simulated data are different violently. This is because of (1) a result of miscalibration or failure of the measuring instrument such a pH-meter, and (2) unfeasibility of drag in-out equalization. However, dynamic data reconciliation (DDR) and robustness test of control strategy can deal these problems effectively. Hence, it seems reasonable to represent this process with the math model as listed in equations (4.2) through (4.5). In order to explore capability of DDR, hereafter an application of control strategy integrated with DDR should be interpreted as referring to the continuous steel pickling process.

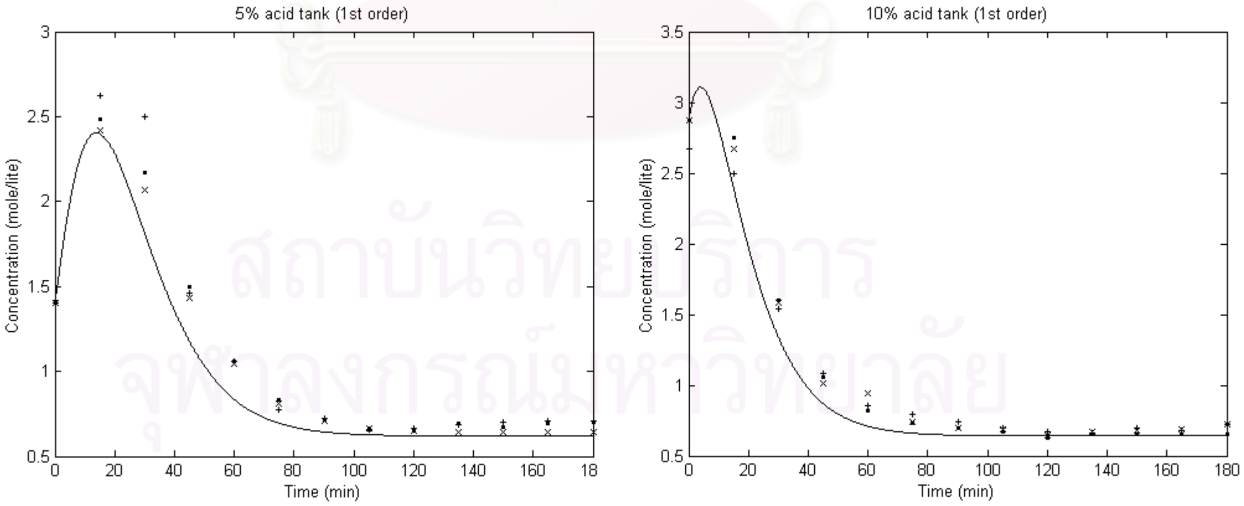

Figure 4.2 - Process performances of 5% (left) and 10% (right) acid tank

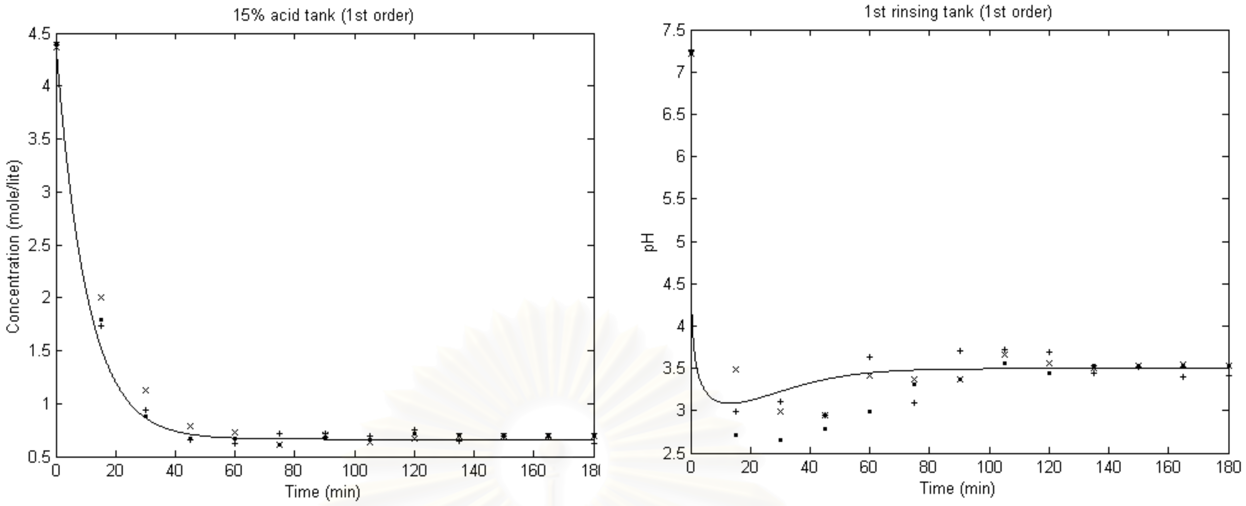

Figure 4.3 - Process performances of 15% acid (left) and 1st (right) ringing tank

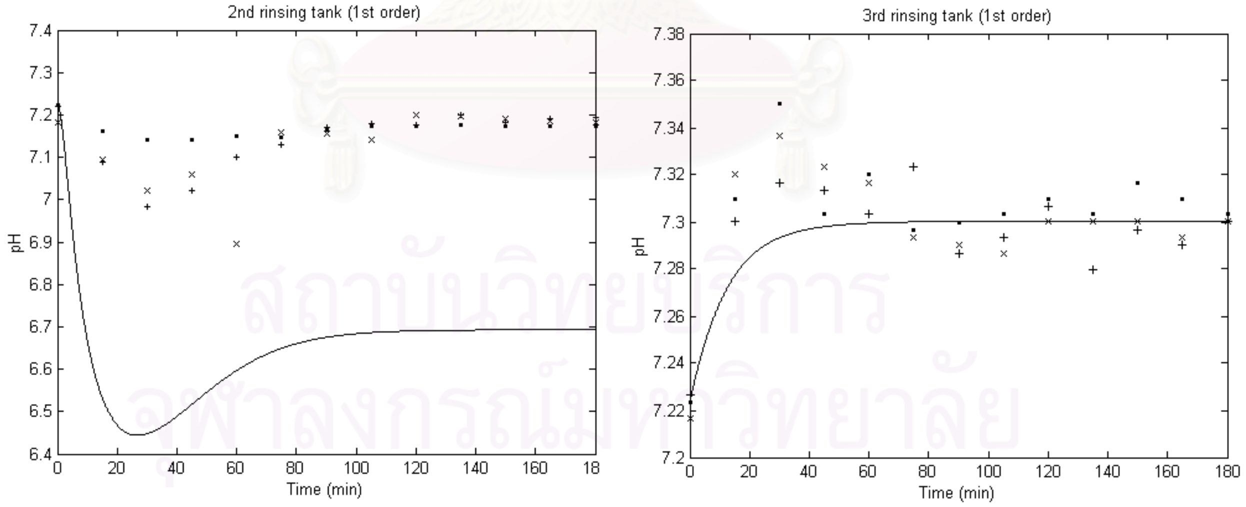

Figure 4.4 - Process performances of 2nd (left) and 3rd (right) rinsing tank

4.1.3 Control configuration

Generic Model Control (GMC) is a control algorithm capable of using nonlinear process model directly. In GMC, mostly, the first principle model derived from dynamic mass, energy and momentum balance is used. When the process is not perfectly known or corrupted by measurement noise, the unknown or noisy parts can be estimated and reconciled by dynamic data reconciliation (DDR).

In continuous steel pickling process, acid concentrations are assumed to be directly measured whereas reaction rates (r_1, r_2, r_3) are unmeasured. Hence, the process has six manipulated variables $(F_2, F_3, F_5, F_6, F_7, F_8)$, one disturbance variable (F_4) and up to six controlled variables $(C_1, C_2, C_3, C_4, C_5, C_6)$. In addition, only drag in-out content (q) is employed as uncertainty parameter. Process control configurations of pickling and rinsing step are shown in figures 4.5 (a) and 4.5 (b), respectively.

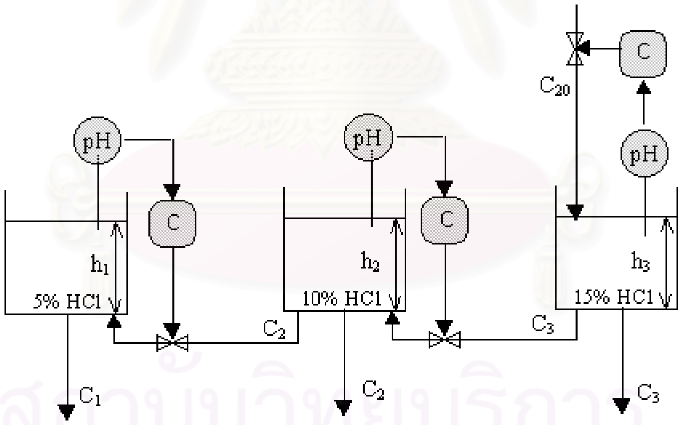

Figure 4.5 (a) - Flow diagram of pickling baths control

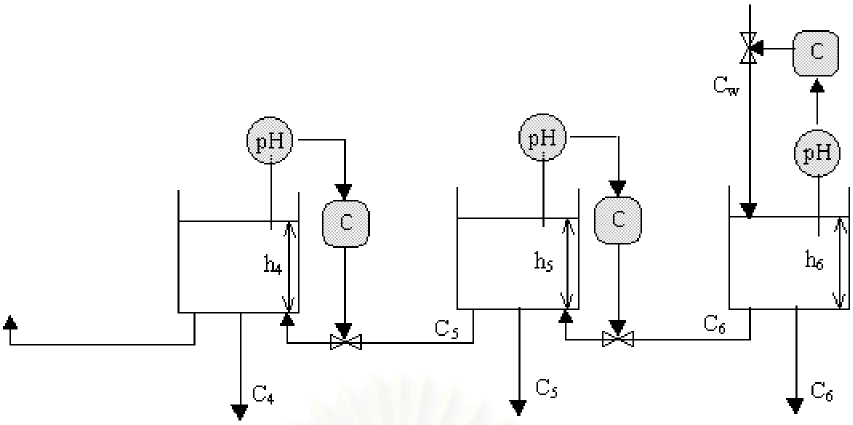

Figure 4.5 (b) - Flow diagram of rinsing baths control

Based on the general form of GMC control algorithm [equation (3.74)], six manipulated equations are finally rearranged in discrete form as shown below in equations (4.7) to (4.12).

$$F_2^{(k)} = \frac{V}{\left(C_2^{(k)} - C_1^{(k)}\right)}\left[K_1^1\left(C_{1,sp} - C_1^{(k)}\right) + \sum_{k=0}^{k} K_1^2 \Delta t\left(C_{1,sp} - C_1^{(k)}\right) + r_1\right] \tag{4.7}$$

$$F_3^{(k)} = \frac{V}{\left(C_3^{(k)} - C_2^{(k)}\right)}\left[K_2^1\left(C_{2,sp} - C_2^{(k)}\right) + \sum_{k=0}^{k} K_2^2 \Delta t\left(C_{2,sp} - C_2^{(k)}\right) - \frac{q}{V}\left(C_1^{(k)} - C_2^{(k)}\right) + r_2\right] \tag{4.8}$$

$$F_5^{(k)} = \frac{V}{\left(C_{20} - C_3^{(k)}\right)}\left[K_3^1\left(C_{3,sp} - C_3^{(k)}\right) + \sum_{k=0}^{k} K_3^2\left(C_{3,sp} - C_3^{(k)}\right)\right]$$

$$- \frac{V}{\left(C_{20} - C_3^{(k)}\right)}\left[\frac{F_4}{V}\left(C_4^{(k)} - C_3^{(k)}\right) + \frac{q}{V}\left(C_2^{(k)} - C_3^{(k)}\right) - r_3\right] \tag{4.9}$$

$$F_6^{(k)} = \frac{V}{\left(C_5^{(k)} - C_4^{(k)}\right)}\left[K_4^1\left(C_{4,sp} - C_4^{(k)}\right) + \sum_{k=0}^{k} K_4^2 \Delta t\left(C_{4,sp} - C_4^{(k)}\right) - \frac{q}{V}\left(C_3^{(k)} - C_4^{(k)}\right)\right] \tag{4.10}$$

$$F_7^{(k)} = \frac{V}{\left(C_6^{(k)} - C_5^{(k)}\right)}\left[K_5^1\left(C_{5,sp} - C_5^{(k)}\right) + \sum_{k=0}^{k} K_5^2 \Delta t\left(C_{5,sp} - C_5^{(k)}\right) - \frac{q}{V}\left(C_4^{(k)} - C_5^{(k)}\right)\right] \tag{4.11}$$

$$F_8^{(k)} = \frac{V}{\left(C_w - C_6^{(k)}\right)}\left[K_6^1\left(C_{6,sp} - C_6^{(k)}\right) + \sum_{k=0}^{k} K_6^2 \Delta t\left(C_{6,sp} - C_6^{(k)}\right) - \frac{q}{V}\left(C_5^{(k)} - C_6^{(k)}\right)\right] \quad (4.12)$$

where Δt = the sampling time of the controller

Figure 4.6 is diagram of the estimation. The unknown reaction rates and uncertainty drag in-out content are estimated which relied upon the reconciled concentrations. Control action is calculated further by GMC controller relied upon these estimated and reconciled information.

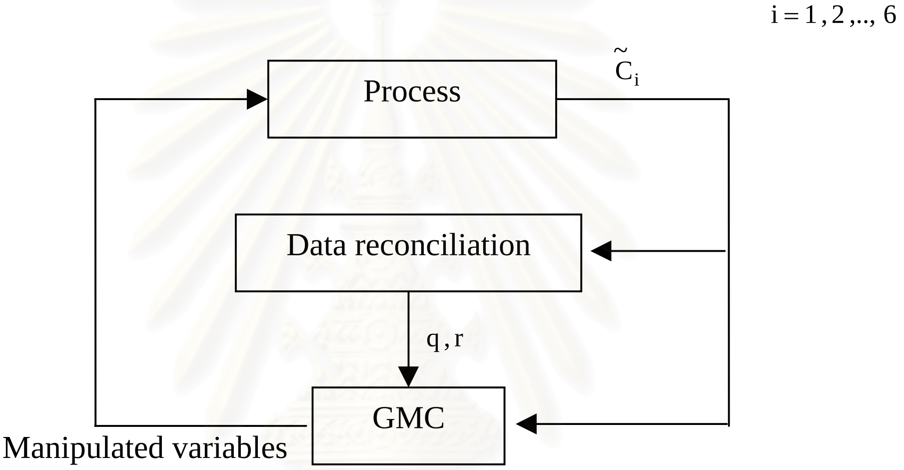

Figure 4.6 –Estimation diagram for the steel pickling process

The physical constants for the model, which are not dependent on the operating conditions, and the appropriate values of GMC tuning parameters are shown in Table 4.1 and 4.2, respectively.

Table 4.1. Physical parameters

q = 0.0005 liter/min A = 0.0729 m^2 V = 14.945 liter	rate constant (k) = 0.003267 C_{20} = 6.034 mole/liter C_w = 5e-008 mole/liter

Table 4.2 Tuning parameters of GMC

Bath	Concentration tuning parameters	
5% HCl	K_1^1	K_1^2
	1.37143	0.05224
10% HCl	K_2^1	K_2^2
	1.2	0.04
15% HCl	K_3^1	K_3^2
	0.274	0.075077
Rinsing 1	K_4^1	K_4^2
	0.05	0.00000625
Rinsing 2	K_5^1	K_5^2
	0.96	0.0256
Rinsing 3	K_6^1	K_6^2
	0.274	0.075077

4.1.4 Simulation results

The concentration measurements of pickling and rinsing baths are simulated with measurement error standard deviation of 1% of the initial values. In this example, DDR algorithm is employed to obtain reconciled estimates of all measured concentrations and to estimate unmeasured reaction rates. After that, GMC controller calculates control action relied upon this reconciled and estimated information. The process simulation is initialized at a steady state operating point as listed in Table 4.3 and 4.4. The ability to handle strong non-linearity of GMC integrated with DDR is discussed in nominal case. In addition, simulation studies are also performed further to analyze the control algorithm with respect to the effects of model and parameter mismatch, and step change of disturbance variable.

Table 4.3. Initial values of concentrations

C_1^0 = 1.4 mole/liter	C_4^0 = 5.979e-008 mole/liter
C_2^0 = 2.87 mole/liter	C_5^0 = 5.979e-008 mole/liter
C_3^0 = 4.408 mole/liter	C_6^0 = 5.979e-008 mole/liter

Table 4.4. Initial values of flow rates

F_1^0 = 0.1445 liter/min	F_7^0 = 1.25 liter/min
F_2^0 = 0.145 liter/min	F_8^0 = 1.25 liter/min
F_3^0 = 0.145 liter/min	F_9^0 = 1.25 liter/min
F_4^0 = 0 liter/min	F_{10}^0 = 0 liter/min
F_5^0 = 0.145 liter/min	F_{11}^0 = 0 liter/min
F_6^0 = 1.25 liter/min	

4.1.4.1 Set point regulation

In this case, a key feature is to remain acid concentrations of pickling baths at 1.4, 2.87 and 4.408 mole per liter, respectively and to handle pH values of individual rinsing bath at desired target; 3, 6.5 and 7.3, respectively.

Table 4.5 IAE and ISE of acid concentrations in pickling baths

Case	$C_{5\%}$		$C_{10\%}$		$C_{15\%}$	
	IAE	ISE	IAE	ISE	IAE	ISE
Nominal	4.479	0.083	7.008	0.209	16.463	1.039
+30% drag	4.647	0.105	7.001	0.215	13.008	0.665
-30%k	4.793	0.099	6.668	0.205	16.677	1.145
Disturbance	4.506	0.085	7.386	0.237	14.446	0.842

Table 4.6 IAE and ISE of acid concentrations in rinsing baths

Case	C_1		C_2		C_3	
	IAE	ISE ($\times 10^{-6}$)	IAE ($\times 10^{-5}$)	ISE ($\times 10^{-12}$)	IAE ($\times 10^{-6}$)	ISE ($\times 10^{-14}$)
Nominal	0.017	7.243	2.123	1.838	1.676	1.577
+30% drag	0.015	5.561	2.048	1.632	1.917	1.739
-30%k	0.017	7.337	2.121	1.845	1.691	1.586
Disturbance	0.017	7.270	2.123	1.841	1.699	1.579

Table 4.7 IAE and ISE of estimated reaction rates

Case	r_1		r_2		r_3	
	IAE	ISE	IAE	ISE	IAE	ISE
Nominal	10.546	0.417	10.683	0.419	10.632	0.416
+30% drag	10.881	0.442	10.542	0.425	10.266	0.397
-30%k	10.777	0.430	10.303	0.401	10.676	0.428
Disturbance	10.900	0.447	10.546	0.416	10.306	0.401

Nominal case

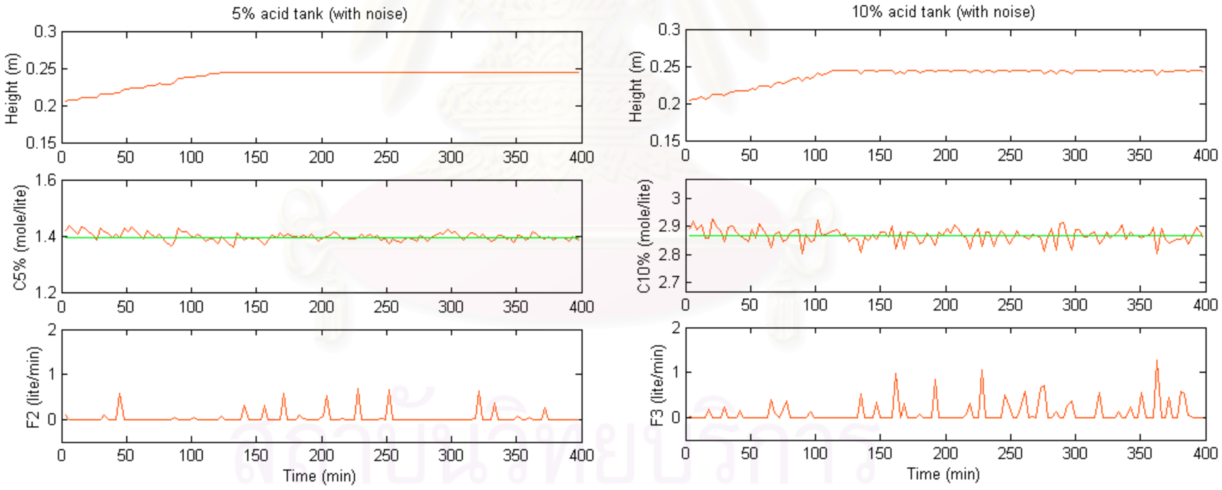

Figure 4.7 – Responses of 5% (left) and 10% (right) acid tank in nominal case

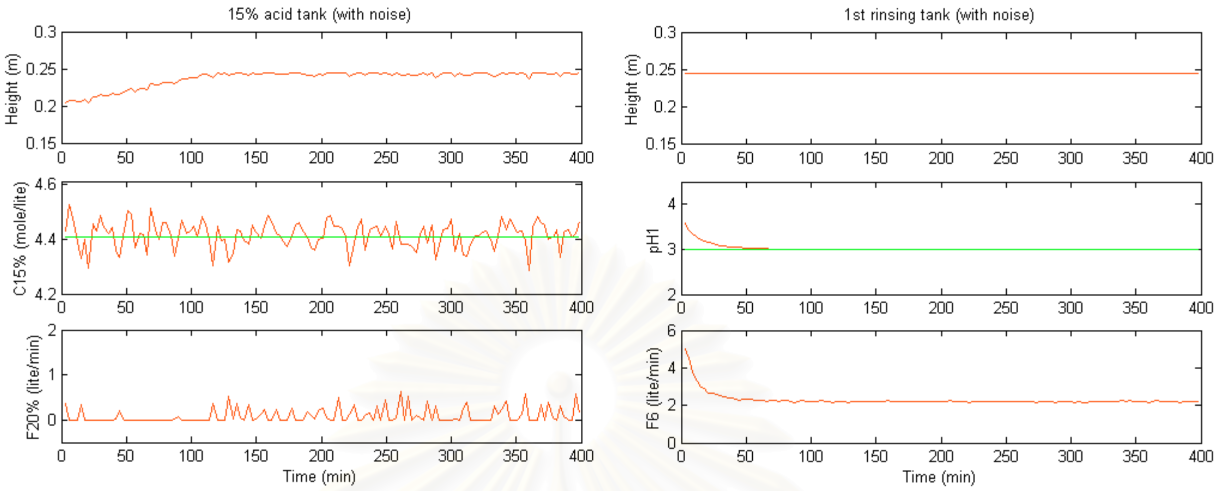

Figure 4.8 – Responses of 15% acid (left) and 1st rinsing (right) tank in nominal case

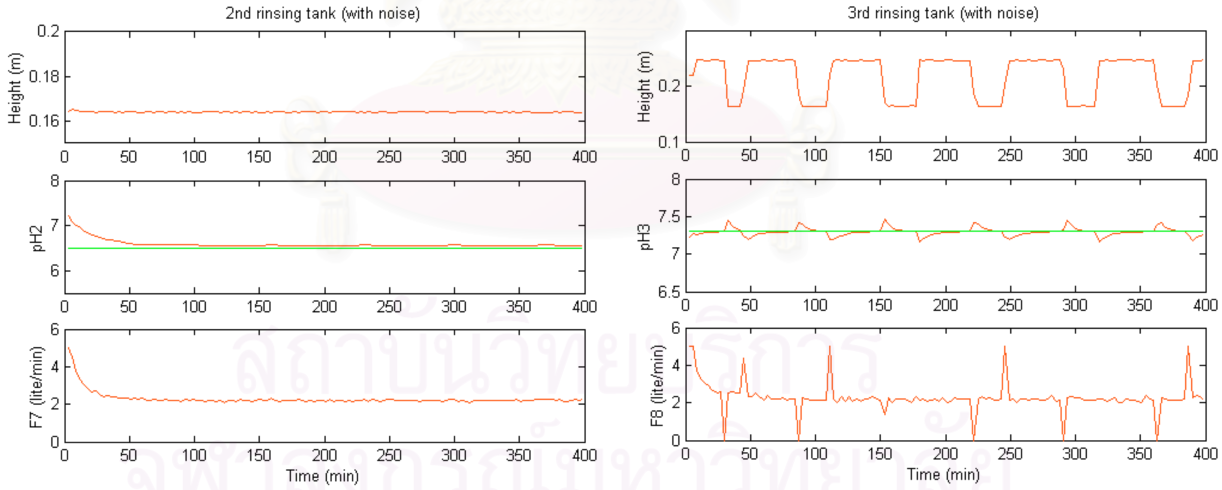

Figure 4.9 – Responses of 2nd (left) and 3rd (right) rinsing tank in nominal case

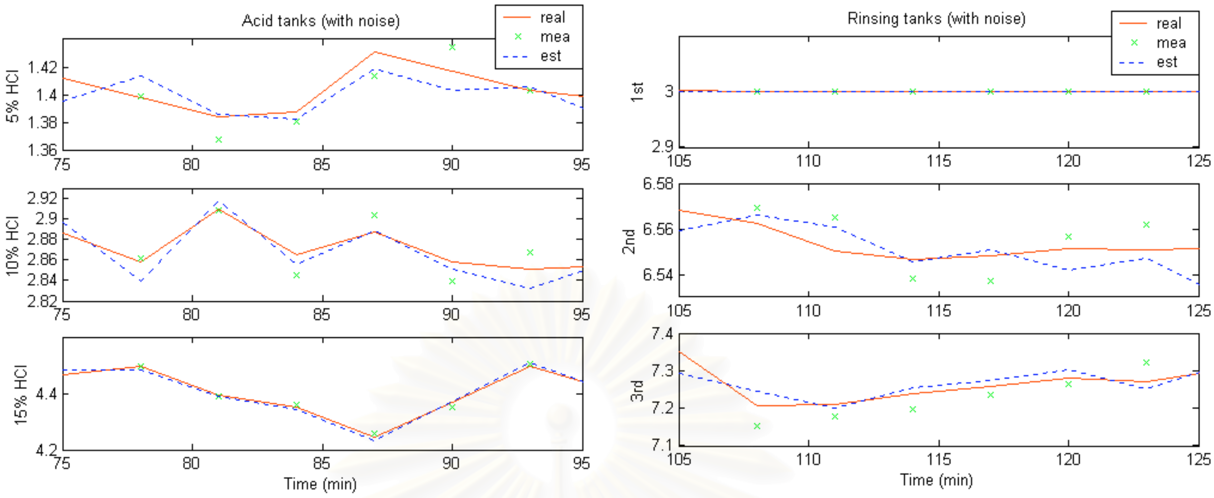

Figure 4.10 – Reconciliation of acid concentrations in nominal case

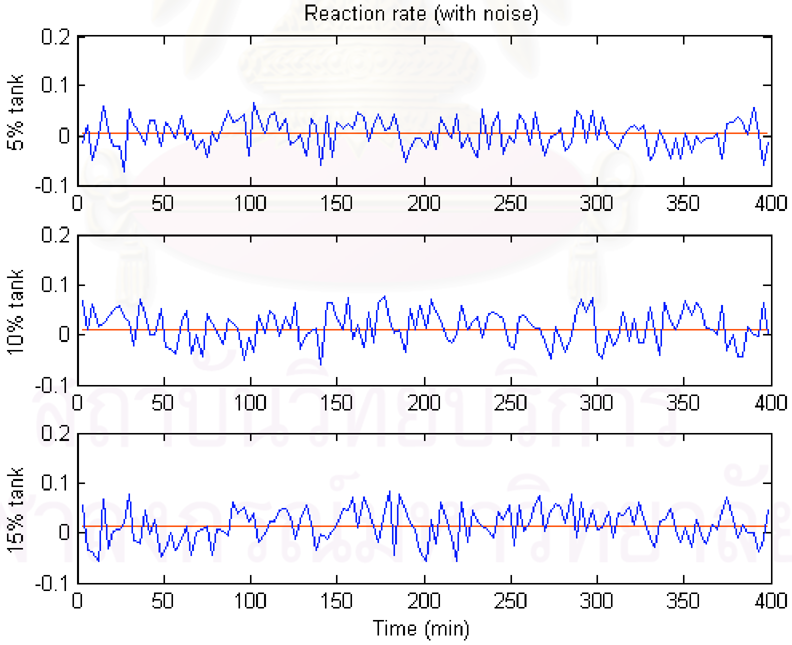

Figure 4.11 – Estimation of reaction rates in nominal case

+30% Drag in-out

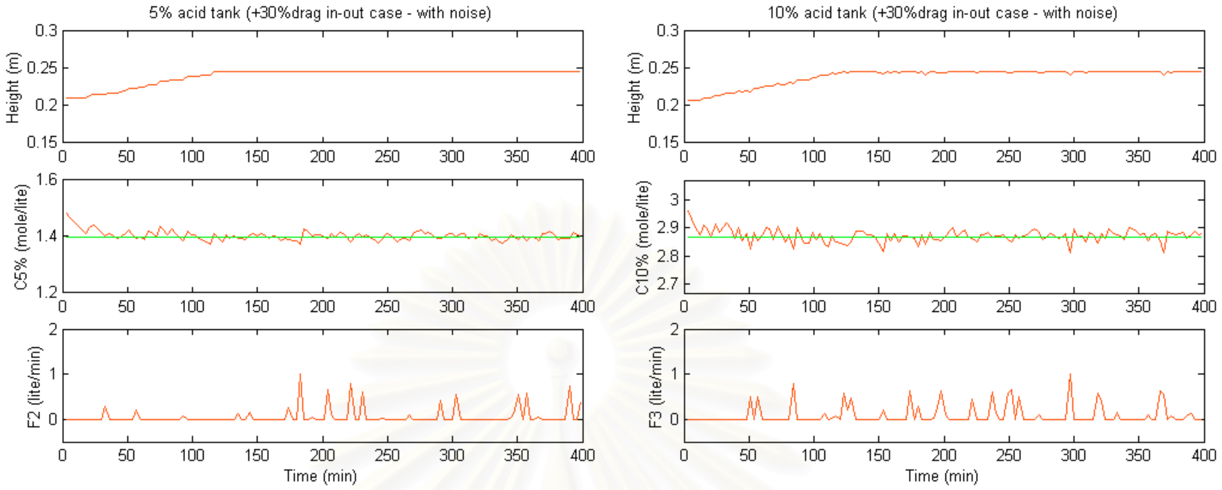

Figure 4.12 – Responses of 5% (left) and 10% (right) acid tank

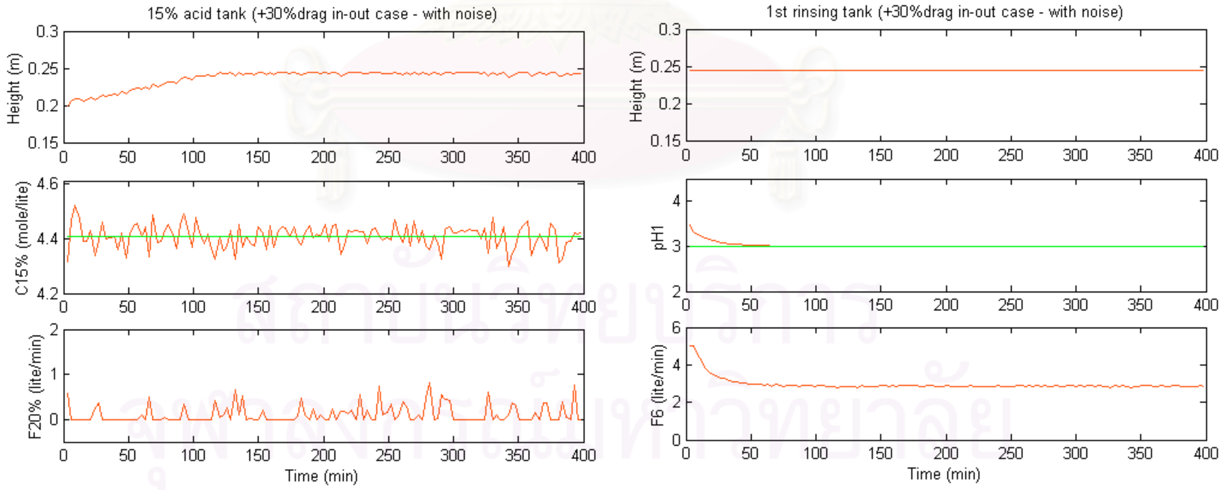

Figure 4.13 – Responses of 15% acid (left) and 1st rinsing (right) tank

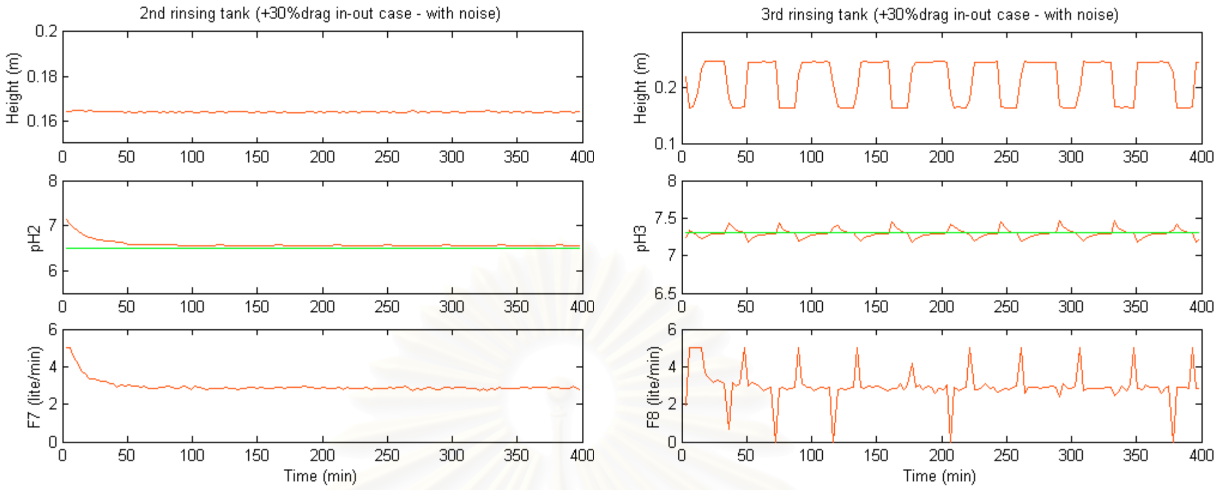

Figure 4.14 – Responses of 2nd (left) and 3rd (right) rinsing tank

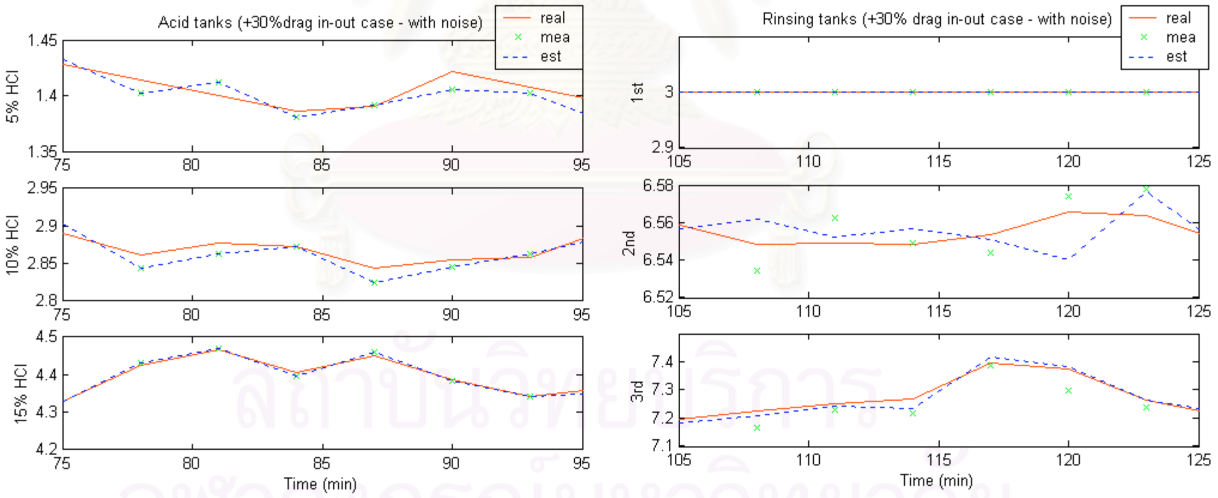

Figure 4.15 – Reconciliation of acid concentrations in +30% drag in-out case

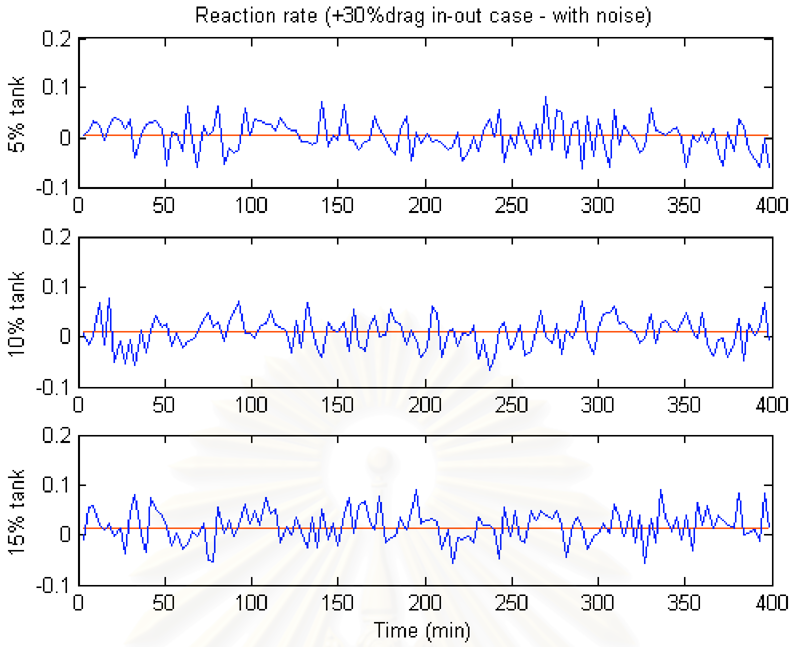

Figure 4.16 – Estimation of reaction rates in +30% drag in-out case

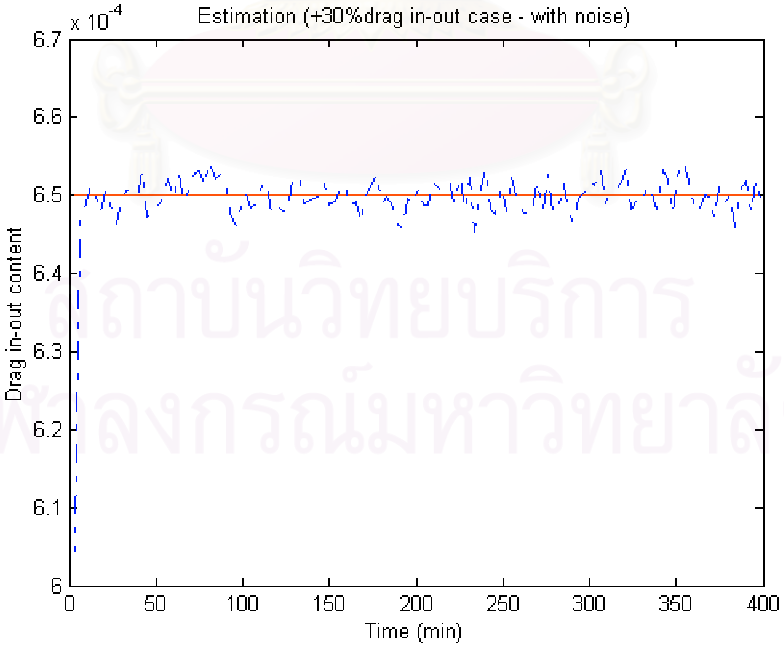

Figure 4.17 – Estimation of drag in-out content in +30% drag in-out case

-30% Reaction rate

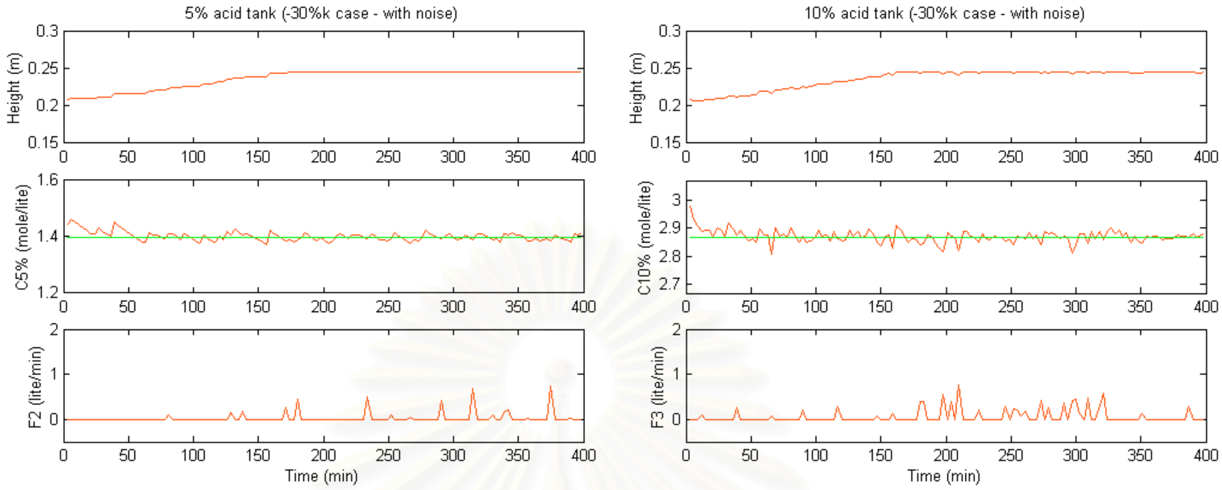

Figure 4.18 – Responses of 5% (left) and 10% (right) acid tank

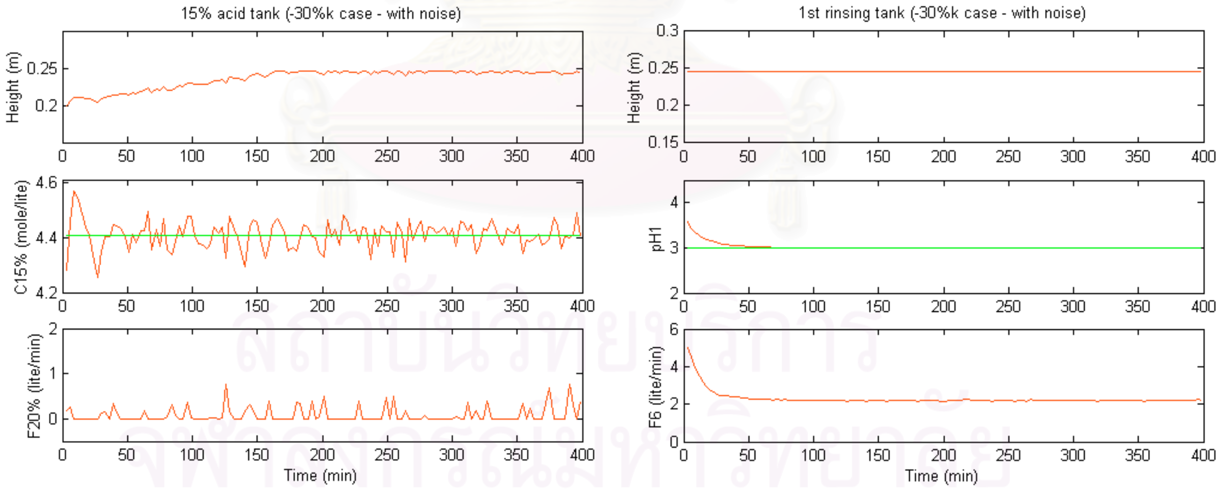

Figure 4.19 – Responses of 15% acid (left) and 1st rinsing (right) tank

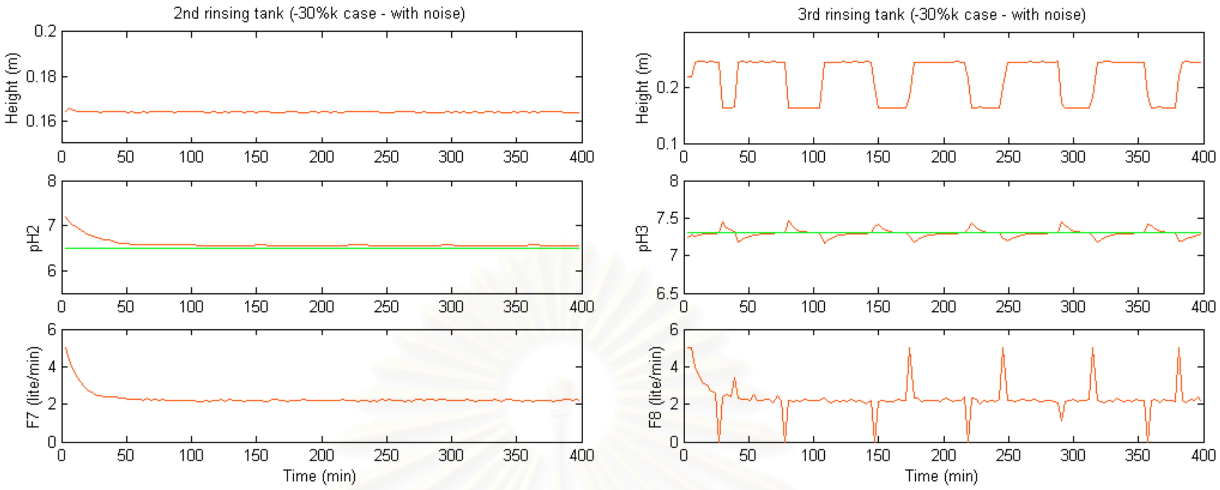

Figure 4.20 – Responses of 2nd (left) and 3rd (right) rinsing tank

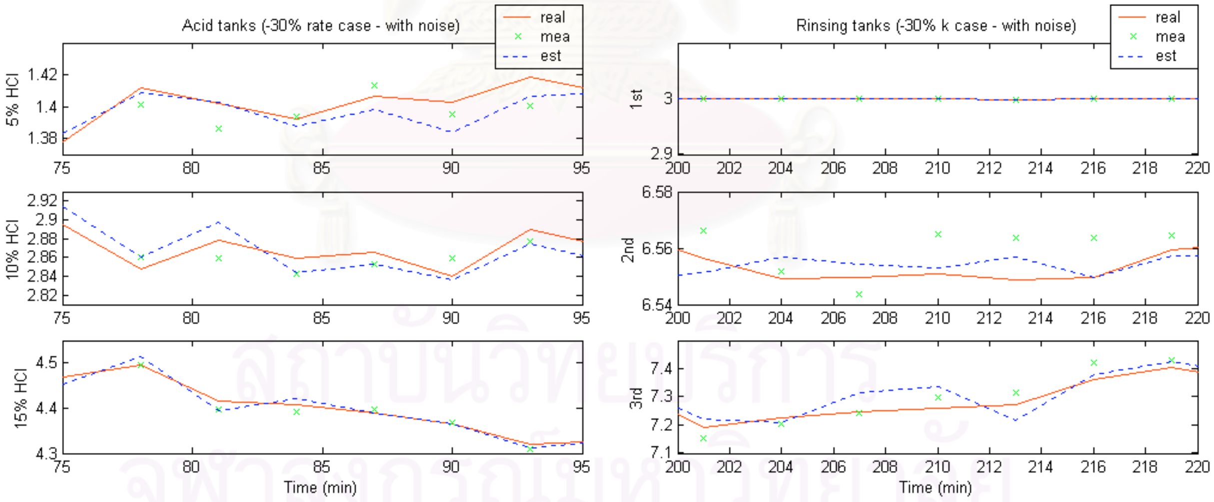

Figure 4.21 – Reconciliation of acid concentrations in -30% reaction rate case

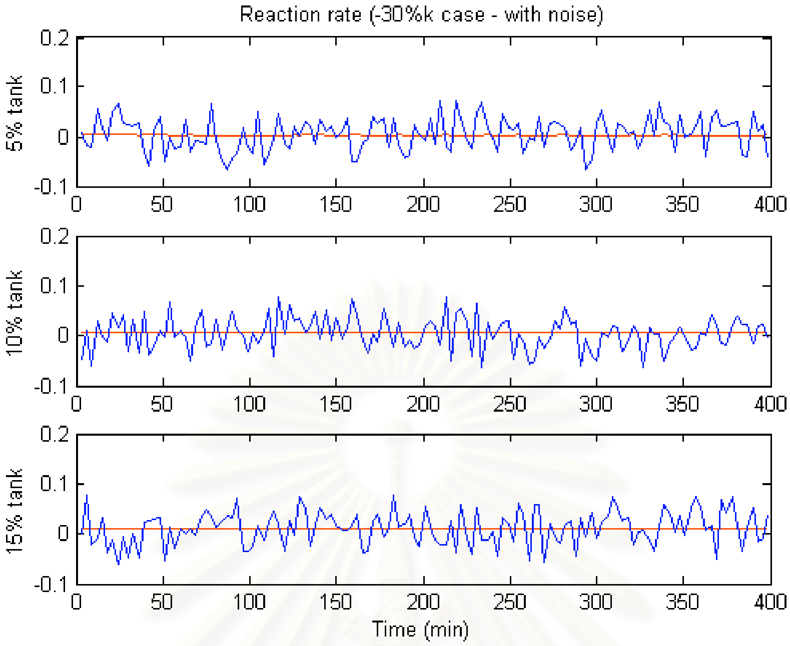

Figure 4.22 – Estimation of reaction rate in –30% reaction rate case

Disturbance case

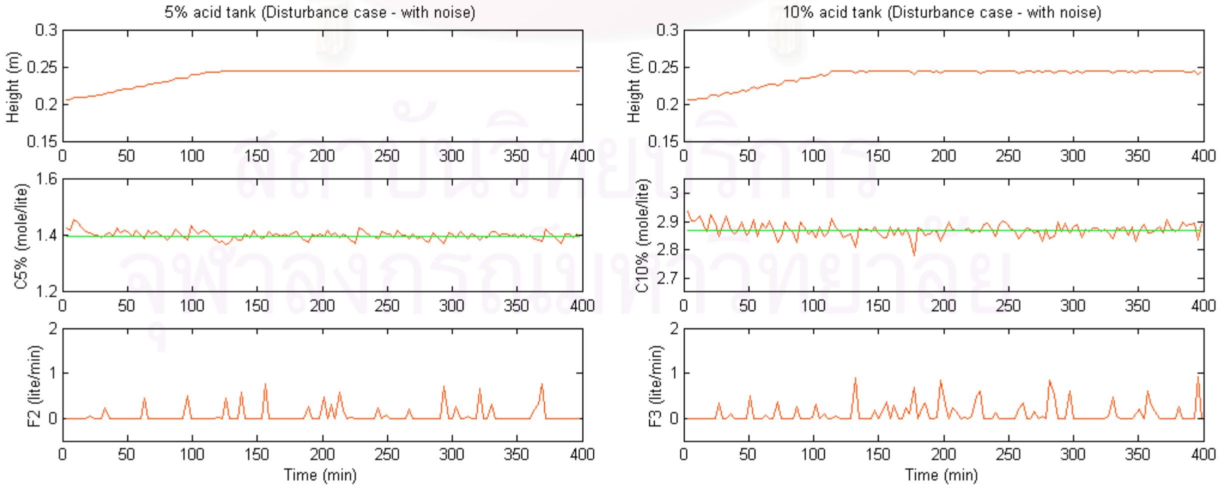

Figure 4.23 – Responses of 5% (left) and 10% (right) acid tank

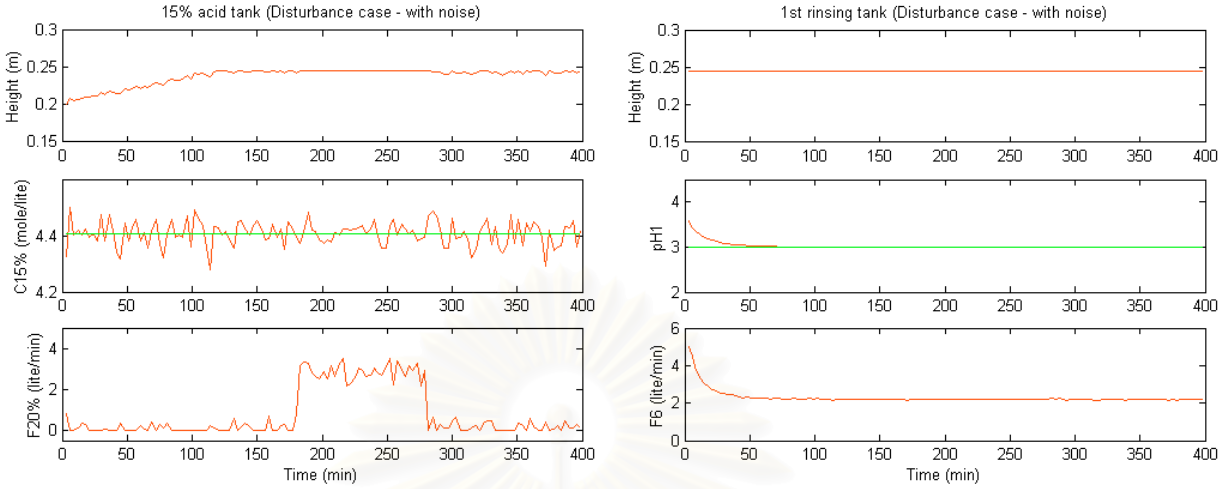

Figure 4.24 – Responses of 15% acid (left) and 1st rinsing (right) tank

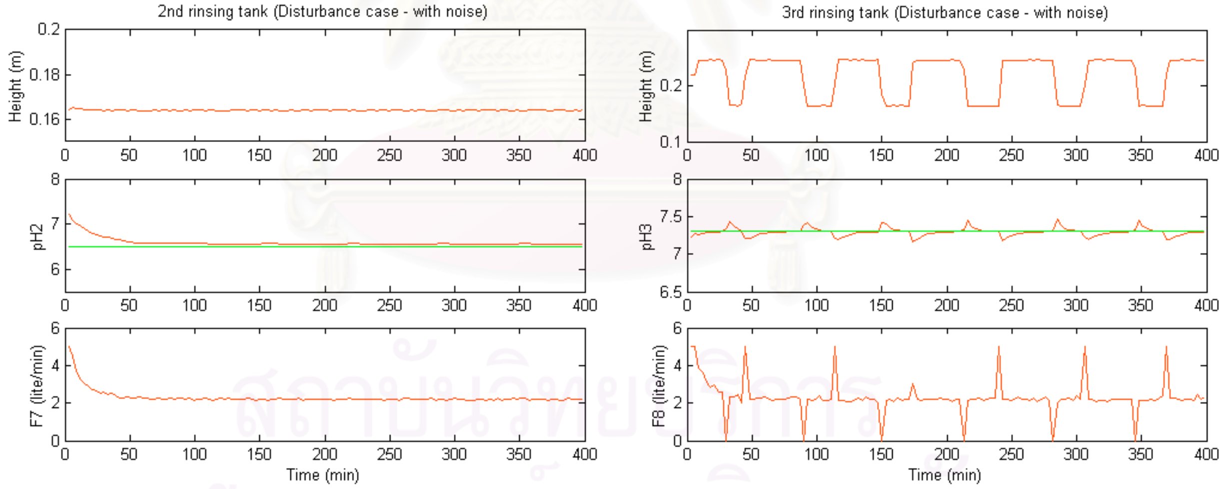

Figure 4.25 – Responses of 2nd (left) and 3rd (right) rinsing tank

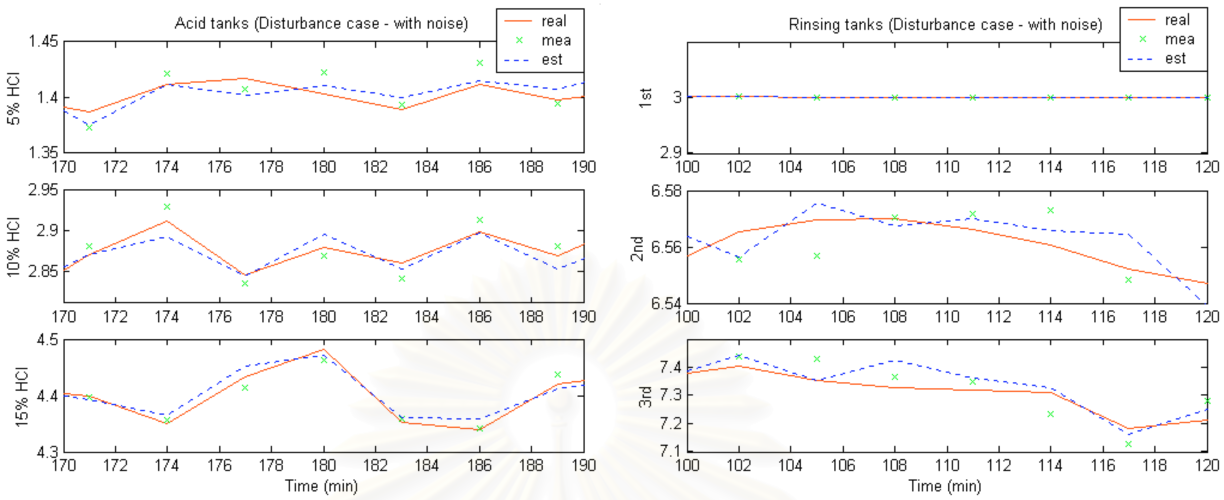

Figure 4.26 – Reconciliation of acid concentration in disturbance case

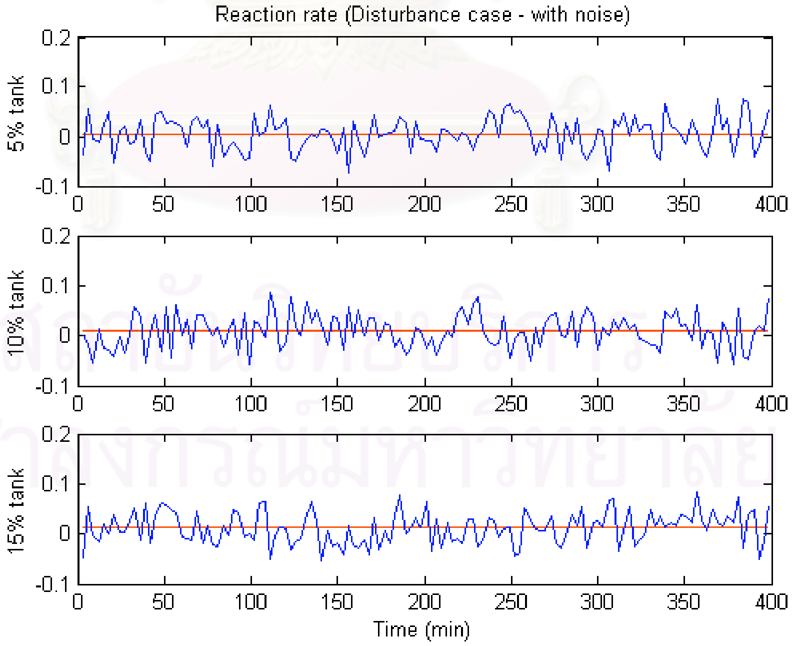

Figure 4.27 – Estimation of reaction rates in disturbance case

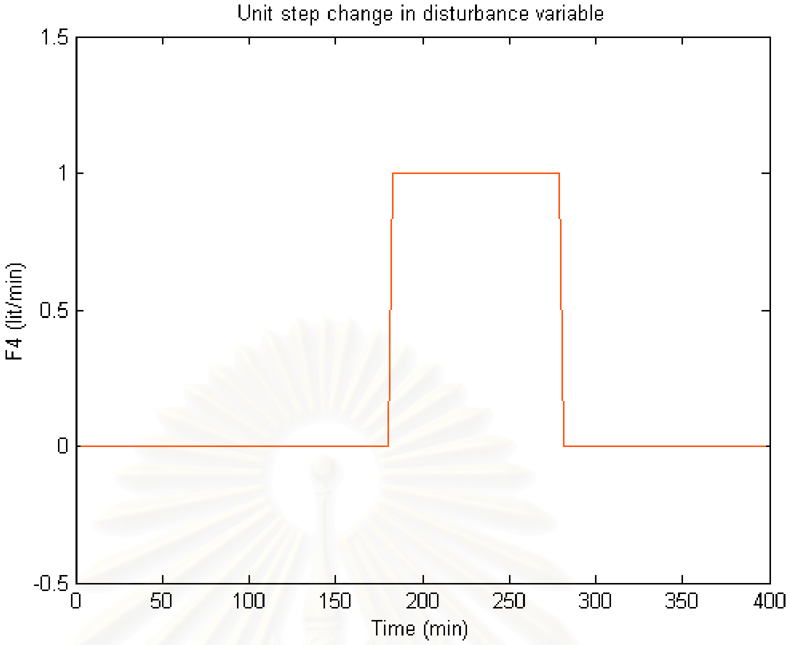

Figure 4.28 – Unit step change in disturbance variable (F_4)

4.1.4.2 Set point tracking

Set point tracking performances of GMC integrated with DDR are tested where set point values of the pickling baths are stepped from the reference values to 1.2, 2.5 and 4, respectively at time step 200 min.

Table 4.8 IAE and ISE of acid concentrations in pickling baths

Case	$C_{5\%}$		$C_{10\%}$		$C_{15\%}$	
	IAE	ISE	IAE	ISE	IAE	ISE
Nominal	12.438	1.003	17.752	2.238	29.494	5.484
+30%drag	12.825	1.056	21.776	3.416	26.958	5.179
-30%k	15.88	1.456	25.308	4.112	35.095	7.839
Disturbance	11.620	0.886	19.656	2.846	17.289	1.507

Table 4.9 IAE and ISE of acid concentrations in rinsing baths

Case	C_1		C_2		C_3	
	IAE	ISE ($\times10^{-6}$)	IAE ($\times10^{-5}$)	ISE ($\times10^{-12}$)	IAE ($\times10^{-6}$)	ISE ($\times10^{-14}$)
Nominal	0.017	7.223	1.711	1.625	1.608	1.487
+30%drag	0.015	5.540	1.585	1.403	1.855	1.679
-30%k	0.017	7.222	1.674	1.619	1.605	1.484
Disturbance	0.017	7.314	1.667	1.608	1.776	1.679

Table 4.10 IAE and ISE of estimated reaction rates

Case	r_1		r_2		r_3	
	IAE	ISE	IAE	ISE	IAE	ISE
Nominal	10.522	0.426	10.943	0.443	11.057	0.453
+30%drag	10.462	0.412	11.112	0.467	10.663	0.433
-30%k	10.772	0.429	10.702	0.432	10.378	0.405
Disturbance	10.696	0.425	10.500	0.408	10.656	0.418

<u>Nominal case</u>

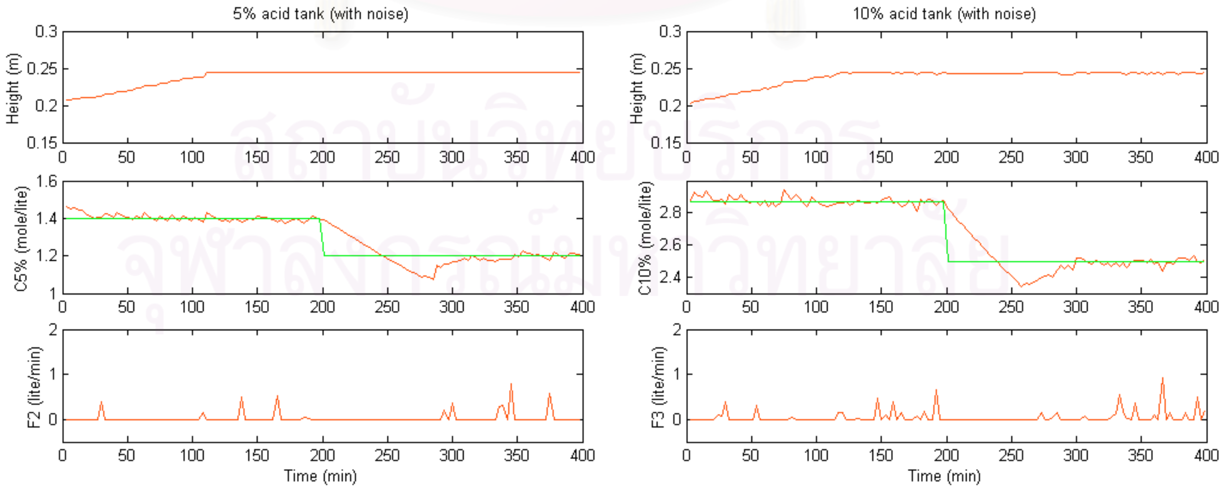

Figure 4.29 – Responses of 5% (left) and 10% (right) acid tank in nominal case

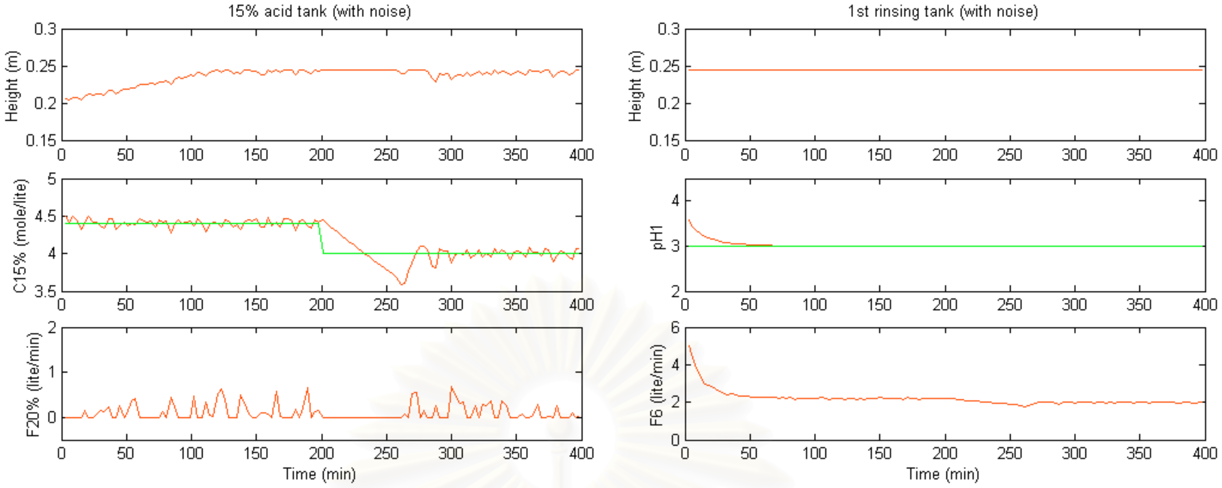

Figure 4.30 – Responses of 15% acid (left) and 1st rinsing (right) tank in nominal case

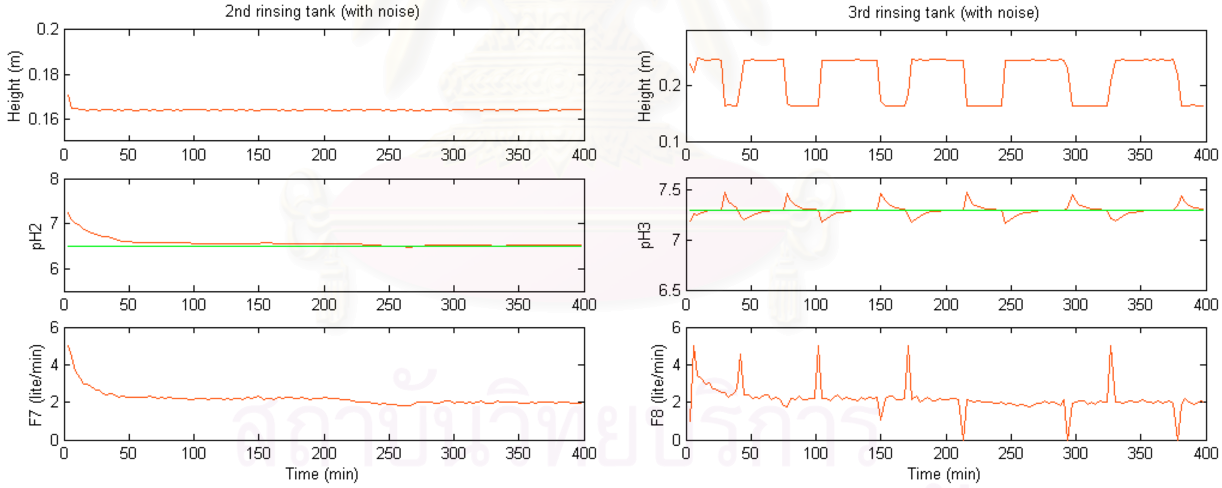

Figure 4.31 – Responses of 2nd (left) and 3rd (right) rinsing tank in nominal case

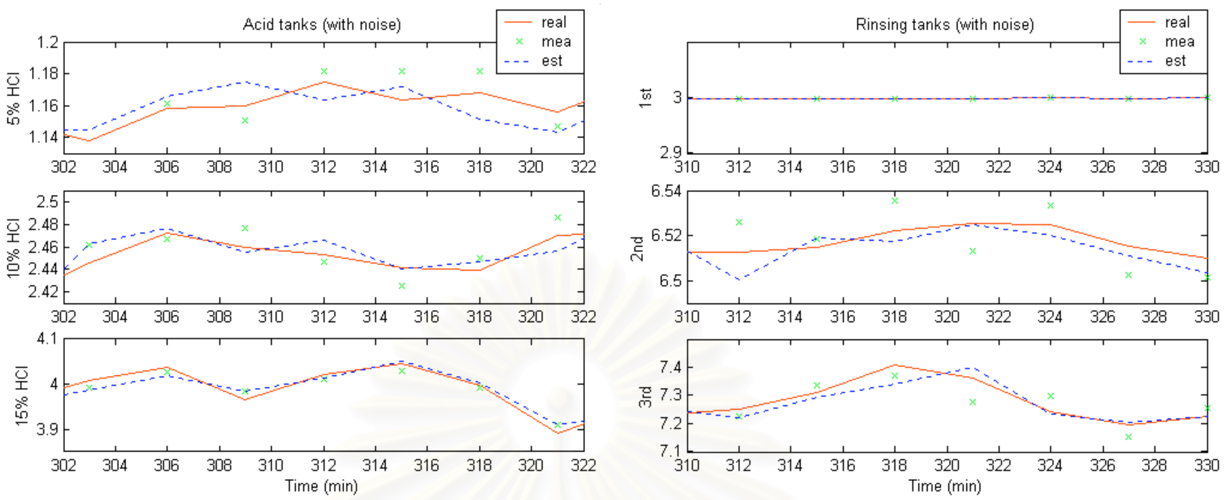

Figure 4.32 – Reconciliation of acid concentrations in nominal case

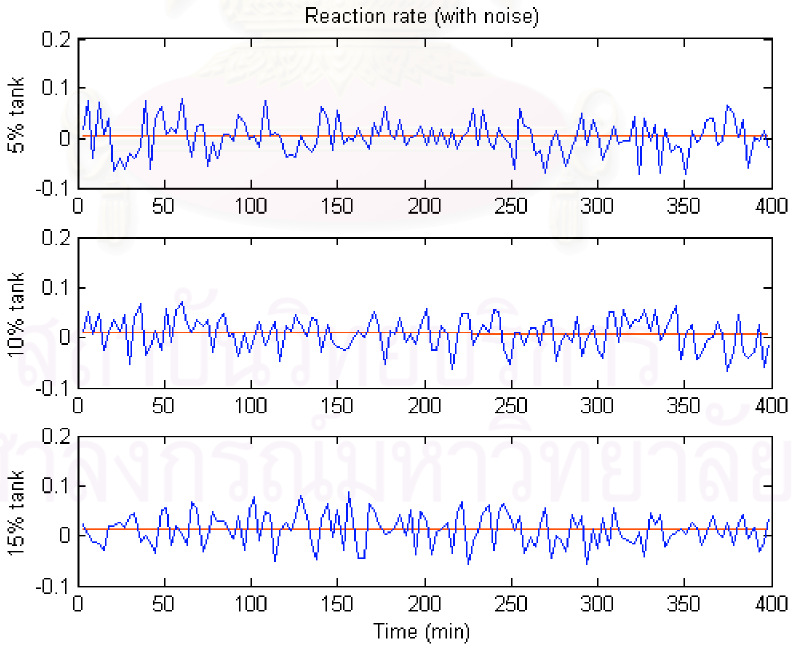

Figure 4.33 – Estimation of reaction rates in nominal case

+30% Drag in-out

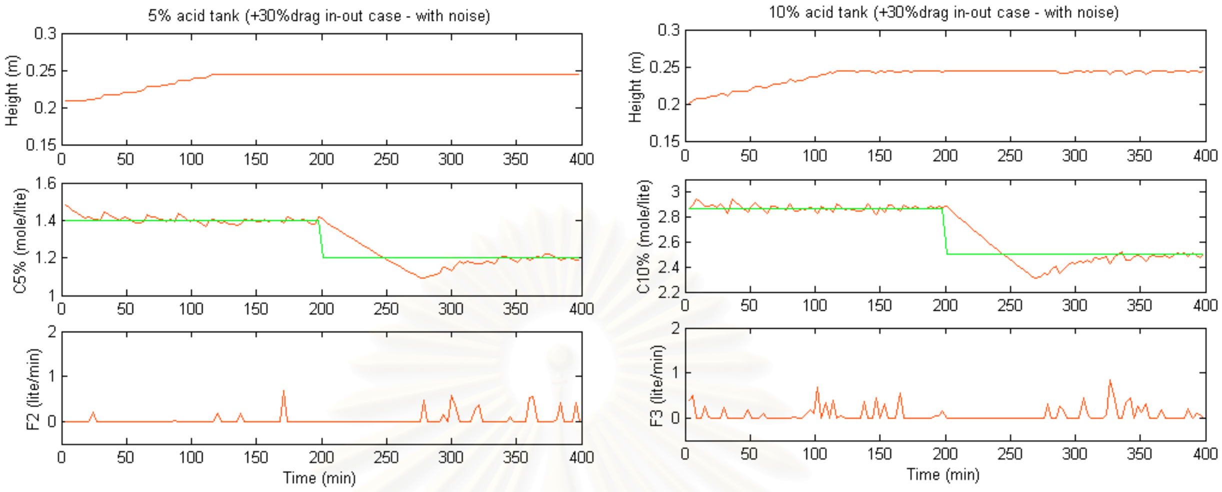

Figure 4.34 – Responses of 5% (left) and 10% (right) acid tank

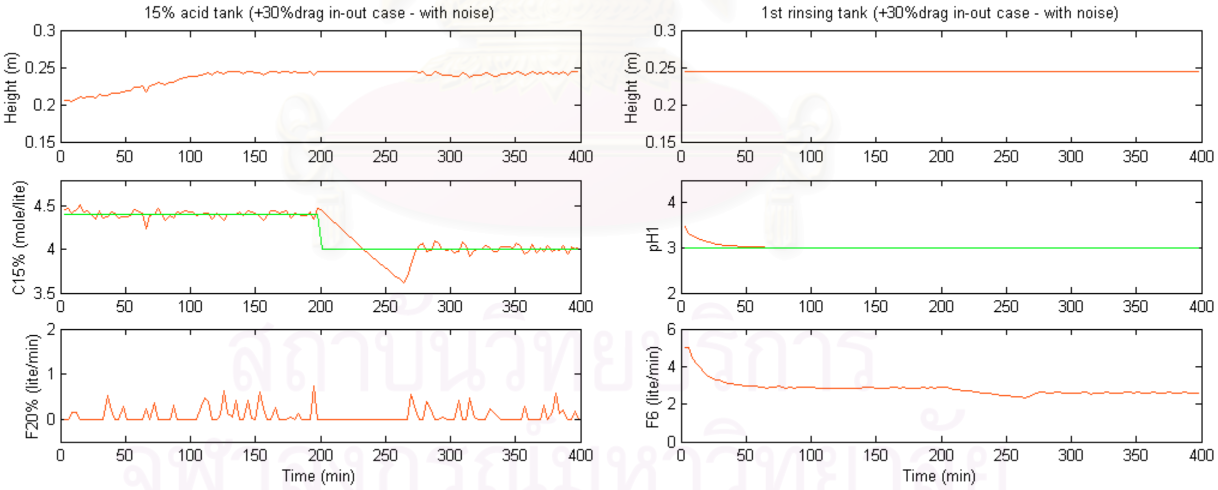

Figure 4.35 – Responses of 15% acid (left) and 1st rinsing (right) tank

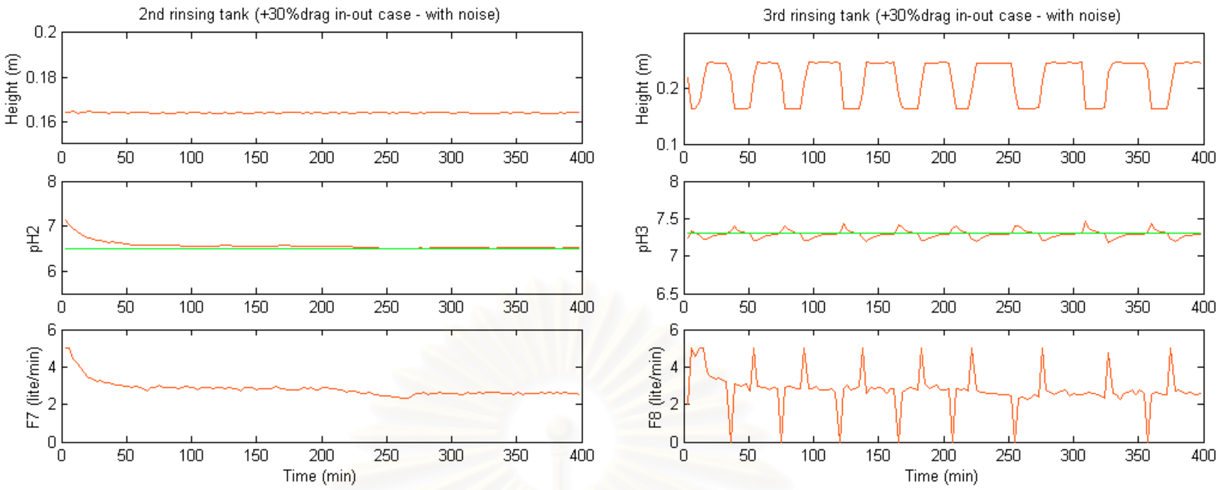

Figure 4.36 – Responses of 2nd (left) and 3rd (right) rinsing tank

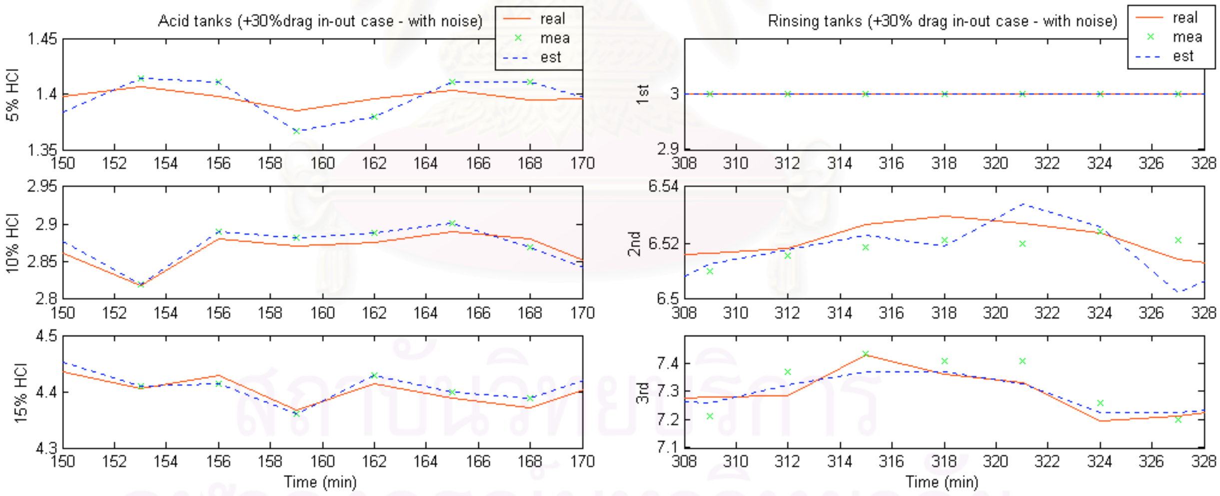

Figure 4.37 – Reconciliation of acid concentrations in +30% drag in-out case

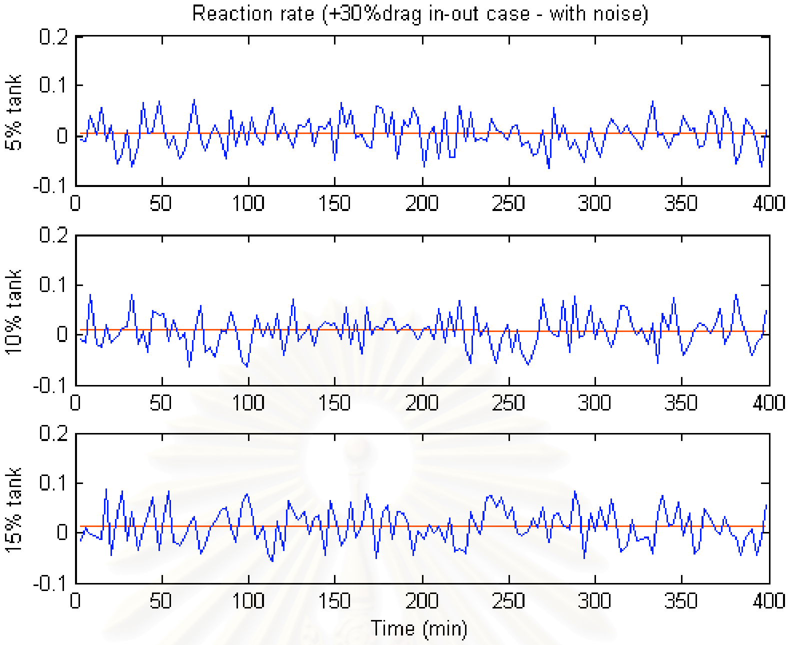

Figure 4.38 – Estimation of reaction rates in +30% drag in-out case

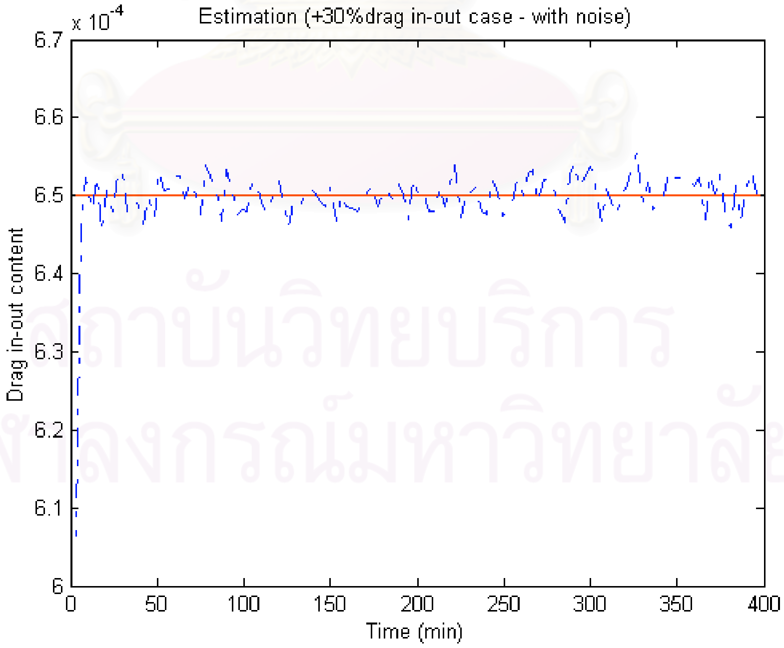

Figure 4.39 – Estimation of drag in-out content in +30% drag in-out case

-30% Reaction rate

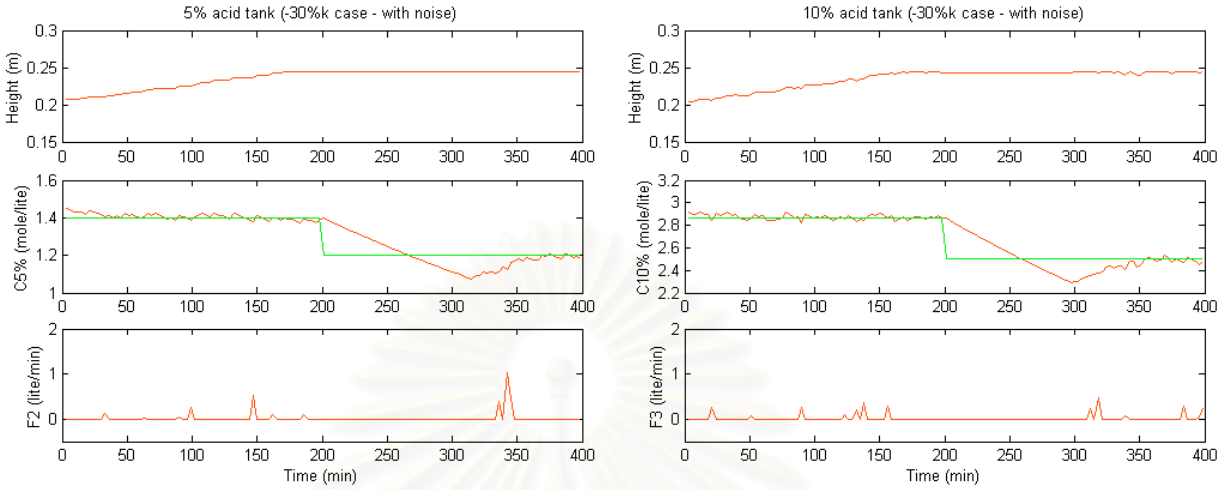

Figure 4.40 – Responses of 5% (left) and 10% (right) acid tank

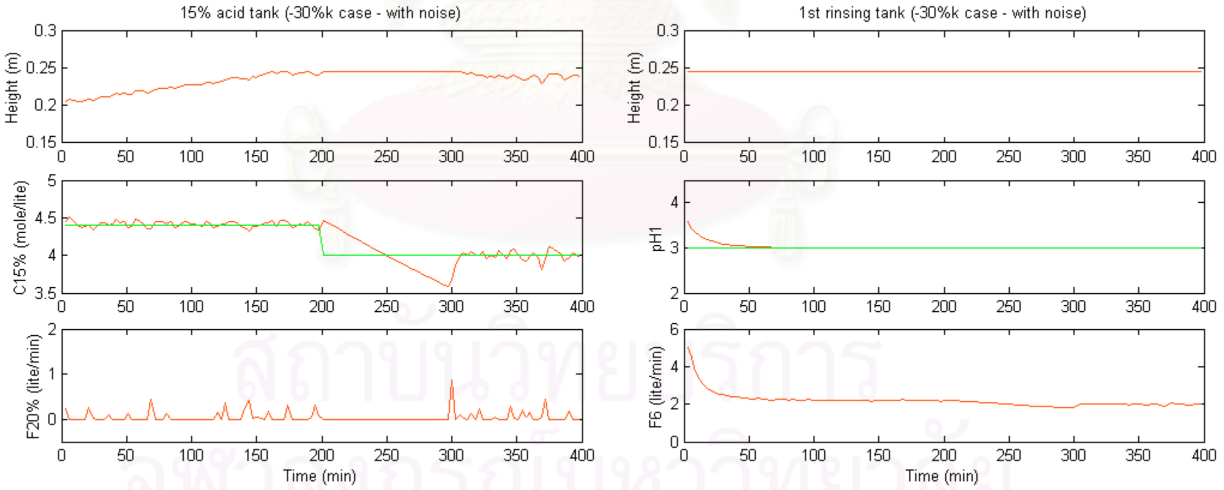

Figure 4.41 – Responses of 15% acid (left) and 1st rinsing (right) tank

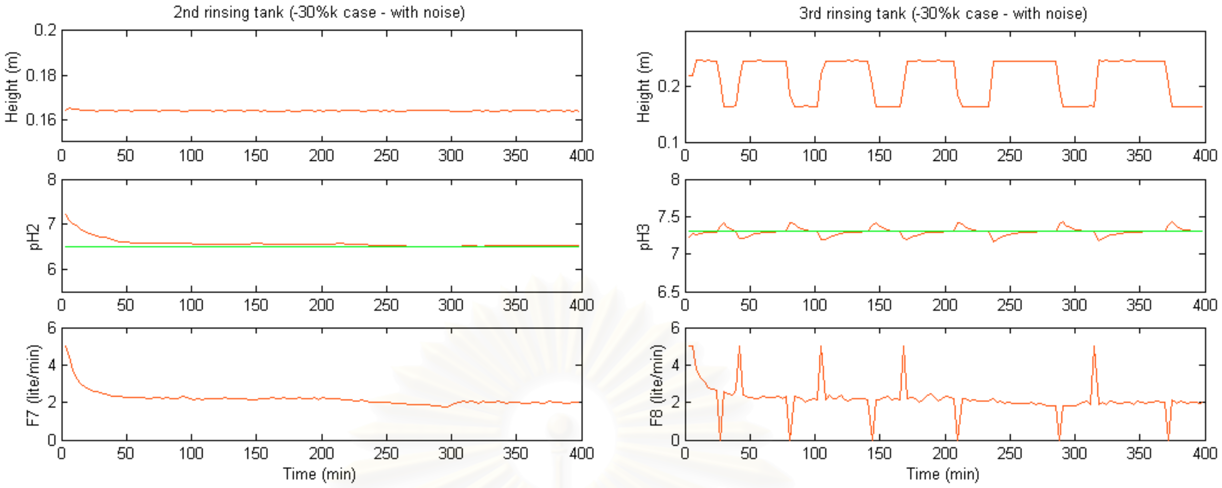

Figure 4.42 – Responses of 2nd (left) and 3rd (right) rinsing tank

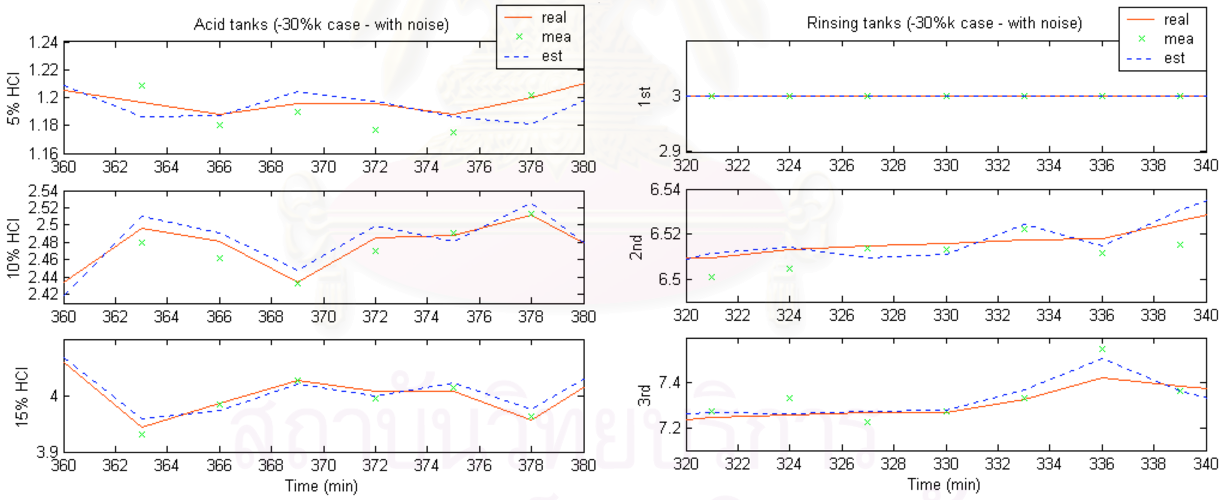

Figure 4.43 – Reconciliation of acid concentrations in -30% reaction rate case

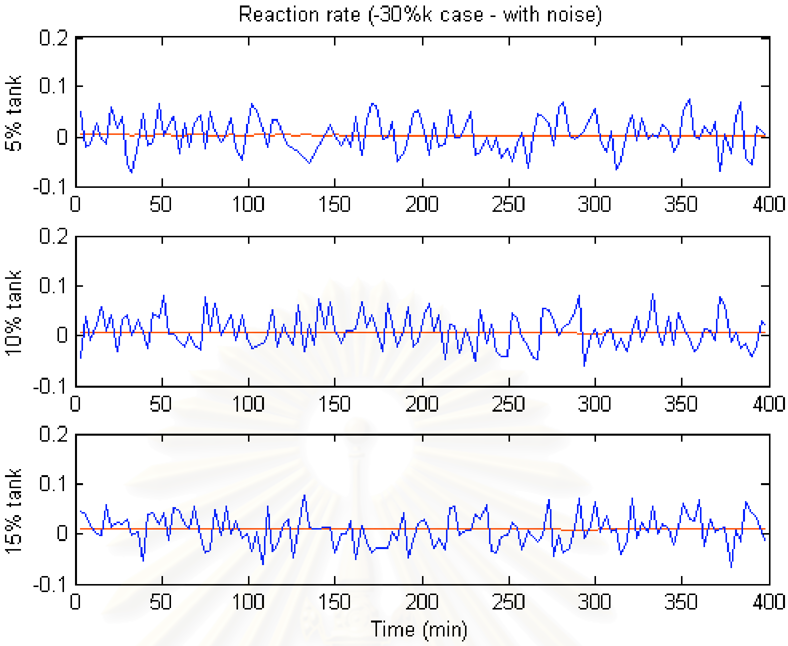

Figure 4.44 – Estimation of reaction rate in –30% reaction rate case

Disturbance case

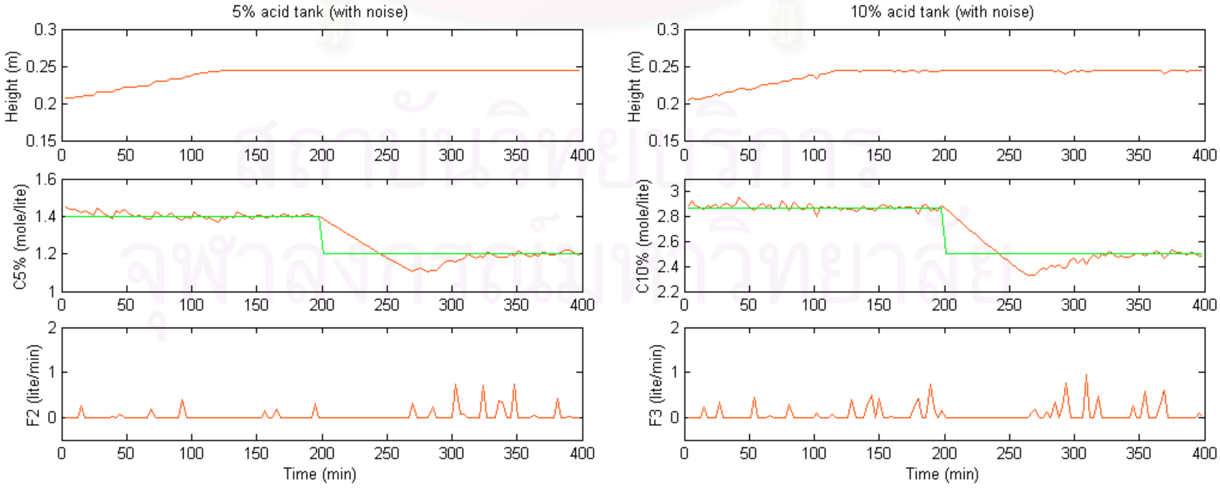

Figure 4.45 – Responses of 5% (left) and 10% (right) acid tank

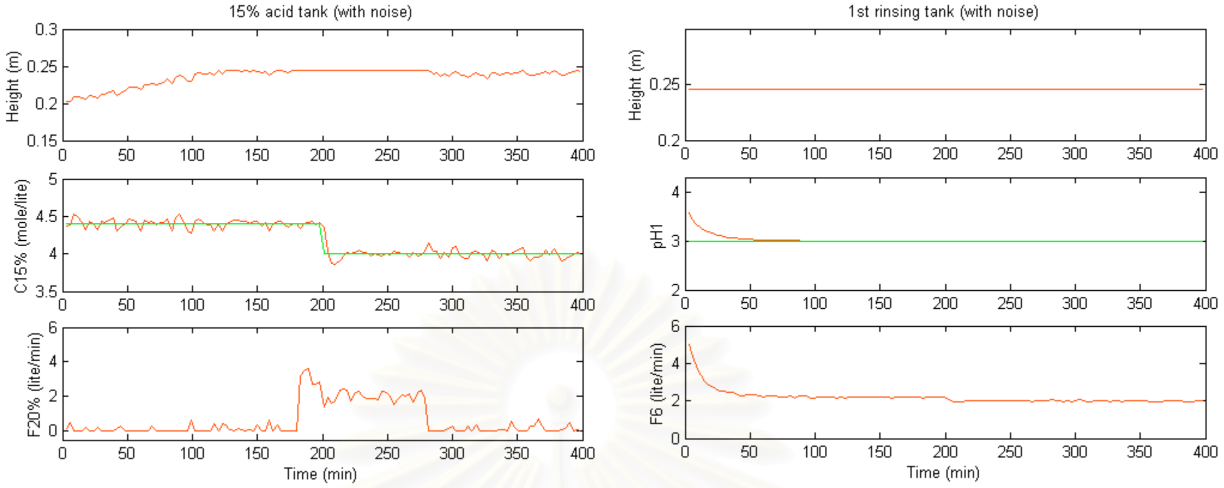

Figure 4.46 – Responses of 15% acid (left) and 1st rinsing (right) tank

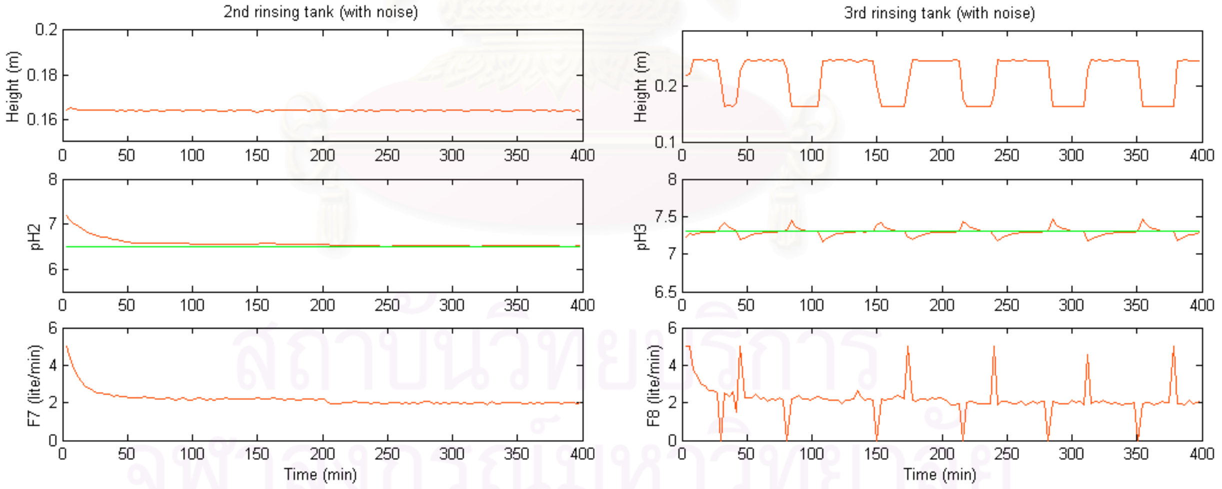

Figure 4.47 – Responses of 2nd (left) and 3rd (right) rinsing tank

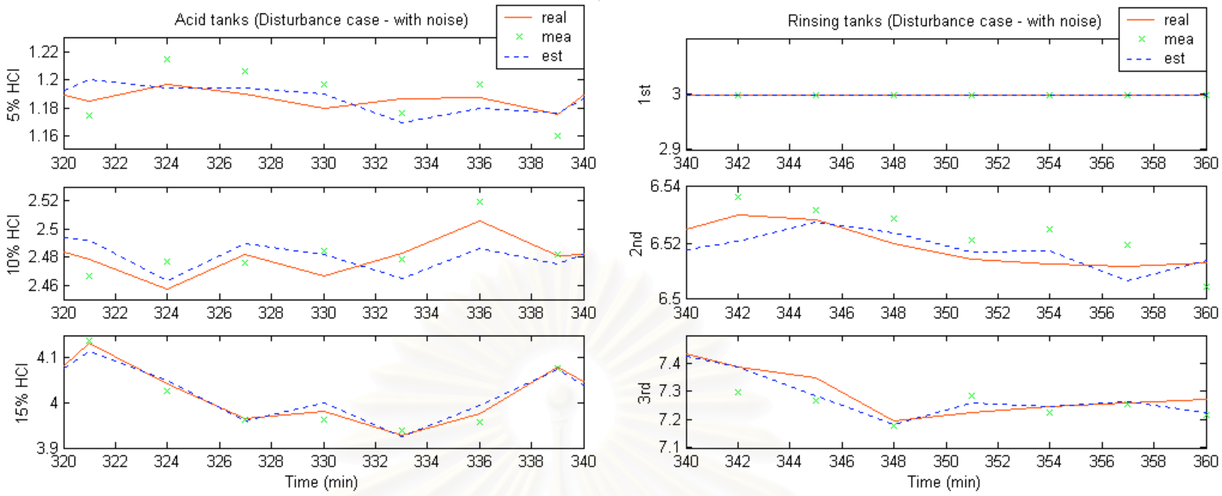

Figure 4.48 – Reconciliation of acid concentration in disturbance case

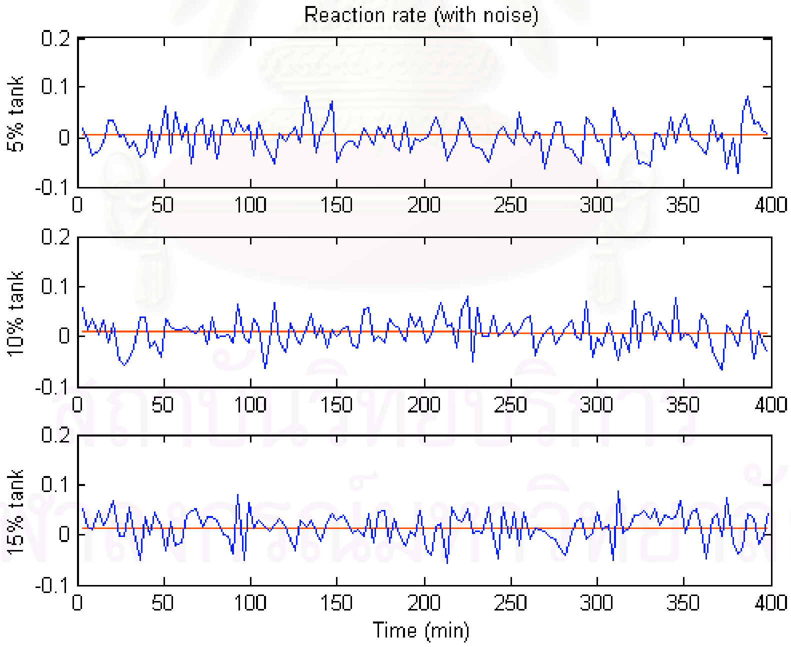

Figure 4.49 – Estimation of reaction rates in disturbance case

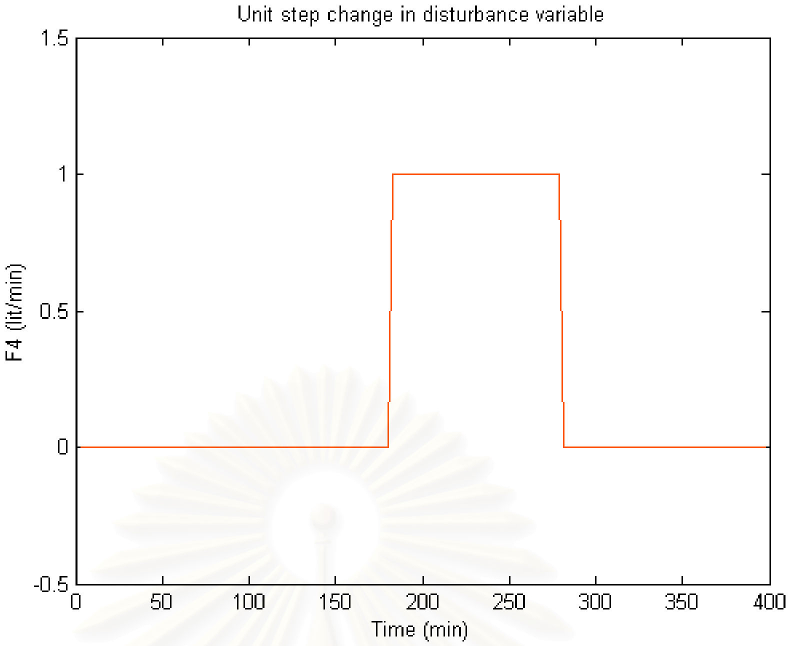

Figure 4.50 – Unit step change in disturbance variable (F_4)

4.1.5 Discussions

4.1.5.1 Set point regulation

Nominal case

Measurements of all concentrations are simulated with a measurement error standard deviation of 1% of the initial values. Figure 4.7 - 4.9 present the control performances of Generic Model Control (GMC) for the nominal case using tuning parameters in Table 4.1 and physical properties listed in Table 4.2. For this case, it is assumed that the amount of drag in-out is known exactly. This assumption will be relaxed in the next section. It can be seen that GMC succeeds to deliver the outputs to their set point values. Estimates of the concentrations appear to be significantly smoother than the corresponding measurements, as shown in Figure 4.10. In the 1st rinsing tank, it can be observed that pH value is unaffected by noise, this is because the magnitude of the error is very small with respect to its pH value. Figure 4.11 shows the estimates of the reaction rates by dynamic data reconciliation (DDR) while operating the continuous process under the nominal conditions.

+30% Drag in-out case

The GMC controller is based on the 1st principle model, so it needs the model parameters. In fact, the amount of drag in-out is never known exactly and what is more it can be changed with time. Therefore, a robustness analysis of GMC formulation needs to be investigated through simulation studies. In this case, drag in-out content is increased to about 1.3 times the original value. . It can be seen that this parameter mismatch significantly affects the accuracy of DDR approach in output reconciliation as illustrated in figure 4.15. Figure 4.17 gives the estimation of drag in-out content in light of a change in this unmeasured parameter. However, GMC controller effectively controls the process concentrations relied upon the small improvement, and estimation of unmeasured quantities.

-30% Reaction rate case

To illustrate the dependency of GMC integrated with DDR on having inaccurate process model, the reduction of reaction rates from their nominal values to ones 30% less is presented. It is found that the performances of GMC controller have changed very little when compared with the nominal responses. DDR approach do a reasonable job of output reconciliation as presented in figure 4.21. Furthermore, the improvements in performances are provided by DDR as it could successfully predict reaction rates of the process as shown in figure 4.22.

Disturbance case

The results of a step change in F_4 (as seen in figure 4.1) clearly illustrate the benefits of DDR. The process simulation is initialized at a steady state operating points, afterward at time step 180 min the disturbance flow rate is stepped form nil to one liter per min. Once again, DDR seems to provide smoother estimates and the GMC controller's performances have remained consistent as seen in figures 4.23 - 4.25. Figure 4.26 shows the estimates by the net of process concentrations, the true values, and the unreconciled original measurements.

4.1.5.2 Set point tracking

Nominal case

The control objective for most systems is regulation of state variables subject to process constraints. For some application, it maybe necessary to make set point changes to controlled variables, and hence the set point tracking performance of the control system is relevant here. The ability of GMC integrated with DDR is tested via applying set point step change in the pickling baths. Estimates of concentrations appear to be significantly smoother than the corresponding measurements, as shown in figure 4.32. Although significant lags are observed in process performances of pickling step, GMC controller is still able to deliver the process to new set point successfully with no overshoot.

+30% Drag in-out case

As mentioned previously that rarely does the amount of drag in-out exactly match the actual content. Hence, simple modifications to DDR formulation used above are made in order to allow additional item to be estimated. The unmeasured amounts of drag in-out and reaction rates are estimated simultaneously with the data reconciliation calculations. The results show that DDR do a reasonable job of estimation but does not do quite as well as for reconciliation as illustrated in figures 4.37 - 4.39. However, the proposed control strategy is much more robust with respect to a change in unmeasured drag in-out content.

-30% Reaction rate case

The difference in outcome could be caused by several factors including model mismatch. Therefore, it is important to examine the robustness with respect to model mismatch such the reduction of reaction rates with 30% change. The overall responses of the GMC controller are slightly slower when compared to the nominal case due to the limitation of tank level. The ability of GMC controller to handle such an extreme model mismatch is due to ability of DDR algorithm for estimation of reaction rates as shown in figure 4.44.

Disturbance case

Figures 4.45 - 4.47 show the resulting process controls. Note that concentration in the last pickling bath is delivered rapidly to new set point value, due to the limitation of tank level the volume of fresh acid flow rate could be increased in equivalent different amount of drained (F_{10}) and disturbance flow rate (F_4). However, the control performances of the others have changed very little when compared with the nominal responses. The estimates of the process measurements are significant smother than the simulated measurements. The majority of the measurement noise is removed. Figure 4.48 shows the ability of DDR algorithm to reconcile tank concentration measurements during dynamic behavior.

The results of process control simulation of continuous pickling process clearly illustrate the benefits of DDR. It is shown that DDR algorithm is capable of removing measurement errors to give a better view of the true state of the continuous process than is provided by the raw measurements. Since the dynamic behavior of batch system is more complex than continuous process, then this research effort also focuses further on the efficiency of the current strategy to reconcile and estimate process variables of the exothermic batch reactor in the following example.

4.2. Exothermic Batch Reactor

The initial heat-up from ambient temperature and the subsequent temperature control of exothermic batch reactors have always proved to be a difficult control problem (Shinskey, 1979). Because the amount of heat released as the reaction mixture is heated up can become very large very quickly, the reaction may become unstable and causes the temperature to run away if the heat generated exceeds the cooling capacity of the reactor. This runaway can obviously cause great risk to plant personnel and equipment and can, even in the best case, result in a loss of the batch. Therefore, careful control of the rate of change of the reactor temperature and minimization of temperature overshoot is required. On the other hand, from a production point of view, the heat-up should be done as quickly as possible in order to reduce the overall cycle time of the reaction process. Therefore, any control strategy for heat-up must balance the needs of production with those of safety and quality.

4.2.1 Process description

The reactor simulation used in this work is largely based upon a dynamic model and process data from Cott and Macchietto (1989). A well mixed, liquid-phase reaction system is considered in which two reactions are modeled:

Reaction1: $A + B \rightarrow C$
Reaction2: $A + C \rightarrow D$

Component C is a desired product while D is an unwanted byproduct, and the general operating objective is to achieve a good conversion of C while minimizing the production of D.

Figure 4.31 presents a diagram of the reactor system. Heating and cooling of the reactor contents is performed through the use of a single-pass jacket system. Control of the jacket temperature is provided using a temperature controller on the jacket inlet stream. The heat exchangers needed to control this temperature are not modeled but are accounted for by basing the time constant of the jacket temperature response on typical figures given by Liptak (1986).

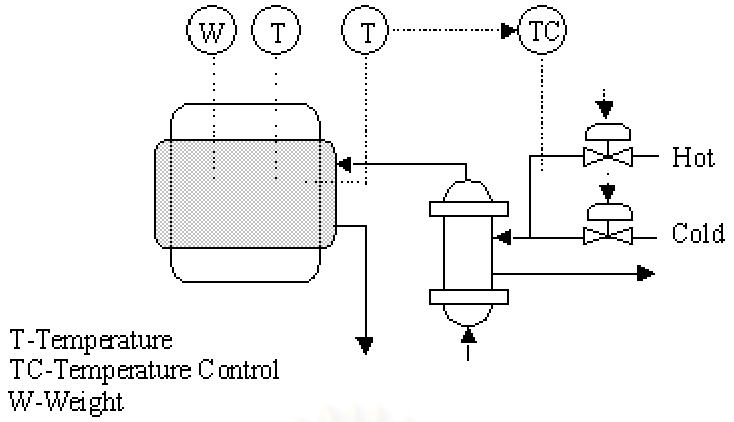

Figure 4.51 - Batch reactor schematic diagram.

4.2.2 Mathematical modeling

The first step in the development of the data reconciliation package is the preparation of a model of the reactor. It is based on mass and energy balances as follows:

$$\frac{dM_A}{dt} = -R_1 - R_2 \qquad (4.13)$$

$$\frac{dM_B}{dt} = -R_1 \qquad (4.14)$$

$$\frac{dM_C}{dt} = R_1 - R_2 \qquad (4.15)$$

$$\frac{dM_D}{dt} = R_2 \qquad (4.16)$$

where

$R_1 = k_1 M_A M_B$ $\quad$ $R_2 = k_2 M_A M_C$

$k_1 = \exp(k_1^1 - k_1^2 / (T_r + 273.15))$ $\quad$ $k_2 = \exp(k_2^1 - k_2^2 / (T_r + 273.15))$

$$\frac{dT_r}{dt} = \frac{Q_r + Q_j}{M_r C_{pr}} \tag{4.17}$$

$$\frac{dT_j}{dt} = \frac{F_j \rho_j C_{pj} (T_j^{sp} - T_j) - Q_j}{V_j \rho_j C_{pj}} \tag{4.18}$$

where

$W_r = MW_A M_A + MW_B M_B + MW_C M_C + MW_D M_D$

$C_{pr} = (C_{pA} M_A + C_{pB} M_B + C_{pC} M_C + C_{pD} M_D) / M_r$

$M_r = M_A + M_B + M_C + M_D$

$V_r = W_r / \rho_r$ $\quad$ $A_r = 2 V_r / r$

$Q_j = U_r A_r (T_j - T_r)$ $\quad$ $Q_r = -\Delta H_1 R_1 - \Delta H_2 R_2$

4.2.3 Control configuration

The formulation of GMC for temperature control of a exothermic batch reactor is quite straightforward. A process model relating the reactor temperature, T_r, to the manipulated variable, the jacket temperature, T_j, is required. The amount of heat retained in the walls of the reactor is assumed to be small in comparison with the heat transferred in the rest of the system, an energy balance around the reactor contents gives the required model:

$$\frac{dT_r}{dt} = \frac{Q_r + U_r A_r (T_j - T_r)}{W_r C_{pr}} \tag{4.19}$$

Substituting T_r for y and T_r^{sp} for y^{sp} in equation (3.32), combining equation (4.19) to the general form of the GMC control algorithm and finally rearranging for the manipulated variable, T_j, obtain:

$$T_j = T_r - \frac{Q_r}{U_r A_r} + \frac{W_r C_{pr}}{U_r A_r}\left[K_1 (T_r^{sp} - T_r)\right] + \frac{W_r C_{pr}}{U_r A_r}\left[K_2 \int_0^t (T_r^{sp} - T_r) dt \right]$$

Therefore, the discrete time version of the above equation is

$$T_j^{(k)} = T_r^{(k)} - \frac{Q_r^{(k)}}{U_r A_r} + \frac{W_r C_{pr}}{U_r A_r}\left[K_1 \left(T_r^{sp} - T_r^{(k)} \right)\right]$$

$$+ \frac{W_r C_{pr}}{U_r A_r}\left[K_2 \sum_0^k \left(T_r^{sp} - T_r^{(k)} \right) \Delta t \right] \tag{4.20}$$

Equation (4.20) gives not the jacket temperature set point, if it is used directly as the set point, then, the resulting control would be sluggish because of the regardless of jacket dynamics in equation (4.20). Therefore, some form of dynamic compensation of the jacket temperature must be used for moving the reactor temperature toward its set point. If the dynamics of the jacket are assumed to be first order (Liptak, 1986), then a difference equation can be used

$$T_j^{(k)} = T_j^{(k-1)} + \frac{\Delta t \left(T_j^{sp\,(k)} - T_j^{(k-1)} \right)}{\tau_j} \tag{4.21}$$

where τ_j is the estimated time constant of the jacket. The jacket temperature set point can be obtained by simply rearranging equation (4.21). Hence, the following dynamic compensator is obtained:

$$T_j^{sp\,(k)} = T_j^{(k-1)} + \frac{\tau_j \left(T_j^{(k)} - T_j^{(k-1)} \right)}{\Delta t} \tag{4.22}$$

The solution of equations (4.20) and (4.22) gives the actual set point value for the jacket temperature controller to be used for the next control interval.

The success of the GMC controller is largely depended upon the ability to measure, estimate, or predict the heat released at any given period of time. Therefore, the data reconciliation is used to estimate this information. Since the sensitivity of the estimation of the heat released by reaction to the heat transfer coefficient change, the data reconciliation is used to estimate the heat transfer coefficient to compensate the mismatch.

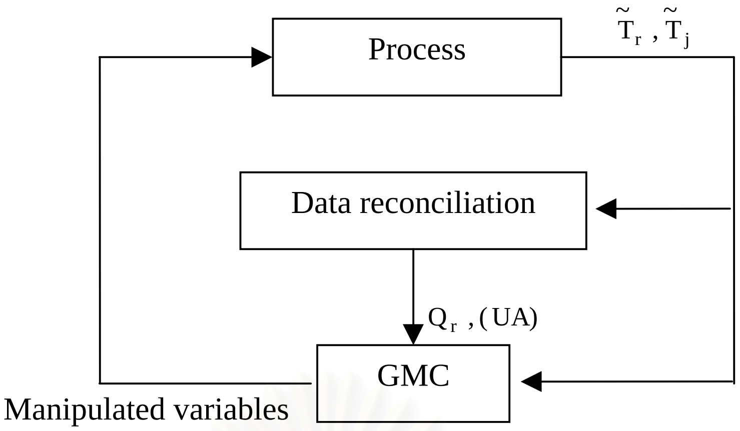

Figure 4.52 –The estimation diagram for the exothermic batch reactor

As seen in figure 4.32, the heat released, which cannot be measured, is needed in the GMC algorithm. Here, dynamic data reconciliation (DDR) algorithm is also applied to estimate the heat released and heat transfer coefficient by using the energy balances on the jacket and reactor, the state equations for purposed of estimation are:

$$\frac{dT_{rest}}{dt} = \frac{Q_{rest} + U_r A_r \, (T_{jrest} - T_{rest})}{M_r C_{pr}} \tag{4.23}$$

$$\frac{dT_{jest}}{dt} = \frac{F_j \rho_j C_{pj} \, (T_j^{sp} - T_{jest})}{V_j \rho_j C_{pj}} - \frac{U_r A_r \, (T_{jest} - T_{rest})}{V_j \rho_j C_{pj}} \tag{4.24}$$

T_{rest} and T_{jest} are measurable and are used to estimate Q_{rest} via the data reconciliation in which the measurement and estimation covariance matrixes used in reconciliation algorithm are defined to be unit matrix. The initial conditions of data reconciliation and tuning parameters of GMC controller are given in Table 4.18 and 4.19, respectively.

Table 4.11 Data reconciliation parameters and initial state estimates

T_{rest}^0 = 20 °C	T_{jest}^0 = 20 °C
Q_{rest}^0 = 0 kJ/min	U_r^0 = 40.842 kJ/(min.m^{2}·°C)

Table 4.12 Tuning parameters of GMC

K_1	K_2
0.25	0.0001

4.2.4 Simulation results

Due to some given cost function, Pulley (1986) determined that the optimal isothermal reaction temperature typically falls in the range 90.0 - 100.0 °C so that the final reaction temperature is set to 95.0 °C. The jacket temperature is assumed to be limited to the range 20.0 - 120.0 °C due to heat-exchanger capacities, and the reaction mixture is assumed to be at 20.0 °C at the starting point.

Because measurement errors are always present when working with real equipment, these are included in the simulation by adding noise (±0.2 °C) to all temperature measurements. DDR is used here to determine the amount and rate of heat released by the reaction, which is unavailable. This information is, in turn, utilized to determine the change in jacket temperature set point in order to keep the reaction temperature on its desired trajectory. Physical parameters and initial conditions used in process model are listed in Table 4.16 and 4.17, respectively.

Table 4.13 Physical properties and process data

MW_A = 30 kg/kmol	MW_B = 100 kg/kmol
MW_C = 130 kg/kmol	MW_D = 160 kg/kmol
C_{pA} = 75.31 kJ/(kmol.°C)	C_{pB} = 167.36 kJ/(kmol.°C)
C_{pC} = 217.57 kJ/(kmol.°C)	C_{pD} = 334.73 kJ/(kmol.°C)
k_1^1 = 20.9057	k_1^2 = 10000
k_2^1 = 38.9057	k_2^2 = 17000
ΔH_1 = - 41840 kJ/kmol	ΔH_2 = - 25105 kJ/kmol
ρ_r = 1000 kg/m^3	r = 0.5 m
U_r = 40.842 kJ/(min.m^{2}·°C)	ρ_j = 1000 kg/m^3
C_{pj} = 1.8828 kJ/(kg.°C)	F_j = 0.348 m^3/min
V_j = 0.6812 m^3	

Table 4.14 Initial conditions

M_A^0 = 12 kmol	M_B^0 = 12 kmol
M_C^0 = 0 kmol	M_D^0 = 0 kmol
T_r^0 = 20 °C	T_j^0 = 20 °C

4.2.4.1 Set point regulation

Estimated heat released by reaction is used to determine the change in jacket temperature set point in order to keep the reaction temperature at 95.0 °C.

Table 4.15 IAE and ISE

Case	Temperature		Heat released	
	IAE	ISE ($\times10^{+4}$)	IAE ($\times10^{+4}$)	ISE ($\times10^{+7}$)
Nominal	779.682	3.687	4.631	2.712
-30%U	950.096	4.565	15.69	29.06
-30%k	789.553	3.711	4.499	2.588
-30%dH	785.857	3.710	4.424	2.469

<u>Nominal case</u>

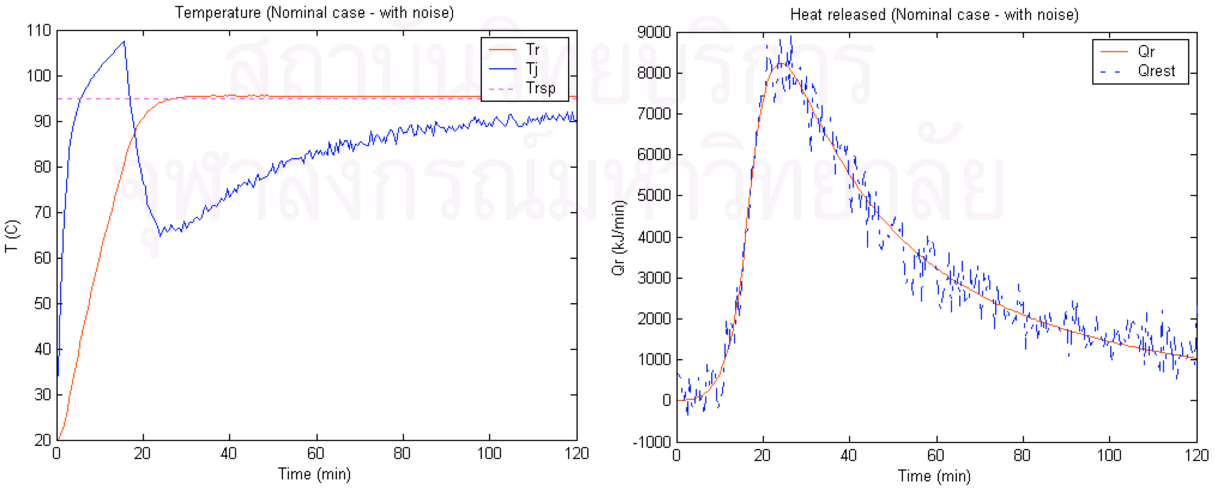

Figure 4.53 - Responses of reactor temperature (left) and heat released (right)

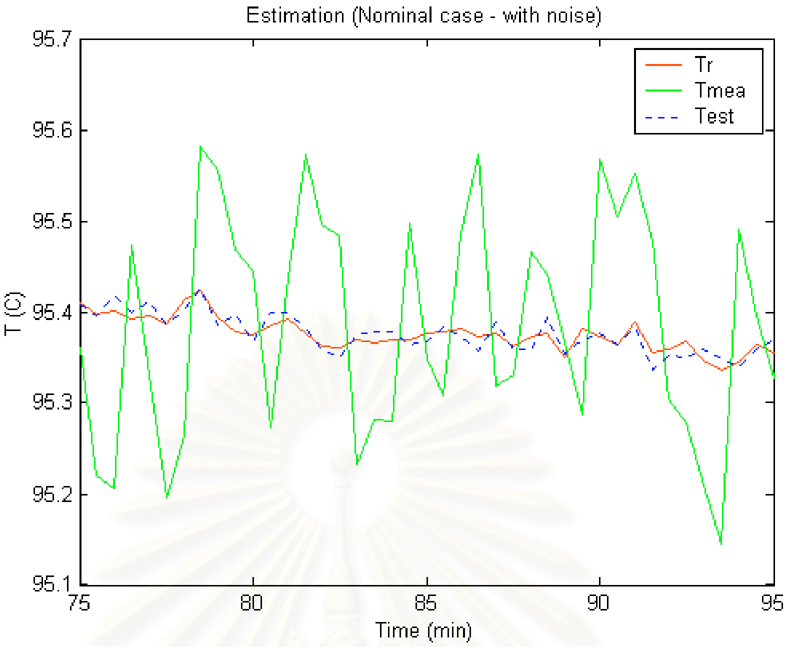

Figure 4.54 – Reconciliation of reactor temperature in nominal case

-30% Heat transfer coefficient case

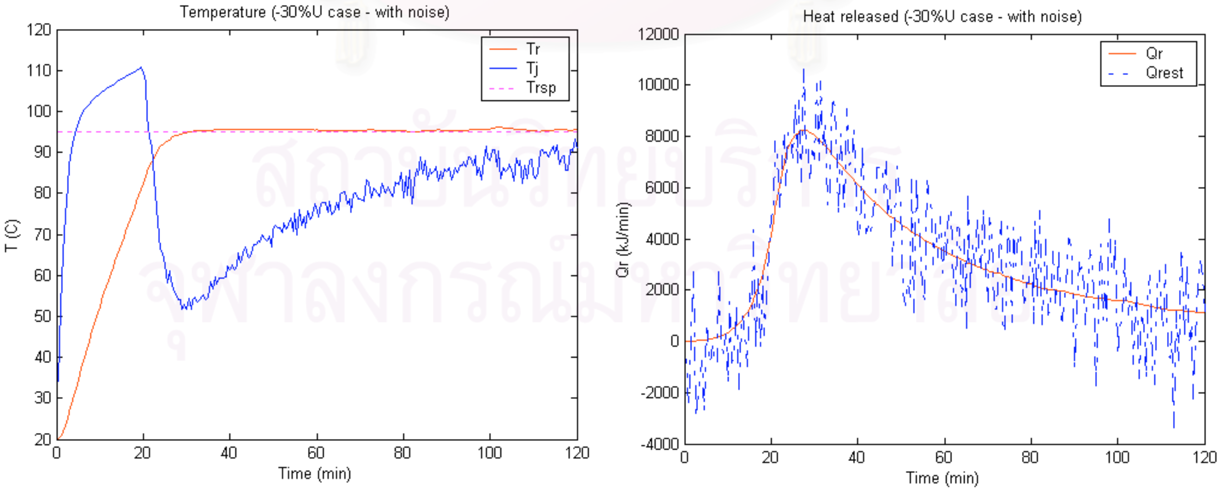

Figure 4.55 - Responses of reactor temperature (left) and the heat released (right)

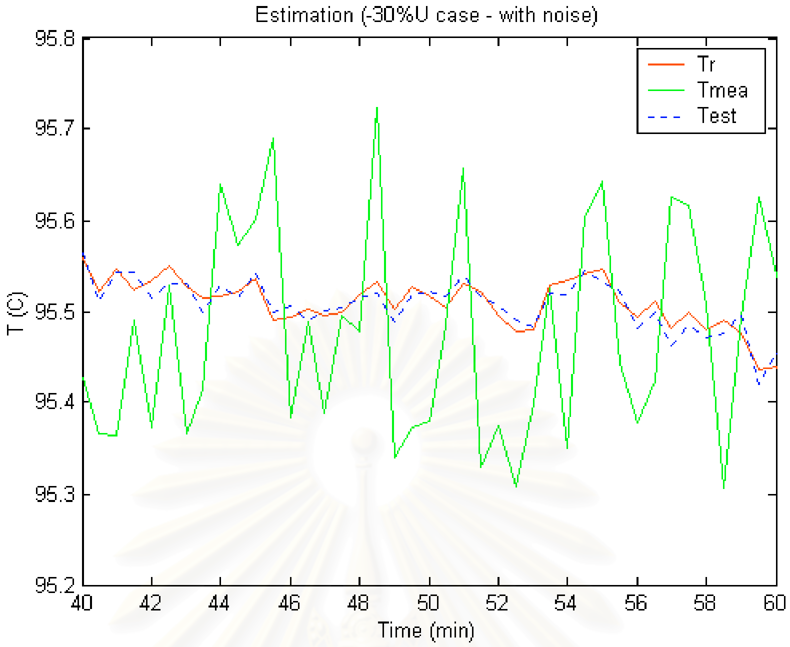

Figure 4.56 – Reconciliation of reactor temperature in -30% U case

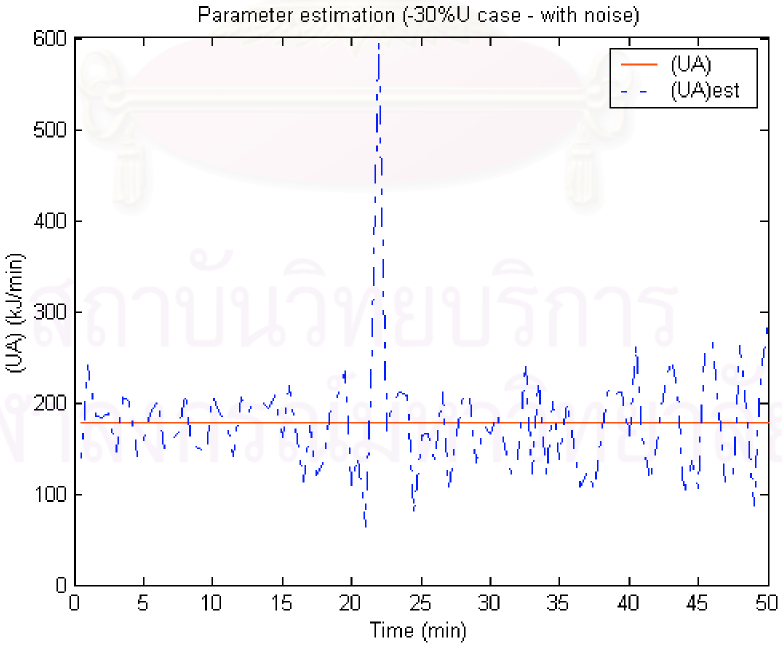

Figure 4.57 – Estimation of heat transfer coefficient in -30% U case

-30% Reaction rate case

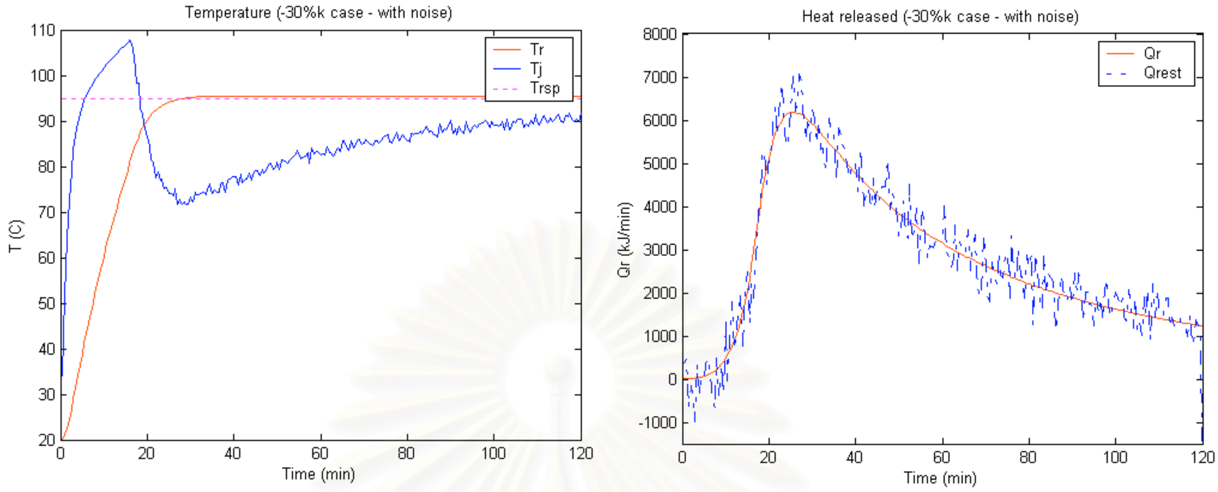

Figure 4.58 – Responses of reactor temperature (left) and heat released (right)

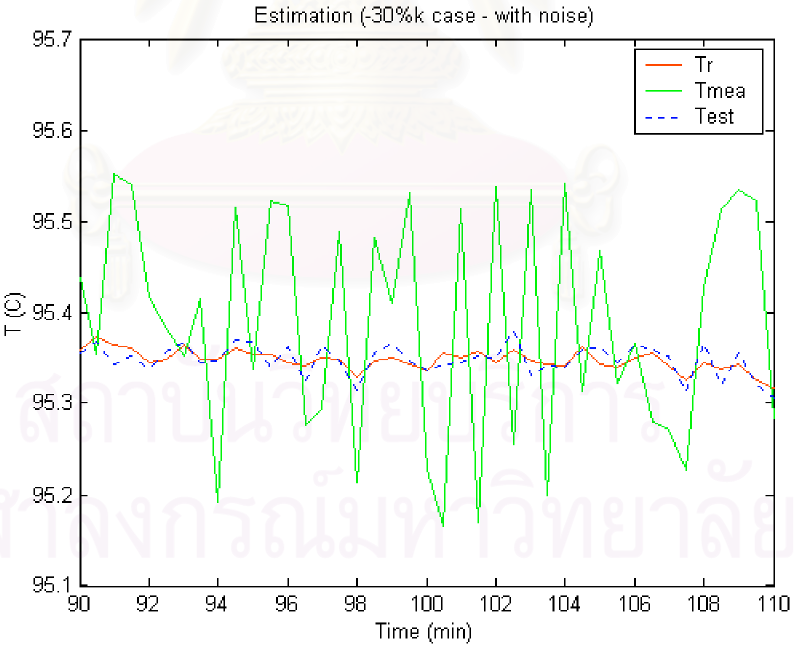

Figure 4.59 – Reconciliation of reactor temperature in -30% k case

-30% Heat case

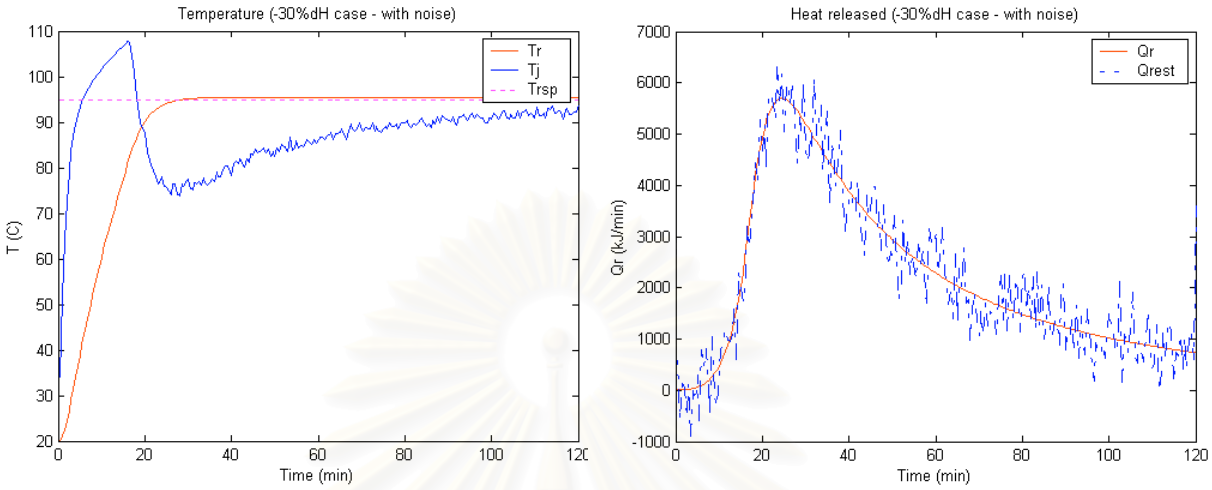

Figure 4.60 – Responses of reactor temperature (left) and the heat released (right)

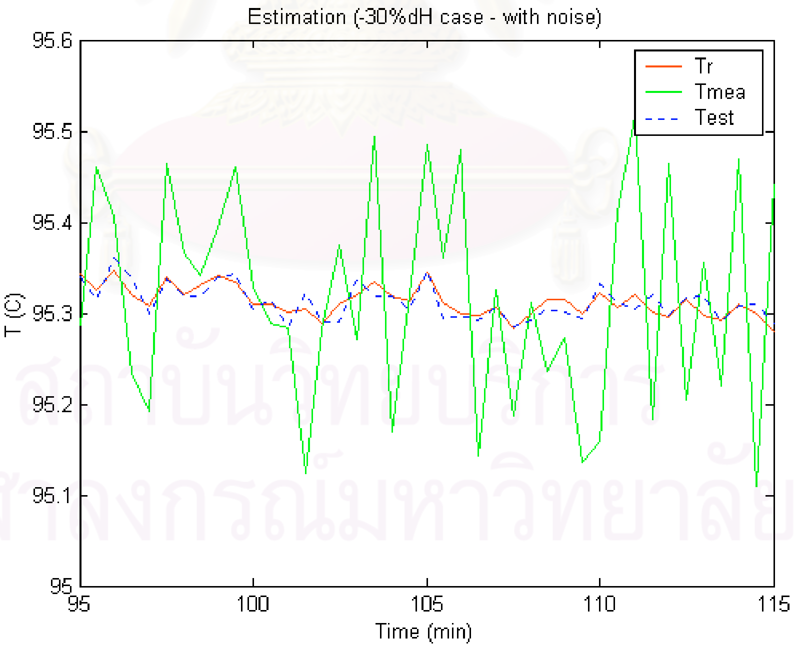

Figure 4.61 – Reconciliation of reactor temperature in -30% dH case

4.2.4.2 Set point tracking

In this case, the estimated information is employed to handle the reaction temperature when the set point is stepped from 95.0 °C to 100.0 °C at time step 60 min.

Table 4.16 IAE and ISE

Case	Temperature		Heat released	
	IAE	ISE $(\times10^{+4})$	IAE $(\times10^{+4})$	ISE $(\times10^{+7})$
Nominal	790.407	3.691	4.510	2.594
-30%U	787.018	3.744	15.95	33.16
-30%k	800.745	3.715	4.709	2.715
-30%dH	797.693	3.715	4.603	2.627

Nominal case

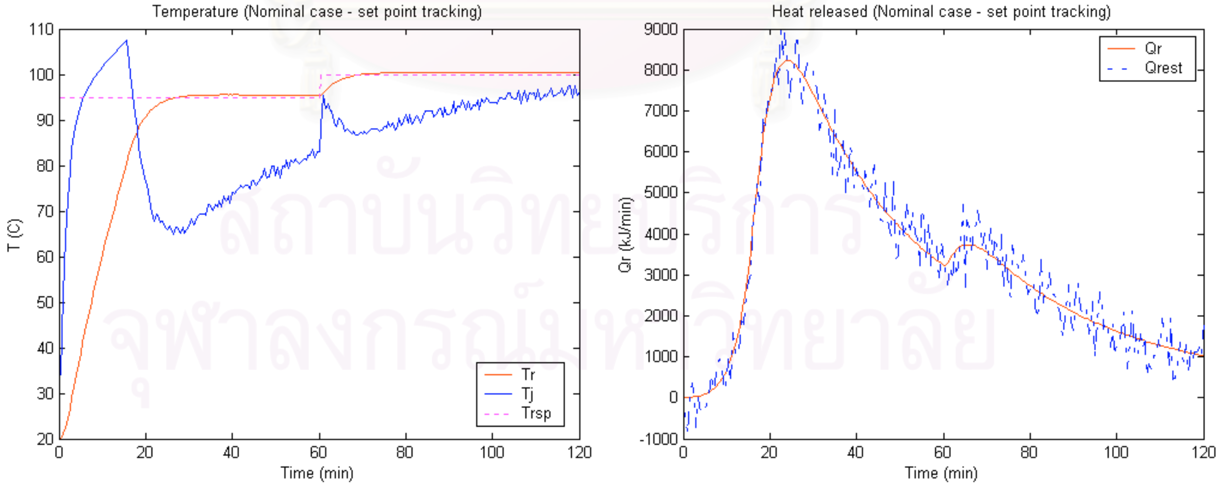

Figure 4.62 - Responses of reactor temperature (left) and heat released (right)

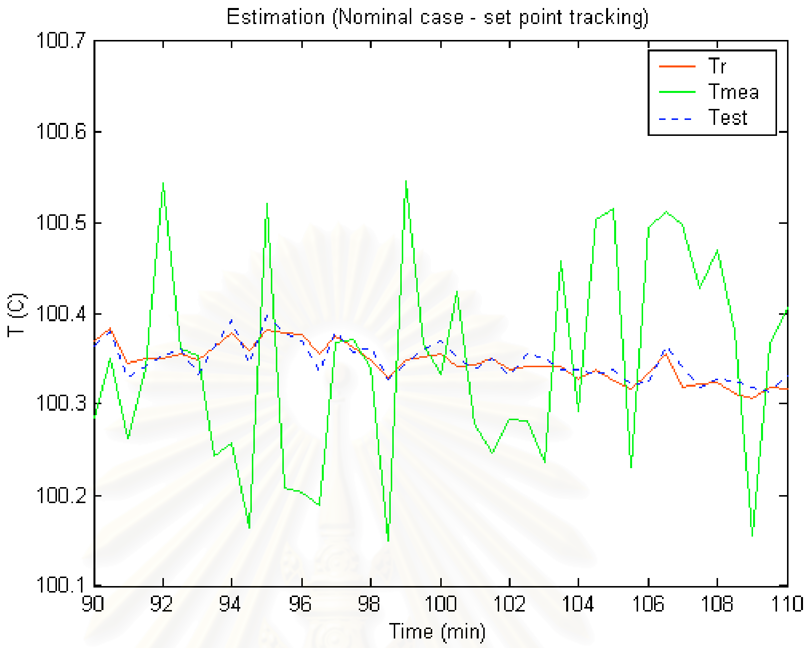

Figure 4.63 - Reconciliation of reactor temperature in nominal case

-30% Heat transfer coefficient case

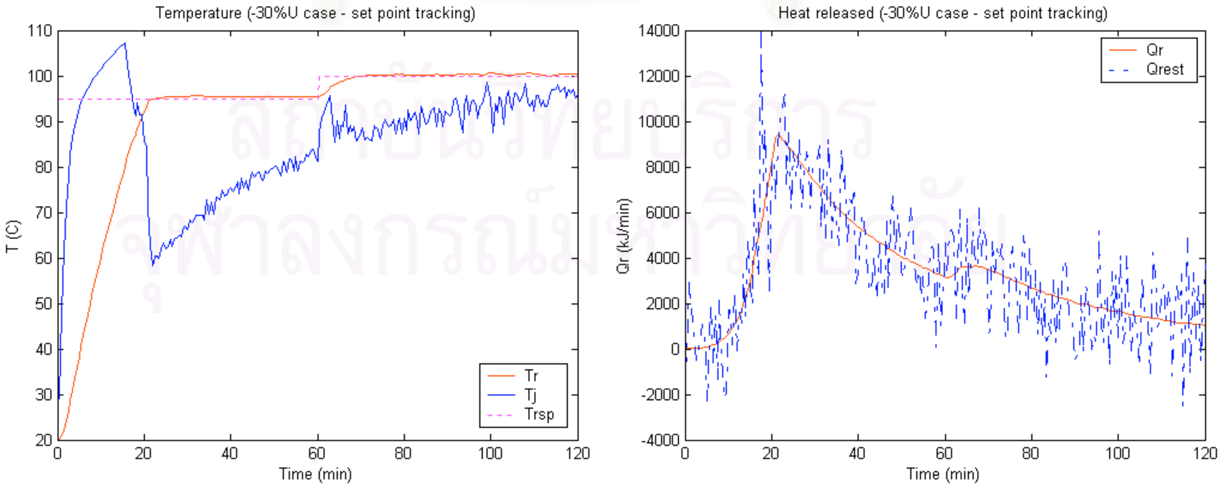

Figure 4.64 - Responses of reactor temperature (left) and heat released (right)

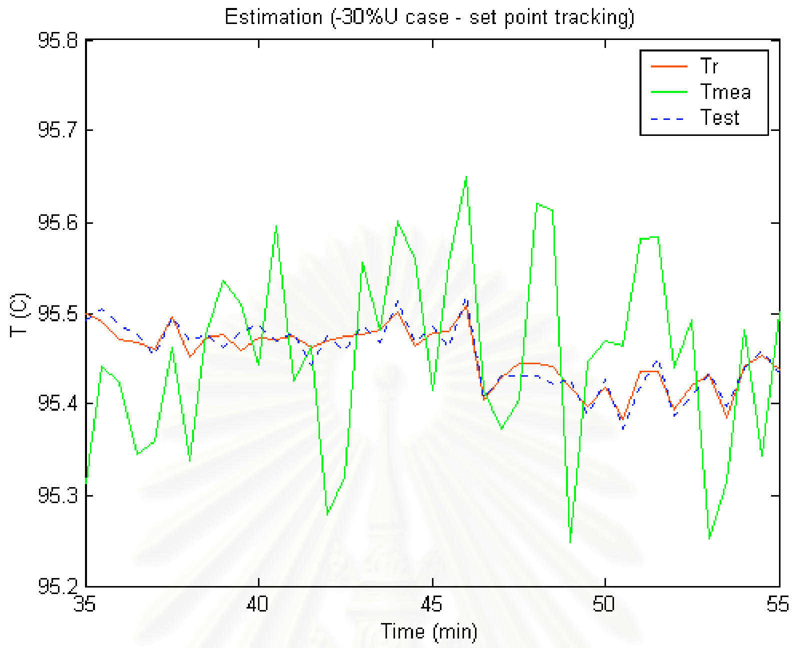

Figure 4.65 - Reconciliation of reactor temperature in –30% U case

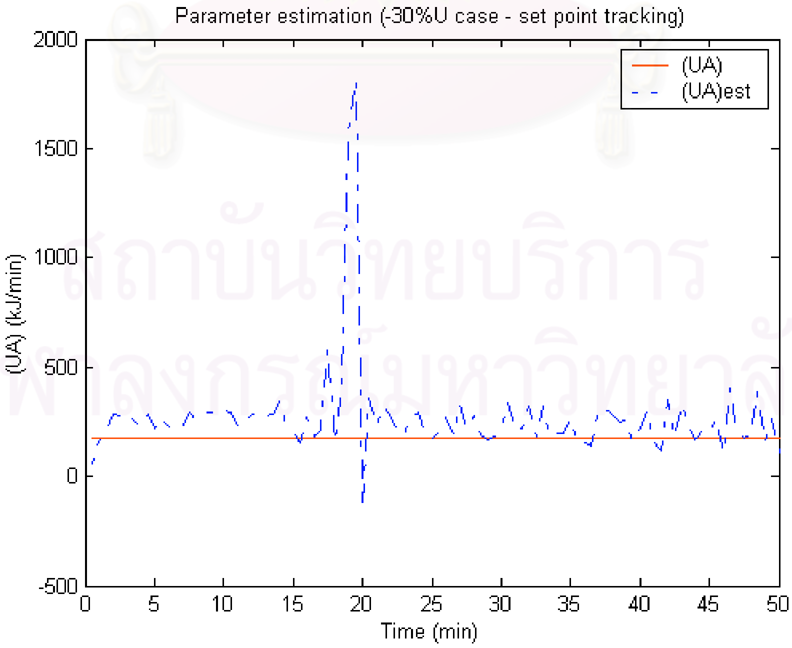

Figure 4.66 - Estimation of heat transfer coefficient in –30% U case

-30% Reaction rate case

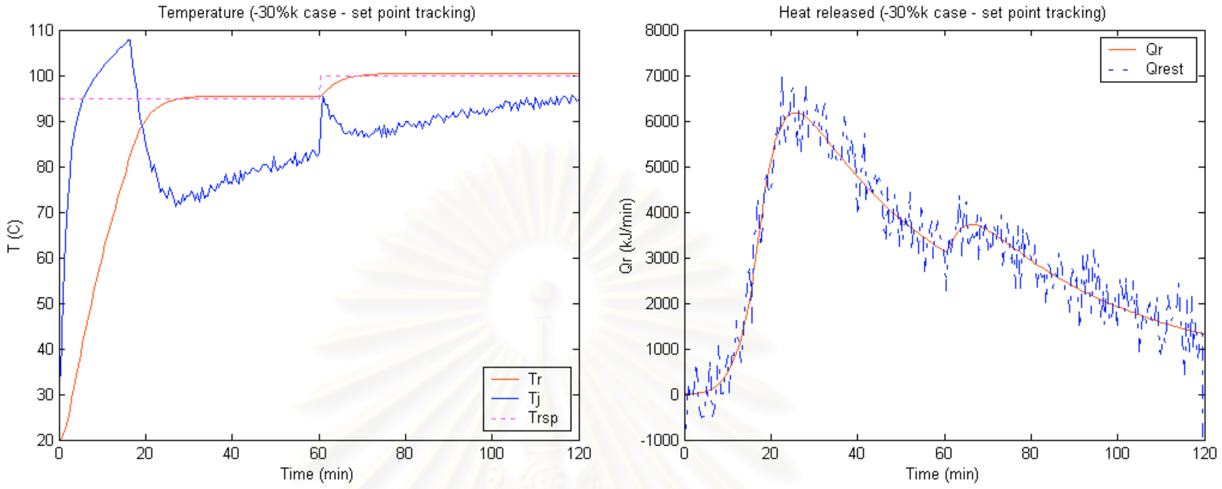

Figure 4.67 - Responses of reactor temperature (left) and heat released (right)

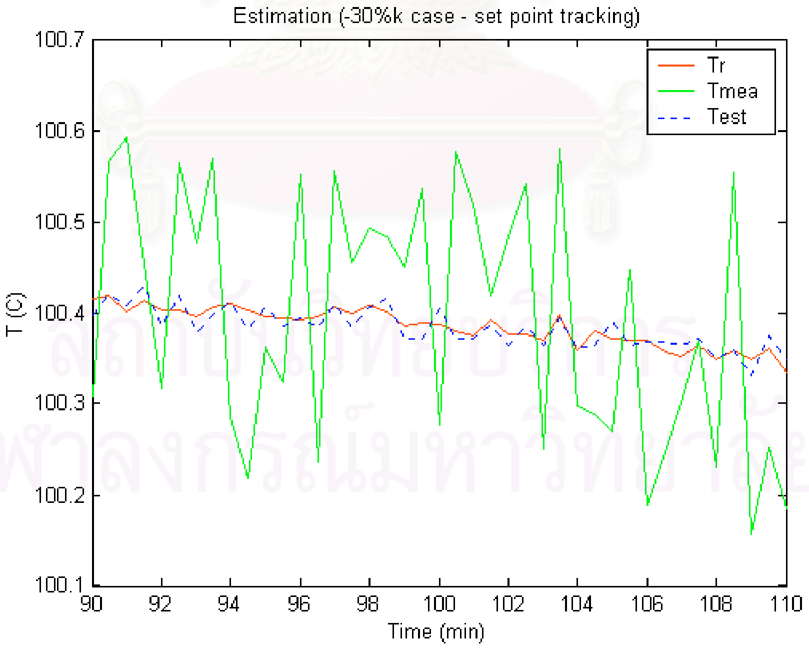

Figure 4.68 - Reconciliation of reactor temperature in –30% k case

-30% Heat case

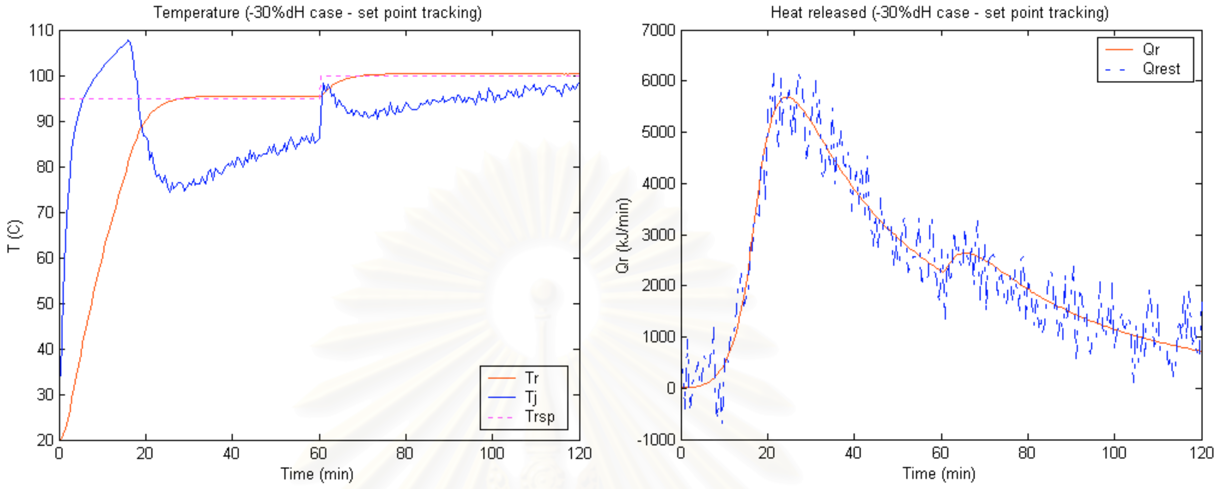

Figure 4.69 - Responses of reactor temperature (left) and heat released (right)

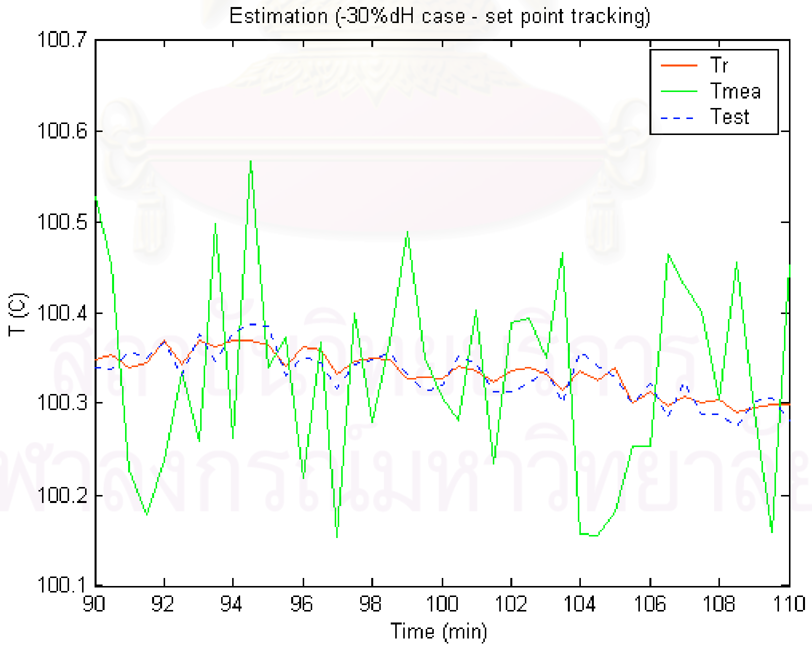

Figure 4.70 - Reconciliation of reactor temperature in –30% dH case

4.2.5 Discussion

4.2.5.1 Set point regulation

Nominal case

In this example, the application of dynamic data reconciliation (DDR) technique is demonstrated on a simulated exothermic batch reactor with two irreversible reactions. The physical constants for the model are shown in Table 4.18 to 4.19. Temperature measurements are simulated with a measurement error standard deviation of 1% of the corresponding initial values. DDR algorithm is used to obtain reconciled estimates of all measured temperature and estimation of unmeasured quality such heat released by reaction. Figure 4.53 (left) presents the control performance of Generic Model Control (GMC) for the nominal case. It can be seen that GMC provides good control performances. Estimates of the reaction temperature contain far less noise than the simulated measurements as shown in figure 4.54. Figure 4.53 (right) shows the estimate of the heat released by using DDR.

-30% Heat transfer coefficient change

The previous case shows that the proposed control strategy effectively control the reactor temperature for the nominal operation. However, it is important to examine the robustness with respect to change in process parameter. In this case, the test involves the reduction of the heat transfer coefficient from its nominal value to one 30% less. This test simulated a change in heat transfer that could be expected due to fouling of the heat transfer surfaces. Figure 4.55 (left) gives the response of GMC controller in response to the changed heat transfer coefficient. The control performances have degraded due to uncertainty of the parameter. Figure 4.55 (right) shows the ability of DDR algorithm to estimate heat released during dynamic behavior. It is significantly degraded the response to the change in the heat transfer coefficient.

-30% Reaction rate change

The robustness of GMC controller in the face of change in the reaction chemistry is tested in this case. The reaction rates of the both reactions are decreased to about 0.7 time the original rates. The results of this test are given in figures 4.58 - 4.59. Once again, it can be seen that GMC controller's performance has changed very little when compared with the nominal case. The improvement in performance is provided by DDR algorithm as it can predict the speed at which heat is being released in the reaction effectively.

-30% Heat of reaction change

This case represents an extreme case of model mismatch where reaction heat of both reactions is decreased from its nominal value to one 30% less. As seen in figure 4.60 (left), GMC controller's performance has remained consistent. The overall response of GMC controller is slightly slower when compared to the nominal case, but this is largely due to the face that the jacket temperature set point is constrained at 120 °C and therefore the amount of heat transfer is limited. Furthermore, significant reductions in the measurement error are achieved through the application of DDR algorithm as seen in figure 4.61.

4.2.5.2 Set point tracking

Nominal case

The set point tracking performances of GMC integrated with DDR are tested in this case study. Figure 4.62 shows the set point tracking for the typical proposed strategy. For the step change to 100 °C, the GMC controller delivers the reactor temperature to new set point rapidly and the estimate of heat released is immediately tracked to the true value with no lag. Figure 4.63 displays that the estimate closely followed the true value.

-30% Heat transfer coefficient change

In this case, heat transfer coefficient calculated using modified DDR approach described in chapter III is shown in figure 4.66. The estimate obtained using DDR strategy is acceptable. In addition, the estimate of heat released, as seen in figure 4.64 (right), remains close to the true value and displays the same dynamic trend. The estimate for the measured reactor temperature rapidly diverges from the measurement as presented in figure 4.65.

-30% Reaction rate change

DDR has been the technique for obtaining state and parameter estimates. As mentioned in the previous chapter, a linear approximation to the nonlinear system is applied in order to provide the estimates in any cases. In this robustness test, GMC coupled with DDR algorithm is tested with respect to change in reaction rates. The simulation resells have been shown to provide similar performances to the nominal responses as seen in figure 4.67. The reconciled estimate for the measured reactor temperature is still much smoother than the original measurements as shown in figure 4.68.

-30% Heat of reaction change

As a final demonstration of the robustness of the proposed control strategy, the reactor temperature is modified so that reaction heat is decreased to about 0.7 time the original value. More significantly, the estimate for the unmeasured heat released is remarkably good as seen in figure 4.69 (right). The reactor temperature is delivered to the new desired set point with no overshoot. In figure 4.70, the estimate obtained using DDR strategy is much more reliable.

CHAPTER V

CONCLUSION AND RECOMMENDATION

5.1. Conclusion

In a modern chemical plant, a wide variety of measurements of the process variables are taken for the purpose of evaluating process control or process performance. However, not all variables needed are generally measured, because of technical infeasibility or cost. Furthermore, the measurements are often contaminated in the sense that random noise may be present due to human error, result of miscalibration, or failure of the measuring instruments. When flawed information is used for state estimation and process control, the state of the system is misrepresented and the resulting control performance may be poor and can lead to sub-optimal and even unsafe process operation. Thus, data reconciliation is frequently required before the data can be used for evaluating process control or process performance.

Data reconciliation has received considerable attention to resolve inconsistencies between plant measurements and balance equations. In this work, dynamic data reconciliation (DDR) presented by Darouach and Zasadzinski (1991) was employed. However, DDR algorithm is linear and deterministic with all the variables measured. Thus, simple modifications to DDR formulation was made in this research in order to allow additional items to be estimated. A matrix projection method proposed by Crowe et.al. (1983) was used to decompose the problem so that the measured and unmeasured variables can be evaluated sequentially by the proposed DDR algorithm as described in chapter III. Later, coupled procedure presented by MacDonald and Howat (1988) was also applied here to extend DDR technique to estimate process parameters. Therefore, parameter estimation proceeds simultaneously with the data reconciliation calculations.

There are several model based control strategies that could be used with DDR, Generic Model Control (GMC) was chosen because it has some appealing properties that are not found in some of the other model based control schemes. In particular, models derived from dynamic mass, energy and momentum balances can be directly used in the controller, and controller tuning is straightforward and easy to understand.

In chapter IV, the benefits of combining DDR with GMC was demonstrated on two example problems for reconciliation and estimation of process data. Firstly, the application of the proposed control strategy to a continuous steel pickling process was discussed. The continuous pickling process incorporates several characteristics typical of many industrial processes, which render it difficult to model and to control. In particular, the process is strongly nonlinear. A mathematical model of the process was developed to allow control of the process to be studied in simulation. A pilot plant of the pickling process was designed and devised during the research project. It is found that the first principle model could provide a feasible representation of the continuous steel pickling process because the model and pilot plant data provided the same behavior. Afterward, the robustness of the proposed control strategy was investigated with respect to changes in process condition, modeling error and disturbance variable. Lastly, this work looked at the application to an exothermic batch reactor, whose dynamic model was presented by Cott and Machietto (1989). The performance of GMC integrated with DDR was further evaluated for set point regulation and set point tracking.

In parameter mismatch, the simulation results of both continuous and batch systems have shown that the performances of DDR deteriorated. This is maybe because the reconciled measurements also highlighted deficiencies in process operation, which reducd its effectiveness. Furthermore, a linear approximation to the nonlinear systems was applied in linear DDR algorithm. However, a rudimentary treatment of measurement errors has proved extremely effective in other cases. On the other hand, linear DDR is shown to be capable of removing random errors to give a better view of the true state of the process than is provided by the raw measurements. In addition, the ability to handle strong non-linearity and estimate unmeasured quantities significantly improved the reconciled estimates. It is therefore an important adjunct to advanced control and optimization.

5.2. Recommendation

Some limitations of this work have been investigated. The various assumptions in simplified process simulations are the limitations in study of dynamic process model and data reconciliation. The assumptions for this work are included as shown below:

1. Negligible gross error.
2. Directly measurable state variables.

3. Well-mixed reaction system.
4. Considering only one unknown parameter.
5. Considering linear dynamic data reconciliation.

It is found that dynamic data reconciliation (DDR), which relied upon steady state algorithm, gives successful estimation and reconciliation as shown in simulation results. Hence, future efforts should focus on application of linear DDR for other size of problems such as the presence of multiple unmeasured variables and unavailable process parameters. Evaluation studies should also be considered in case of indirectly measurable state variables. In addition, non-linear DDR approach including gross error detection to verify more accuracy of the response predictions could be achieved.

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APPENDICES

Appendix A

TUNING OF GMC CONTROLLER FOR STEEL PICKLING PROCESS CONTROL

Lee and Sullivan (1988) outline a system for tuning GMC controller based on choosing a target profile of the controlled variable, $y^{sp}(t)$. This profile is characterized by two values, ξ and τ. Lee and Sullivan present a figure that outlines the relative control performances of different combinations of ξ and τ as shown in figure A.1. The similar plots to the classical second-order response showing the normalized response of the system y/y^{sp} vs. normalized time t/τ with ξ as a parameter can be produced.

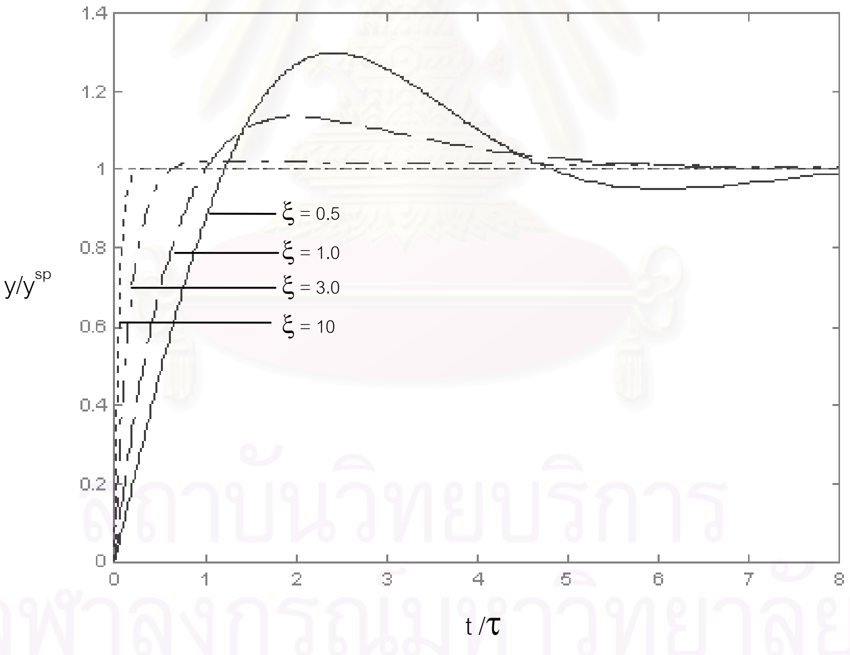


Figure A.1 - Generalized GMC profile specification.

The general form of GMC control algorithm can be written as

$$\dot{y} = K_1 (y^{sp} - y) + K_2 \int (y^{sp} - y)\,dt \qquad \text{(A.1)}$$

The value of two tuning constants, K_1 and K_2 are obtained using the following relationships:

$$K_1 = \frac{2\xi}{\tau}$$

$$K_2 = \frac{1}{\tau^2}$$

In tuning the GMC controller, because overshoot is undesirable, ξ is set to the expected value. After that the value of τ is obtained by examining the tuning charts given by Lee and Sullivan. In this work, six controllers are considered here to control the concentrations of three acid and three rinsing baths, then each tuning parameter are outlined as these follows.

Since there are two major steps in this process, the pickling step and the rinsing step, then each step is considered separately to evaluate the tuning parameters of GMC controller. The first one is the pickling step, as seen in the figure A.2, manipulated of the last acid tank, 15% HCl, is independent stream then this tank is the first one that be tuned to provide the desired set point. After that the 10% and 5% HCl tanks are tuned respectively.

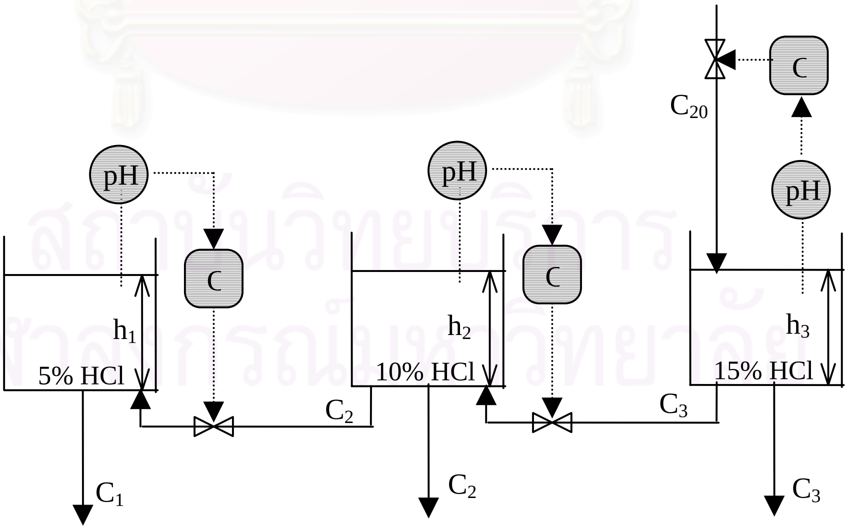


Figure A.2 - Flow diagram of pickling bath controls

1. 15% acid tank

In this tank, ξ and t are set to be 0.5 and 5, respectively then τ is evaluated from this relationship, $t = 1.37\,\tau$, as this follow.

$$t = 5 \text{ min. gives } \tau = \frac{5}{1.37} = 3.6496 \,,$$

$$K_1 = \frac{2 \times 0.5}{3.6496} = 0.274 \qquad \text{and} \qquad K_2 = \frac{1}{3.6496^{\,2}} = 0.075077$$

2. 10% acid tank

ξ is set to be 3 then the controlled variable shall cross the set point at approximately $0.8\,\tau$. The expected time to the desired trajectory is chosen at 4 minutes, then

$$t = 4 \text{ min. gives } \tau = \frac{4}{0.8} = 5 \,,$$

$$K_1 = \frac{2 \times 3}{5} = 1.2 \qquad \text{and} \qquad K_2 = \frac{1}{5^{2}} = 0.04$$

3. 5% acid tank

ξ is set to be 3, same as 10% acid tank then the expected time is also around $0.8\,\tau$. But the expected time to the desired trajectory is chosen at 4 minutes, then

$$t = 3.5 \text{ min. gives } \tau = \frac{3.5}{0.8} = 4.375 \,,$$

$$K_1 = \frac{2 \times 3}{4.375} = 1.37143 \qquad \text{and} \qquad K_2 = \frac{1}{4.375^{\,2}} = 0.05224$$

The pickling and the rinsing steps are considered separately, this is because each step is independent with each other then it is easier to evaluate the tuning parameters separately to provide the desired target. With the same consideration as the former step, the last rinsing tank is the first one to be tuned.

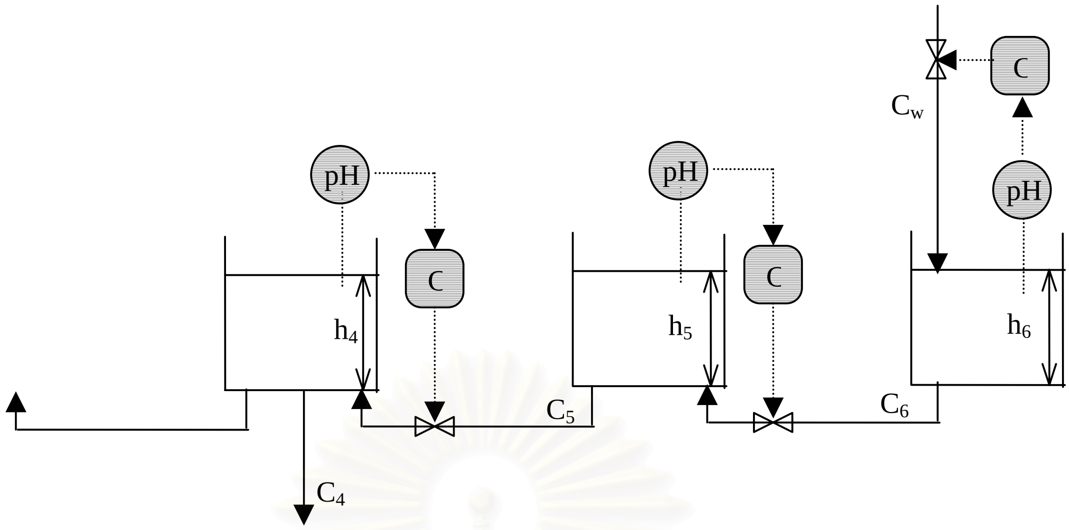


Figure A.3 - Flow diagram of rinsing bath controls

1. The 3rd rinsing tank

ξ is set to be 10 then the controlled variable shall cross the set point at approximately $0.25\,\tau$. The expected time to the desired trajectory is chosen at 100 minutes, then

$$t = 100 \text{ min. gives } \tau = \frac{100}{0.25} = 400\ ,$$

$$K_1 = \frac{2 \times 10}{400} = 0.05 \qquad \text{and} \qquad K_2 = \frac{1}{400^2} = 0.00000625$$

2. The 2nd rinsing tank

ξ is set to be 3 , from the figure A.1 time is approximated at $0.8\,\tau$. The expected time to the desired trajectory is chosen at 5 minutes, then

$$t = 5 \text{ min. gives } \tau = \frac{5}{0.8} = 6.25\ ,$$

$$K_1 = \frac{2 \times 3}{6.25} = 0.96 \qquad \text{and} \qquad K_2 = \frac{1}{6.25^2} = 0.0256$$

3. The 1st rinsing tank

Same as above, ξ and t are set to be 0.5 and 5, respectively then τ is evaluated from this relationship, $t = 1.37\,\tau$, as this follow.

$$t = 5 \text{ min. gives } \tau = \frac{5}{1.37} = 3.6496 \;,$$

$$K_1 = \frac{2 \times 0.5}{3.6496} = 0.274 \qquad \text{and} \qquad K_2 = \frac{1}{3.6496^{\,2}} = 0.075077$$

From equation (A.1), the first expression is to bring the process back to steady state due to change in ${dy}/{dt}$. The last expression is introduced in order to make the process have a zero offset. In this work, the appropriate values of the tuning parameters of each GMC controller to control the concentrations to the desired targets are presented above. With these parameters the control strategy is able to hold the process without offset.

Appendix B

LABORATORY PROCESS

It is important to show that the 1st principle model could provide an accurate representation of continuous steel pickling process before the project progressed to the control simulation. For this purpose, pilot plant of the continuous pickling process is designed and devised at an early stage of the project as seen in figure B.1.

Figure B.1 – Pilot plant for continuous steel pickling process

The moving direction of the workpieces is opposite to the process flow as described in section 4.1.1 (chapter IV). The physical constants for this plant and operating conditions are listed in Table B.1, B.2 and B.3, respectively.

Table B.1. Physical parameters

q = 0.0005 liter/min A = 0.0729 m^2 V = 14.945 liter	rate constant (k) = 0.003267 C_{20} = 6.034 mole/liter C_w = 5e-008 mole/liter

Table B.2. Initial values of concentrations

C_1^0 = 1.4 mole/liter	C_4^0 = 5.979e-008 mole/liter
C_2^0 = 2.87 mole/liter	C_5^0 = 5.979e-008 mole/liter
C_3^0 = 4.408 mole/liter	C_6^0 = 5.979e-008 mole/liter

Table B.3. Initial values of flow rates for experiment

F_1^0 = 1.3945 liter/min	F_7^0 = 1.25 liter/min
F_2^0 = 1.395 liter/min	F_8^0 = 1.25 liter/min
F_3^0 = 1.395 liter/min	F_9^0 = 0 liter/min
F_4^0 = 1.25 liter/min	F_{10}^0 = 0 liter/min
F_5^0 = 0.145 liter/min	F_{11}^0 = 0 liter/min
F_6^0 = 1.25 liter/min	

In this case the determination of acid concentrations in hydrochloric acid pickling solutions iss carried out by acid-base titration, whereas pH values of rinsing water are monitored via using a pH electrode along with a pH meter. For acid-base titration, two or three drops of methyl orange indicator are added to 2 mL sample. A burette containing 0.5 M sodium hydroxide solution is used to titrate until the red color changes to yellow. The calculation follows from the stoichiometric relationships between the reactant and product.

$$C_{HCl}(\text{mole}/\text{liter}) = \frac{0.5 \times \text{NaOH(mL)}}{2}$$

Appendix C

COMPUTER SOURCE CODE

Some computer source codes for estimating the process variables using steady state and dynamic data reconciliation (DDR) are listed in this chapter. The first part shows basic calculation of general matrix that the source codes of the estimation are discussed later.

C.1. Basic calculation of matrix

```
procedure  CountRow ( Mat: StrMat; var row: integer ) ;
begin
        for n : = 0 to  410  do  begin
            try  StrToFloat ( Mat[n,0] ) ;
            except
            on  EAccessViolation   do  begin   Row := n;   exit;  end;
            on  EConvertError       do  begin   Row := n;   exit;  end;
            on  EMathError          do  begin   Row := n;   exit;  end;
            else  begin   Row := n;   exit;     end;
            end;
        end;
end;

procedure  CountColumn ( Mat: StrMat ; var column: integer ) ;
begin
        for  n := 0  to  410  do   begin
            try  StrToFloat( Mat[0,n] ) ;
            except
            on  EAccessViolation  do   begin   column := n;     exit;  end;
            on  EConvertError      do   begin   column := n;     exit;  end;
            on  EMathError          do   begin    column := n;     exit;  end;
            else   begin   column := n;     exit;   end;
            end;
        end;
end;
```

```
procedure   FindDet ( Mat: StrMat ; dimension: integer ; var  Det: real ) ;
var   procedure  DetOfThreeDimension ( Mat: StrMat ; var  Det: real ) ;
        var    Minor11, Minor12, Minor13: real ;
        begin
                Minor11 := [ StrToFloat( Mat[1,1] ) * StrToFloat( Mat[2,2] ) ]
                                - [ StrToFloat( Mat[2,1] ) * StrToFloat( Mat[1,2] ) ] ;
                Minor12 := [ StrToFloat( Mat[1,0] ) * StrToFloat( Mat[1,2] ) ]
                                - [ StrToFloat( Mat[2,0] ) * StrToFloat( Mat[2,2] ) ];
                Minor13 := [ StrToFloat( Mat[1,0] ) * StrToFloat( Mat[1,1] ) ]
                                - [ StrToFloat( Mat[2,0] ) * StrToFloat( Mat[2,1] ) ];
                Det := [ StrToFloat( Mat[0,0] ) * Minor11 ] – [ StrToFloat( Mat[0,1] ) *
                                Minor12 ] + [ StrToFloat( Mat[0,2] ) * Minor13 ] ;
        end;
begin
            case  dimension  of
            1:  Det := StrToFloat( Mat[0,0] ) ;
            2:  Det := [ StrToFloat( Mat[0,0] ) * StrToFloat( Mat[1,1] ) ]
                        - [ StrToFloat( Mat[0,1] ) * StrToFloat( Mat[1,0] ) ] ;
            3:  DetOfThreeDimension( Mat, Det ) ;
            else  begin     sum:=0;
                for  j := 0  to  (dimension-1)  do  begin
                    FindMinor( 0, j, Mat, Minor, DetMinor ) ;
                    sum := sum + ( StrToFloat( Mat[0,j] ) * power((-1),(2+j))*DetMinor) ;
                end;
                Det := sum ;    end;
            end;
end;

procedure FindInverseDiagonal(Mat:StrMat; dimension:integer;var InvMat:StrMat);
begin
        SetLength( InvMat, dimension ) ;
        for   i:=0   to   dimension-1   do   begin
            SetLength( InvMat[i], dimension ) ;
            for   j:=0   to   dimension-1   do
                if   i=j   then   InvMat[i,j] := FloatToStr( 1/StrToFloat( Mat[i, j] ) )
                else   InvMat[i,j] := FloatToStr(0) ;
        end;
end;
```

```
procedure FindMinor(a,b:integer;Mat:StrMat ; var Minor:StrMat;var DetMinor:real);
begin
    CountRow( Mat, row ) ;              CountColumn( Mat, column ) ;
    SetLength( Minor, row-1 ) ;         a1 := 0 ;
    for  i := 0  to  (row-1)  do  begin
      if  i <> a  then   begin              { Cut row }
        if  i = 0  then   SetLength( Minor[0], column-1 )
        else    SetLength( Minor[i-1], column-1 ) ;
        b1 := 0 ;
        for  j := 0   to   (column-1)   do   begin
          if  j <> b  then     begin     { Cut column }
            Minor[a1, b1] := Mat[i, j] ;           b1 := b1 + 1 ;
          end;
        end;
        a1 := a1 + 1 ;
      end;
    end;
    FindDet( Minor,row-1,DetMinor ) ;
end;


procedure   FindInverse( Mat:StrMat; dimension:integer; var InvMat:StrMat ) ;
begin
    FindDet(Mat,dimension,Det);         SetLength(InvMat,dimension);
    if   dimension = 1   then    begin
      SetLength(InvMat[0],dimension);
      if   Det <> 0   then   InvMat[0,0] := FloatToStr( 1/Det )
      else   InvMat[0,0] := FloatToStr(0)
    end   else
      for   i:=0   to   (dimension-1)   do    begin
        for   j:=0   to   (dimension-1)   do    begin
          SetLength( InvMat[j], dimension ) ;
          FindMinor( i, j, Mat, Minor, DetMinor ) ;
          num := power( -1, i+j+2 ) * DetMinor/Det ;
          InvMat[j,i] := FloatToStr( num ) ;
        end;
      end;
end;
```

```
procedure FindAdd( Mat1, Mat2:StrMat; row1, column1, row2, column2: integer;
                        var  Mat12: StrMat ) ;
begin
      SetLength( Mat12 , row1 ) ;
      if   row1 = row2    then    begin
         if  column1 <> column2   then  ShowMessage( 'Two Matrixs are not equal.' )
         else   begin
            for   i:=0   to   (row1-1)   do     begin
               SetLength(Mat12[i],column1);
               for   j:=0   to   (column1-1)   do    begin
                  num := StrToFloat( Mat1[i,j] ) + StrToFloat( Mat2[i,j] ) ;
                  Mat12[i,j] := FloatToStr( num ) ;
               end;
            end;
         end;
      end  else   ShowMessage( 'Two Matrixs are not equal.' ) ;
end;


procedure FindMinus( Mat1,Mat2: StrMat; row1,column1,row2,column2: integer;
                          var Mat12:StrMat ) ;
begin
      SetLength( Mat12, row1 ) ;
      if   row1 = row2    then  begin
         if  column1 <> column2  then  ShowMessage('Two Matrixs are not equal.')
         else   begin
            for   i:=0   to   (row1-1)   do     begin
               SetLength( Mat12[i], column1 ) ;
               for   j:=0   to (column1-1)   do     begin
                  num := StrToFloat( Mat1[i,j] ) - StrToFloat( Mat2[i,j] ) ;
                  Mat12[i,j] := FloatToStr( num ) ;
               end;
            end;
         end;
      end   else   ShowMessage( 'Two Matrixs are not equal.' ) ;
end;
```

```
procedure FindMulti(Mat1,Mat2:StrMat;row1,column1,row2,column2:integer;
                    var Mat12:StrMat);
begin
    SetLength( Mat12, row1 ) ;
    if  column1 <> row2  then
      ShowMessage('Column of Matrix 1 is not equal with row of Matrix 2')
    else  begin
      for  k:=0  to  (column2-1)  do begin
        for  i:=0  to  (row1-1)  do begin
          SetLength( Mat12[i], column2 ) ;          sum:=0;
          for  j:=0  to  (column1-1)  do
            sum := StrToFloat( Mat1[i,j] ) * StrToFloat( Mat2[j,k] ) + sum ;
          Mat12[i,k] := FloatToStr( sum ) ;
        end;
      end;
    end;
end;
```

```
procedure  FindTranpose( Mat: StrMat; row,column: integer; var TMat: StrMat ) ;
begin
    SetLength( TMat, column ) ;
    for  i:=0  to  (row-1)  do
      for  j:=0  to  (column-1)  do  begin
        SetLength( TMat[j], row ) ;
        TMat[j,i] := Mat[i,j] ;
      end;
end;
```

The procedures above are routines to access matrix calculation in the developed computer software. These are matured via using Delphi scheme that can be applied to other program with some transformation. Some computer source codes, which used for accomplishing steady state and dynamic data reconciliation technique, are listed in next section.

C.2. Data reconciliation algorithm

```
procedure   ProjectionMatrix( UMJacobian: StrMat; var  Projection: StrMat ) ;
begin
   SubProjection( Tunit ,NumUnMea, C1, C2 ) ;

   try    StrToFloat( C1[0,0] ) ;
   except
   on  EAccessViolation  do  begin
         FindUnitMat( TUnit, Projection );  exit;
   end;
   else   begin    FindUnitMat( TUnit, Projection ) ;     exit;    end;
   end;

   FindUnitMat( TUnit-NumUnMea, Umat ) ;

   if   ProcessStudy <>  'Pickling'    then
         FindInverse( C1, NumUnMea, InvC )
   else   FindInverseDiagonal( C1, NumUnMea, InvC ) ;

   FindMulti(C2,InvC,TUnit-NumUnMea,NumUnMea,NumUnMea,NumUnMea,P);
   SetLength( Proj, TUnit-NumUnMea ) ;

   for   i:=0   to   TUnit-NumUnMea-1   do   begin
      SetLength( Proj[i], Tunit ) ;
      for   j:=0   to   TUnit-1   do  begin
         if   j <   NumUnMea   then
               Proj[i,j] := FloatToStr((-1)*StrToFloat(P[i,j]))
         else   Proj[i,j] := UMat[i,j-NumUnMea] ;
      end;
   end;

   FindTranpose( Proj, TUnit-NumUnMea, TUnit, Projection ) ;
end;
```

```
procedure  SubProjection( row,column: integer; var  C1,C2: StrMat ) ;
begin
        try  StrToFloat( UMJacobian[0,0] ) ;
        except   on  EAccessViolation  do   exit;
                 on   EMathError        do   exit;
        else    exit;    end;
        if  column<row  then  begin          { Find C1 }
           For  i:=0  to  column-1  do  begin
               SetLength( C1, column ) ;              SetLength( C1[i], column ) ;
               For   j:=0   to   column-1   do   C1[i,j] := UMJacobian[i,j] ;
           end;
        end;
        n := row - column ;                           SetLength( C2, n ) ;
        For   i:=(row-n)   to (row-1)   do  begin
            SetLength( C2[i-row+n], column ) ;
            For   j:=0   to   column-1   do    C2[i-row+n,j] := UMJacobian[i,j] ;
        end;
end;


procedure SteadyDataReconciliation( AAA, BBB, CCC, MeaX: StrMat ;
                                                     var  Xest, UAest: StrMat ) ;
begin
{Find projection matrix}
    ProjectionMatrix( BBB, Projection ) ;

{Eliminate un-known variable}
    FindTranpose( Projection, TUnit, TUnit-NumUnMea, Tprojection ) ;
    FindMulti( TProjection,AAA,TUnit-NumUnMea,TUnit,TUnit,NumMea,MatA ) ;
    FindMulti( TProjection, CCC, TUnit-NumUnMea, TUnit, TUnit, 1, MatC ) ;

{Find inter-covariance}
    FindUnitMat( NumMea, MeaCov ) ;
    FindTranpose( MatA, TUnit-NumUnMea, NumMea, TMatA ) ;
    FindMulti( MatA, MeaCov, TUnit-NumUnMea, NumMea, NumMea,
                    NumMea, MatAEstCov ) ;
    FindMulti( MatAEstCov, TMatA, TUnit-NumUnMea, NumMea, NumMea,
                    TUnit-NumUnMea, InterCov ) ;
```

```
   FindInverse( InterCov, TUnit-NumUnMea, InvInterCov ) ;

{Find function}
   FindMulti( MatA, MeaX, TUnit-NumUnMea, NumMea, NumMea, 1, MatAX_k ) ;
   FindMinus( MatC, MatAX_k, TUnit-NumUnMea, 1, TUnit-NumUnMea, 1, Fn ) ;

{ reconcile Mea variables_k }
   FindMulti( MeaCov, TMatA, NumMea, NumMea, NumMea, TUnit-NumUnMea,
                  EstCovTMatA ) ;
   FindMulti( EstCovTMatA, InvInterCov, NumMea, TUnit-NumUnMea,
                  TUnit-NumUnMea, TUnit-NumUnMea, EstCovInterCov ) ;
   FindMulti( EstCovInterCov, Fn, NumMea, TUnit-NumUnMea,TUnit-NumUnMea,
                  1, AddX_k ) ;
   FindAdd( MeaX, AddX_k, NumMea, 1, NumMea, 1, Xest ) ;

{ estimate un-mea variable }
   if   NumUnMea  <> 0   then   begin
      { FFn =(CCC-AAA*Xest) }
      FindMulti( AAA, Xest, TUnit, NumMea, NumMea, 1, Ffnpart ) ;
      FindMinus( CCC, FFnpart, TUnit, 1, TUnit, 1, FFn ) ;

      { Uest_k = inv(TBBB*BBB)*TBBB*FFn}
      FindTranpose( BBB, TUnit, NumUnMea, TBBB ) ;
      FindMulti( TBBB, BBB, NumUnMea, TUnit, TUnit, NumUnMea, TBB ) ;
      FindInverse( TBB, NumUnMea, InvTBB ) ;
      FindMulti( InvTBB, TBBB, NumUnMea, NumUnMea, NumUnMea, TUnit,
                     InvTBTB ) ;
      FindMulti( InvTBTB, FFn, NumUnMea, TUnit, TUnit, 1, UAest ) ;
   end;
end;
```

```
procedure  DataReconciliation( it:integer; EEE, AAA, BBB, CCC, DDD, X_k1,
                    X_k, parameter_k, EstCov: StrMat;  var  Xest_k1, Xest_k,
                    UAest_k, Estparameter, NewEstCov: StrMat ) ;
begin
{Find projection matrix}
   ProjectionMatrix( BBB, Projection ) ;

{Eliminate un-known variable}
   FindTranpose( Projection, TUnit, TUnit-NumUnMea, TProjection ) ;
   FindMulti( TProjection, EEE, TUnit-NumUnMea, TUnit, TUnit, NumMea, MatE);
   FindMulti( TProjection, AAA, TUnit-NumUnMea, TUnit, TUnit,NumMea,MatA);
   FindMulti( TProjection, CCC, TUnit-NumUnMea, TUnit, TUnit, 1, MatC ) ;
   FindMulti( TProjection, DDD, TUnit-NumUnMea, TUnit, TUnit,
               NumParameter, MatD ) ;

{Find inter-covariance}
{InterCov=(MatA*EstCov*TMatA)+(MatE*MeaCov*TMatE)}
   FindUnitMat( NumMea, MeaCov ) ;
   FindTranpose( MatA, TUnit-NumUnMea, NumMea, TMatA ) ;
   FindTranpose( MatE, TUnit-NumUnMea, NumMea, TMatE ) ;
   FindMulti( MatA, EstCov, TUnit-NumUnMea, NumMea, NumMea,
               NumMea, MatAEstCov ) ;
   FindMulti( MatAEstCov, TMatA, TUnit-NumUnMea, NumMea, NumMea,
               TUnit-NumUnMea, part1 ) ;
   FindMulti( MatE, MeaCov, TUnit-NumUnMea, NumMea, NumMea,
               NumMea, MatEMeaCov ) ;
   FindMulti( MatEMeaCov, TMatE, TUnit-NumUnMea, NumMea, NumMea,
               TUnit-NumUnMea, part2 ) ;
   FindAdd( part1,part2,TUnit-NumUnMea,TUnit-NumUnMea,TUnit-NumUnMea,
               TUnit-NumUnMea,InterCov ) ;

{Find function}
{Fn=(MatE*X_k1)-MatC-(MatA*X_k)}
   FindMulti( MatE,X_k1, TUnit-NumUnMea, NumMea, NumMea, 1, MatEX_k1 ) ;
   FindMulti( MatA, X_k, TUnit-NumUnMea, NumMea, NumMea, 1, MatAX_k ) ;
   FindMinus( MatEX_k1, MatC, TUnit-NumUnMea, 1, TUnit-NumUnMea,1,ppart);
   FindMinus( ppart, MatAX_k, TUnit-NumUnMea, 1, TUnit-NumUnMea, 1 , Fn );
```

```
{parameter estimation}
{par_est=par_+inv(TMatD*InvInterCov*MatD)*TMatD*InvInterCov*Fn}
   FindInverseDiagonal( InterCov, TUnit-NumUnMea, InvInterCov ) ;
   if   NumParameter   <>   0     then   begin
      if   it=0   then    Estparameter := parameter_k
      else    begin
         FindTranpose( MatD, TUnit-NumUnMea, NumParameter, TMatD ) ;
         FindMulti( TMatD, InvInterCov, NumParameter, TUnit-NumUnMea,
                        TUnit-NumUnMea, TUnit-NumUnMea, TDInvCov ) ;
         FindMulti( TDInvCov, MatD, NumParameter, TUnit-NumUnMea,
                        TUnit-NumUnMea, NumParameter, InterInv ) ;
         FindInverse( InterInv, NumParameter, InvInterInv ) ;
         FindMulti(InvInterInv,TMatD,NumParameter,NumParameter,NumParameter
                        ,TUnit-NumUnMea,InvTMatD);
         FindMulti( InvTMatD, InvInterCov, NumParameter, TUnit-NumUnMea,
                        TUnit-NumUnMea, TUnit-NumUnMea, InvInv ) ;
         FindMulti(InvInv,Fn,NumParameter,TUnit-NumUnMea,TUnit-NumUnMea,
                        1,AddFn);
         FindAdd( parameter_k, AddFn, Numparameter, 1, Numparameter, 1 ,
                        Estparameter ) ;
      end;
   end;

{ reconcile Mea variables_k }
{ Xest_k = X_k +EstCov*TMatA*InvInterCov*Fn }
   FindMulti( EstCov, TMatA, NumMea, NumMea, NumMea, TUnit-NumUnMea,
                  EstCovTMatA ) ;
   FindMulti( EstCovTMatA, InvInterCov, NumMea, TUnit-NumUnMea,
                  TUnit-NumUnMea, TUnit-NumUnMea, EstCovInterCov ) ;
   FindMulti( EstCovInterCov,Fn,NumMea,TUnit-NumUnMea,TUnit-NumUnMea,
                  1,AddX_k ) ;
   FindAdd( X_k, AddX_k, NumMea, 1, NumMea, 1, Xest_k ) ;

{ reconcile Mea variables_k1 }
{ Xest_k1 = X_k1 -MeaCov*TMatE*InvInterCov*Fn }
   FindMulti( MeaCov, TMatE, NumMea, NumMea, NumMea, TUnit-NumUnMea,
                  MeaCovTMatE ) ;
```

```
 FindMulti( MeaCovTMatE, InvInterCov, NumMea, TUnit-NumUnMea,
               TUnit-NumUnMea, TUnit-NumUnMea, MeaCovInterCov ) ;
 FindMulti(MeaCovInterCov,Fn,NumMea,TUnit-NumUnMea,TUnit-NumUnMea,
               1,AddX_k1);
 FindMinus( X_k1, AddX_k1, NumMea, 1, NumMea, 1, Xest_k1 ) ;

{ estimate un-mea variable }
 if   NumUnMea  <>  0     then   begin
    { FFn =(EEE*X_k1-AAA*X_k-CCC) }
    FindMulti( EEE, X_k1, TUnit, NumMea, NumMea, 1, FFnpart1 ) ;
    FindMulti( AAA, X_k, TUnit, NumMea, NumMea, 1, FFnpart2 ) ;
    FindMinus( FFnpart1, FFnpart2, TUnit,1, TUnit, 1, FFnpart ) ;
    FindMinus( FFnpart, CCC, TUnit, 1, TUnit, 1, FFn ) ;

    { Uest_k = inv(TBBB*BBB)*TBBB*FFn}
    FindTranpose( BBB, TUnit, NumUnMea, TBBB ) ;
    FindMulti(TBBB,BBB,NumUnMea,TUnit,TUnit,NumUnMea,TBB);
    FindInverseDiagonal(TBB,NumUnMea,InvTBB);
    FindMulti(InvTBB,TBBB,NumUnMea,NumUnMea,NumUnMea,TUnit,
                  InvTBTB);
    FindMulti(InvTBTB,FFn,NumUnMea,TUnit,TUnit,1,UAest_k);
 end;

{ calculate new covariance }
{ NewEstCov = MeaCov - MeaCov*TMatE*InvInterCov*MatE*MeaCov}
FindMulti(MeaCovInterCov,MatE,NumMea,TUnit-NumUnMea,TUnit-NumUnMea,
              NumMea,MMMatE);
FindMulti(MMMatE,MeaCov,NumMea,NumMea,NumMea,NumMea,AddMeaCov);
FindMinus( MeaCov, AddMeaCov, NumMea, NumMea, NumMea, NumMea,
              NewEstCov ) ;
end;
```

Appendix D

DATA RECONCILIATION PROGRAM MANUAL

Data reconciliation program is the example software, which developed here for students of chemical engineering to more understanding the main role of data reconciliation as estimator to chemical process plant in both cases of steady state and dynamic conditions. Users proceed the program by adding just needed information of considered process such as set point and initial values, tuning parameter etc. In this chapter, user guide of this program is mentioned briefly for easy access. As seen in figure D.1, it shows main window of this program. It is clear that Generic Model Control (GMC) integrated with data reconciliation is applied here to control the interested process in which four examples are considered in this program as following:

1. Exothermic batch reactor
2. Pervaporative membrane reactor
3. Steel pickling process
4. Steady state flow system

The first three processes are simulated under the dynamic conditions to explain the application of dynamic data reconciliation as stated before in Chapter IV. The last one is exemplified to illustrate the efficiency of the proposed control strategy in case of steady state.

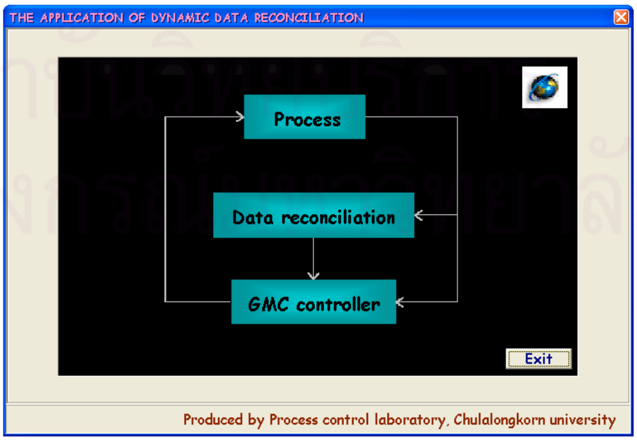


Figure D.1 – Main window

By this reason, the developed program is divided into four main sections according to the four interested processes as stated above. The users can select the process as needed by right click of the mouse button on process button in main window of this program as seen in figure D.2.

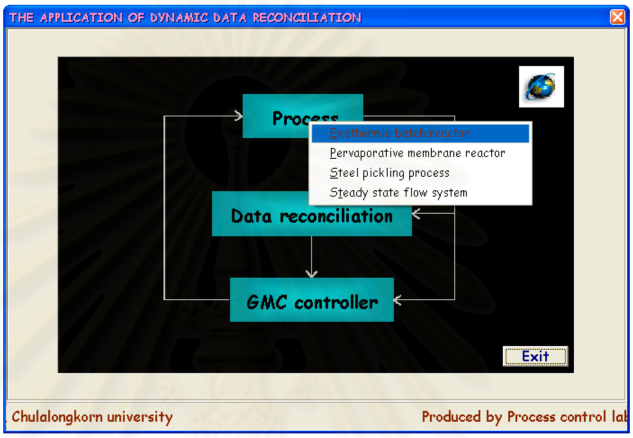


Figure D.2 – Selecting the process

By the reason of completely different window of each process, this chapter is also divided into four major sections according to the four examples in the program. Each section is presented in a step-by-step manner including of nominal case and other tests, for example parameter and model mismatch, disturbance case. The simulation results are performed in dynamic charts and also in sense of Integral Absolute Error (IAE) and Integral Square Error (ISE) values.

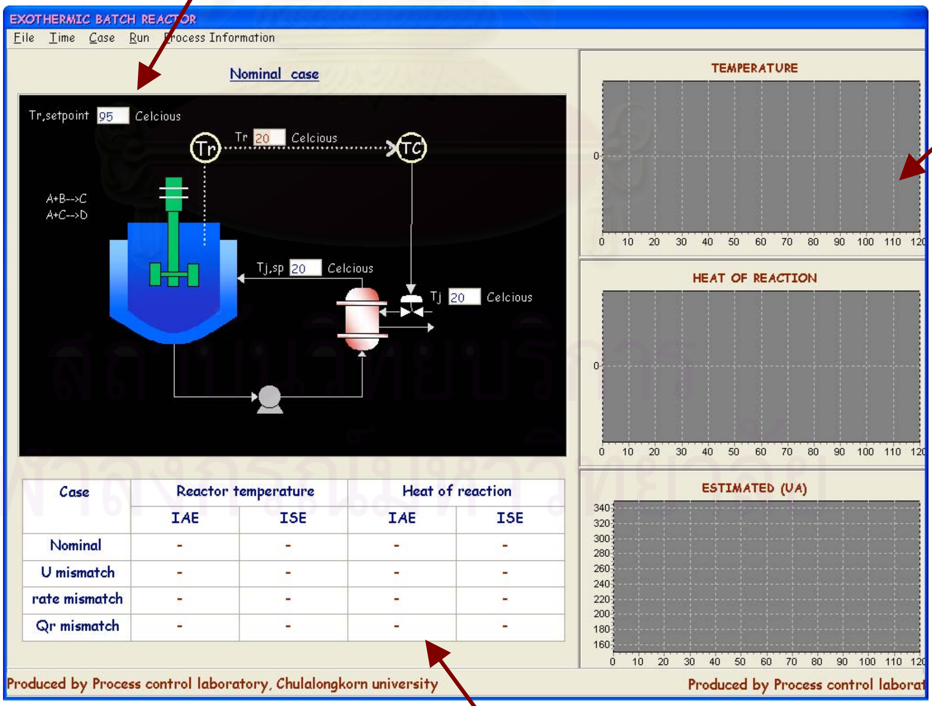
For the first three examples, the users can not change all properties of reactor and components but for the last one, the steady state flow system, the configuration of flow system can be designed differently depend on the users. Each flow can be either measured or unmeasured then the estimated values of flow rates are shown in result table in which the users can see in the fourth section of this chapter.

1. Exothermic batch reactor

As seen in figure D.2, exothermic batch reactor (Cott and Macchietto, 1989) is selected here to focus process performances. Figure D.3 shows window of the exothermic batch reactor case of this program. Two reactions that are occurred in this process are assumed to be well-mixed liquid phase system as seen in picture. Component C is a desired product while D is an unwanted by product. The optimal reactor temperature that provides the maximum desired product is 95°C as seen in default value.

The reactor temperature (T_r) is controlled as desired value via adjusting the jacket temperature (T_j) for moving the controlled state toward its set point with regarding jacket dynamic (Liptak, 1986). Dynamic data reconciliation algorithm is used for evaluating unmeasured heat released by reaction and reconciling measured temperatures; T_r and T_j, after that these estimates are sent to advanced controller, Generic Model Control (GMC) to handle the process as desired target.

Process diagram



Tr,setpoint 95 Celcious

Tr 20 Celcious

Tj,sp 20 Celcious

Tj 20 Celcious

Case	Reactor temperature		Heat of reaction	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
U mismatch	-	-	-	-
rate mismatch	-	-	-	-
Qr mismatch	-	-	-	-

Process chart

IAE & ISE table

Figure D.3 – Exothermic batch reactor window

As seen in the figure D.3, there are three major parts in the exothermic batch reactor window. Firstly, process diagram shows control configuration of the process, at the same time some information is defined by users. Secondly, simulation results display in process chart. Temperature chart shows reactor, desired reactor, and jacket, desired jacket temperatures. Heat of reaction chart shows the actual and estimated heat released by reaction and the last one displays the actual and estimated UA (the multiple of heat transfer coefficient, U, and reactor area, A) in case of the heat transfer coefficient change. And the last part shows IAE and ISE of the controlled reactor temperature and the estimated heat released by reaction in any cases. Then, the users can change just only in the first part which is outlined next below.

The process parameters and variables are set at their default values so that the users can immediately accomplish the simulation without changing. But if the users want to study in the other case, the following suggestion will guide the users for optimal proceeding.

1.1. Process input

The first step in building the process simulation is the definition of set point and initial values of process variables.

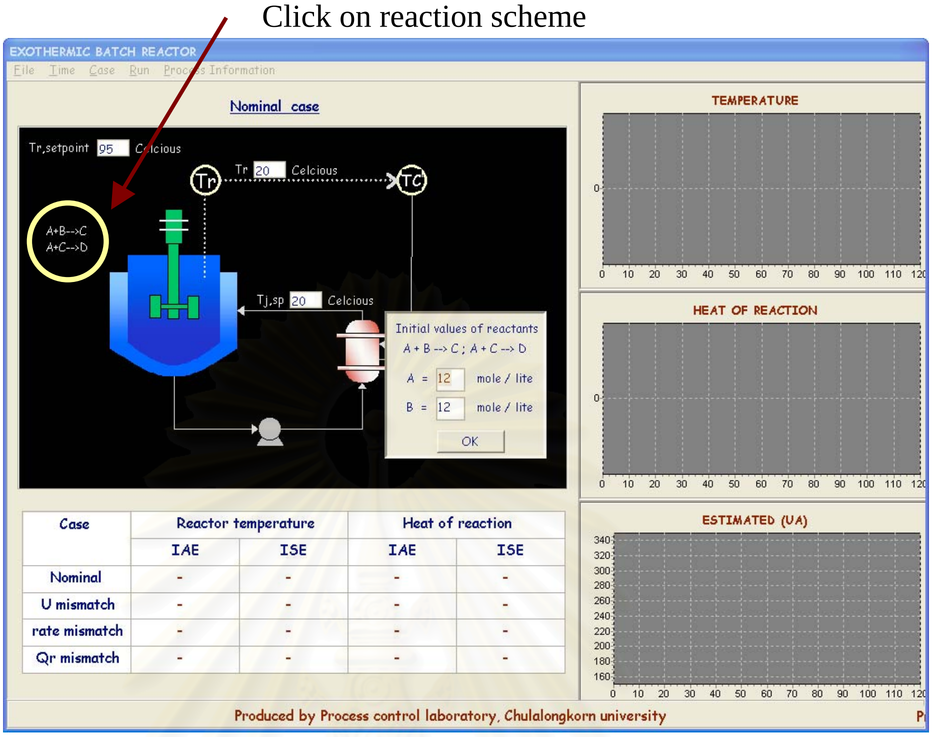
Temperature

It is clear that the users can define the set point of reactor temperature and the initial values of other temperatures directly on the process diagram as seen in figure D.3. For this system, the optimal reactor temperature falls in the range 90.0 – 100.0 °C then the desired temperature is limited in this range. For the other temperatures, they are limited to the range 20.0 – 120.0 °C.

Material

To specify the initial values of reactants:

1. Click on reaction scheme at the left side of the process diagram, and the input initial value of reactant view appears.
2. Change the initial values of component A and B, for this case the initial value of component C is set to be zero.



Click on reaction scheme

EXOTHERMIC BATCH REACTOR

Tr,setpoint 95 Celcious

Tr 20 Celcious

Tj,sp 20 Celcious

Initial values of reactants
A + B --> C ; A + C --> D
A = 12 mole / lite
B = 12 mole / lite

Case	Reactor temperature		Heat of reaction	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
U mismatch	-	-	-	-
rate mismatch	-	-	-	-
Qr mismatch	-	-	-	-

Produced by Process control laboratory, Chulalongkorn university

As seen in figure, the default initial values of reactants are 12 mole/lit for both component A and B.

3. Click the **OK** button to close the view and return to the process view.

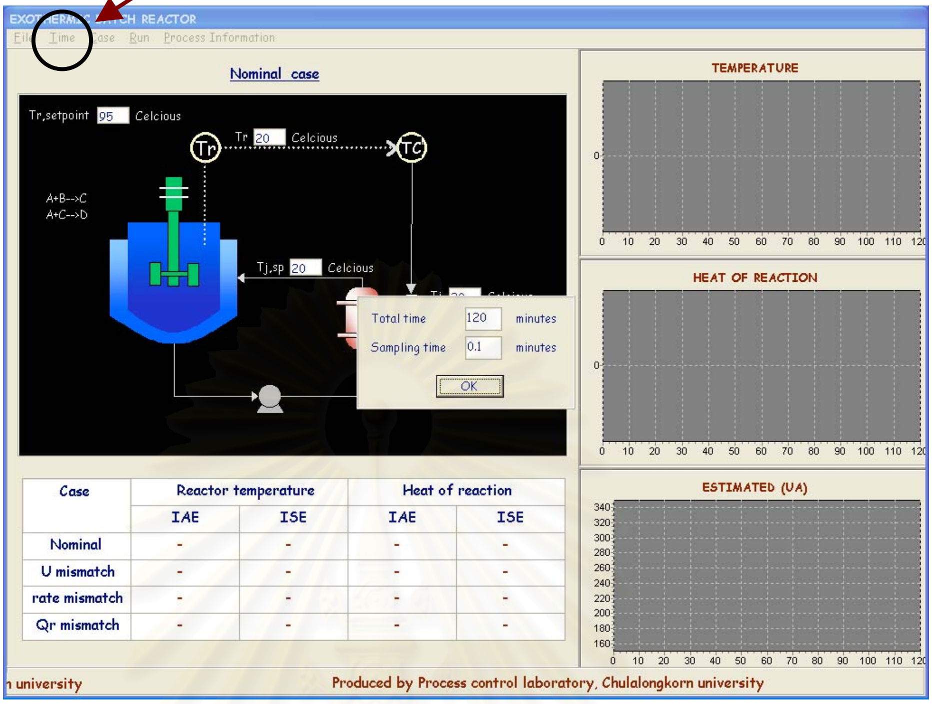
1.2. Control input

The next step is to set the parameter and variable values of the controller. For this program, the initial values of the controller and the estimator are set to be equal to of process input. This is because the convenience of the users.

Time

To specify the total and sampling time of the simulation:

1. Click on the **Time** menu to open the input time view.



Click on the **Time** menu

Tr,setpoint 95 Celcious

Tr 20 Celcious

Tj,sp 20 Celcious

Total time 120 minutes

Sampling time 0.1 minutes

Case	Reactor temperature		Heat of reaction	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
U mismatch	-	-	-	-
rate mismatch	-	-	-	-
Qr mismatch	-	-	-	-

The default values of total time and sampling time are 120 and 0.1 minutes, respectively.

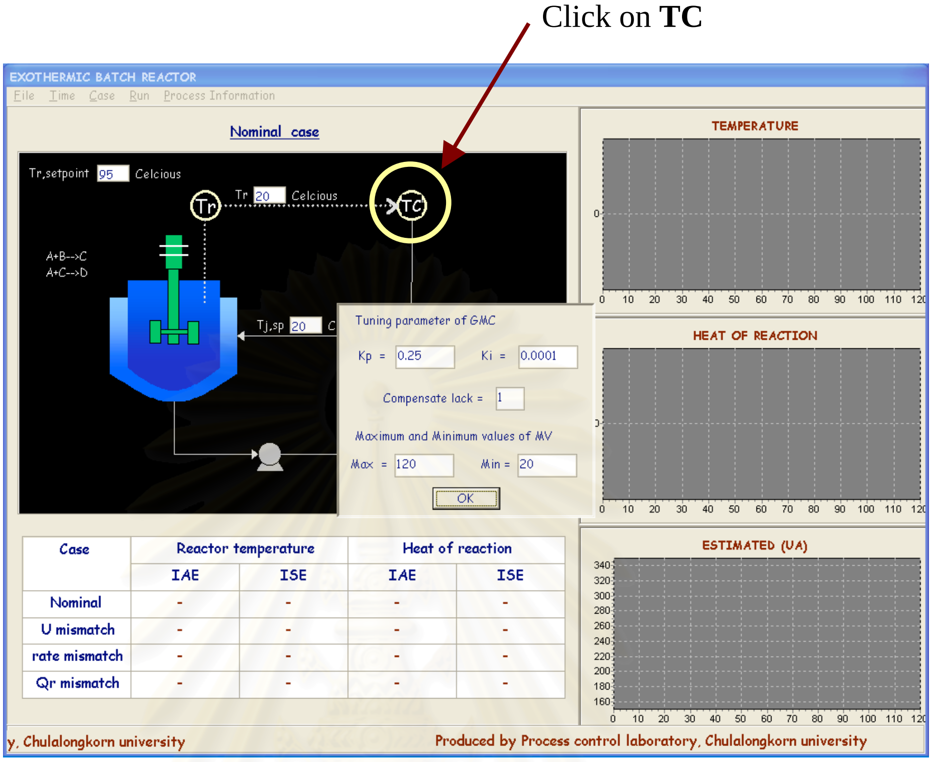
2. Set total time and sampling time for simulating this process.
3. Click the **OK** button to close the view and return to the process view.

Controller parameters and variables

To specify tuning parameters, compensate lack, maximum and minimum values of manipulated variable:

1. Move the mouse on the **TC** (Temperature Control) which is on the process diagram, hand cursor will be appeared, and click on it to open the input controller parameter view.
2. Enter the following values:
    - Tuning parameters, K_p and K_i of GMC controller, they are set at 0.25 and 0.0001 as default values, respectively.
    - Compensate lack, to eliminate the sluggish control performance resulted the jacket dynamic, it is set at 1 as default value.
    - Maximum and minimum values of the manipulated variable, they are set at 120 and 20°C as default values.

Click on **TC**



Tr,setpoint 95 Celcious

Tr 20 Celcious

Tj,sp 20

Tuning parameter of GMC

Kp = 0.25 Ki = 0.0001

Compensate lack = 1

Maximum and Minimum values of MV

Max = 120 Min = 20

Case	Reactor temperature		Heat of reaction	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
U mismatch	-	-	-	-
rate mismatch	-	-	-	-
Qr mismatch	-	-	-	-

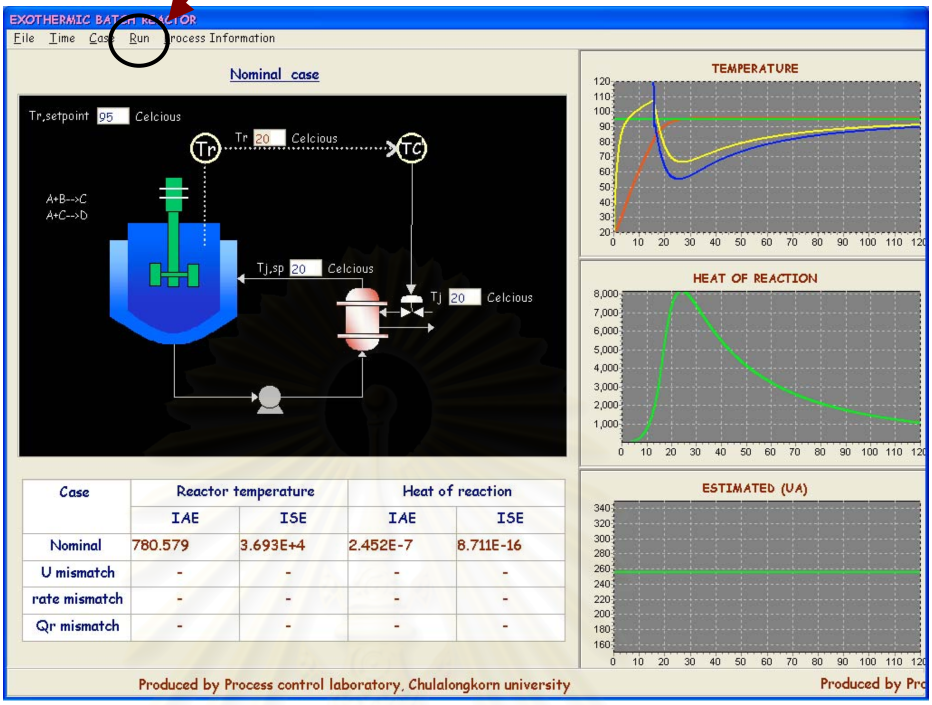
3. Click the **OK** button to close the view and return to the process view.

1.3. Run

Nominal case

To run the simulation in nominal case:

1. Click on the **Case** menu and select the **Nomimal case**, it will appear right mark in front of the context to ensure that the program is concentrating in nominal case.
2. Click on the **Run** menu to simulate the process.



Click on **Run** menu

Case	Reactor temperature		Heat of reaction	
	IAE	ISE	IAE	ISE
Nominal	780.579	3.693E+4	2.452E-7	8.711E-16
U mismatch	-	-	-	-
rate mismatch	-	-	-	-
Qr mismatch	-	-	-	-

While the program is simulating the process in nominal case, the charts will be moving along the actual trajectory as shown in figure. At the same time, IAE and ISE are calculated through the simulation. These values are shown in the table as seen in the window. As seen in the results, it is found that the process trajectories, IAE and ISE are similar as in chapter IV.

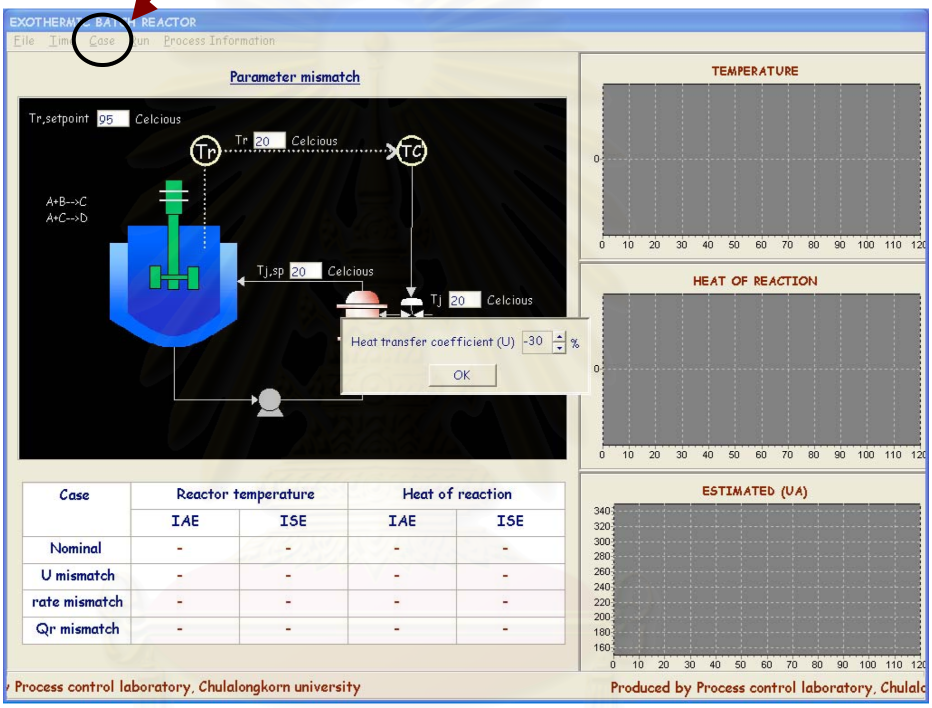
Parameter mismatch

Now that the exothermic batch reactor has been simulated in nominal case, the next step is to test robustness of this control strategy in parameter mismatch. In this system, the interested parameter is the heat transfer coefficient then this program focus only on this parameter change:

1. Click on the **Case** menu and move to the **Other case**.
2. Select the **Parameter mismatch**, then the input mismatch view appears for receiving the percentage of the heat transfer coefficient (U) change as shown below.

For this program the parameter change is limited to the range –30% to +30% from the actual value (the users can view the actual value by selecting the **Process Information** menu). As the example in Chapter IV, the percentage of this parameter change is changed to be –30% here.

Click on **Case** menu and select **Parameter mismatch**



Tr,setpoint 95 Celcious

Tr 20 Celcious

Tj,sp 20 Celcious

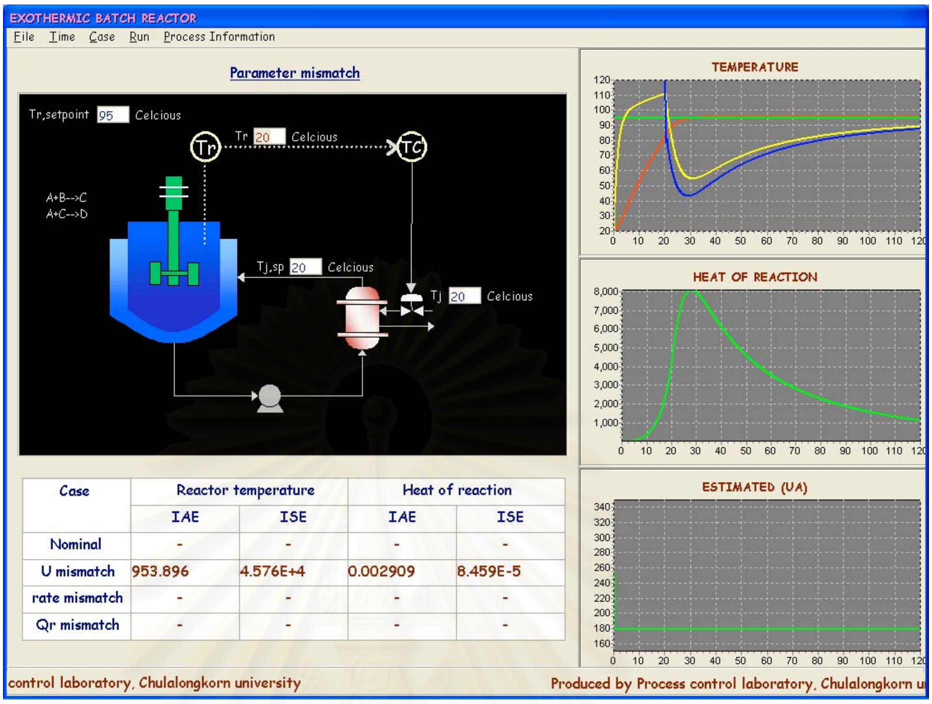
Tj 20 Celcious

Heat transfer coefficient (U) -30 %

Case	Reactor temperature		Heat of reaction	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
U mismatch	-	-	-	-
rate mismatch	-	-	-	-
Qr mismatch	-	-	-	-

3. Close the input parameter mismatch view to return to the process view.
4. Click on the **Run** menu to simulate the process.

It is also found that the simulation results in this case are not different from the results in Chapter IV. It points out that this program is work for studying the performance of this process.



Parameter mismatch

Tr,setpoint 95 Celcious

Tr 20 Celcious

Tj,sp 20 Celcious

Tj 20 Celcious

Case	Reactor temperature		Heat of reaction	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
U mismatch	953.896	4.576E+4	0.002909	8.459E-5
rate mismatch	-	-	-	-
Qr mismatch	-	-	-	-

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Produced by Process control laboratory, Chulalongkorn u

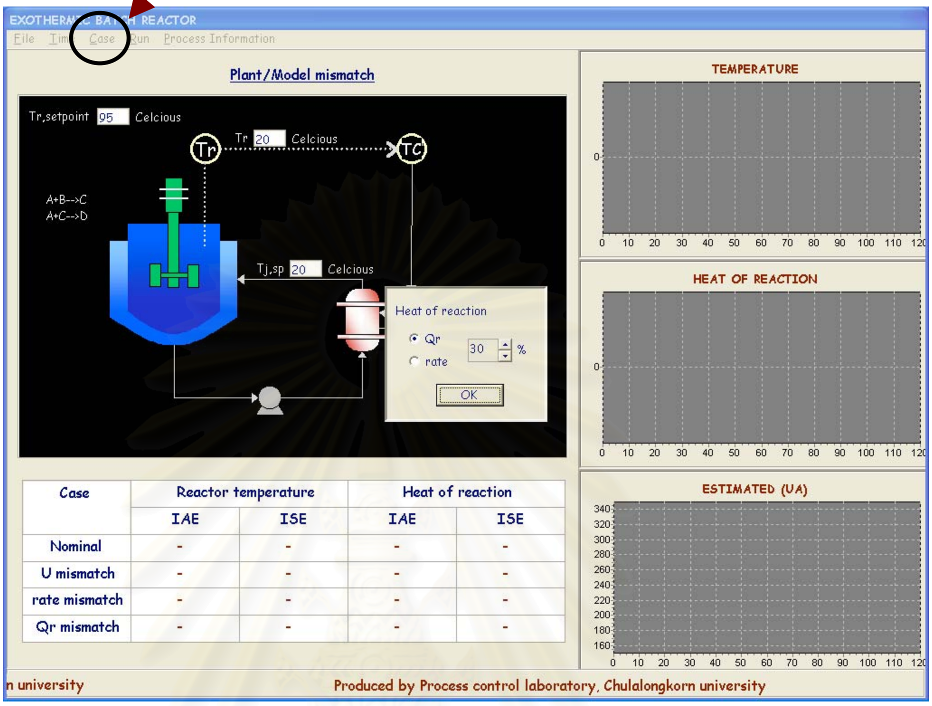
<u>Plant/Model mismatch</u>

The case of plant/model mismatch is considered now, this test also shows the robustness of the control strategy. For this process, the change of two variables is studied in this case as stated before in Chapter IV. The first one is the heat released by reaction (Qr) and the last one is the reaction rate (rate) occurred in the reactor.

1. Click on the **Case** menu and move to the **Other case**.
2. Select the **Plant/model mismatch**, then the input mismatch view appears for receiving the percentage of the change as shown below.

For this program the variable change is limited to the range –30% to +30% from the actual value (the users can view the actual value by selecting the **Process Information** menu).

Click on **Case** menu and select **Plant/model mismatch**



Plant/Model mismatch

Tr,setpoint 95 Celcious

Tr 20 Celcious

Tj,sp 20 Celcious

Heat of reaction

● Qr 30 %

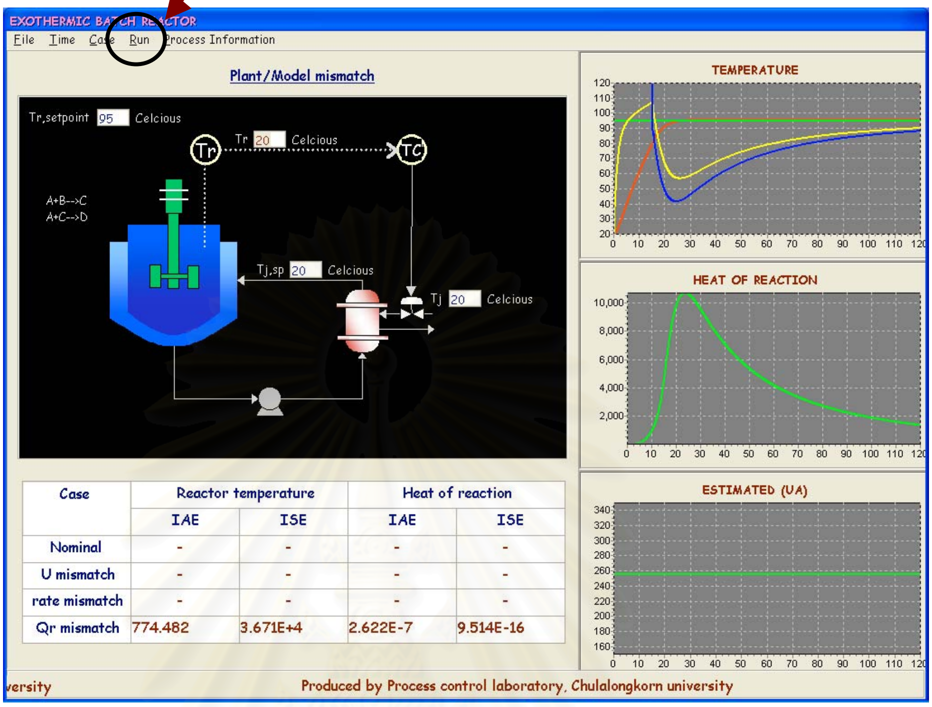
○ rate

Case	Reactor temperature		Heat of reaction	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
U mismatch	-	-	-	-
rate mismatch	-	-	-	-
Qr mismatch	-	-	-	-

3. Select the considered variable, the heat released by the reaction (Qr) is selected here as example, and change the percentage of the mismatch.
4. Click on the **OK** button to close the input view and return to the process window.
5. Click on the **Run** menu to simulate the process.

If the users want to study in case of the reaction rate change, the users just repeat steps 1 and 2 to open the input mismatch view. But in step 3, the reaction rate (rate) has to been selected and replaced the percentage as wanted. After that the instructions steps 4 and 5 are repeated.

Click on **Run**



Tr,setpoint 95 Celcious

Tr 20 Celcious

Tj,sp 20 Celcious

Tj 20 Celcious

Case	Reactor temperature		Heat of reaction	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
U mismatch	-	-	-	-
rate mismatch	-	-	-	-
Qr mismatch	774.482	3.671E+4	2.622E-7	9.514E-16

1.4. Other

From the menu bar, it can be seen that there are still two menu buttons that are not mentioned before such as the **File** menu and the **Process Information** menu. The prior one is used for clearing and closing the current window, the last one gives the information of the considered process.

Menu File

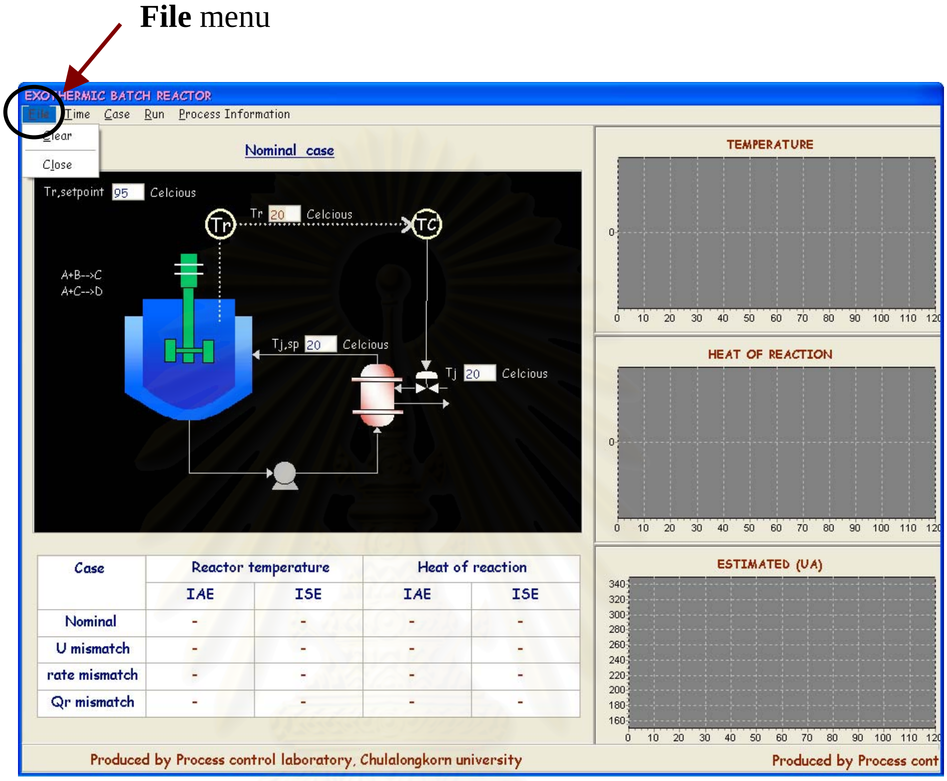
This menu button contains two submenus such as the Clear menu and the Close menu as seen in the figure.

1. The **Clear** menu

This submenu is used for clearing all prior simulation results and retun all values to the default values.

2. The **Close** menu

This one is used for closing the current process window and return to the main window for new process selection.



File menu

Tr,setpoint 95 Celcious

Tr 20 Celcious

Tj,sp 20 Celcious

Tj 20 Celcious

Case	Reactor temperature		Heat of reaction	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
U mismatch	-	-	-	-
rate mismatch	-	-	-	-
Qr mismatch	-	-	-	-

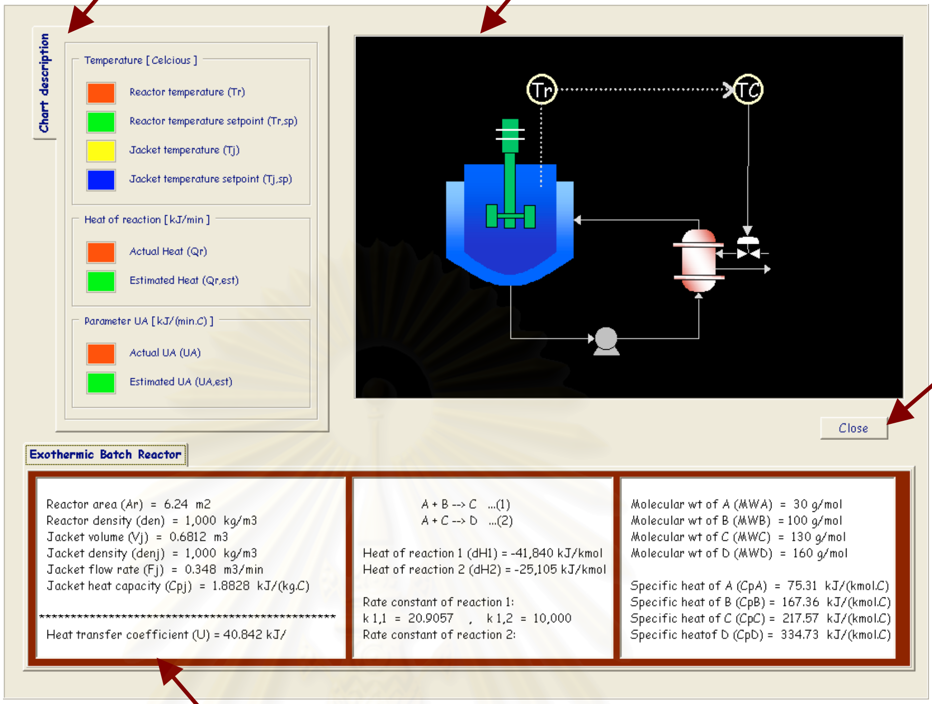
Process Information

This menu button gives the important information of the current process, for example the properties of the reactor and the materials, chart description. In case of parameter mismatch, the initial value of the process parameter can be found in this window.

1. Click on the Process Information menu to open the view of process information.
2. As seen in the process information window, there are three parts in this view.
    - The first one is a process diagram to describe the process control configuration.
    - The second is the chart description to inform the meaning of each line in the charts.
    - The last one is the properties of reactor and materials to display details of the process.

Chart description

Process diagram



Reactor area (Ar) = 6.24 m2
Reactor density (den) = 1,000 kg/m3
Jacket volume (Vj) = 0.6812 m3
Jacket density (denj) = 1,000 kg/m3
Jacket flow rate (Fj) = 0.348 m3/min
Jacket heat capacity (Cpj) = 1.8828 kJ/(kg.C)
****
Heat transfer coefficient (U) = 40.842 kJ/

A + B --> C ...(1)
A + C --> D ...(2)

Heat of reaction 1 (dH1) = -41,840 kJ/kmol
Heat of reaction 2 (dH2) = -25,105 kJ/kmol

Rate constant of reaction 1:
k 1,1 = 20.9057 , k 1,2 = 10,000
Rate constant of reaction 2:

Molecular wt of A (MWA) = 30 g/mol
Molecular wt of B (MWB) = 100 g/mol
Molecular wt of C (MWC) = 130 g/mol
Molecular wt of D (MWD) = 160 g/mol

Specific heat of A (CpA) = 75.31 kJ/(kmol.C)
Specific heat of B (CpB) = 167.36 kJ/(kmol.C)
Specific heat of C (CpC) = 217.57 kJ/(kmol.C)
Specific heatof D (CpD) = 334.73 kJ/(kmol.C)

Close button

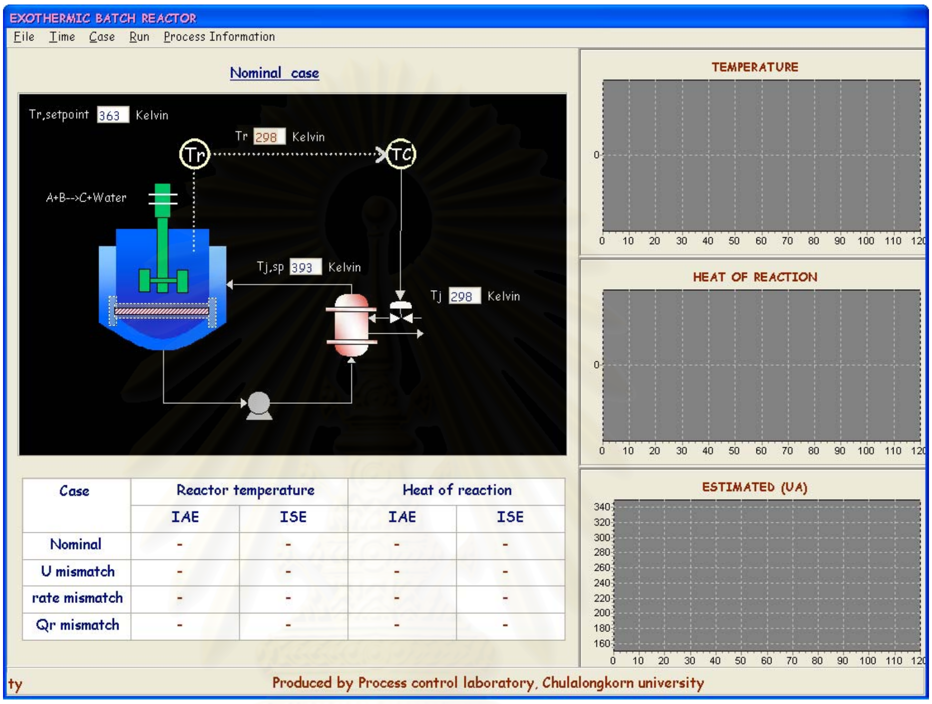
Process properties

3. Click on the **Close** button to close this view.

2. Pervaporative membrane reactor

From the figure D.2, pervaporative membrane reactor (Feng and Huang, 1996) is selected now to study process performance. The esterification of acetic acid with n-butanol in the presence of Zr(SO4)2 developed by Liu et at.(2001) is considered in this system. Butyl acetate (denoted as C) is a desired product and water needs to be removed via the membrane. The optimal temperature for this system is at 363 K then the temperature of the pervaporative membrane reactor (Tr) is handled at this value by adjusting a jacket temperature (Tj).

The jacket temperature is assumed to be limited to the range 298 – 393 K because of the heat-exchange capacities. Here, heat released by the reaction is also estimated via data reconciliation algorithm and GMC is implemented to control reaction temperature. As stated in the exothermic batch reactor, some form of dynamic compensation of the jacket temperature (Liptak, 1986) must be also used to provide a jacket temperature set point (Tj,sp).



Tr,setpoint 363 Kelvin

Tr 298 Kelvin

Tj,sp 393 Kelvin

Tj 298 Kelvin

Case	Reactor temperature		Heat of reaction	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
U mismatch	-	-	-	-
rate mismatch	-	-	-	-
Qr mismatch	-	-	-	-

Figure D.4 – Pervaporative membrane reactor window

Since the windows of both exothermic batch reactor and pervaporative membrane reactor are same then the proceeding guides of this process is shortly outlined here.

2.1. Process input

Set point and initial values of the process need to be specified by changing the default values as following suggestions.

Temperature

The operating temperature of the membrane reactor is defaulted at 363 K, which the optimal reactor temperature falls in the range 363 – 373 K. The other temperature is assumed to be limited to the range 298 – 393 K. It can be seen that the widows of both exothermic batch reactor and pervaporative membrane reactor are not different. Then the users can simply change the temperatures.

Material

To specify the initial values of reactants, the users accomplish this task by follow the suggestions as stated in the exothermic case.

2.2. Control input

In this step, sampling time and the parameter and variable values of the controller are set to building the simulation. The users can access this step by follow as in the exothermic case.

2.3. Run

The simulation of the pervaporative membrane reactor in nominal, parameter mismatch, heat transfer coefficient (U), change and plant/model mismatch, heat released by the reaction (Q_r) and reaction rate (rate) change, can be done by proceeding the same way as in the exothermic batch reactor.

2.4. Other

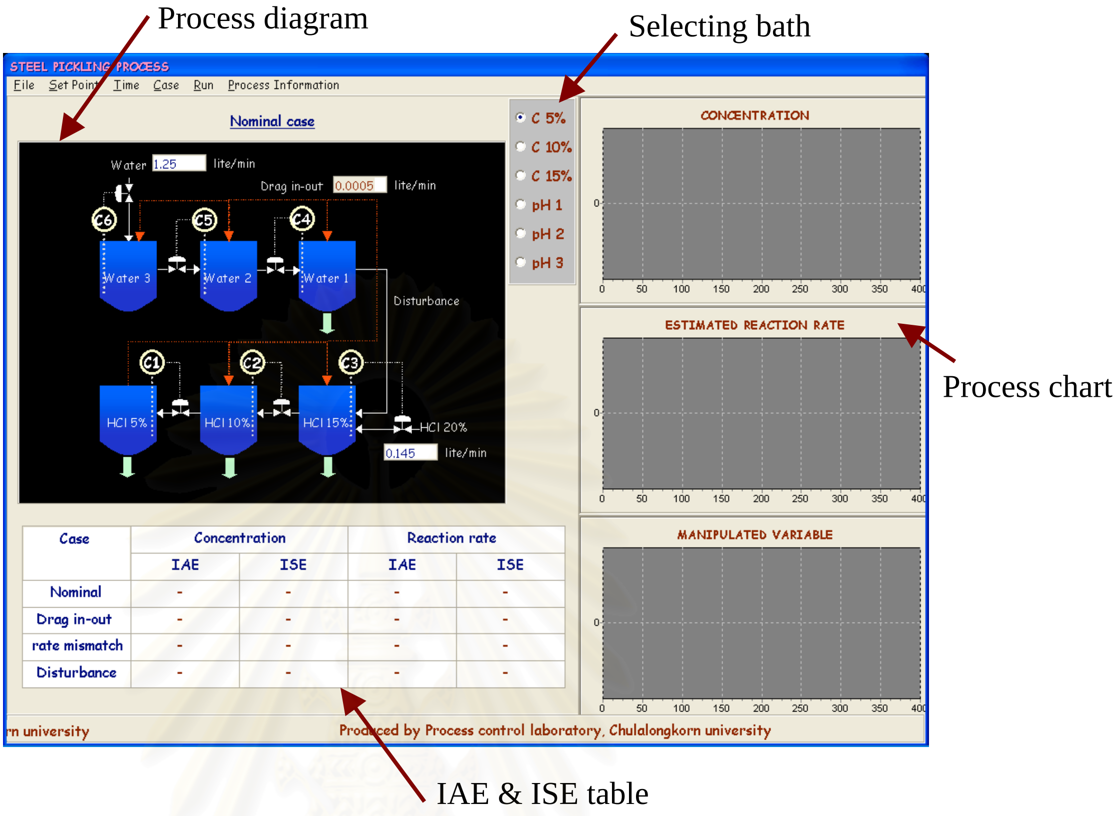
In figure 4, this process window can be cleared and closed by clicking on the **File** menu and selecting the expected button. Furthermore, the process information can be found by clicking the **Process Information** menu button.

3. Steel pickling process

To selecting a steel pickling process, the **Steel pickling process** is clicked as seen in the figure D.2. This process is designed and developed by Pornsiri (2002) to illustrate an application of the control strategy, which consists of Generic Model Control (GMC) and Dynamic Data Reconciliation (DDR). There are six tanks for this process containing of three acid tanks and three rinsing tanks. Surface oxides (scales) and other contaminants of metals are removed by immersing the samples into aqueous acid solution with 5%, 10% and 15% HCl by wt. in the first three tanks. The irreversible reaction in the pickling step is described as seen in the **Process Information**.

Each tank is controlled to maintain pH value at a desired target with regardless of batch level. The desired concentration of the acid baths are set at 1.4, 2.87 and 4.408 mole/lit respectively by adjusting return acid stream as shown in process diagram of the steel pickling process window (figure D.5). For rinsing bath the pH values are handled at 3, 6.5 and 7.3 respectively by adjusting return water flow stream. By unfeasible measurement, the reaction rates (rate) in the three acid tanks are unavailable so that these values are estimated via DDR. For simplification, flow rate of drag in-out is assumed to be constant at 0.0005 lit/min then this parameter needs to be tested as parameter mismatch. Furthermore, for this process disturbance case is studied to test the robustness of the proposed control strategy.

As seen in the figure D.5, there are four major parts in the steel pickling process window. Firstly, process diagram shows control configuration of the process. Secondly, the process result of each bath is displayed by selecting the considered bath. Next, simulation results show in process chart. Concentration chart shows the actual pH or concentration of the considered bath. Estimated reaction rate chart shows the actual and estimated reaction rate occurred in acid tanks and the last one displays the flow rate of manipulated variable of the considered bath. In the last part, IAE and ISE of the controlled concentration and estimated reaction rate in any cases are listed in the table.



Water 1.25 lite/min

Drag in-out 0.0005 lite/min

0.145 lite/min

Case	Concentration		Reaction rate	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
Drag in-out	-	-	-	-
rate mismatch	-	-	-	-
Disturbance	-	-	-	-

Figure D.5 – Steel pickling process window

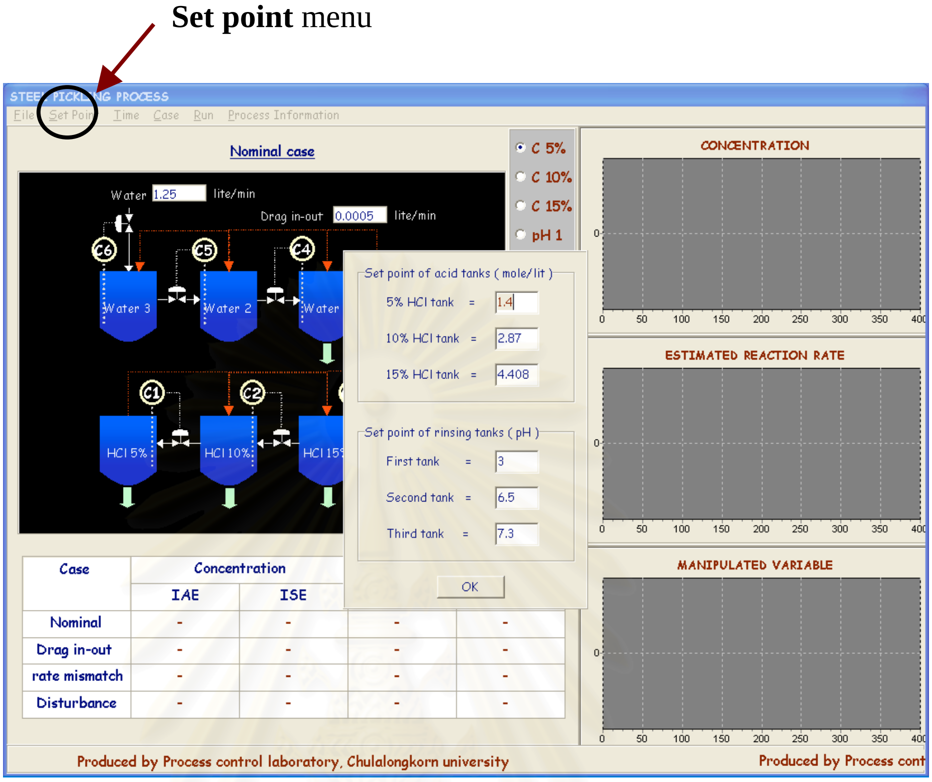
3.1. Process input

The users can define the initial flow rates of input water and 20% HCl, and an amount of drag in-out directly on the process window. For this process, the initial concentrations of each bath can not be changed. These values can be found by clicking the **Process Information** menu.

Set point

To specify the set point value of each tank:

1. Click on the **Set point** menu to open input set point view.
2. Enter the expected desired values of acid and rinsing tanks.


Set point menu

Water 1.25 lite/min

Drag in-out 0.0005 lite/min

Set point of acid tanks (mole/lit)

5% HCl tank = 1.4

10% HCl tank = 2.87

15% HCl tank = 4.408

Set point of rinsing tanks (pH)

First tank = 3

Second tank = 6.5

Third tank = 7.3

Case	Concentration			
	IAE	ISE		
Nominal	-	-	-	-
Drag in-out	-	-	-	-
rate mismatch	-	-	-	-
Disturbance	-	-	-	-

The default concentrations of acid tanks are 1.4, 2.87 and 4.408 mole/lit respectively, and the default pH values of rinsing tanks are 3, 6.5 and 7.3 respectively.

3. Close the view by clicking the **OK** button.

3.2. Control input

Time

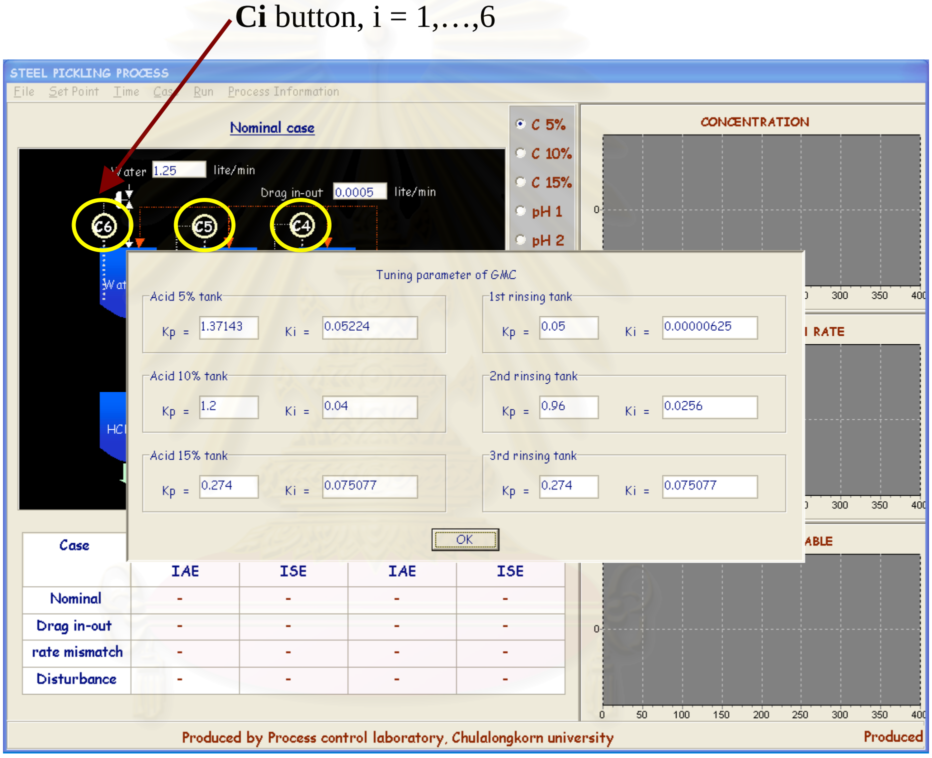
To specify the total and sampling time of the simulation:

1. Click on the **Time** menu to open the input time view.
2. Change the default total and sampling time as desired. The default values are 400 and 0.5 minutes.
3. Click the **OK** button to close the view and return to the process view.

Controller parameters and variables

To specify tuning parameters of Generic Model Control (GMC):

1. Move the mouse on the **C1** or **C2...C6** which is on the process diagram, hand cursor will be appeared, and click on it to open the input controller parameter view.
2. Enter the tuning parameter values (K_p and K_i) of GMC controller of each tank.



Ci button, i = 1,…,6

Water 1.25 lite/min

Drag in-out 0.0005 lite/min

Tuning parameter of GMC

Acid 5% tank: Kp = 1.37143 Ki = 0.05224

Acid 10% tank: Kp = 1.2 Ki = 0.04

Acid 15% tank: Kp = 0.274 Ki = 0.075077

1st rinsing tank: Kp = 0.05 Ki = 0.00000625

2nd rinsing tank: Kp = 0.96 Ki = 0.0256

3rd rinsing tank: Kp = 0.274 Ki = 0.075077

Case	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
Drag in-out	-	-	-	-
rate mismatch	-	-	-	-
Disturbance	-	-	-	-

3. Click on the **OK** button to close the input view and return to the process window.

3.3. Run

Nominal case

To run the simulation in nominal case:

1. Click on the **Case** menu and select the **Nomimal case**, it will appear right mark in front of the context to ensure that the program is concentrating in nominal case.
2. Click on the **Run** menu to simulate the process.

The chart line will be moving along the actual trajectory, at the same time IAE and ISE are calculated through the simulation. These values are shown in the table as seen in the window. It can be also seen that the process trajectories, IAE and ISE are similar as in chapter IV.

3. The simulation results of the first acid tank (5%HCl) will display in both Charts and Table. If the users want to focus in other tanks, just clicking on the expected bath near the concentration chart.

Click on **Run** menu

Water 1.25 lite/min

Drag in-out 0.0005 lite/min

HCl 20% 0.145 lite/min

Case	Concentration		Reaction rate	
	IAE	ISE	IAE	ISE
Nominal	0.08379	9.696E-5	3.18E-12	3.864E-26
Drag in-out	-	-	-	-
rate mismatch	-	-	-	-
Disturbance	-	-	-	-

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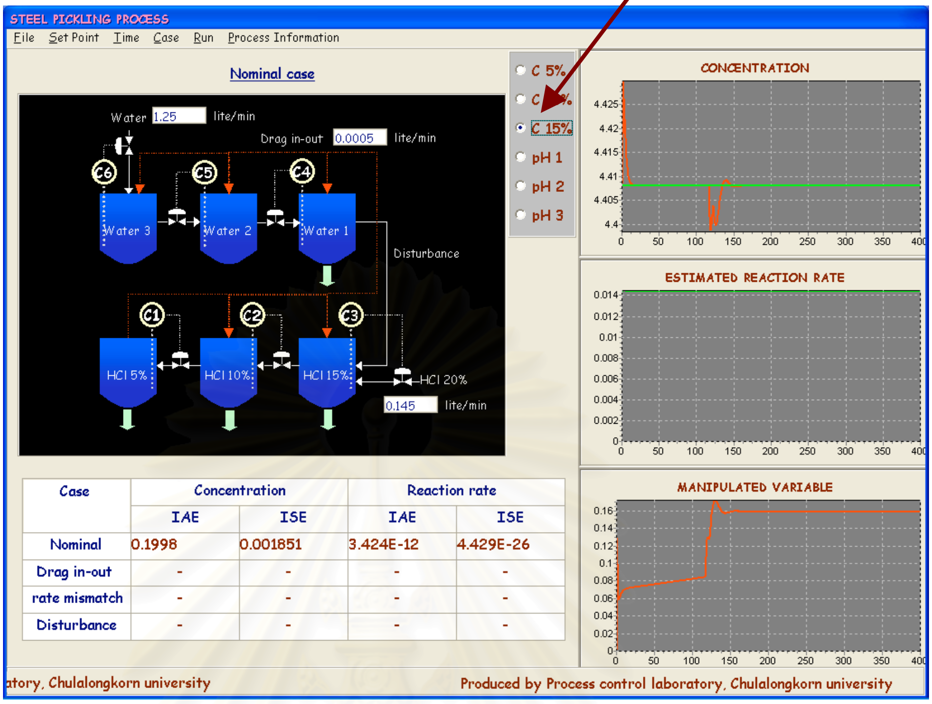
Selecting 15%HCl tank



Water 1.25 lite/min

Drag in-out 0.0005 lite/min

0.145 lite/min

Case	Concentration		Reaction rate	
	IAE	ISE	IAE	ISE
Nominal	0.1998	0.001851	3.424E-12	4.429E-26
Drag in-out	-	-	-	-
rate mismatch	-	-	-	-
Disturbance	-	-	-	-

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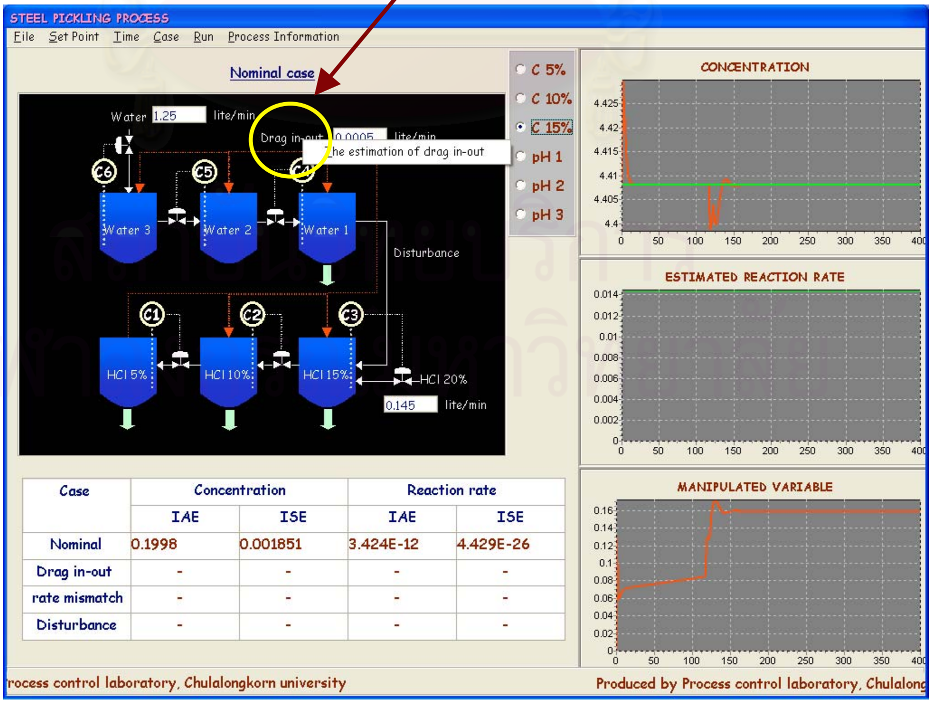
4. Move the mouse to **Drag in-out** text on the process diagram, hand cursor will be appear and right click on it.

Right click on **Drag in-out** text



Water 1.25 lite/min

Drag in-out 0.0005 lite/min

0.145 lite/min

Case	Concentration		Reaction rate	
	IAE	ISE	IAE	ISE
Nominal	0.1998	0.001851	3.424E-12	4.429E-26
Drag in-out	-	-	-	-
rate mismatch	-	-	-	-
Disturbance	-	-	-	-

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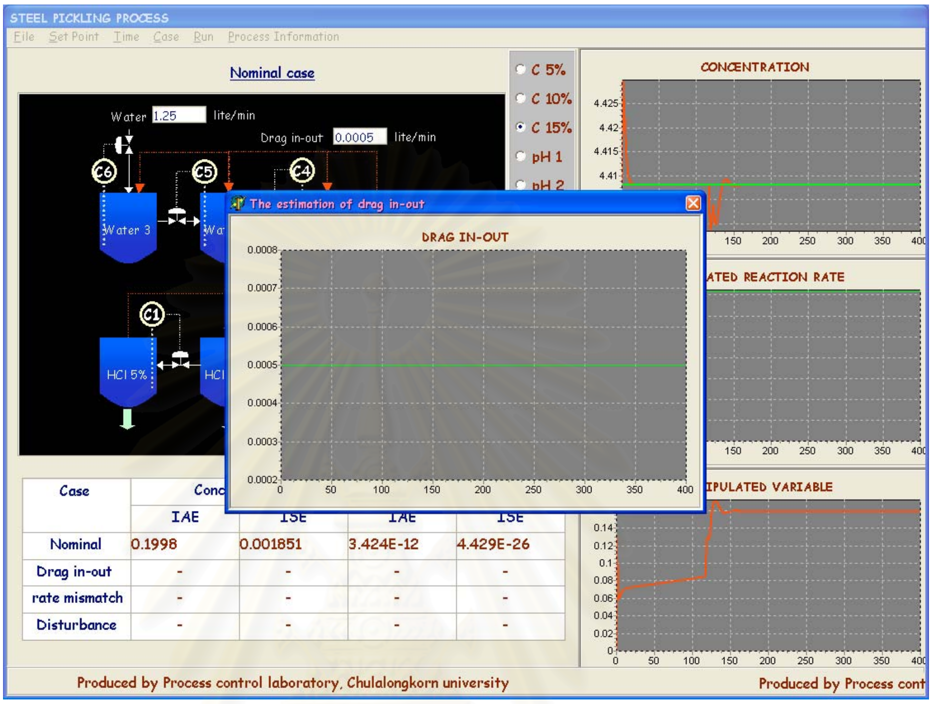
5. Select the popup menu to open the estimation result view of drag in-out content.



Water 1.25 lite/min

Drag in-out 0.0005 lite/min

Case	Conc			
	IAE	ISE	IAE	ISE
Nominal	0.1998	0.001851	3.424E-12	4.429E-26
Drag in-out	-	-	-	-
rate mismatch	-	-	-	-
Disturbance	-	-	-	-

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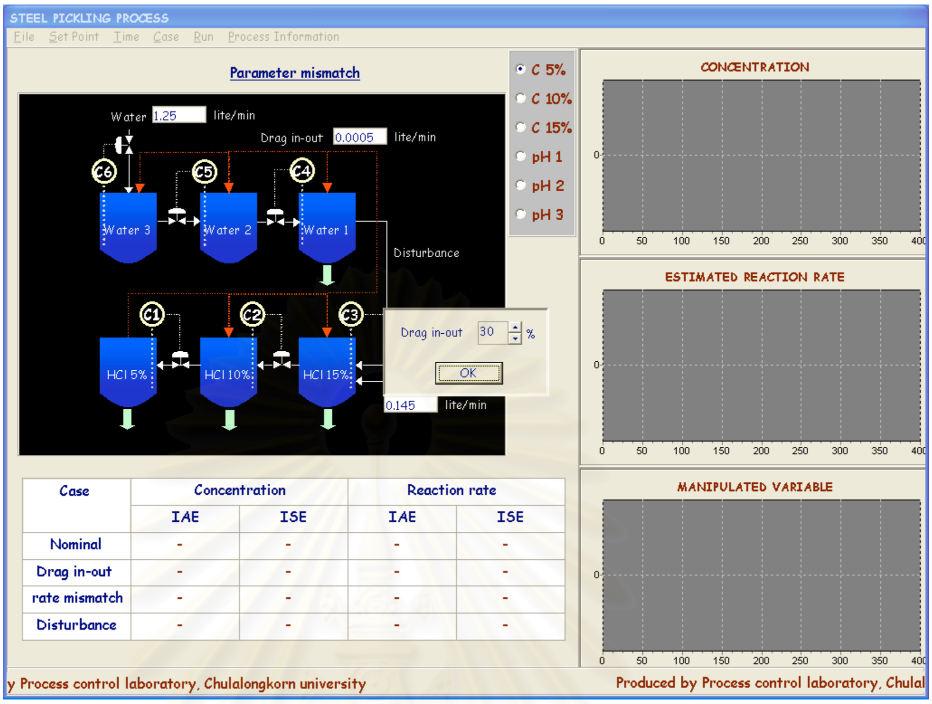
<u>Parameter mismatch</u>

To test the efficiency of the estimator and controller, now the process simulation in case of parameter change (an amount of drag in-out) is considered.

1. Click on the **Case** menu and move to the **Other case**.
2. Select the **Parameter mismatch** to open the input mismatch view for receiving the percentage of the drag in-out content change.



Water 1.25 lite/min

Drag in-out 0.0005 lite/min

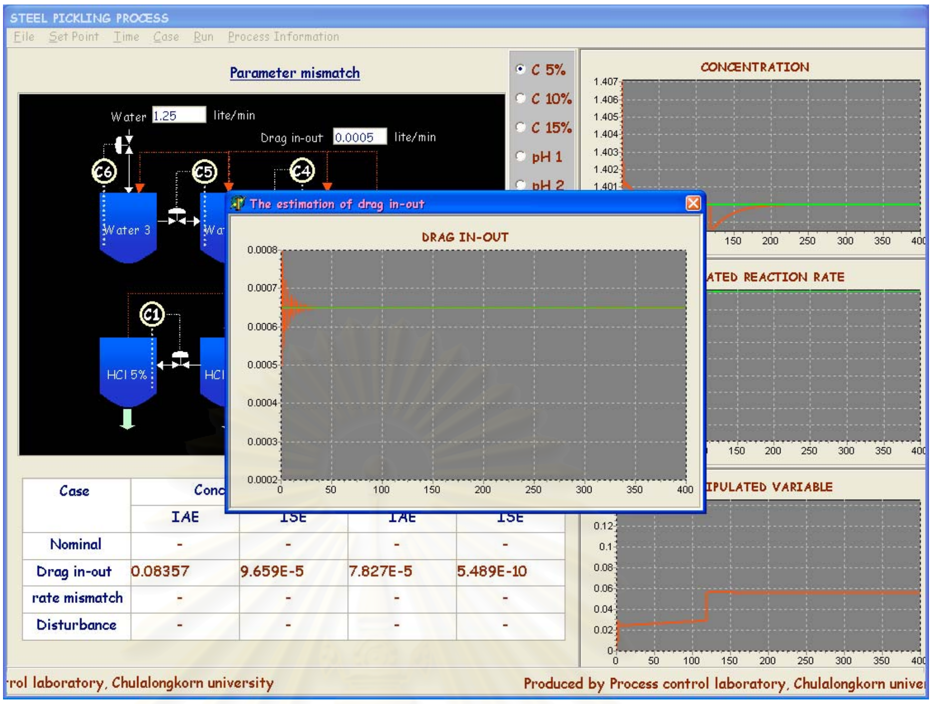
Drag in-out 30 %

0.145 lite/min

Case	Concentration		Reaction rate	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
Drag in-out	-	-	-	-
rate mismatch	-	-	-	-
Disturbance	-	-	-	-

The parameter change is limited to the range –30% to +30% from the initial value. Here, the percentage of this parameter change is changed to be +30%.

3. Click on the **OK** button to close the input view and return to the steel pickling process view.
4. To simulate the process performance in this case, click on the **Run** menu. The simulation results of 5% HCl tank will be shown first.
5. Select the expected bath to see its simulation results.
6. Click on the **Drag in-out** text on the process diagram to view the result of the drag in-out content estimation via the dynamic data reconciliation (DDR).
7. Close the estimation result and return to the process view.



Case	Conc			
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
Drag in-out	0.08357	9.659E-5	7.827E-5	5.489E-10
rate mismatch	-	-	-	-
Disturbance	-	-	-	-

Plant/Model mismatch

To test the robustness of the proposed control strategy, the change of reaction rate is considered in this case.

1. Click on the **Case** menu and move to the **Other case**.
2. Select the **Plant/model mismatch** to open the input mismatch view for receiving the percentage of the reaction rate (rate) change as shown below.

In this case, it is assumed that the defined percentage of this mismatch will effect to the reaction rate changes in the whole acid tanks. Here, the percentage of the reaction rate changes is changed to -30% from the actual values.

3. Click on the **OK** button to close the input view and return to the process view.
4. Click on the **Run** menu to simulate the process performance in this case.

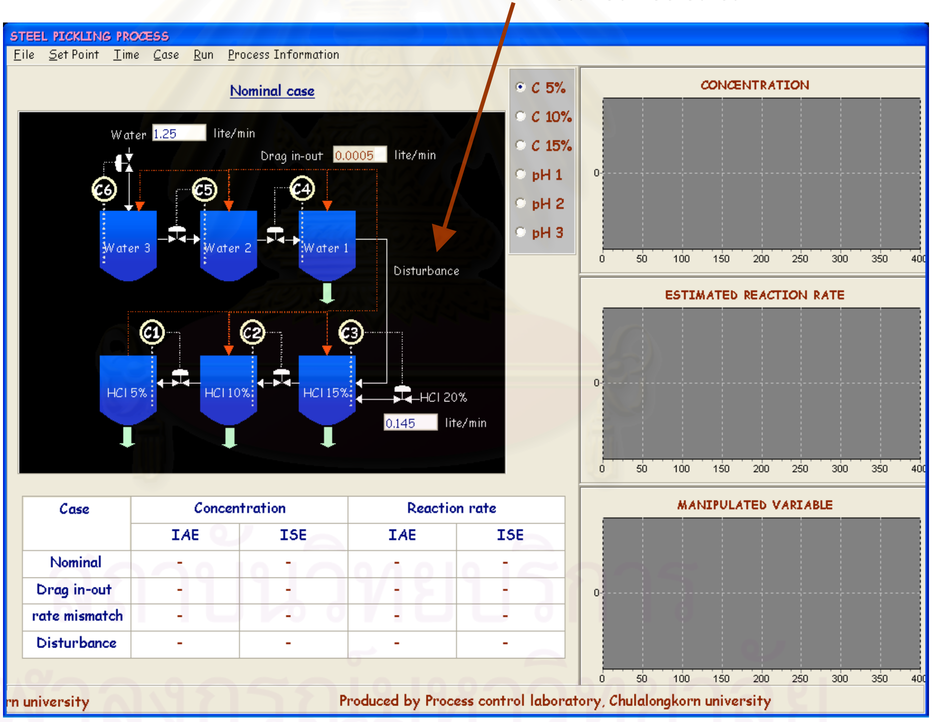
The simulation results of 5% HCl tank will be shown first. It can be seen that the reaction rate of 5% HCl is smaller than in nominal case, these process results are same as seen in Chapter IV.

5. Select the expected bath to see its simulation results.
6. Click on the **Drag in-out** text on the process diagram to view the result of the drag in-out content estimation via the dynamic data reconciliation (DDR).
7. Close the estimation result and return to the process view.

Disturbance

For the steel pickling process, the proposed control strategy is also tested in disturbance case. The flow stream of disturbance for this process can be seen in the process diagram. The flow rate of the disturbance stream is assumed to be zero in other cases but in this case it is not zero in the expected time interval.

Disturbance stream



● C 5%

Water 1.25 lite/min

Drag in-out 0.0005 lite/min

0.145 lite/min

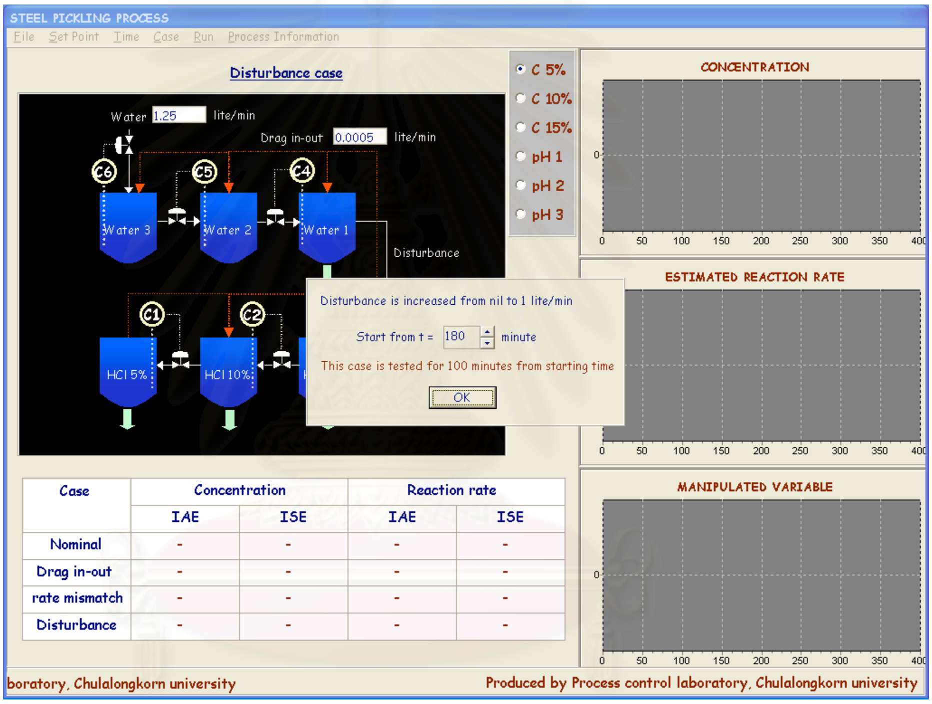
Case	Concentration		Reaction rate	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
Drag in-out	-	-	-	-
rate mismatch	-	-	-	-
Disturbance	-	-	-	-

1. Click on the **Case** menu and move to the **Other case**.
2. Select the **Disturbance case** to open the input time view for receiving the starting time of the disturbance as shown in the figure.

It is assumed that the value of the disturbance flow rate increases from zero to be one lit/min at the defined starting time. This flow rate will has been one lit/min for 100 minutes from the starting time, after that it will be zero lit/min through the simulation.

3. Enter the starting time to be 180 minute.

It means that the disturbance flow rate will increase from zero to one lit/min at t = 180 until t = 280, after that it will be decreased to be zero again.



Water 1.25 lite/min

Drag in-out 0.0005 lite/min

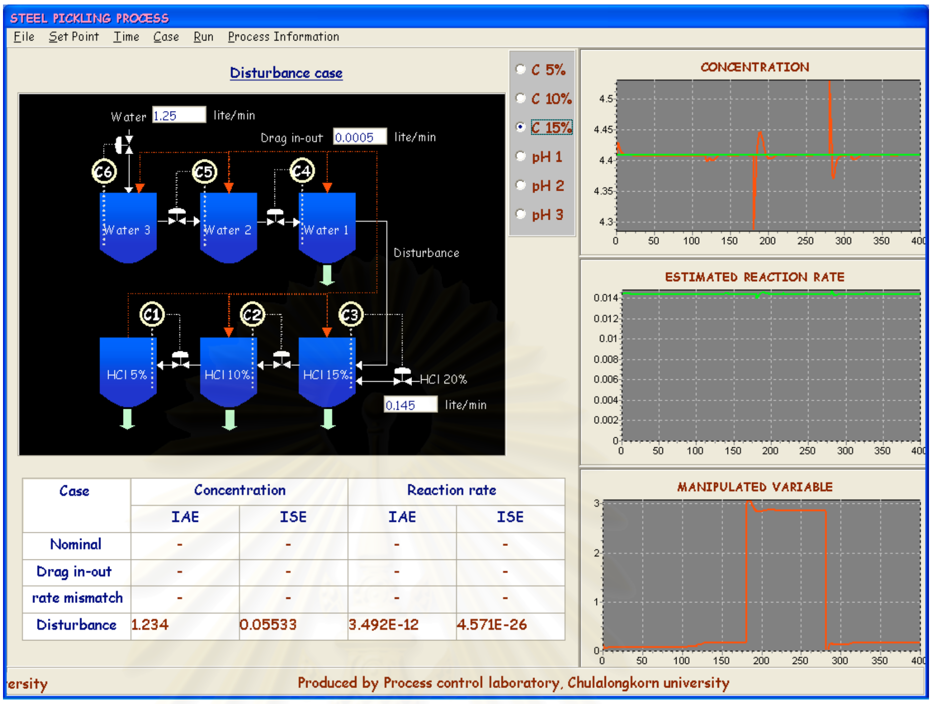
Disturbance is increased from nil to 1 lite/min

Start from t = 180 minute

This case is tested for 100 minutes from starting time

Case	Concentration		Reaction rate	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
Drag in-out	-	-	-	-
rate mismatch	-	-	-	-
Disturbance	-	-	-	-

4. Click on the **OK** button to close the input view and return to the process view.
5. Click on the **Run** menu to simulate the process performance in this case.
6. Select the expected bath to see its simulation results.



Case	Concentration		Reaction rate	
	IAE	ISE	IAE	ISE
Nominal	-	-	-	-
Drag in-out	-	-	-	-
rate mismatch	-	-	-	-
Disturbance	1.234	0.05533	3.492E-12	4.571E-26

3.4. Other

Menu File

1. The **Clear** menu

This submenu is used for clearing all prior simulation results and returns all values to the default values.

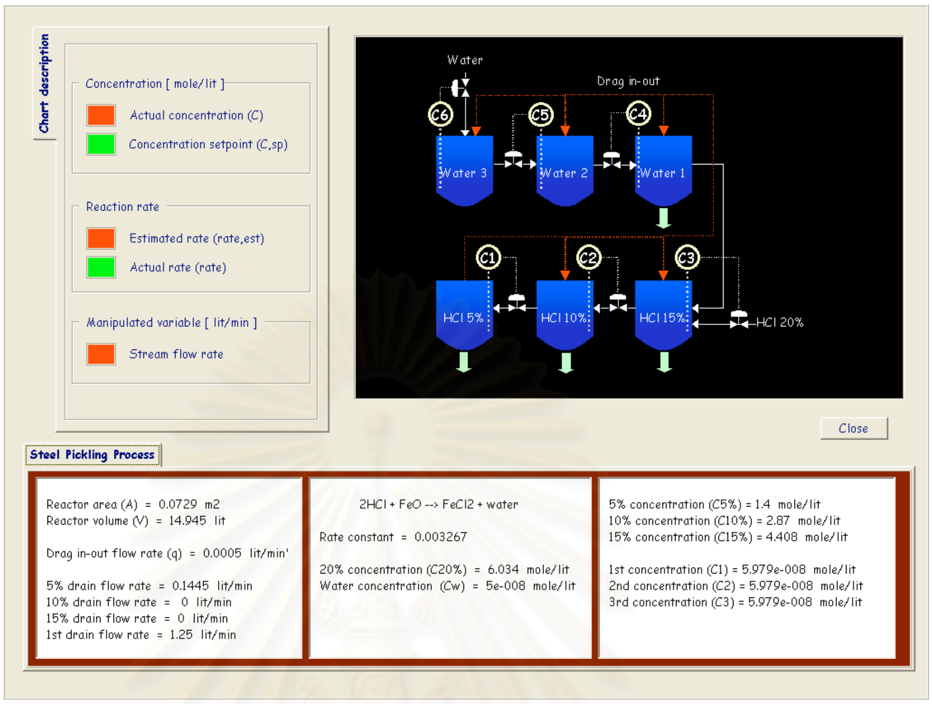
2. The **Close** menu

This one is used for closing the current process window and returns to the main window for new process selection.

Process Information

To illustrate the information of the steel pickling process:

1. Click on the **Process Information** menu to open the view of process information.



Concentration [mole/lit]

🟥 Actual concentration (C)
🟩 Concentration setpoint (C,sp)

Reaction rate

🟥 Estimated rate (rate,est)
🟩 Actual rate (rate)

Manipulated variable [lit/min]

🟥 Stream flow rate

Reactor area (A) = 0.0729 m2
Reactor volume (V) = 14.945 lit

Drag in-out flow rate (q) = 0.0005 lit/min'

5% drain flow rate = 0.1445 lit/min
10% drain flow rate = 0 lit/min
15% drain flow rate = 0 lit/min
1st drain flow rate = 1.25 lit/min

2HCl + FeO --> FeCl2 + water

Rate constant = 0.003267

20% concentration (C20%) = 6.034 mole/lit
Water concentration (Cw) = 5e-008 mole/lit

5% concentration (C5%) = 1.4 mole/lit
10% concentration (C10%) = 2.87 mole/lit
15% concentration (C15%) = 4.408 mole/lit

1st concentration (C1) = 5.979e-008 mole/lit
2nd concentration (C2) = 5.979e-008 mole/lit
3rd concentration (C3) = 5.979e-008 mole/lit

As stated in the exothermic batch reactor manual, there are three parts in this window: process diagram, chart description and details of the steel pickling process.

2. Close the information view and return to the process window.

4. Steady state flow system

The last section of this developed computer software is to illustrate an application of steady state data reconciliation to a flow system. The steady state flow process is generalized in this section.

1. This system is selected by clicking on the **Steady state flow system** from popup menu as seen figure D.2, the input view appears.
2. Enter a number of total tanks in the expected process, the number of tanks is limited not more than seven.

As example, The flow process proposed by Romagnoli J. (1983) is discussed here. There is not chemical reaction in this system. As seen in process diagram, the process contains four units and nine flow streams.

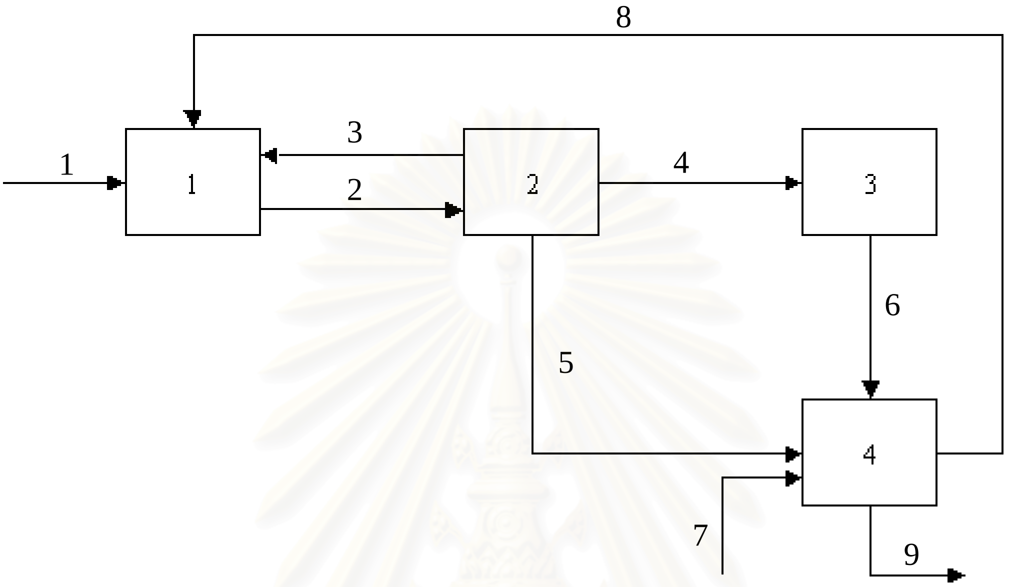
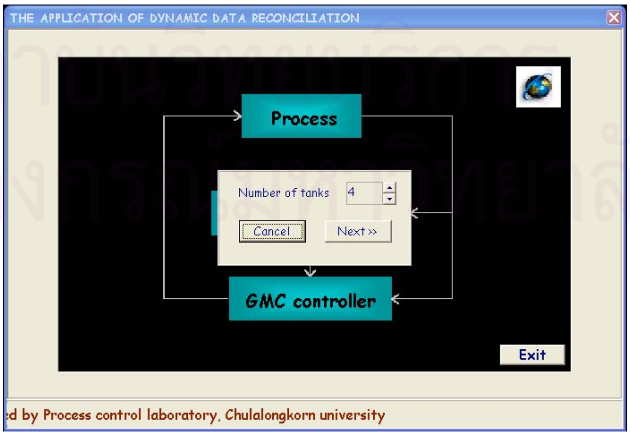


Figure D.6 – Steady state flow process (Romagnoli, 1983)

Then the number of total units is set to be 4 in this example.

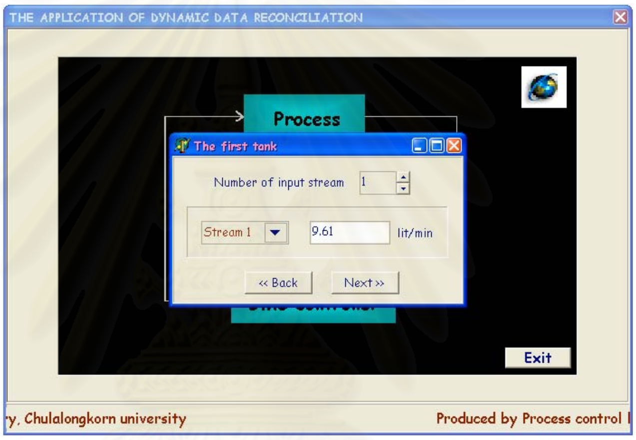

THE APPLICATION OF DYNAMIC DATA RECONCILIATION

Number of tanks 4

d by Process control laboratory, Chulalongkorn university

3. Click on the **Next** button to continuous or click on the **Cancel** button to close all flow system and return to the main window.
4. After click on the **Next** button, the input flow rate of the first unit view appears to receiving the values of input flow rate.
5. Enter the number and values of input stream of the first unit as following:

Number of input stream = 1
Flow rate of the first flow stream = 9.61 lit/min (the 1st stream)

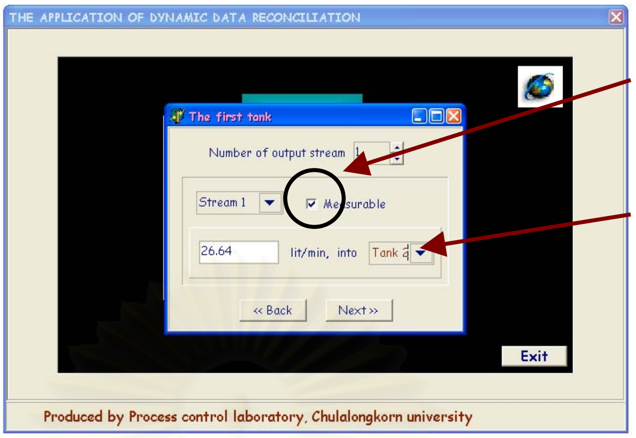


Number of input stream 1
Stream 1 9.61 lit/min

For this computer software, the number of input and output flow stream is limited not more than five streams.

6. Click on the **Next** button to open the output flow view of the first unit and enter the number and values of output flow rate as follows:

Number of output stream = 1
Flow rate of the first flow stream = 26.64 lit/min (the 2nd stream)



Number of output stream 1

Stream 1 ☑ Measurable

26.64 lit/min, into Tank 2

Measurable is checked

The 2nd stream flows into the 2nd unit

7. Click on the **Next** button to continuous enter the flow streams of the 2nd until the 4th unit as below:

Input flow streams			
The 1st unit	The 2nd unit	The 3rd unit	The 4th unit
Number = 1 1st stream = 9.61	Number = 0	Number = 0	Number = 1 7th stream = 12.87

Output flow streams							
The 1st unit				The 2nd unit			
Stream	Value	Measurable	To tank	Stream	Value	Measurable	To tank
2nd	26.64	Checked	2	3rd	8.48	Checked	1
				4th	-	Not checked	3
				5th	2.2	Checked	4
The 3rd unit				The 4th unit			
Stream	Value	Measurable	To tank	Stream	Value	Measurable	To tank
6th	12.45	Checked	4	8th	-	Not checked	1
				9th	23.75	Checked	Envi

8. After finish enter all streams; click on the **OK** button to open the flow process view.

As seen in the steady state flow system view, there are two major parts in the window. The first one is flow chart of process containing the number of input and output stream of each tank, and the direction of output stream (including recycle stream). There are two sections in the report part. The left side displays the flow rate values of each tank including the unmeasured flow rate as seen in the figure.

- Tank 1
  - Number of input stream = 1
  - Number of output stream = 1
    - Stream 1 to Tank 2
- Tank 2
  - Number of input stream = 0
  - Number of output stream = 3
    - Stream 1 to Tank 1
    - Stream 2 to Tank 3
    - Stream 3 to Tank 4
- Tank 3
  - Number of input stream = 0
  - Number of output stream = 1
    - Stream 1 to Tank 4
- Tank 4
  - Number of input stream = 1
  - Number of output stream = 2
    - Stream 1 to Tank 1
    - Stream 2 to environment

- Tank 1
  - Input
    - Stream 1 = 9.61
  - Output
    - Stream 1 = 26.64
- Tank 2
  - Input
  - Output
    - Stream 1 = 8.48
    - Stream 2 = un-measurable
    - Stream 3 = 2.2
- Tank 3
  - Input
  - Output
    - Stream 1 = 12.45
- Tank 4
  - Input
    - Stream 1 = 12.87
  - Output
    - Stream 1 = un-measurable
    - Stream 2 = 23.75

- Tank 1
- Tank 2
- Tank 3
- Tank 4

9. Click on the **Run** menu to estimate the un-measurable flow streams and reconcile the measured flow streams.

Click on the **Run** menu

```
Tank 1
    Number of input stream = 1
    Number of output stream = 1
        Stream 1 to Tank 2
Tank 2
    Number of input stream = 0
    Number of output stream = 3
        Stream 1 to Tank 1
        Stream 2 to Tank 3
        Stream 3 to Tank 4
Tank 3
    Number of input stream = 0
    Number of output stream = 1
        Stream 1 to Tank 4
Tank 4
    Number of input stream = 1
    Number of output stream = 2
        Stream 1 to Tank 1
        Stream 2 to environment
```

```
Tank 1
    Input
        Stream 1 = 9.61
    Output
        Stream 1 = 26.64
Tank 2
    Input
    Output
        Stream 1 = 8.48
        Stream 2 = un-measurable
        Stream 3 = 2.2
Tank 3
    Input
    Output
        Stream 1 = 12.45
Tank 4
    Input
        Stream 1 = 12.87
    Output
        Stream 1 = un-measurable
        Stream 2 = 23.75
```

```
Tank 1
    Input
        Stream 1 = 10.033
    Output
        Stream 1 = 25.762
Tank 2
    Input
    Output
        Stream 1 = 9.357
        Stream 2 = 13.328
        Stream 3 = 3.078
Tank 3
    Input
    Output
        Stream 1 = 13.328
Tank 4
    Input
        Stream 1 = 13.293
    Output
        Stream 1 = 6.372
        Stream 2 = 23.327
```

The values of estimates are reported in the right side of the report part. It is found that the estimated flow rates are similar to the actual values as seen in the table below.

Stream	Measured	Actual	Estimated	Measured error (%)	Estimated error (%)
1	9.61	10.11	10.033	4.946	0.762
2	26.64	25.86	25.762	3.016	0.379
3	8.48	9.35	9.357	9.305	0.075
4	-	13.4	13.328	-	0.537
5	2.2	3.11	3.078	29.260	1.029
6	12.45	13.4	13.328	7.090	0.537
7	12.87	13.20	13.293	2.500	0.705
8	-	6.4	6.372	-	0.438
9	23.75	23.31	23.327	1.888	0.073

From the estimated results, it shows that the estimated errors are much smaller than the measured errors.

10. Click on the **Close** menu to close the steady state flow process window and return to the main view.

As described above, this computer software is designed with respect to the considered processes as example in Chapter IV. The application of steady state and dynamic data reconciliation is considered and incorporated into control strategy, Generic Model Control (GMC). The producer ensures that the users will realize the greatest benefit to illustrate the application of data reconciliation as estimator from the developed program.

VITA

Miss Pornsiri Kaewpradit was born in Haddyai, Songkhla, on July 22, 1976. After completing her senior high school at Haddyai-Vittayalai school in 1995, she graduated her Bachelor Degree of Engineering in Chemical Engineering from Srinakarinvirot University in 1999. In 2002, she completed her Master Degree of Engineering in Chemical Engineering, Chulalongkorn University.