APPLICATION OF REAL TIME OPTIMISATION FOR FATTY ACID FRACTIONATION PROCESS

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To my FAMILY

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ABSTRACT

This thesis discusses the application of Real Time Optimisation (RTO) in improving process plant profitability. The RTO cycle consisting of five major components, namely, plant model in steady state and dynamic modes, steady state detection, data reconciliation, gross error detection and economic optimisation routines were developed and tested on a selected base–case operating condition of a fatty acid fractionation (FAF) process. The cycle of RTO implementation began with collection of selected process data from the plant, represented by a dynamic simulation model developed using HYSYS.Plant™ version 2.4. The measured data were then evaluated by the steady state detection mechanism to ascertain that the process had reached steady state operating condition prior to the evaluation by the data reconciliation and gross error detection stages. Following these data validation phases, the search for optimal operating conditions was executed by the HYSYS.Plant™ optimiser, facilitated by the steady state model of the plant. Successful implementation with profit improvement of 5.61% over the base-case condition was obtained. Larger profitability was difficult to realise due to tight constraints imposed on this low pressure fractionation plant. The RTO scheme was then tested for robustness by introducing four types of process uncertainties. These were the variation in product prices, measurement noise, leakage in process streams and process disturbances. In all cases, errors introduced by these uncertainties were successfully detected and rectified and successful process optimisations were obtained. The results obtained in this study proved the capability of the RTO scheme in improving the profitability of process plant operation.

ABSTRAK

Tesis ini membincangkan penggunaaan pengoptimuman masa nyata (RTO) dalam meningkatkan keuntungan loji proses. Kitaran RTO yang mempunyai 5 komponen utama, iaitu model loji dalam bentuk dinamik dan keadaan mantap, pengesanan keadaan mantap, penyesuaian data, pengesanan ralat kasar dan pengotimuman ekonomi telah dibangun dan diuji ke atas loji asid lelemak pada keadaan operasi kes asas yang dipilih. Pelaksanaan kitaran RTO bermula dengan pengumpulan data pembolehubah yang dipilih dari loji yang diwakili oleh model penyelakuan dinamik yang dibangunkan menggunakan perisian HYSYS.Plant™ versi 2.4. Data yang diukur ini dinilai oleh pengesan keadaan mantap bagi memastikan proses telah mencapai keadaan mantap sebelum penyesuaian data dan pengesanan ralat kasar dilaksanakan. Ekoran daripada fasa validasi data ini, pencarian keadaan optimum dilaksanakan dengan pengoptimum HYSYS.Plant™ dengan dibantu oleh model kedaan mantap. Kejayaan dicapai dalam perlaksanaan tersebut dan peningkatan keuntungan sebanyak 5.61% daripada operasi keadaan asas telah dicapai. Keuntungan yang lebih besar sukar untuk dicapai kerana loji pemecahan asid lelemak ini beroperasi pada tekanan rendah dan tertakluk kepada kekangan yang ketat. Seterusnya, ketegapan skim RTO ini diuji dengan memperkenalkan 4 jenis ketidakpastian proses yang terdiri daripada variasi dalam harga produk, hingar pengukuran, kebocoran dalam aliran proses, dan gangguan proses. Dalam semua kes, ralat yang dihasilkan oleh ketidakpastian proses berjaya dikenalpasti dan pengoptimuman proses berjaya dicapai. Keputusan yang terhasil dalam kajian ini telah membuktikan keupayaan skim RTO dalam meningkatkan keuntungan operasi loji proses.

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SYMBOLS

a_{ij}	–	Non-temperature dependent energy parameter between components i and j
A	–	Coefficient matrix of the linear process model.
$\underline{A}_k$	–	$N - 1$ time the sample covariance matrix
A_w	–	Van der Waals area
b_{ij}	–	Temperature dependent energy parameter between components i and j
B	–	Coefficient matrix of the linear process model as the suspected measurement is excluding
c_a	–	Mass conversion from tons to kilograms
c_b	–	Heat conversion from megajoules to kilojoules
c_c	–	Time conversion from hours to seconds
C	–	Critical value
C_{cw}	–	Utility cost of the cooling water for the cooler
C_e	–	Utility cost of the electricity for the pumps
C_{feed}	–	Feed stream cost
C_{fo}	–	Utility cost of the fuel oil for the reboilers
$c_{p,cw}$	–	Heat capacity of cooling water
$C_{utilities}$	–	Total utilities costs
d	**–**	**V**ector **v**ariable as the suspected measurement.
$\underline{d}$	–	Difference of average value of measurements between two periods.
D_{cw}	–	Cooling water unit price

D_e	–	Electricity unit price
D_{feed}	–	Feed stream unit price
D_{fo}	–	Fuel oil unit price
D_i	–	Product streams unit price
f	–	Vector of equality constraints
f_a, f_b	–	Denominator degrees of freedom for Composite Statistical Test.
f_i	–	Outlet flow of the i_{th} stream
$F_{p,f}$	–	F distribution with degrees of freedom p and f.
F	–	Feed flowrate
g	–	Vector of inequality constraints
h	–	Specific enthalpy
H	–	Enthalpy or heat flow
H_o, H_1	–	Hypothesis
L	–	Liquid flowrate
m	–	Rank of matrix of the linear process model.
m_{feed}	–	Mass flow rate of the feed stream
m_i	–	Mass flow rate of the product stream
m_{high}	–	Upper limit of manipulated variables
m_{low}	–	Lower limit of manipulated variables
m_{norm}	–	Normalized of manipulated variables
M	–	Process Fluid Flowrate
MW	–	Molecular weight of the fluid
n	–	Total number of component
N	–	Number of measurement in period minus 1.
N_m	–	Dynamic degrees of freedom
N_{om}	–	Number of manipulated variable with no steady state effect
N_{oy}	–	Number of variable that need to controlled, but with no steady state effect
N_{ss}	–	Steady State degrees of freedom
p	–	Number of Variable in a subset
P	–	Projection Matrix
P_i	–	Product stream values

P_1	–	Pressure of the inlet stream
P_2	–	Pressure of the exit stream
q_i	–	Van der Waals area parameter minus van der Waals area and divided by 2.5E9.
Q_{cooler}	–	Cooler duty
Q_{fo}	–	Heat capacity of fuel oil per 1 centimeter cube
Q_{heater}	–	Heater duty
Q_{pump}	–	Total duty of the pumps
Q_{reb}	–	Total duty of the reboilers (KJ/h)
Q_o, Q_1	–	Covariance Matrices
r	–	Vector of balance residuals
r_i	–	Van der Waals volume parameter minus van der Waals volume and divide by 15.17
R_i	–	Flow ratio of the i_{th} stream
S	–	Suspected measurement contain gross error
$\underline{S}_k$	–	Sample Covariance Matrices.
$S.D.$	–	Standard Deviation
T	–	Temperature (K)
$T^2_{p,f}$	–	T^2 distribution with degrees of freedom p and f.
u	–	Unmeasured Variables
v	–	Covariance matrix r
V	–	Vapour flowrate
V_w	–	Van der Waals volume
w	–	Weighting factor of measured variables.
W	–	Test Statistic for the Stage 1 of Composite Statistical Test
W_r	–	Random Variable of W.
$\hat{x}$	–	True values of the measured variables
x	–	Measured Variables
x_i	–	Liquid mole fraction of component i
$\bar{\underline{x}}_k$	–	Average value of Measurements
y	–	Vector of N measurements
y_i	–	Vapour mole fraction of component

z	–	Feed mole fraction of component i
$z_{e,i}$	–	Measurement Test Statistic
$z_{r,i}$	–	Nodal Test Statistic
Z	–	10.0 co-ordination number

GREEK SYMBOLS

α	–	Level of significant for overall measurements
β	–	Level of significant for individual measurement
ε	–	Vector of unknown random error
σ_i	–	Standard deviation of measurement i
γ	–	Global test statistic calculated
γ_i	–	Activity coefficient of component i
ρ	–	Density of the inlet stream
ρ_{cw}	–	Density of the cooling water
Σ	–	Variance-covariance matrix.

ABBREVIATIONS

APC	–	Advanced Process Control
BGLR	–	Bounded Generalized Likelihood Ratio
DCS	–	Distributed Control System
DMC	–	Dynamic Matrix Control
EOS	–	Equation of State
FAF	–	Fatty Acid Fractionation
FCCUs	–	Fluid Catalytic Cracking Units
GAMS	–	General Algebraic Modeling System
GLR	–	Generalised Likelihood Ratio
GT	–	Global Test
HDA	–	Hierarchical Decomposition Approach

IMT	–	Iterative Measurement test
LC	–	Light-cut Column
LLE	–	Liquid / Liquid Equilibrium
MC	–	Middle-cut Column
MIMT	–	Modified Iterative Measurement Test
MT	–	Measurement Test
MTE	–	Mathematical Theory of Evidence
NLP	–	Nonlinear Programming
NT	–	Nodal Test
ODE	–	Ordinary Differential Equation
PC	–	Pre-cut Column
PKO	–	Palm Kernel Oil
PSHFA	–	Palm Stearine Hydrogenated Fatty Acid
RSC	–	Residue Still-cut Column
RTO	–	Real Time Optimisation
SC	–	Still-cut Column
SQP	–	Sequential Quadratic Programming
UNIQUAC	–	Universal Quasi Chemical
VLE	–	Vapor / Liquid Equilibrium
VLLE	–	Vapor / Liquid / Liquid Equilibrium

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CHAPTER 1

INTRODUCTION

1.1 Challenges in Plant Operations

Process industries have been undergoing substantial changes in order to cope with new challenges resulting from high energy and manpower costs, strict safety and environmental regulations, stringent product specification and scarcity of reduced variation feedstock as well as stiff competition from new players. The challenge is particularly serious for plants producing intermediate products where the overall economic potentials are low with small differences between products and raw materials pricing. An increase in raw materials prices and utility costs can sometimes push the plant to operate at a very slim profit margin which may in turn, lead to overall losses if not properly managed.

The situation is further exacerbated by the fact that most of these large scale chemical processes are time–varying in nature. Process changes such as heat exchanger fouling, reactor catalyst decay and feedstock composition variations contribute to the complexity of the process characteristics. Consequently, process plants of this nature are often operated near various constraints governed by limitations of process units as well as the dynamics of the process involved. It is also quite common for a process plant operating in the vicinity of intersections among constraints in order to push for higher economic returns. Such practices impart serious intricacies to plant operators as dealing with simultaneous multiple constraints is not easy to realise. This demands better practices in plant operations.

Along with the development of computer and software technologies, advanced process control (APC) and real-time optimisation (RTO) have been brought forward for chemical industries as potential solutions to the increasingly intense production challenges. Whilst APC software concentrate on solving difficult control problems, RTO packages focus on the improvement of the overall economy of plant operations. The aim of RTO is to search for optimal operating conditions so that the plant profitability is increased by reducing the operating costs. Marlin and Hrymak (1997) listed the features of process plants that favour the application of RTO as follows:

- Adjustable optimisation variables exist after higher priority safety, quality and production rate objectivities have been achieved.
- Profit changes significantly as values of the optimisation variables are changed.
- Disturbances occur frequently.
- Determination of the proper values for the optimisation variables is too complex to be achieved by selecting from several standard operating procedures.

RTO is also useful as it provides detailed operation information that can be highly valuable for plant improvement efforts especially during process debottlenecking and troubleshooting. Abnormalities detected by the gross error detection mechanism, which is a part of the RTO package, may serve as a guide to the process and instruments engineers to troubleshoot the plant errors. Process parameters estimated from the parameter estimation package facilitate process engineers to evaluate equipment conditions and to identify sources of problems. Based on these insights, maintenance can be planned and upgrading can be proposed.

RTO moves processes from one steady state operating condition to another setting that are more profitable. During operation, the RTO software runs a steady state model of the plant based on the current operating conditions to detect the desired steady state values of the process responses. These, along with the actual operation data are used by the steady state detection mechanism to check whether or not the plant is at steady state. This is then followed by two other data validation stages known as data reconciliation and gross error detection where adjustment of measurements and rectification of gross errors are performed. To facilitate the system to cope with changing operating conditions, the software is also supported by parameter estimation package that updates the model parameters. All these features assist to achieve proper conditions required for economic optimisation to be executed. When these are established, the optimisation algorithm then searches for the optimal operating setpoints to be implemented by the plant control system.

1.2 Problem Statement

In this research, a fatty acid fractionation (FAF) process in a local oleochemical plant located in Pasir Gudang, Johor is considered. The plant produces various grades of fatty acids from palm kernel oil and palm hydrogenated stearine. Similar to other plants producing intermediate products, the profit margin is fairly small. The use of multiple feedstock as well as fluctuations in raw material costs and product prices qualify the plant as a candidate for RTO implementations. Here, the aim is to periodically push the plant profit to the most optimal operating zones so that overall profitability is periodically increased.

1.3 Objectives and Scope of Work

This research addresses issues relevant to the implementation of Real Time Optimisation (RTO) to the FAF process aiming at improving the plant economy. The scope of work covers:

i. Development of steady state model of FAF process using HYSY.Plant™ software to support various aspects of RTO implementations.
ii. Development of dynamic model of the FAF process using HYSY.Plant™ software to represent the process throughout the study.

iii. Development of steady state detection using the mathematical theory of evidence.

iv. Development of data reconciliation using the weighted least square technique to ensure the measurements are consistent with the material and energy balances.

v. Development of gross error detection using the Measurement Test (MT) method to eliminate gross error from the measurement.

vi. Development of economic optimisation scheme based on the profit objective function to generate the optimal setpoints for the controllers. HYSYS.Plant^{TM} optimiser is used and sequential quadratic programming (SQP) is chosen to solve the optimisation problem.

In addition to HYSYS.Plant software used to generate both the dynamic and steady state plant operation data, MATLAB software is used for data validation stages. The required software integration can be implemented with the availability of specially built software interface drivers.

1.4 Contribution of the Thesis

This work addresses the development of real time optimisation (RTO) cycle for a tight profit margin process. The cycle that consists of 5 major components, namely steady state and dynamic models, steady state detection, data reconciliation, gross error detection and economic optimisation was tested on a fatty acid fractionation plant, a process with some tight constraints and low operating pressure. Dynamic model was used to represent the real plant. This is thought to be better than the typical strategy of using steady state model with noise added; to represent actual plant condition. The performances of this RTO methodology were further tested by introducing some uncertainties that normally happen in the plant were studied. These include the measurement noises, process disturbances, process leakages and changes of product prices.

1.5 Layout of This Thesis

The thesis is organised as follows. Chapter 2 presents the theoretical foundations of various topics related to the research. Chapter 3 discusses the development of the plant simulation and optimisation model of the FAF process. Chapter 4 describes the development of RTO components, which include the steady state detection, data reconciliation, gross error detection and the economic optimisation. This is then followed by further discussions on the performance of RTO cycle when subjected to the uncertainties such as product price variation, measurement noises, and the process disturbances. Finally, in Chapter 6 overall findings of the research are summarised, conclusions are drawn and recommended further works are listed.

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