FRAMEWORK OF COMPUTER-AIDED SUSTAINABLE INTEGRATED PROCESS DESIGN AND CONTROL FOR REACTOR SYSTEMS

SITI AMINAH BINTI ZAKARIA

UNIVERSITI TEKNOLOGI MALAYSIA

FRAMEWORK OF COMPUTER-AIDED SUSTAINABLE INTEGRATED PROCESS DESIGN AND CONTROL FOR REACTOR SYSTEMS

SITI AMINAH BINTI ZAKARIA

A thesis submitted in fulfillment of the
requirements for the award of the degree of
Master of Engineering (Chemical)

Faculty of Chemical Engineering
Universiti Teknologi Malaysia

JUNE 2015

To my beloved husband, little calliph, parents and family.

ACKNOWLEDGEMENT

First of all, I would like to give a greatest thanks to Allah the Almighty when lastly I finished this project. This project has been carried out at Process System Engineering Centre (*PROSPECT*) at Department of Chemical Engineering from August 2013 until January 2015, under the supervision of Dr Mohd Kamaruddin Abd. Hamid. This work has been supported by Zamalah Universiti Teknologi Malaysia (*UTM*).

I would like to give my sincerest thanks to my supervisor, Dr Mohd Kamaruddin Abd. Hamid who has been provided all the support, help and guidance whenever required. I am also grateful to him for this continuously guidance, academic support and also weekly discussion that has been go through along the journey in finishing this work.

A lot of thanks for my husband, Mohd Jufri bin Zakaria for his limitless support and encouragement that he give to me. Futhermore, I also like to thanks my little calliph, Muhammad Fateh Hizqil bin Mohd Jufri. Thank you for your love and support. Importantly, I like to thanks my dad, mom, my mother in law and father in law, Zakaria Awang, Sobil Yatu Aslamiah Junoh, Jora Kassim and Zakaria Husin for their countless support, love and understanding during the work and thesis done. Not to forget all of my family members for their support and doa'. Thank you.

ABSTRACT

An integrated process design and control (*IPDC*) methodology has been developed which is able to identify and obtain an optimal solution for the *IPDC* problem for chemical processes in an easy, simple and efficient way. However, the developed *IPDC* methodology does not consider any sustainability aspect in the analysis. This study aims to develop a framework of computer-aided sustainable integrated process design and control (Sustain*IPDC*) for reactor systems. This new framework methodology was developed in order to ensure that the process is more economical, controllable as well as sustainable to meet the product quality specifications. The Sustain-*IPDC* problem for reactor systems, typically formulated as a generic optimization problem was solved by decomposing it into six hierarchical stages: (i) pre-analysis, (ii) design analysis, (iii) controller design analysis, (iv) economic analysis, (v) sustainability analysis, and (vi) final selection and verification. Using thermodynamics and process insights, a bounded search space was first identified. This feasible solution space was further reduced to satisfy the process design, controller design and economic constraints in stages 2, 3 and 4, respectively. The sustainability aspect was then analyzed in stage 5 to satisfy the sustainability constraints, until in the final stage all feasible solutions (candidates) were ordered according to the defined performance criteria (objective function). The final selected design was then verified through rigorous simulations or experiments. In the first stage, the concept of the attainable region (AR) was used to locate the optimal solution. The target for this optimal solution was defined and selected at the maximum point of the *AR* diagram. It is expected that the solution target will show higher value of the objective function, hence verifying the optimal solution for the Sustain*IPDC* problem for reactor systems. In addition, the sustainability calculator (called SustainPlus©) was also developed in this study in which the simultaneous calculation of three sustainability indices (one-dimensional, two-dimensional, and three-dimensional) can be performed in one single analysis. Then, the developed methodology were verified by using two different case studies; (i) production of cyclohexanone in a continuous-stirred tank reactor system, and (ii) biomass production in two continuous bioreactor system. Based on two different case studies that have been performed, the results have shown that the optimal solution in terms of design, controller design, economic and sustainability is the best at the highest point of the *AR* diagram. It also shows that the proposed Sustain*IPDC* methodology is able to find the optimal solution that satisfies design, controller, economics and sustainability criteria in an easy, efficient and systematic way.

ABSTRAK

Kaedah proses rekabentuk dan kawalan bersepadu (*IPDC*) telah dihasilkan yang mana ianya mampu mengenalpasti penyelesaian yang optimum untuk masalah *IPDC* bagi proses kimia dengan mudah, cekap dan sistematik. Tetapi, kaedah *IPDC* yang dihasilkan tidak mengambilkira sebarang aspek kelestarian di dalam analisisnya. Kajian ini bertujuan untuk menghasilkan satu kaedah bantuan computer bagi proses rekabentuk dan kawalan bersepadu (menampung*IPDC*) bagi sistem reaktor. Kaedah sistematik ini dihasilkan bagi memastikan bahawa proses ini adalah lebih ekonomi, boleh dikawal dan mampan bagi memenuhi spesifikasi kualiti produk. Masalah menampung*IPDC* bagi system reaktor, biasanya dirumuskan sebagai masalah pengoptimuman generik yang diselesaikan dengan dibahagikan kepada enam peringkat: (i) pra-analisis, (ii) analisis rekabentuk, (iii) analisis rekabentuk pengawal, (iv) analisis ekonomi, (v) analisis kemampanan, dan (vi) pemilihan akhir dan pengesahan. Menggunakan termodinamik dan gambaran proses, ruang carian terbatas dikenalpasti. Ruang penyelesaian ini dikurangkan lagi untuk memenuhi kekangan rekabentuk proses, kawalan dan ekonomi di peringkat 2, 3 dan 4. Aspek kelestarian kemudiannya dianalisis di peringkat 5 untuk memenuhi kekangan kemampanan, sehingga di peringkat akhir semua penyelesaian (calon) disusun mengikut kriteria prestasi tertentu (fungsi objektif). Rekabentuk terakhir yang dipilih kemudiannya disahkan melalui simulasi atau eksperimen. Di peringkat pertama, konsep rantau tercapai (*AR*) ini digunakan untuk mencari penyelesaian yang optimum dari segi keadaan operasi. Sasaran bagi penyelesaian optimum ini ditakrifkan dan dipilih pada titik maksimum rajah AR. Ia dijangka bahawa calon pada titik maksimum rajah ini akan menunjukkan nilai yang lebih tinggi, oleh itu pengesahan penyelesaian optimum bagi masalah menampung*IPDC* untuk sistem reaktor. Selain itu, kalkulator kemampanan (SustainPlus©) juga dibangunkan dalam kajian ini di mana pengiraan serentak tiga indeks kelestarian (satu-dimensi, dua-dimensi dan tiga-dimensi) boleh dilakukan dalam satu analisis tunggal. Kemudian, kaedah ini diuji dengan menggunakan dua kes yang berbeza; (i) penghasilan sikloheksanon dalam sistem tangki reaktor pengacau berterusan, dan (ii) penghasilan biomass dalam dua sistem bioreaktor berterusan. Berdasarkan dua kajian kesini, keputusan menunjukkan bahawa penyelesaian optimum dari segi rekabentuk, rekabentuk pengawal, ekonomi dan kemampanan adalah yang terbaik pada titik tertinggi rajah AR. Ia menunjukkan bahawa kaedah menampung*IPDC* yang dicadangkan mampu untuk mencari penyelesaian optimum yang memenuhi rekabentuk, pengawal, ekonomi dan kemampanan kriteria dengan cara yang mudah, cekap dan sistematik.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

AIChE	-	American Institute of Chemical Engineers
AR	-	Attainable Region
ASW	-	Aspen Simulation Workbook
CEI	-	Chemical Exposure Index
CSTR	-	Continuous-stirred tank reactor
DS	-	Decision Support
EIA	-	Equipment and Inventory Analysis
FTA	-	Fault Tree Assessment
HAZOP	-	Hazard and Operability
HAZOPExpert	-	Software in HAZOP Analysis
IChemE	-	Institution of Chemical Engineers
IPDC	-	Integrated Process Design and Process Control
LCA	-	Life Cycle Analysis/Assessment
MINLP	-	Mixed Integer Non-Linear Programming
MIDO	-	Mixed Integer Dynamic Optimization
m-SAS	-	Modular-based Sustainability Assessment and Selection
NPEI	-	Net Potential Economic Impact
NPV	-	Net Present Value
ROR	-	Rate of Return
SA	-	Sustainability Analysis
Sustain*IPDC*	-	Sustainable Integrated Process Design and Process Control
SustainPlus	-	Sustainability Calculator
SustainPRO	-	Sustainability Tool in retrofitting the chemical processes
WAR	-	Waste Reduction
WBCSD	-	World Business Council for Sustainable Development

1D	-	One-Dimension
2D	-	Two-Dimension
3D	-	Three-Dimension

LIST OF SYMBOLS

A	-	Area
CS	-	Controller structure
d	-	Disturbance variables
dy/dd	-	Sensitivity of controlled variable respect to disturbance
dy/du	-	Sensitivity of controlled variable respect to manipulated
G	-	Set of independent variables
i	-	Category of objective function
j	-	Specific term of each category
J	-	Multi-objective function
T	-	Temperature
u	-	Manipulated (design)variables
v	-	Set of chemical system variables
x	-	Set of process state variables
y	-	Set of controlled variable
Y	-	Set of binary decison variables
θ	-	Set of constitutive variables
$C_{a,f}$	-	Feed concentration of component a
$C_{b,f}$	-	Feed concentration of component b
$C_{c,f}$	-	Feed concentration of component c
$C_{d,f}$	-	Feed concentration of component d
C_D	-	Cost of depreciation per year
F_f	-	Feed flowrate
h_r	-	Reactor height
I_1	-	Income of the product
I_2	-	Cost of raw material

k_1	-	Kinetic Rate
$P_{i,j}$	-	Objective term
$Price_i$	-	Price of product *i* ($/kg)
Price*j*	-	Price of raw material *j* ($/kg)
$Prod_i$	-	Draw rate of product *i* (kg/year)
Prod*j*	-	Feed of rate of raw material *j* (kg/year)
P_1	-	Process design objective
$P_{2,1}$	-	Sensitivity of dy/dd objective
$P_{2,2}$	-	Sensitivity of dy/du objective
P_3	-	Profit function objective
P_4	-	Sustainability objective
R_a	-	Rate law of component a
T_{min}	-	Minimum temperature
T_{max}	-	Maximum temperature
V_R	-	Reactor Volume
$w_{i,j}$	-	Weight factor af each objective term
x_i	-	Mole fraction of feed component i
T_b^i	-	Boiling point temperature
T_m^i	-	Melting point temperature

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Research Background

Chemical processes have been traditionally designed by a sequential approach consisting of initial process design, which is based on steady state economic calculations followed by the synthesis of a controller structure that is generally based on heuristic controllability measures. Thus, the process design and process control aspects have been generally studied independently. This traditional sequential design approach is often inadequate since the process design can significantly affect the process control of the systems (Malcom *et al.*, 2007). Another drawback has to do with how process design decisions influence the controllability of the process to assure that design decisions give the optimum economic and the best control performance, controller design issues need to be considered simultaneously with the process design issues (Miranda *et al.*, 2008). The research area of combining process design and controller design considerations is referred here as integrated process design and controller design (*IPDC*).

Integrated Process Design and Control (*IPDC*) methodology was developed which is able to identify and obtain an optimal solution for the *IPDC* problem for chemical processes in an easy, simple and efficient way (Hamid, 2011). However, the developed methodology for the *IPDC* did not consider sustainability aspect in the early chemical processes design stage. Designing controllable and also sustainable process is one of the key challenges for sustainable development of chemical processes. Chemical process design can be further improved by including sustainability aspect within the developed *IPDC* method to ensure that the design is more cost efficient and controllable, as well as sustainable to meet product quality specifications. This can be achieved by extending the developed model-based *IPDC* method encompasses sustainability aspect.

Sustainability is based on balancing three principal objectives: environmental protection, economic growth, and societal equity. Metrics and indicators are used to assess the sustainability performance of a process or a system, to evaluate the progress toward enhancing sustainability, and to assist decision makers in evaluating alternatives. There are one-dimensional (*1D*), two-dimensional (*2D*) and three-dimensional (*3D*) sustainability indices that will be used in this study. In order to make it more easily in measuring the sustainability in chemical processes, a new computer-aided tool that combined all three dimension of sustainability index has been successfully developed.

Solving *IPDC* problem together with the sustainability criteria may cause complexity in the optimization problem. To obtain solutions for this problem will require a huge computational effort which makes this approach impractical for solving real industrial problems. In order to overcome the complexity of the Sustain-*IPDC* problem and obtain an achievable optimal solution, a decomposition approach is used in this study. The decomposition approach has been applied in managing and solving the complexity of different optimization problems in chemical engineering (Hamid, 2011). The basic idea is that in optimization problems with constraints, the search space is defined by the constraints within which all feasible solutions lie and the objective function helps to identify one or more of the optimal solutions. The constraint equations are solved in a pre-determined sequence such that after every sequential sub-problem, the search space for feasible solutions is reduced and a subset of decision variables are fixed. When all the constraints are satisfied, it remains to calculate the objective function for all the identified feasible solutions to locate the optimal solution. In this study, the decomposition solution strategy has been adopted to develop a new framework of model-based methodology for solving Sustain-*IPDC* problem.

1.2 Problem Statement

Previously, *IPDC* methodology was developed which is able to identify and obtain an optimal solution for the *IPDC* problem for reactor systems in an easy, simple and efficient way (Hamid, 2011). However, the developed methodology for the *IPDC* did not consider sustainability aspect. Designing controllable and also sustainable process is one of the key challenges for sustainable development of reactor systems since reactor is the hard part of the chemical design before any other parts of the design. Reactor system process design can be further improved by including sustainability aspect within the developed *IPDC* method to ensure that the design is more cost efficient and controllable, as well as sustainable to meet product quality specifications. This can be achieved by extending the developed model-based *IPDC* method for reactor systems encompass sustainability aspect.

1.3 Objectives of the Study

The objective for this study is to develop a new framework of model-based methodology, which is able to identify and obtain an optimal solution for the Sustain-*IPDC* problem for reactor systems.

1.4 Scope of the Study

In order to achieve the abovementioned objective, several scopes have been planned:

1. Developing a new model-based methodology for Sustain-IPDC for reactor systems.
2. Developing a sustainability calculator called SustainPlus© for reactor systems that simultaneously calculate three sustainability indexes (*1D*, *2D*, *3D*) in one single analysis.
3. Integrating different available tools in every single stage (such as Microsoft excel, Aspen HYSYS and MATLAB) in the proposed Sustain-IPDC methodology.
4. Testing the performance of the proposed Sustain-IPDC methodology in solving complex reactor system problems.

1.5 Significant of the Study

The significant of this study is that the proposed methodology allows the process engineer in finding the optimal solution for a Sustain-*IPDC* problem for reactor systems in a systematic, efficient and fast. In addition, the proposed methodology can be used not only for industrial purpose but also for academic purpose.

1.6 Thesis Organization

The thesis is organized into six chapters which are (1) introduction, (2) literature review, (3) sustainable integrated process design and control methodology for reactor systems, (4) SustainPlus©: a software for calculating sustainability index of reactor systems, (5) result and discussion, and (6) conclusion and recommendation. In Chapter one, the background of research, problem statement, research objectives, research scopes, significant of the research are presented. Then, in Chapter two, the literature review on the previous research activities is discussed in more details, which includes the development of the *IPDC* methodology, sustainability indices that have been measured by the previous researchers and the *IPDC* methodology upgrading. The methodology development for the Sustain-*IPDC* is detailed out in Chapter three which consists of problem formulation and the decomposition-based solution strategy. In addition, the SustainPlus© software, a computer-aided tool used to calculate the sustainability index is discussed in Chapter four, which includes the overview, framework, implementation and application of the tool. In Chapter five, there are two case studies are presented to test the performance of Sustain-*IPDC* methodology with the help of the developed SustainPlus© tool; the design of the single reactor system and the retrofitting of two reactors system. Finally, the conclusion and recommendation of the research are presented in Chapter six.

REFERENCES

Achour M., Haroun A., Schult C., and Gasem K. (2005). A New Method to Access the Environmental Risk of a Chemical Process. *Chemical Engineering and Processing,* 44, 901-909.

Adams W. (2006). The Future of Sustainability: Re-thinking Environment and Development in the Twenty-first Century. *Report of the IUCN Reowned Thinkers Meeting*.

AfganN., Carvalho M., and Hovanov N. (2000). Energy System Assessment with Sustainability Indicator. *Energy Policy,* 28, 603-612.

Azapagic A., Millington A., and Collett A. (2006, June). A Methodology for Integrating Sustainability Considerations into Process Design. *Chemical Engineering Research and Design, Trans IChemE, Part A, 84*, 439-452.

Alvarado-Morales M., Hamid M. K. A., Sin G., Gernaey K. J., Woodley J. M., and Gani R.(2010).A Model-based Methodology for Simultaneous Design andControl of a Bioethanol Production Process.*Computers and Chemical Engineering,* 34, 2043–2061.

Bare J. (2002). Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI): User's guide and Systems Documentation..

Carvalho A., Matos H. A., and Gani R. (2009). Design of Batch Operations: Systematic Methodology for Generation and Analysis of Sustainable Alterantives. *Computers and Chemical Engineering*, *33*, 2075-2090.

Carvalho A., Matos H. A., and Gani R.(2008). Design of Sustainable Chemical Processes: Systematic Retrofit Analysis Generation and Evaluation of Alternatives. *Process Safety and Environmental Protection, 86*(5), 328-346.

Constable D., Curzons D., and Cunningham V. (2002). Metrics to 'Green' Chemistry-Which are the Best?.*Green Chemistry,* 4, 521-527.

Douglas J. M.(1998). Conceptual Design of Chemical Processes. New York: McGraw-Hill.

Halim I., Carvalho A., Srinivasan R., Matos H. A., and Gani R. (2011). A Combined Heuristic and Indicator-Based Methodology for Methodology for Design of Sustainable Chemical Process Plant. *Computers and Chemical Engineering, 35*, 1343-1358.

Halim I. and Srinivasan R. (2008). Designing Sustainable Alternative for Batch Operations Using an Intelligent Simulation-Optimization Framework. *Chemical Engineering Research and Design, IChemE, 86*, 809-822.

Halim I. and Srinivasan R. (2011). A Knowledge-Based Simulation-Optimization Framework and System for Sustainable Process Operations. *Computers and Chemical Engineering, 35*, 92-105.

Hamid M. K. A. (2011).*Model-Based Integrated Process Design and Controller Design of Chemical Processes*. PhD. Thesis, Technical University of Denmark

Hamid M. K. A., Sin G., and Gani R. (2010).Integration of Process Design and ControllerDesign for Chemical Processes using Model-based Methodology.*Computers andChemical Engineering*, 34, 683–699.

Heikkila A. (1999). *Inherent Safety in Process Plant Design: An Index-based Approach.*Doctor of Science in Technology (132),Espoo: Department of Chemical Technology, Helsinki University of Technology.

Karunanithi A. P. T., Achenie L. E. K., and Gani R. (2006). A Computer-aided Molecular Design Framework for Crystallization Solvent Design. *Chemical Engineering Science*, 61 (4), 1247-1260.

Krotscheck C. and Narodoslawsky M. (1996). The Sustainable Process Index: A New Dimension in Ecological Evaluation. *Ecological Engineering*,6, 241-258.

Malcom, A., Polan, J., Zhang, L., Ogunnaike, B. A., and Linninger, A. (2007). Integrating systems design and control using dynamic flexibility analysis. *AIChE Journal*, 53(8), 2048-2061.

Martins A., Mata T., Costa C., and Sikdar S. (2007). Framework for Sustainability Metrics. *Industrial and Engineering Chemistry Research*, 46, 2962-2973.

Miranda, M., Reneaume, J. M., Meyer, X., Meyer, M., and Szigeti, F. (2008). Integrating process design and control: An application of optimal control to chemical processes. *Chemical Engineering and Processing*, 47, 2004-2018.

Morales-Alvarado M., Terra J., Gernaey K. V., Woodley J. M., and Gani R. (2009). Biorefining Computer Aided Tools for Sustainable Design and Analysis of Bioethanol Production. *Chemical Engineering Research and Design, 87*, 1171-1183.

Othman M., Repke J., Wozny G., and Huang Y. (2010). A Modular Approach to Sustainability Assessment and Decision Support in Chemical Process Design. *Induxtrial and Engineering Chemistry Research*, 49, 7870-7881.

Sailing P., Maisch R., Silvani M., and KonigN. (2005). Assessing the Environmental-Hazard Potential for Life Cycle Assessment, Eco-efficiency and SEEbalance. *The International Journal of Life Cycle Assessment,* 10, 364-371.

Sakizlis, V.,Perlins, J. D., and Pistikopoulos, E. N. (2004). Recent advances in optimization-based simultaneous process design and control design, *Computers and Chemical Engineering*, 28, 2069-2086.

Seferlis P., and Georgiadis, M. C. (2004). The integration of process design and control. Amsterdam: Elsevier B.V.

Shadiya O. O., and High A. K. (2012). Sustainability Evaluator: Tool for Evaluating Process Sustainability. *Environmental Progress and* Sustain*able Energy,* 32 (3), 749-761.

Singh A., and Lou H. (2006). Hierarchical Pareto Optimization for the Sustainable Development of Industrial Ecosystems, *Industrial and Engineering Chemistry Research*, 45, 3265-3279.

Tanzil D. and Beloff B. (2006). Assessing Impacts: Overview on Sustainability Indicators and Metrics. *Environmental Quality Management,* 15, 41-56.

Tallis B. (2002). The Sustainability Metrics: Sustainable Development Progress Metrics Recommended for use in the Process Industry, Warwickshire, UK: Institution of Chemical Engineer (IChemE).

Uhlman, B. W., &Saling, P. 2010. Measuring and communicating sustainability through eco-efficiency analysis. *Chemical Engineering Progress*, December, 17-26.

Vanavil B., Harikumar M. P., and Rao A. S. (2014). Bifurcation analysis of two continuous bioreactors operated in series. *Chemical Engineering Research and Design*, http://doi.org/10.1016/j.cherd.2014.01.013.

Venkatasubramanian V., Zhao J., and Viswanathan S. (2000). Intelligent Systems for HAZOP Analysis of Complex Process Plants. *Computers and Chemical Engineering*, 24, 2291-2302.

Vincent R., Bonthoux F., Mallet G., Ipurraquirre J. F., and Rio S. (2005). MethodologieD'evaluationSimplifiee du RisqueChimique: UnOutild'Aide a la Decision. INRS Hyg. Secur. Travail, 195.

Zakaria S. A, Zakaria M. J., and Hamid M. K. A. (2014). Sustainable Integrated Process Design and Control for a Continuous-Stirred Tank Reactor System. *Applied Mechanics and Materials*, 625, 466-469.