



<http://researchspace.auckland.ac.nz>

## ***ResearchSpace@Auckland***

### **Copyright Statement**

The digital copy of this thesis is protected by the Copyright Act 1994 (New Zealand).

This thesis may be consulted by you, provided you comply with the provisions of the Act and the following conditions of use:

- Any use you make of these documents or images must be for research or private study purposes only, and you may not make them available to any other person.
- Authors control the copyright of their thesis. You will recognise the author's right to be identified as the author of this thesis, and due acknowledgement will be made to the author where appropriate.
- You will obtain the author's permission before publishing any material from their thesis.

To request permissions please use the Feedback form on our webpage.

<http://researchspace.auckland.ac.nz/feedback>

### **General copyright and disclaimer**

In addition to the above conditions, authors give their consent for the digital copy of their work to be used subject to the conditions specified on the [Library Thesis Consent Form](#) and [Deposit Licence](#).

### **Note : Masters Theses**

The digital copy of a masters thesis is as submitted for examination and contains no corrections. The print copy, usually available in the University Library, may contain corrections made by hand, which have been requested by the supervisor.



# The Development of a Controllability Index based on RGA and Exergy for Plant-wide Control Problems

---

**M. Tajammal Munir**

*A thesis submitted in partial fulfilment of the requirements for the degree of Doctor of Philosophy in Chemical and Materials Engineering,*

*The University of Auckland, 2012.*

This thesis is for examination purposes only and may not be consulted or referred to by any persons other than those involved in the examination process.

## **Abstract**

Process design is a complex activity and has many levels and stages. The information and knowledge required at every level of the design increases through the process design sequence. As the design process is constrained by control and thermodynamics (eco-efficiency), for efficient and easily controllable process design, an integrated approach involving process design, control and thermodynamics (eco-efficiency) must be used during early design stages. An integrated approach has many advantages over previous approaches in which process control was only considered during the late stages of the process design.

For an easily controllable process, the controllability of the process should be determined as early as possible in the process design sequence. Thus there is a need for tools which can evaluate the controllability of the process before detailed design or construction commences. For the selection of the best control configuration, there are many mathematical formulations and systematic strategies, such as; the relative gain array (RGA), the Niederlinski index (NI), singular value decomposition (SVD), the condition number (CN) and Morari's resiliency index (MRI).

In the wake of the energy crises, control system structure selection must focus, not only on controllability, but also on energy cost and environmental impact (eco-efficiency). For the integration of controllability and eco-efficiency, the potential of the thermodynamic property exergy is used. The combination of the 1<sup>st</sup> and 2<sup>nd</sup> laws of thermodynamics gives rise to the concept of Exergy. Exergy combines control scheme selection and eco-efficiency into a single domain.

Exergy has many valuable uses in process design and control for the facilitation of these complex tasks. There are many exergy based tools and methods, such as; the efficiency concept, the exergy flow diagram, the relative exergy array (REA), the exergy eco-efficiency factor (EEF) and the relative exergy destroyed array (REDA). These tools/methods can be used to describe, analyze, optimize and control the process.

In this research project, tools and methods were developed to determine plantwide controllability/control scheme interactions (plantwide RGA/REA), a process exergy calculator, whole process eco-efficiency analysis tools (EEF and REDA), and tools to integrate process design, control and eco-efficiency. These newly-developed tools (the REA,

EEF and the REDA) combined with classical controllability tools (the RGA, NI, SVD and the CN) help in deciding on controllable and eco-efficient control schemes for an entire process/plant.

## **Acknowledgements**

I express my deepest gratitude to my supervisor Prof. Brent R. Young for his careful supervision throughout the course of my PhD research work. His excellent guidance, encouragement, support and advice from the early phase of my PhD work to the final phase facilitated me not only to produce this thesis but also to produce a number of journal articles and conference papers. For this, I owe my sincere appreciation to him. I would also like to thank my co-supervisor Prof. John JJ Chen for his devotion to the project during the first year of my PhD.

I would like to express my special thanks to Dr Wei Yu for his suggestions and valuable explanations about the potential problems in this research, to the members of Industrial Information and Control Centre (I<sup>2</sup>C<sup>2</sup>), and the Chemical and Materials Engineering department for their support. I would also like to thank Margaret Stiles for proofreading.

Finally, I would like to thank my parents and family for their patience, encouragement, love and prayers, for their support and love from a far distance, and my friends for their friendship.

Thank you very much.

# Table of Contents

Abstract.....	ii
Acknowledgements.....	iv
List of Figures .....	ix
List of Tables .....	xi
Chapter 1. Introduction.....	1
1.1. Process control.....	1
1.2. Eco-efficiency .....	4
1.3. Objective(s) .....	6
1.4. Research Organisation .....	8
1.5. Expected Contributions.....	9
1.6. Thesis Structure .....	11
1.7. Summary .....	13
References .....	15
Chapter 2. Literature Review .....	17
2.1. Process Design .....	17
2.2. Process Control .....	19
2.3. Thermodynamics.....	21
2.4. Integration of Process design, Control and Thermodynamics.....	23
2.4.1. Process control and Thermodynamics (Region a).....	23
2.4.2. Process design and control (Region b).....	25
2.4.3. Process design and Thermodynamics (Region c).....	26
2.5. The Need for New Tools .....	26
2.6. Summary .....	27
References .....	28
Chapter 3. Determination of Plant-wide control loop configuration and Eco-efficiency .....	34
Abstract.....	34
3.1. Introduction .....	34
3.2. RGA and REA .....	36
3.2.1. RGA.....	36
3.2.2. REA .....	38
3.3. Exergy Calculation Procedure .....	42

3.4. Case Studies .....	45
3.4.1. Case Study 1: Distillation Column .....	45
3.4.2. Case Study 2: Ethylene Glycol Production Plant .....	49
3.5. Summary .....	53
References .....	54
Chapter 4. Recycle effect on the Relative Exergy Array.....	58
Abstract.....	58
4.1. Introduction .....	58
4.2. Relative Gain Array (RGA) and Relative Exergy Gain Array (REA).....	61
4.2.1. Relative Gain Array (RGA) .....	61
4.2.2. Exergy and Relative Exergy Array (REA).....	62
4.3. Exergy Calculation.....	66
4.3.1. Exergy Calculation Programme .....	68
4.4. Case Studies .....	68
4.4.1. Case Study 1: Ethyl Benzene Production .....	68
4.4.2. Case Study 2: Ethylene Glycol Production .....	75
4.5. Summary .....	79
References .....	80
Chapter 5. Plant-wide control: Eco-efficiency and control loop configuration .....	84
Abstract.....	84
5.1. Introduction .....	84
5.2. Control loop configuration.....	87
5.2.1. Methods based on controllability .....	87
5.2.2. Methods based on eco-efficiency .....	88
5.3. Case study – MCB separation plant .....	93
5.3.1. Process description .....	94
5.3.2. Results and Discussions .....	95
5.3.3. Validation of EEF Results.....	97
5.4. Summary .....	99
5.5. Conclusions .....	100
References .....	101
Chapter 6. Eco-efficiency and control loop configuration for recycle systems .....	106
Abstract.....	106
6.1. Introduction .....	106

6.2. Control loop configuration.....	109
6.2.1. Methods based on controllability.....	109
6.2.2. Methods based on Eco-efficiency.....	109
6.3. Case study – MCB separation plant.....	114
6.3.1. An Isolated distillation column.....	115
6.3.2. MCB distillation column with recycle.....	117
6.3.3. MCB plant with distillation column without recycle.....	124
6.3.4. MCB plant with distillation column and recycle.....	126
6.4. Summary.....	129
6.5. Conclusions.....	129
References.....	130
Chapter 7. A software algorithm/package for control loop configuration and eco-efficiency.....	134
Abstract.....	134
7.1. Introduction.....	134
7.2. Eco-efficiency and Exergy Eco-efficiency factor (EEF).....	136
7.2.1. Eco-efficiency.....	136
7.2.2. Exergy eco-efficiency factor (EEF).....	137
7.3. Software algorithm/package for EEF calculation.....	138
7.4. Case study.....	142
7.5. EEF calculation software algorithm/package.....	144
7.6. Summary.....	148
7.7. Conclusions.....	148
References.....	149
Chapter 8. The Relative exergy-destroyed array: A new tool for process design and control.....	152
Abstract.....	152
8.1. Introduction.....	152
8.2. Eco-efficiency, Exergy eco-efficiency factor (EEF) and RGA.....	155
8.2.1. Eco-efficiency.....	155
8.2.2. Exergy eco-efficiency factor (EEF).....	156
8.2.3. The Relative Gain Array (RGA).....	157
8.3. Relative Exergy Destroyed Array (REDA) – A new tool.....	157
8.3.1. REDA definition.....	157
8.3.2. Interpretation of the REDA.....	159
8.3.3. Rank based on the REDA.....	160

8.3.4. An illustrative example .....	161
8.4. Case studies .....	163
8.4.1. MCB separation process description .....	163
8.4.2. MCB distillation column .....	165
8.4.3. Heat exchanger networks (HEN).....	167
8.4.4. MCB whole plant.....	170
8.5. Summary .....	172
8.6. Conclusions .....	172
References .....	173
Chapter 9. Discussion, conclusions and recommendations for future work .....	175
9.1. Discussion.....	175
9.1.1. Process simulator based Exergy Calculator .....	175
9.1.2. Plantwide RGA and REA .....	176
9.1.3. Exergy Eco-efficiency Factor (EEF) .....	176
9.1.4. Relative Exergy Destroyed Array (REDA) .....	177
9.2. Conclusions .....	177
9.3. Limitations.....	179
9.4. Recommendations for future work .....	180
Appendix A: List of Publications.....	183
A.1. Journal articles and Book Chapters .....	183
A.2. Conference articles.....	183

## List of Figures

Figure 1-1. Overall research organisation/stages .....	8
Figure 1-2. Overall thesis structure.....	11
Figure 2-1. General process design procedure.....	18
Figure 2-2. Control loop interactions for a 2x2 system .....	20
Figure 2-3. Energy and Exergy .....	22
Figure 2-4. Integration of process design, control and thermodynamics .....	23
Figure 3-1. A general thermodynamic process .....	38
Figure 3-2. Steps involved in exergy calculation.....	44
Figure 3-3. Distillation column schematic for case study 1 .....	46
Figure 3-4. Ethylene glycol plant schematic for case study 2 (Svrcek et al. 2006) .....	49
Figure 4-1. General thermodynamic process .....	62
Figure 4-2. Case study 1 Ethyl benzene production schematic .....	69
Figure 4-3. Case study 2 Ethylene glycol production schematic .....	76
Figure 5-1. A general thermodynamic process .....	89
Figure 5-2. Exergy flows for a general process .....	91
Figure 5-3. MCB separation process schematic.....	93
Figure 5-4. Variation of Exergy In and Out of MCB plant due to composition set point changes for the $LVQ_{cw}$ configuration (a) Exergy variation due to step change in $x_D$ (b) Exergy variation due to step change in $x_B$ (c) Exergy variation due to step change in $x_{HCl}$ .....	98
Figure 5-5. Variation of Exergy In and Out of MCB plant due to composition set point changes for the $DVQ_{cw}$ configuration (a) Exergy variation due to step change in $x_D$ (b) Exergy variation due to step change in $x_B$ (c) Exergy variation due to step change in $x_{HCl}$ .....	98
Figure 6-1. Exergy flows for a general process .....	111
Figure 6-2. MCB separation process schematic.....	114
Figure 6-3. Variation of Exergy In and Out of the isolated MCB column due to composition set point changes for the $LB$ configuration (a) Exergy variation due to step change in $x_D$ (b) Exergy variation due to step change in $x_B$ .....	116
Figure 6-4. Variation of Exergy In and Out of the isolated MCB column due to composition set point changes for the $DV$ configuration (a) Exergy variation due to step change in $x_D$ (b) Exergy variation due to step change in $x_B$ .....	117
Figure 6-5. Variation of Exergy In and Out due to composition set point changes for the $LVQ_{cw}$ configuration (a) Exergy variation due to step change in $x_D$ (b) Exergy variation due to step change in $x_B$ .....	122
Figure 6-6. Variation of Exergy In and Out due to composition set point changes for the $DVQ_{cw}$ configuration (a) Exergy variation due to step change in $x_D$ (b) Exergy variation due to step change in $x_B$ .....	122
Figure 6-7. Variation of Exergy In and Out of MCB plant without recycle due to composition set point changes for the $LB$ configuration (a) Exergy variation due to step change in $x_D$ (b) Exergy variation due to step change in $x_B$ .....	125
Figure 6-8. Variation of Exergy In and Out of MCB plant without recycle due to composition set point changes for the $DV$ configuration (a) Exergy variation due to step change in $x_D$ (b) Exergy variation due to step change in $x_B$ .....	125

Figure 6-9. Variation of Exergy In and Out of MCB plant due to composition set point changes for the $LVQ_{cw}$ configuration (a) Exergy variation due to step change in $x_D$ (b) Exergy variation due to step change in $x_B$ (c) Exergy variation due to step change in $x_{HCl}$ .....	127
Figure 6-10. Variation of Exergy In and Out of MCB plant due to composition set point changes for the $DVQ_{cw}$ configuration (a) Exergy variation due to step change in $x_D$ (b) Exergy variation due to step change in $x_B$ (c) Exergy variation due to step change in $x_{HCl}$ .....	127
Figure 7-1. Exergy flows for a general process .....	137
Figure 7-2. A generalized EEF calculation algorithm .....	138
Figure 7-3. EEF calculation algorithm for 3x3 system.....	140
Figure 7-4. A simple CSTR with a hypothetical reaction, $A \rightarrow B$ .....	141
Figure 7-5. MCB separation process schematic.....	143
Figure 7-6. Schematic of EEF calculation software algorithm/package.....	145
Figure 8-1. Exergy flows for a general process .....	156
Figure 8-2. A simple CSTR with a hypothetical reaction, $A \rightarrow B$ .....	161
Figure 8-3. Schematic of MCB separation process.....	164
Figure 8-4. Heat exchanger networks (a) original configuration and (b) modified configuration with bypass.....	167

## List of Tables

Table 3-1. Feed and distillation column specifications for case study 1.....	46
Table 3-2. Control loop pairing nomenclature.....	47
Table 3-3. Variable pairing of different control configurations for case study 1.....	47
Table 3-4. Configurations for step change experiments for case study 1.....	47
Table 3-5. Feed, column and simulation model specifications for case study 2.....	50
Table 3-6. Control pairings of different control configurations for case study 2.....	51
Table 4-1. Distillation columns details and specifications.....	70
Table 4-2. Loop pairing nomenclature.....	70
Table 4-3. Variable pairing of different control configurations for case study 1.....	71
Table 4-4. Description of the 4 simulations performed for case study 1.....	71
Table 4-5. Configurations for step change experiments for case study 1.....	72
Table 4-6. RGA results for distillation column T1.....	72
Table 4-7. REA results for distillation column T1.....	73
Table 4-8. Selection of control configuration for column T1 based on the RGA and REA values from models 1-4.....	74
Table 4-9. RGA results for distillation column T2.....	74
Table 4-10. REA results for distillation column T2.....	75
Table 4-11. Selection of control configuration for column T2 based on the RGA and REA values from models 1-4.....	75
Table 4-12. Feed, column and simulation model specifications for case study 2.....	76
Table 4-13. Control pairings of different control configurations for case study 2.....	77
Table 4-14. RGA results for the study case 2.....	78
Table 4-15. REA results for the study case 2.....	78
Table 5-1. The RGA, DRGA, REA, NI and CN results for the whole MCB plant.....	95
Table 5-2. The EEFs for the MCB plant.....	97
Table 5-3. Total Exergy used by the whole MCB plant with the two control configurations $LVQ_{cw}$ and $DVQ_{cw}$ .....	99
Table 6-1. The RGA, DRGA, NI and CN Results for the MCB distillation column alone (T2).....	115
Table 6-2. The EEFs for the MCB column alone.....	116
Table 6-3. Exergy used by the two control configurations $LB$ and $DV$ on the isolated MCB column.....	117
Table 6-4. The RGA, DRGA, NI and CN Results for the whole MCB plant.....	119
Table 6-5. EEFs for the MCB column in the plantwide layout.....	120
Table 6-6. PI controllers for the MCB distillation column.....	121
Table 6-7. Exergy used by the two control configurations $LVQ_{cw}$ and $DVQ_{cw}$ on the column within the MCB plantwide layout.....	123
Table 6-8. EEFs for MCB plant with and without recycle.....	124
Table 6-9. Exergy used by control configurations $LB$ and $DV$ in MCB plant without recycle.....	126
Table 6-10. Total Exergy used by the whole MCB plant with the two control configurations $LVQ_{cw}$ and $DVQ_{cw}$ .....	128
Table 7-1. Hypothetical components and reaction information.....	141
Table 7-2. EEFs for reactor, R1.....	142
Table 7-3. EEFs for MCB plant with and without recycle.....	147

Table 8-1. REDA ranks for selecting control configuration .....	160
Table 8-2. Hypothetical components and reaction information .....	161
Table 8-3. The EEFs for an illustrative example .....	162
Table 8-4. The RGA, REEFA and REDA results for an illustrative example.....	162
Table 8-5. The EEFs for the MCB distillation column .....	165
Table 8-6. The RGA, REEFA and REDA results for the MCB distillation column .....	165
Table 8-7. The RGA, REEFA and REDA results for the HEN .....	168
Table 8-8. The EEFs for the HEN.....	169
Table 8-9. The RGA, REEFA and REDA results for the whole MCB plant.....	170
Table 8-10. The EEFs for the whole MCB plant .....	171

## **Chapter 1. Introduction**

This chapter presents a basic introduction and the background to major topics related to this research. The goal of this chapter is to provide an introduction to the relevant aspects of process control, control scheme selection, exergy, eco-efficiency and an integrated approach to process design, control and eco-efficiency. The chapter also provides motivation for the development of; tools to determine plant-wide controllability/control scheme interactions, a process exergy calculator, whole process eco-efficiency analysis tools, and tools to integrate process design, control and eco-efficiency.

### **1.1. Process control**

The operation of a chemical/petrochemical process depends on important aspects like process control. Process control is an engineering discipline that deals with algorithms, mechanisms and strategies for controlling the output of a process within a desired range. No process can constantly maintain a steady state due to the presence of measured and unmeasured disturbances which are responsible for driving the process variables away from their desired set points. A well designed process control system uses a control strategy to maintain the process variables close to the designed set points while maintaining an apparently steady state.

Normally process plants are dynamic in nature and cannot be treated as being in a steady state, as there will always be a variation in variables with the passage of time. Under these circumstances, it is required that the variables are controlled within certain limits. These variations act as disturbances for a process plant. The disturbances can be internal, such as an incidence of fouling inside a heat exchanger, or can be external, such as a change in the temperature of the surroundings. To handle these disturbances in a process, it is necessary to have a process control system that can control the variables in order that an apparently steady state can be maintained; such a steady state is compulsory for safe running and in accordance with the design of a plant. Process control uses sensors, signals, control variables and manipulated variables to do its job. Otherwise the safe operation of a process plant is impossible.

Process control is a complex and multi-faceted task having five main phases/stages: i) process design; ii) control system structure design; iii) controller algorithm/configuration

selection; iv) controller tuning; and v) control hardware/infrastructure. The process design stage involves: the construction of a steady state process flow sheet; the selection of a particular flow sheet structure; the selection of design parameters; the selection of equipment, and the selection of operating conditions. Control loop configuration/control pair selection occurs during the control system structure stage. The selection of the controller type of (e.g. a proportional, integral and derivative type) pertains to the controller algorithm/configuration stage. The next stage of the process control involves dealing with controller tuning. The selection of control hardware such as, sensors, control valves and final control elements is the last stage of process control (Luyben et al. 1998; Marlin 2000).

The gamut of process control starts with the aim of an easily controllable design of the process. As the process design is constrained by process control, an integrated approach to process design and control must be used. Due its importance, process control should be considered during the early design stages of a new or improved process. However, this is still rarely the case in process design practice (Luyben et al. 1998; Kookos and Perkins 2001; Koolen 2001).

The Integrated approach to process design and control has many advantages over the previous approach in which process control was considered during late stages of the process design. For example, applying an integrated approach means being able to change the flow sheet structure, employ different types of equipment and to use alternative design parameters more easily and cost effectively. This integrated approach simultaneously allows changes to be made in the configuration of the process to permit easier control and evaluation of the many control structure candidates. An integrated approach results in better process design and an easily controllable process with low additional capital expenditure and few lost sales opportunities (Luyben et al. 1998).

After the initial process design stage, the next stage of process control involves the determination of the control system structure. The selection of control system structure is based on the type of control used for the process/plant. A centralized multi-input multi-output (MIMO) controller or a set of single-input single-output (SISO) controllers is used to control a process. A decentralized type of control system is more common than the centralized type of control system in the process industry, as it has more captivating advantages: it is easy to understand, uses uncomplicated hardware, and employs simple working algorithms (Morari and Evangelhos 1989; Marlin 2000).

For a decentralized type of control system, the control system structure decides the best control scheme. Control scheme selection pertains to the pairing of manipulated (MV) and controlled variables (CV). For a process/plant, control scheme selection is a straightforward task, provided that no interactions are present between the various control loops in multi-loop control schemes of that process/plant. However, this is rarely the case in process control design practice. A well performing control scheme selection is essential because the incorrect pairing of MV and CV will result in poor performance.

There are several techniques/methods for designing/selecting decentralized MIMO control schemes, such as the relative gain array (RGA), the Niederlinski index (NI), singular value decomposition (SVD), the condition number (CN) and Morari's resiliency index (MRI) (Seborg et al. 1989; Svrcek et al. 2006; Seborg et al. 2010).

The RGA, proposed by Bristol (1966), is a popular tool used for a quantitative comparison of the effect of a control loop on other control loops. The RGA is used to determine possible interactions between multiple SISO control loops. The RGA helps to select well performing control schemes/control pairings. The NI is a handy tool for analyzing and testing the stability of an RGA selected control scheme. The use of NI is more common for lower order systems (2x2). In the instance of higher order systems, the NI can evaluate only control loop instability (Niederlinski 1971). SVD is another useful tool for predicting the directional sensitivity of a process. SVD is used to analyze the sensitivity of the control loop interaction to process gain errors. SVD also helps to evaluate the decoupling of the control loops. The CN is used to determine the feasibility of implementing a decoupling controller. The CN is the ratio of the largest to the smallest eigenvalues of the diagonal eigenvalues matrix in the SVD of the process gain matrix. The value of this ratio (CN) is very important in determining whether decoupling is feasible or not (McAvoy 1983). These techniques/methods (RGA, NI, SVD and CN) predict possible interactive effects between multiple SISO control loops, based on steady state information.

In some cases, these steady state information based techniques (RGA, NI, SVD and CN) can lead to incorrect conclusions concerning the control scheme selection. Dynamic effects are also included in some techniques/methods to minimize the deficiency of these steady state techniques. For example, this happens in dynamic relative gain array (DRGA), internal model control (IMC) and effective relative gain array (ERGA). Using the steady state (RGA, NI, SVD and CN) and dynamic (DRGA, IMC and ERGA) techniques, well performing control

schemes are further selected. The viability of a well performing/selected control scheme is further validated by the dynamic simulation of responses to the various process disturbances.

In spite of all the advantages of RGA (simple and easy to use), its results can change significantly when a single isolated unit is connected with other units in a plant-wide layout through recycles, this can result in a different control configuration from that on an isolated unit without recycles (Papadourakis et al. 1987). To improve the rate of materials usage and energy efficiency, material and energy streams are recycled from downstream units to upstream units in the chemical process industry. However, this recycling of material/energy streams from a unit can have a significant effect on the controllability of that unit.

## **1.2. Eco-efficiency**

Steady state/dynamic techniques for selecting MIMO control schemes focus on controllability and control loop stability. Control system structure/control scheme selection is a large part of process control. In this ubiquitous age of industrialization and in the wake of decreasing energy resources, increasing energy costs and energy crises, special attention must be paid to the control system structure/control scheme selection, as a poorly structured control scheme can lose a great deal of energy from a process/plant. In the wake of energy crises, control scheme selection must also consider energy usage, cost and ecological impacts. This can be achieved by integrating control scheme selection and energy cost/energy usage/environmental impacts.

Thermodynamic properties such as exergy have the potential to amalgamate several elements into a single domain, these include; control system structure/control scheme selection and energy cost/energy usage/environmental impacts. The concept of exergy indicates what is wasted in terms of energy or the eco-efficiency of the process/plant. Exergy is the component of energy which is available for useful work. Kotas (1985, pp 7) defines exergy as “The maximum amount of work/useful energy drawn from a process/material stream as it comes from its original state (process condition) to the ultimate dead state (reference state) during which it interacts only with the environment”. At the ultimate dead state, the process/material stream is in thermodynamic (thermal, mechanical and chemical) equilibrium with the environment (Kotas 1985).

Exergy accounts for the quality of energy/fraction of energy that can be fully converted into useful work and/or other types of energies. Every irreversible process causes exergy

destruction leading to an increased exergy/energy requirement or entropy production. Since exergy can detect and evaluate the causes of the thermodynamic imperfections of the considered process/material stream, it can therefore be used as a measure to evaluate the eco-efficiency of the process.

Eco-efficiency is also a measure of progress in green chemical engineering growth. The concept of eco-efficiency can be traced back to the 1960s as the concept of environmental efficiency, or as a business when linked to sustainable development. Eco-efficiency has a role in expressing how efficient economic activity is with regard to nature's goods/services. The concept of eco-efficiency focuses on methods of resource use, obtaining economic and environmental progress through efficient use of resources and lower pollution/emissions.

The World Business Council for Sustainable Development (WBCSD) states that eco-efficiency is achieved through the practice of producing "valuable goods and services that satisfy human needs and bring quality of life with reduced environmental impacts and resource intensity in line with the Earth's estimated carrying capacity." In other words eco-efficiency means producing more with less. An eco-efficient process is ecologically friendly and economically viable. Ecologically friendly practices signify a process with reduced consumption of energy/destroyed exergy. This diminution in energy utilization reduces the operational expenses of that process. Efficient use of energy/exergy plays an important role for sustainability and minimizing environmental impacts.

Exergy has many valuable uses in process design and control to facilitate these complex tasks. There are many exergy based tools and methods, such as; efficiency concepts, exergy flow diagrams, relative exergy array (REA), exergy eco-efficiency factor (EEF) and relative exergy destroyed array (REDA). These tools/methods can be used to describe, analyze, optimize and control the process. REA, EEF and REDA are also explained in Section 1.5 of this chapter.

Inefficient parts of a process/plant are identified by using the concepts of exergy/exergy analysis and exergetic efficiency (efficiency concepts). Exergetic efficiency is the ratio of the total exergy going out to the total exergy going into a process. The exergetic efficiency ratio of a process is equivalent to its eco-efficiency and is used to measure the exergy efficiency of a process (Szargut et al. 1988).

As, in practice, individual units are connected with other units of a plant in a plant-wide layout through recycles, so the control scheme selection criteria (RGA, NI, SVD and CN) and eco-efficiency measures (EEF and REDA) should be based on the plant-wide layout with the consideration of recycles.

This chapter is further organized as follows. After this general and brief introduction related to this research project, the objectives of the project are discussed and explained. Following this, the research's approach to the accomplishment of these objectives is discussed. The major contributions achieved in this project are then discussed. Next, the thesis structure and contributing research papers are outlined. Finally, all the details and discussions are summarized.

### **1.3. Objective(s)**

The objectives of this research project were: i) development of a process exergy calculator using a commercial simulator VMGSim; ii) to develop tools for the evaluation of plantwide controllability/ control scheme interactions (plantwide RGA/REA); iii) use of exergy for the eco-efficiency analysis of the whole unit/process or even the plant (EEF); and iv) to explore the use of exergy as a tool to develop controllability index/control scheme interactions/relative eco-efficiency of a MIMO process (REA, REEFA and REDA).

During the initial stages of this work our intentions were to develop a process exergy calculator using a commercial simulator, VMGSim. An exergy calculator was required to calculate exergy of the material streams, necessary to develop eco-efficiency tools such as REA, EEF and REDA. In this work the VMGSim was used; this is one of the latest commercial process simulators. The VMGSim has the most recent and up to date thermodynamic engine, called VMGThermo, for the prediction of thermodynamic data. The use of VMGSim facilitates the calculation of accurate material exergy values (Virtual Materials Group Inc. 2009).

In this work, after developing an exergy calculator, the focus moved towards the extending of RGA to include the plant-wide control problem. Plantwide RGA was then extended to plant-wide REA by using the concept of exergy. As, in practice, individual units are connected with other units of the plant in plant-wide layout through recycles, in this work tools were developed for the evaluation of plant-wide controllability (plant-wide RGA) and eco-

efficiency/exergy interactions (plantwide REA). The effect of recycles on the REA results was also studied in this work.

As the REA only measures eco-efficiency within the scope of control loops, in this work, a new measure of eco-efficiency, EEF, was developed for the eco-efficiency analysis of the whole unit/process/plant. EEF helps to select the best control configuration for eco-efficiency of the whole process/plant. Since the recycling of material and energy streams from downstream units to upstream units is a common practice in the process industry, the effect of recycles on the EEF results was also studied in this project. In this work, the controllability/eco-efficiency assessments (RGA, REA, and EEF) of different designs (i.e. different plant topology with or without recycle) were performed manually because for complex actual plants the strategies available for automatic selection of the best plant design by using different measures are difficult or impossible to implement and are not done in practice (Young, 2012). Having said that, manual strategies for the manual testing of each possible design/topology can be very time consuming task especially for large scale systems.

The development of a new tool, REDA, was also proposed for the measurement of the relative eco-efficiency of a MIMO process for possible alternative control schemes. The REDA is used to compare the eco-efficiencies of a process under different possible control schemes. The REDA tool is simple and easy to use to quickly find an optimal and eco-efficient control design during early design stages, as it is based on steady state information.

EEF and REDA can both be used to determine the most eco-efficient control configuration. Both tools (EEF and REDA) have the same objective but differ in their methods of application to determine the most eco-efficient control configuration. For example, EEF determines the most eco-efficient control configuration by considering one control configuration at a time. EEF results also require dynamic simulation validation because they are based on steady state information. Dynamic simulation validation of EEF increases the computation load on practicing engineers.

REDA is simpler than EEF as it helps to develop a rank for selecting a control configuration that is based on controllability and eco-efficiency. As REDA measures the relative eco-efficiency of a MIMO process for different combinations of control structure, REDA can therefore also be used as a screening tool to preliminarily select eco-efficient control schemes for their further evaluation of eco-efficiency. REDA results are verified with the results of steady state EEF. Dynamic simulation validation can also be used for the validation of REDA

results. The interpretation of REDA results (closeness of diagonal elements to zero) can help to quantify eco-efficiency differences due to the varying combinations of control structures. Like EEF, REDA also integrates the controllability and measurements of the eco-efficiency of a process.

In this work, the methodologies used are mostly based on simple linear models of the system except for a few cases of distillation columns and complicated case studies (non-linear model systems). The linearization of the system introduces uncertainty in the results for complicated nonlinear case studies. This work does not refer to the complexities that such uncertainty introduces into the validity of the proposed methodology because in this work, the main objective was to find relation between controllability and eco-efficiency. So the assumption was that if the plant was assessed as controllable, then these non-linearities would not be significant because the plant can be easily controlled at the operating/linearization point. The proposed REA, EEF and REDA measures are only applicable to stable systems and an extension to unstable systems needs to consider for applying these tools to more complex systems – fortunately most actual process systems are open loop stable.

### 1.4. Research Organisation

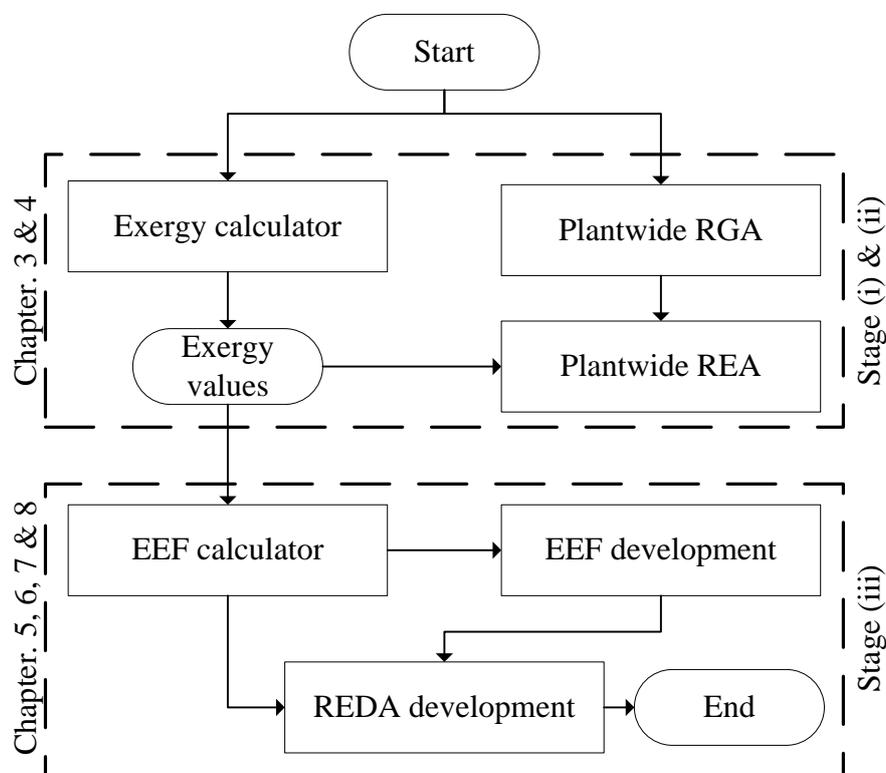


Figure 1-1. Overall research organisation/stages

In order to address the proposed research objectives, this research is divided into three key areas/stages: i) development of a process exergy calculator using VMGSim; ii) development of tools for the evaluation of plant-wide controllability/control scheme interactions (plant-wide RGA/REA); and, iii) use of exergy for the whole process eco-efficiency analysis (EEF) and the relative eco-efficiency of a MIMO process for different combinations of control schemes (REDA). The overall organisation of this research is also shown in Figure 1-1.

In this research, stages (i) and (ii) involve the development of an exergy calculator and plantwide RGA/REA. An exergy calculator is required for computing the exergy values of material streams for plant-wide REA analysis. Chapters 3 and 4 present all the details of stages (i) and (ii). Stage (iii) presents the eco-efficiency analysis (EEF and REDA) for the whole process. Chapters 5, 6, 7 and 8 present all the details of stage (iii) of this research.

## **1.5. Expected Contributions**

There are six main contributions that have been achieved in this research project: i) development of an exergy calculator; ii) determination of plantwide control loop configuration and efficiency; iii) examination of the recycle effect on REA; iv) development of a new measure of eco-efficiency, EEF; v) development of an algorithm/software package for EEF calculation; and, vi) development of a new tool, REDA, to compare the eco-efficiency of a process under different control schemes.

The development of an exergy calculator is useful for the calculation of the exergy of material streams. For exergy calculations of a material stream, a VBA (Visual Basics for applications) programme is integrated with a GUI and VMGSim with an embedded Microsoft Excel unit operation (Munir et al. 2010; Munir et al. 2011). The calculation of material stream exergies is required for the REA, EEF and REDA development. The developed exergy calculator/exergy analysis can also facilitate identification of inefficient parts of the process/plant during the design of a new process or when analyzing/improving the operating process.

The second and third major contributions of this research project are the determination of plant-wide control loop configuration/efficiency and examination of the recycle effect on REA. The REA is an extension of the RGA concept into the exergy domain. The exergy thermodynamic property is placed in the place of gain in the RGA analysis for the definition of the REA. The REA can be used for measurements of the control scheme exergy

interactions and exergetic efficiency for different possible control schemes during the early process design stages (Montelongo-Luna et al. 2010; Munir et al. 2011). In this research, REA was used with RGA to determine plant-wide controllability and efficiency (Munir et al. 2011). The recycle loop effect was also studied in this research (Munir et al. 2012). More details of RGA and REA are discussed in chapters 3 and 4.

The fourth major contribution of this research project is the development of a new measure of eco-efficiency, EEF. As REA only measures the eco-efficiency within the scope of control loops, it was therefore necessary to develop a new measure of eco-efficiency for the eco-efficiency analysis of the whole process. The REA is a simple tool based on steady state exergy information. For the eco-efficiency analysis of the whole unit/process or even the plant, a new measure of eco-efficiency, EEF was developed in this work. EEF integrates control scheme selection and eco-efficiency to help engineers select the best control configuration for eco-efficiency of the whole process/plant. As EEF is also based on steady state exergy information, the results for EEF need to be validated by dynamic simulation. The control scheme selection techniques (RGA, NI, SVD and CN) are combined with the eco-efficiency measure (EEF) to select the best control configuration for both controllability and eco-efficiency (Munir et al. 2011; Munir et al. 2012). More details of EEF are discussed in chapters 5 and 6.

EEF calculation for different cases with all possible control schemes is difficult. It increases the computational load on process design engineers. The fifth major contribution of this research project is the development of an algorithm/software package for EEF calculation. This package combines together a commercial simulator, VMGSim and Excel to calculate the EEF. In this objective for the research project, the intention was to show the potential help obtainable in EEF calculation by using a commercial simulator VMGSim (Munir et al. 2012).

The EEF was further utilized in the development of another new tool that has been developed in this research. REDA is a tool to measure the relative eco-efficiency of a MIMO process for the differing combinations of control schemes. REDA is obtained by the multiplication of RGA and relative exergy eco-efficiency array (REEFA). REEFA is an array of relative EEF for all possible pairing combinations of the control scheme. REDA compares the eco-efficiency of a process/unit under differing control schemes with the inclusion of exergy interactions. REDA can assist process designers in quickly finding an optimal control design scheme with low operating cost and high eco-efficiency. The REDA is simple and easy to use

during early process design stages as it is based on steady state information. More details of REDA are presented in chapter 8.

The sixth major contribution of this research project is the development of REDA to compare the eco-efficiency of a process under different control schemes. As EEF results require dynamic simulation validation, the development of a simple tool to create a rank for selecting a controllable and eco-efficient control scheme was therefore required. The REDA is simple and easy to use, although it requires verification from steady state EEF results and dynamic simulations.

### 1.6. Thesis Structure

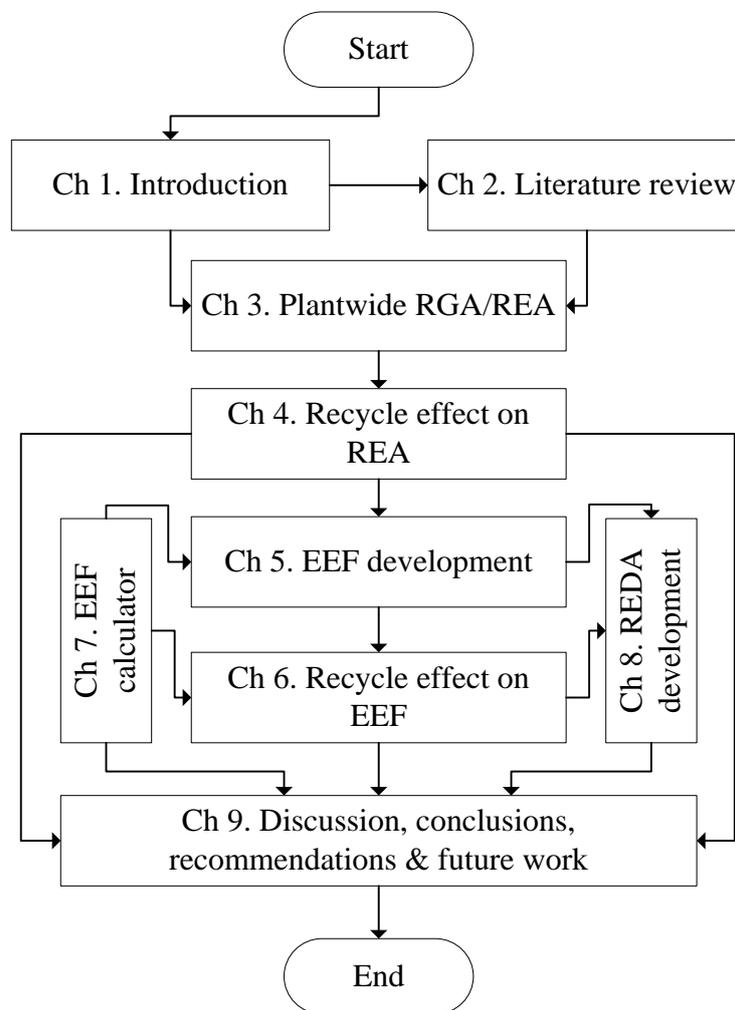


Figure 1-2. Overall thesis structure

A brief, broad overview of the major topics related to this research project has been presented and explained in this introductory chapter. In this chapter, key areas and questions relating to this research project are discussed. This chapter also includes sections on research objectives,

research organisation, expected contributions/scope and thesis structure. Finally, summaries of the contributing research papers are discussed below. The overall thesis structure of thesis is also shown in Figure 1-2.

Chapter 2 (Literature review) presents a brief and an up-to-date literature review pertaining to; process control, control scheme selection, exergy, eco-efficiency and also to an integrated approach to process design/control and eco-efficiency.

Chapter 3 (Determination of plantwide controllability and eco-efficiency) presents the thermodynamic concept of exergy, exergy calculation procedures, the REA details, the visual basic exergy calculator and two case studies for the application of RGA and REA. In this chapter it is emphasized that RGA provides a quantitative comparison of interactions between control loops and REA compares the thermodynamic efficiency for differing control schemes. In chapter 3, the intention is to show that the amalgamation of RGA and REA can provide the measure of controllability and eco-efficiency of the process under a certain design.

Chapter 4 (Recycle effect on the relative exergy array) presents the effect of recycles on the REA. As recycle systems are common in the process industry, it is necessary to study the effect of recycle loops on the REA results. Chapter 4 is the continuation of Chapter 3, and mainly focuses on the unit/process with some recycle loops. Two simulation case studies are also discussed in this chapter.

Chapter 5 (Plant-wide control: Eco-efficiency and control loop configuration) presents the extension of the eco-efficiency of the control scheme (configuration) to the whole process. In this chapter, a new measure of eco-efficiency, EEF, is proposed, explained and implemented for three simulation case studies. EEF was necessary to develop as the REA, discussed in chapter 3 and chapter 4, measures the eco-efficiency only within the scope of control loops. In chapter 5, the simulation results show that EEF can provide a qualitative and quantitative measure for the selection of the most eco-efficient control scheme.

Chapter 6 (Eco-efficiency and control loop configuration for recycle systems) is a continuation of Chapter 5, and is based on the effect of recycle loops on EEF results. In this chapter, the intention is to show the further investigation of the EEF (proposed/discussed in chapter 5) for the whole plant, which also includes recycles. It is necessary to study the effect of recycle loops on the EEF results as recycle loops are common in the process industry and

consideration of recycle loops can have a significant effect on EEF results. The EEF value decreases due to recycle/reuse of material and energy.

Chapter 7 (An algorithm/software package for control loop configuration and eco-efficiency) is linked with Chapters 5 and 6. Chapter 7 presents all the details of an algorithm/software package (EEF calculator) for EEF calculation. In this chapter, the EEF calculator combines a commercial simulator, VMGSim, and Excel together for EEF calculation. EEF calculations are required in Chapters 5, 6, 7 and 8.

In Chapter 8 (The relative exergy destroyed: A new tool for process design and control) a new tool, REDA, is proposed for process design and control and guidelines for interpreting its results are explained. REDA provides a means to compare the eco-efficiency of MIMO processes for various combinations of control scheme. Chapter 8 is also a continuation of Chapters 5, 6, and 7. In this chapter, REDA is also implemented for various simulation case studies.

Finally, in chapter 9 (Discussions, conclusions, recommendations and future research), the main focus is on a general discussion of the proposed tools (plantwide RGA, plantwide REA, EEF and REDA) and on their use in facilitating the process design, control and achieving eco-efficiency in the early stages of design without the need for more advanced and intricate mathematical tools. In Chapter 9, conclusions regarding the exergy calculator, plantwide RGA/REA, EEF and REDA, are also discussed. Finally recommendations for expected future work are also presented.

## **1.7. Summary**

Control structure selection/control scheme selection is an important task in process control. The control system structure selection process decides the best control scheme (easily controllable) for which there are a number of techniques, such as RGA, NI, SVD, CN and MRI. In the wake of energy crises, control system structure selection must not only focus on controllability and control quality but should also include energy cost and environmental impacts (eco-efficiency). For integrating control quality and eco-efficiency, the potential of the thermodynamic property exergy is used. Exergy combines the control scheme selection and eco-efficiency into a single domain. There are many tools developed in this research project such as REA, EEF and REDA to integrate control scheme selection and eco-

efficiency. These developed tools help in deciding controllable and eco-efficient control schemes for the whole process/plant.

## References

- Bristol, E. (1966). "On a new measure of interaction for multivariable process control." Automatic Control, IEEE Transactions on **11**(1): 133-134.
- Kookos, I. K. and J. D. Perkins (2001). "An Algorithm for Simultaneous Process Design and Control." Industrial & Engineering Chemistry Research **40**(19): 4079-4088.
- Koolen, J. L. A. (2001). Design of Simple and Robust Process Plants. Weinheim, Germany, WILEY-VCH.
- Kotas, T. J. (1985). The exergy concept and exergy losses. The exergy method of thermal plant analysis. London, Butterworth-Heinemann Ltd.
- Kotas, T. J. (1985). The exergy method of thermal plant analysis. London, Butterworths.
- Luyben, W. L., B. D. Tyreus. and M. L. Luyben. (1998). Plantwide Process Control. New York, McGraw-Hill.
- Marlin, T. E. (2000). Process control: design process and control system for dynamic performance. New York, McGraw Hill.
- McAvoy, T. J. (1983). Interaction Analysis: Principles and Applications. Research Triangle Park, NC, Instrument Society of America.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2010). "The relative exergy array—a new measure for interactions in process design and control." The Canadian Journal of Chemical Engineering **89**(3): 545-549.
- Morari, M. and Z. Evangelhos (1989). Robust Process Control. Englewood Cliffs, NJ, Prentice Hall.
- Munir, M. T., J. J. Chen and B. R. Young (2010). A computer program to calculate the stream exergy using the visual basic graphical interface. Chemeca 2010. Adelaide, Australia.
- Munir, M. T., W. Yu and B. R. Young (2011). Determination of Plant-wide Control Loop Configuration and Eco-Efficiency. Plantwide Control: Recent Developments and Applications, G. P. Rangaiah and V. Kariwala, John Wiley & Sons (accepted).
- Munir, M. T., W. Yu and B. R. Young (2011). "Plant-wide Control: Eco-efficiency and Control loop configuration." Industrial & Engineering Chemistry Research:(Submitted).
- Munir, M. T., W. Yu and B. R. Young (2012). Control loop configuration and eco-efficiency. FOCAPO/CPC-VIII. Savannah, Georgia, USA.
- Munir, M. T., W. Yu and B. R. Young (2012). "Recycle effect on the relative exergy array." Chemical Engineering Research and Design **90**(1): 110-118.
- Munir, M. T., W. Yu and B. R. Young (2012). "A software algorithm/package for control loop configuration and eco-efficiency " IEEE Transactions on Industrial Informatics:(Submitted).
- Niederlinski, A. (1971). "A heuristic approach to the design of linear multivariable interacting control systems." Automatica **7**(6): 691.
- Papadourakis, A., M. F. Doherty and J. M. Douglas (1987). "Relative gain array for units in plants with recycle." Industrial & Engineering Chemistry Research **26**(6): 1259-1262.

## Chapter 1 - References

- Seborg, D. E., T. F. Edgar and D. A. Mellichamp (1989). Process Dynamics and Control. New York, John Wiley & Sons.
- Seborg, D. E., T. F. Edgar, D. A. Mellichamp and F. J. Doyle (2010). Process Dynamics and Control. New York, John Wiley & Sons.
- Svrcek, W. Y., D. P. Mahoney and B. R. Young (2006). A Real-Time Approach to Process Control. Chichester, John Wiley & Sons Ltd.
- Szargut, J., D. R. Morris. and F. R. Steward (1988). Exergy analysis of thermal, chemical, and metallurgical processes. New York, Hemisphere.
- Virtual Materials Group Inc. (2009). "VMGSim V5.0 User's Manual."

## **Chapter 2. Literature Review**

This chapter presents an up-to-date literature review of the major topics related to this research and the relevant aspects of; process design, process control, control scheme selection, exergy, eco-efficiency, and the integrated approach of process design/control and eco-efficiency. This literature review sheds light on the necessity for simple, but practical, tools/methods to determine plantwide controllability/control scheme interactions, eco-efficiency of the whole process and the relative eco-efficiency of a MIMO process. This chapter also presents the need for the development of a process exergy calculator using VMGSim and a review of the efforts made in this research aimed at integrating process design, control and eco-efficiency. This research attempts to fill the process design, control and eco-efficiency integration knowledge gap by proposing new tools (plantwide RGA/REA, EEF and REDA) for eco-efficient design and control evaluation at the early stages of design.

### **2.1. Process Design**

Process design practice is a major activity in a chemical process plant. It requires a deep understanding and knowledge of all the subjects of chemical engineering, such as; design, process control, and thermodynamics. It also requires empirical knowledge, practical knowledge and rules of thumb (estimation based on long term experience as well as scientific knowledge).

The purpose of a process plant is to convert lower value raw materials into useful, higher value, products. The same product can be produced by different arrangements and configurations of unit operations. These selections are dictated by economics, the thermodynamic efficiency of the process, and environmental regulation. The purpose of a process design is to economically convert raw materials into useful higher value products without violating environmental rules and regulations. Environmental regulations have varying forms in terms of intensity targets and emission limits (Seider et al. 2009).

Process design is a complex task with different stages and sub-tasks. Each level of process design has its own depth of knowledge and understanding. The level of detail increases with every stage of process design. During early design stages, the plant operation is viewed in general terms and the detailed dynamics of the process are not considered even in the

presence of modern simulation tools (Douglas 1988; Peters and Timmerhaus 1991; Ulrich and Vasudevan 2004; Sinnott 2005).

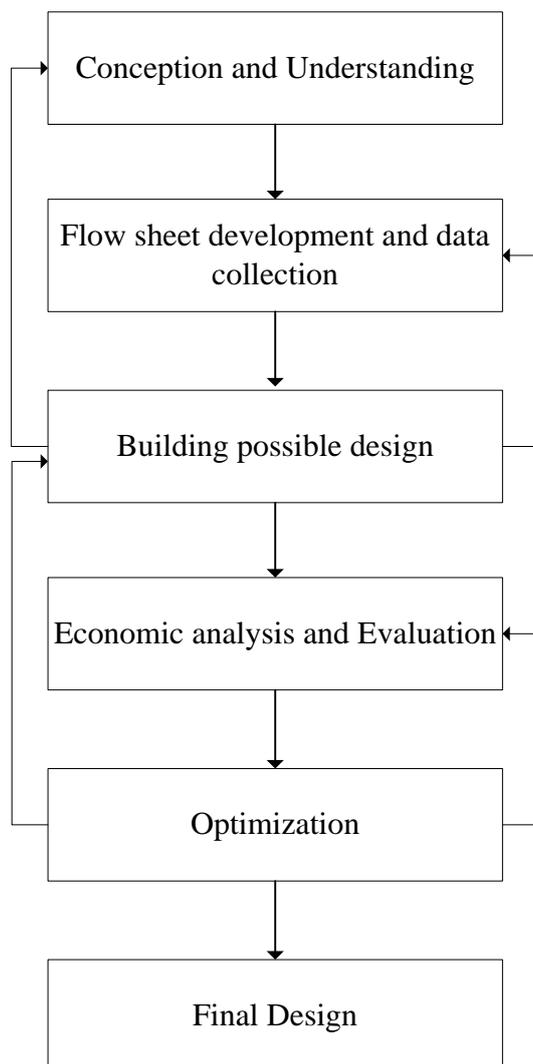


Figure 2-1. General process design procedure

The process design philosophy is creative and iterative in nature. It starts with a conceptual understanding of the process followed by the process synthesis and collection of data. Optimization and changes are made at the end of the design procedure. At the end of every stage of the process, the design is evaluated in terms of economics (Ulrich and Vasudevan 2004; Sinnott 2005). A general process design procedure is also shown in Figure 2-1. The hierarchical sequence of process design is also given in an onion diagram. An onion diagram shows that the process design moves outwards from the reacting core of process to the design of the utility (Smith 2005; Kemp 2007).

Process design has a close connection with process control because the fundamental design of a process determines its inherent controllability. The inherent controllability of a process design determines its disturbance rejection (robustness) and the ease with which the process moves between operating conditions. Thus, process control must be considered during the early process design stages (process synthesis and design activities) (Luyben et al. 1998; Seferlis and M. C. Georgiadis 2004). More details of process design and control integration are given in section 2.4 of this chapter.

## 2.2. Process Control

In process control design, control scheme selection involves determining the control system structure. Control scheme selection is normally dealt with after completing the process design, which constrains control scheme selection to a given process topology. This approach of control scheme selection during the late stages of design causes additional capital expense, lost sales opportunities and, for simple process modifications, can have a large impact on the control of the process. Control scheme selection is constrained to a particular process topology as the process topology has an impact on the process dynamics (Papadourakis et al. 1987; Luyben and Floudas 1994a; Luyben and Floudas 1994b). As the control scheme selection is constrained to a particular process topology, an integrated approach of process design and control must therefore be used.

Control scheme selection is the next stage of process control after the process design stage. Generally, units presented in chemical/petrochemical plants are complex and MIMO in nature. Decentralized control is normally preferred to centralized MIMO control due to its many advantages, as already discussed in chapter 1. The control systems that control multiple CVs by determining and manipulating multiple MVs simultaneously are called centralized multivariable controllers. The control of MIMO systems is more difficult than the control of SISO systems because, in a MIMO system, a step change in an MV causes changes in many CVs due to the interactive effects between the control loops. These control loop interaction effects can be large, small or zero, and must be considered in order to obtain a well performing control design (Stephanopoulos 1983; Zeghal and Palazoglu 1993). The interactive effects depicted in Figure 2-2 give a basic understanding of how a control loop affects other loops. Figure 2-2 shows the interactions that can occur between two inputs ( $u_1$ ,  $u_2$ ) and two output variables ( $y_1$ ,  $y_2$ ) of a 2x2 system. The controllers and the process parts of the control loops are shown by dotted boundaries.

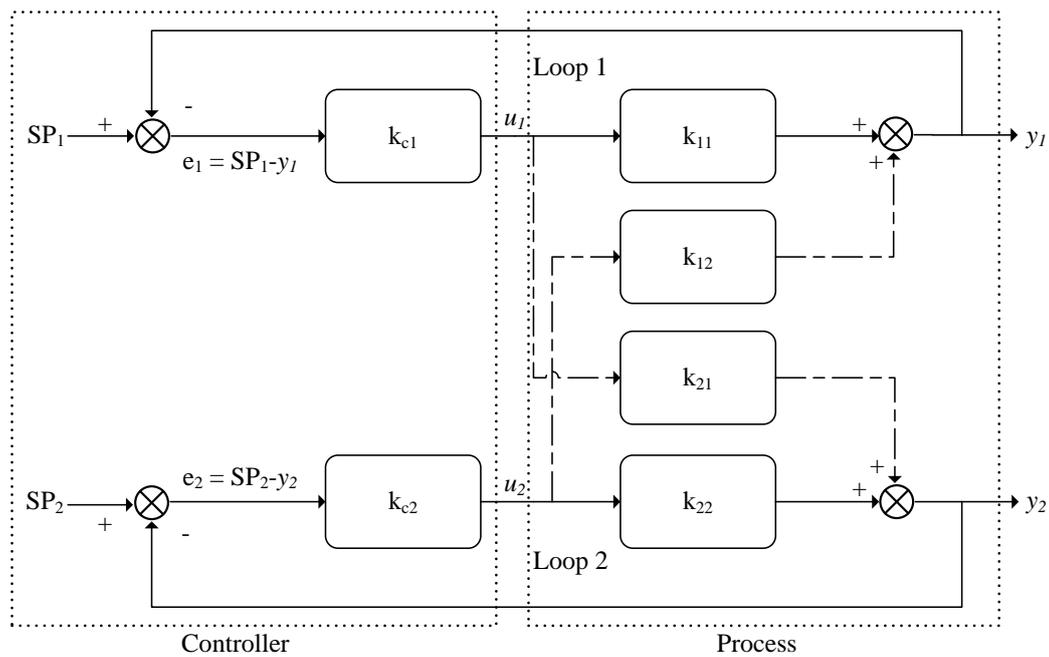


Figure 2-2. Control loop interactions for a 2x2 system

The loop degree of interactions between control loops must be considered for a well performing control design. There are many tools and methodologies to determine the interactive effects of a proposed decentralized MIMO control structure such as: RGA; NI; SVD; CN and MRI (Morari and Evangelhos 1989; Svrcek et al. 2006).

The RGA is a popular, simple and attractive tool to many practitioners. In 1966 Bristol introduced the concept of RGA, which is used to test the controllability of a process. It shows steady state interactions between control loops, and is defined as “The ratio of process gain in an isolated loop to apparent process gain in the same loop when all other control loops are closed” (Bristol 1966, pp 133). Since the work of Bristol (1966), an extensive amount of research has been done in this field. For example, most of the properties of the RGA have been proved theoretically (McAvoy 1981; McAvoy 1983), the effect of recycle loop on RGA results has been studied (Papadourakis et al. 1987) and RGA has been used as a controllability index (Arkun and Downs 1990; Cao and Rossiter 1997; Westphalen et al. 2003; Svrcek et al. 2006). More details of RGA and its rule interpretations are given and discussed in chapters 3 and 4. Chapters 5 and 6 present the details of NI, SVD and CN.

The combination of RGA, NI, SVD and CN predicts possible loop interactions, tests the stability of control scheme, analyzes the sensitivity of the control loop interaction to process gain errors, and determines whether decoupling is feasible. As these techniques are based on steady state information and can lead to incorrect conclusions concerning control structure

selection, dynamic effects must also be included in these techniques. Dynamic effects have been added into steady state RGA: for example, DRGA (McAvoy 1983; McAvoy et al. 2003), IMC (Meeuse and Huesman 2002) and ERGA (Xiong et al. 2005). The selection of control scheme is further validated by dynamic simulation.

The recycling of materials and energy is frequently used to utilize materials and energy more efficiently. A recycle is a positive feedback but it can cause catastrophic problems to control, because recycle systems can show dynamic behaviour that is significantly different from the equivalent process units without recycle. As the need for efficient use of energy and materials is increasing, the necessity for a comprehensive investigation of the problems/effects of recycling and controllability has also increased. For example, a recycle loop can affect controllability /RGA (Papadourakis et al. 1987; Munir et al. 2011), the dynamics of the units in a recycle loop and loop gain determine the stability of the recycle system (Luyben 1993a; Luyben 1993b; Luyben 1993c), a recycle loop is responsible for the snowball affect (Luyben 1994; Luyben et al. 1998), the recycle loop gain is responsible for the stability of the whole system (Mizsey and Kalmar 1996), and the various effects of the recycle are systematically classified (Morud and Skogestad 1994). As individual process units are attached with other units of the plant in a plantwide layout, so control scheme selection criteria (RGA, NI, SVD and CN) should be based on the plantwide layout.

As process engineers strive to make a process controllable and efficient, process control also has an increasing connection with thermodynamics. The efficiency of a process is normally dictated by steady state economics. However, a higher level of efficiency is obtained if a process is controllable and thermodynamically efficient, which provides another trade-off to consider during early process design stages (Luyben et al. 1998). Further details of the integration of process control and thermodynamics are given in section 2.4 of this chapter.

### **2.3. Thermodynamics**

In every chemical process there is material coming in or going out. Similarly, every process needs some energy to perform its work and/or the process rejects energy to the surroundings. So the process has a material and energy balance which gives an idea about how much material or energy is coming in and going out and how much is going into waste. For energy balance calculations, chemical engineers generally only focus on the 1<sup>st</sup> Law of Thermodynamics (Himmelblau and Riggs 2004). When the 2<sup>nd</sup> Law of Thermodynamics is

included in this analysis, this combination gives a more realistic understanding of energy usage and wastage (Denbigh 1956; Szargut et al. 1988; Theodore et al. 2009).

The combination of the 1<sup>st</sup> and 2<sup>nd</sup> laws of thermodynamics gives rise to the concept of exergy. Exergy is the maximum possible amount of work which can be drawn from a process/material stream when it interacts only with the environment; this comes from its initial state to its final dead state. At the dead state the material stream is in thermal, mechanical, and chemical equilibrium with the environment. In other words exergy accounts for the quality of energy (Kotas 1985).

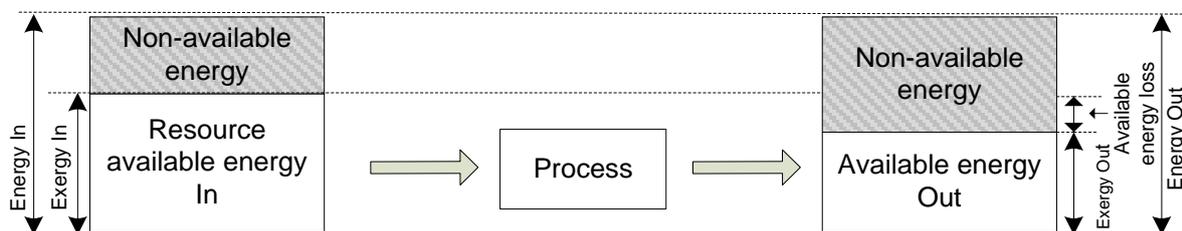


Figure 2-3. Energy and Exergy

The total energy of a material stream has two main parts (available energy and unavailable energy). The exergy of a material stream accounts for the quality of energy or available energy. According to the 1<sup>st</sup> law of thermodynamics, energy flowing in and out of a process is equal at steady state. According to the 2<sup>nd</sup> law of thermodynamics, exergy flowing in is greater than exergy flowing out due to entropy generation or exergy destruction. The fraction of non-available energy normally increases from input to output due to exergy destruction. The increase in non-available energy is also called available energy loss, as shown in Figure 2-3. More details of exergy and its components are given in chapters 3 and 4.

The energy efficiency of a process is calculated by the 1<sup>st</sup> law of thermodynamics. In such a case, the inputs, outputs and losses are defined in terms of energy. Although it is not a true efficiency of the process, it can still give some idea about the efficiency of the process (Smith J. M. et al. 2005; Smith 2005). The exergetic efficiency of a process is a true efficiency based on the exergy balance. It uses the concept of quality of energy or available energy. Exergetic efficiency is defined as the ratio of the exergy going out to the exergy going into a process (Szargut et al. 1988).

The exergy has many other valuable uses in the process industry. There are many exergy based concepts and methods such as efficiency concepts and exergy flow diagrams which can be used to describe, analyse and optimize systems (Wall 2003). A brief history of exergy use is given in Enrico and Goran (2007). Thermodynamics/exergy has a connection with both process design and control, as shown below in section 2.4.

## 2.4. Integration of Process design, Control and Thermodynamics

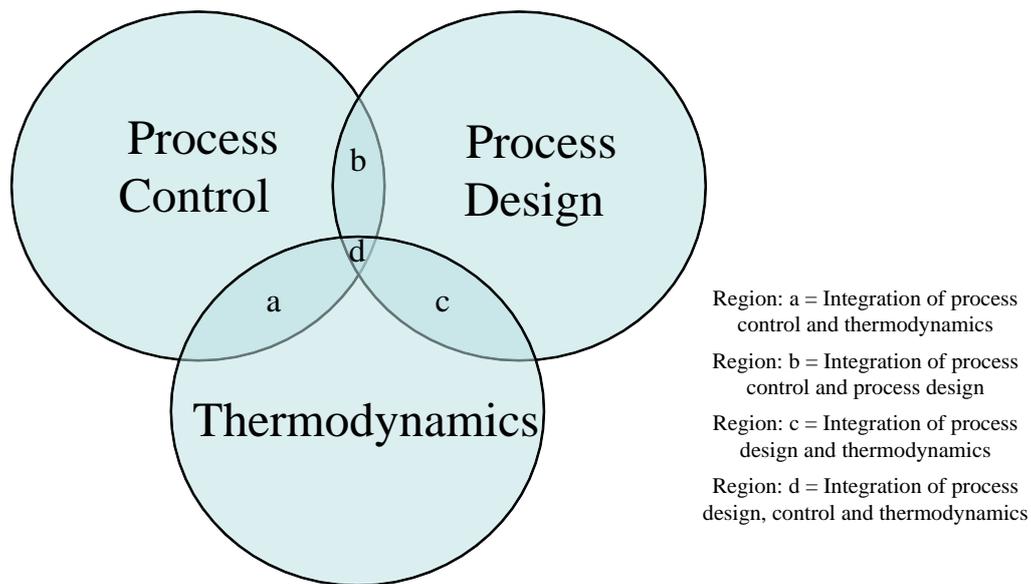


Figure 2-4. Integration of process design, control and thermodynamics

As stated above, process design is a complex task having many stages, and process control combined with thermodynamics must be considered during initial process design stages. The integration of process design, control and thermodynamics, with overlapping shaded intersections (regions a, b, c and d), is shown in Figure 2-4. The integration of process design, control and thermodynamics is divided into three main regions. Region a shows the integration of process control and thermodynamics, while region b shows the integration of process control and process design. Region c shows the integration of process design and thermodynamics, and region d shows the integration of process design, control and thermodynamics. Each of these topics is discussed below in detail.

### 2.4.1. Process control and Thermodynamics (Region a)

Along with controllability, process energy/exergy consumption plays an important role in the economics of a process. For minimizing energy/exergy consumption, process integration and

efficient energy use are needed. In process integration, energy/exergy consumption is saved by integrating heat producing units with heat consuming units, moving surplus energy in one part of the plant to another part of the plant where the energy is required. This can reduce the consumption/cost of the required energy/exergy, but with this technique, the process becomes more complex and it becomes more difficult to operate and control. Energy can efficiently be used by applying the concept of thermodynamic efficiency (energy/exergetic efficiency) based on thermodynamic laws (1<sup>st</sup> and 2<sup>nd</sup>) (Luyben et al. 1998; Kemp 2007).

Control scheme selection/controllability must also include energy usage and ecological impact to integrate the control scheme selection and eco-efficiency of the process. The integration of control scheme selection/controllability and eco-efficiency is necessary due to increases in energy demand/cost and government regulation regarding ecological impacts. Thermodynamic properties such as exergy can be used to integrate the control scheme selection and eco-efficiency of the process because the exergy destruction rate is linked with the dynamic state of the process, and controllability is an issue of process dynamics. More details of exergy, eco-efficiency and the integration of controllability/eco-efficiency are also given in chapters 1, 3, 4 and 5.

Thermodynamic properties such as exergy can also be used for the development of control structures because exergy plays a role in evaluating the controllability of a process/plant. Luyben et al. (1998) added an appendix in their book which acts as a basic framework for the development of a dynamic exergy balance for process control evaluation.

As exergy destruction is directly proportional to entropy production, actual/spontaneous processes normally occur in the direction of decreasing exergy or increasing entropy (Dincer and Cengel 2001). Some research has also been done on the theoretical development and application of process control linked to entropy production (Alonso et al. 2002; Ydstie 2002; Ruszkowski et al. 2005; Antelo et al. 2007).

Exergy also helps to develop many tools for the facilitation of process design and control, such as exergetic efficiency, REA, EEF and REDA. Exergetic efficiency is equivalent to the eco-efficiency of the process and is used to locate inefficient parts of the plant (Szargut et al. 1988; Moran and Sciubba 1994; Montelongo-Luna et al. 2007). The REA is used to measure control scheme interactions and exergetic efficiency for the various possible MIMO control schemes (Montelongo-Luna et al. 2010; Munir et al. 2012; 2012). More details of REA and recycle effect on REA results are presented in chapters 3 and 4. However, the REA only

measures the eco-efficiency within the scope of single, decentralized control loops. To overcome this deficiency in REA, the EEF is defined and employed for the eco-efficiency analysis of the whole process. More details on the EEF and the recycle effect on the EEF are given in chapters 5 and 6. REDA is another tool based on the EEF and RGA, and is used to measure the relative eco-efficiency of an MIMO process. More details of REDA are presented in chapter 8.

#### **2.4.2. Process design and control (Region b)**

The integration of process design and control combines steady state design and dynamic control into a single optimization step. Process design has a strong connection with process control/controllability. Process design also has a substantial effect on the ability of a controller to respond to disturbances and parametric uncertainty. For example, in the presence of large disturbances, a control valve can quickly saturate with a small range of control action (Ricardez-Sandoval et al. 2009).

Process control is usually delayed to the late stages of a process design as it requires a great deal of process information. With this approach to process design, changes in design are difficult and costly during the start-up and operational periods. Sometimes it can lead to processes which are not controllable, or are difficult to control because small design changes can have a large impact on the process control. To avoid these problems, an integrated approach to process design and control in the early process design stages is recommended. Such an approach simultaneously allows for changes in the process configuration of a process for easier control and evaluation of many control structure candidates. This integrated approach results in better process design and control in a cost effective manner (Luyben et al. 1998; Koolen 2001; Seferlis and M. C. Georgiadis 2004).

With all the advantages of an integrated process design and control approach, there are also some disadvantages. For example, many complexities arise due to simultaneous process design and control, which is also one of the factors in the slow pace of research in this area (Kookos and Perkins 2001). Furthermore, integration of process design and control can also have conflicting objectives (Luyben et al. 2004).

A summary of, and future work directions for, the integration of process design and control are also given by Seferlis and Georgiadis (2004). A more recent review of process design and control integration literature is given by Ricardez-Sandoval et al. (2009).

### **2.4.3. Process design and Thermodynamics (Region c)**

A process plant converts higher content exergy raw materials into lower exergy content products, often with the requirement of a substantial amount of energy input. If the exergy of products is close to the exergy of reactants then the process is highly thermodynamically efficient. Total exergy input/output analysis is used for the exergy analysis of a process by comparing the amount of exergy coming in and going out of the process (Moran and Sciubba 1994; Hinderink et al. 1996; Hammond and Stapleton 2001; Chan et al. 2002; Wall 2003; Camdali and Tunc 2005; Sencan et al. 2005; Araújo et al. 2007; Montelongo-Luna et al. 2007; Muangnoi et al. 2007; Aljundi 2009; Niksiar and Rahimi 2009). Exergy analysis helps to identify inefficient parts of the plant, which improves the efficiency of the plant. This approach helps with eco-efficient process design.

Thermodynamic properties such as exergy have also been used to develop a systematic approach to optimal process design with low exergy destruction. Objective functions in terms of energy and exergy were constructed (Fan and Shieh 1980). Sorin et al. (2000) explained that process design with reduced energy consumption is a function of three aspects of process design: energy efficiency, efficient use of raw materials and waste reduction. Process design alternatives can also be evaluated quickly by using the exergetic efficiency tools developed by Wall (2003).

## **2.5. The Need for New Tools**

As stated above, efforts have been made to integrate process design, control and thermodynamics into a unified domain. There are some well explored research areas, namely the integration of process design and control and integration of process design and thermodynamics (regions b and c, respectively, of Figure 2-4). From the literature discussed above, it is clear that tools and methods available for region a (integration of process control and thermodynamics) and region d (integration of process design, control and thermodynamics) of Figure 2-4 lack the capability to fully integrate these concepts. As it is a complex and difficult task, there are therefore significant contributions yet to be made.

The development of new tools that can integrate the concepts of process design, control and thermodynamics within an understandable framework would be welcomed by the process industry and practising design engineers. Specifically, these tools would help them in developing controllable and eco-efficient process designs in a cost effective manner without a

large amount of additional capital investment and the loss of sales opportunities. The main objective of this research is to minimize this gap.

The profitability of designs/operations (as a major objective in the selection of design) can also be integrated into the proposed methods of assessments. This is an optimization problem that is usually done separately in process design practice. So in this research, the main objective was to integrate the concepts of process design, control and thermodynamics. The integration of profitability/optimization into the proposed assessments is a potential next step in this research area.

## **2.6. Summary**

In this chapter, an up-to-date literature review of the major topics related to this research and relevant aspects of process design, control, control scheme selection, thermodynamics, exergy, eco-efficiency and integration of process design/control/thermodynamics has been presented. This chapter also shows the necessity for filling the knowledge gap of integrating concepts of process design, control and thermodynamics.

The chapter also emphasizes that, in this research, the knowledge gap relating to the integrating process design, control and eco-efficiency/thermodynamics is addressed by the proposal of new tools/methods, such as plantwide RGA/REA, EEF and REDA. These tools help to design eco-efficient and controllable processes at the early process design stage.

## References

- Aljundi, I. H. (2009). "Energy and exergy analysis of a steam power plant in Jordan." Applied Thermal Engineering **29**(2-3): 324-328.
- Alonso, A. A., B. E. Ydstie and J. R. Banga (2002). "From irreversible thermodynamics to a robust control theory for distributed process systems." Journal of Process Control **12**(4): 507-517.
- Antelo, L. T., I. Otero-Muras, J. R. Banga and A. A. Alonso (2007). "A systematic approach to plant-wide control based on thermodynamics." Computers and Chemical Engineering **31**: 677-691.
- Araújo, A. C. B., L. G. S. Vasconcelos, M. F. Fossy and R. P. Brito (2007). "Exergetic and economic analysis of an industrial distillation column." Brazilian Journal of Chemical Engineering **24**: 461-469.
- Arkun, Y. and J. Downs (1990). "A general method to calculate input-output gains and the relative gain array for integrating processes." Computers & Chemical Engineering **14**(10): 1101-1110.
- Bristol, E. (1966). "On a new measure of interaction for multivariable process control." Automatic Control, IEEE Transactions on **11**(1): 133-134.
- Camdali, U. and M. Tunc (2005). "Computation of Chemical Exergy Potential in an Industrial AC Electric ARC Furnace." Journal of Energy Resources Technology **127**(1): 66-70.
- Cao, Y. and D. Rossiter (1997). "An input pre-screening technique for control structure selection." Computers & Chemical Engineering **21**(6): 563-569.
- Chan, S. H., C. F. Low and O. L. Ding (2002). "Energy and exergy analysis of simple solid-oxide fuel-cell power systems." Journal of Power Sources **103**(2): 188-200.
- Denbigh, K. G. (1956). "The second-law efficiency of chemical processes." Chemical Engineering Science **6**(1): 1-9.
- Dincer, I. and Y. A. Cengel (2001). "Energy, entropy and exergy concepts and their roles in thermal engineering." Journal of entropy **3**(3): 116-149.
- Enrico, S. and W. Goran (2007). "A brief commented history of Exergy from the beginning to 2004." Int. J. Thermodynamics **10** (1): 1-26.
- Fan, L. T. and J. H. Shieh (1980). "Thermodynamically based analysis and synthesis of chemical process systems." Energy **5**(8-9): 955-966.
- Hammond, G. and A. Stapleton (2001). "Exergy analysis of the United Kingdom energy system." Proceedings of the Institution of Mechanical Engineers, Part A: Journal of Power and Energy **215**(2): 141-162.
- Himmelblau, D. M. and J. B. Riggs (2004). Basic Principles and Calculations in Chemical Engineering. Upper Saddle River, New Jersey, Prentice Hall.
- Hinderink, A. P., F. P. J. M. Kerkhof, A. B. K. Lie, J. De Swaan Arons and H. J. Van Der Kooi (1996). "Exergy analysis with a flowsheeting simulator - I. Theory; calculating exergies of material streams." Chemical Engineering Science **51**(20): 4693-4700.

- Kemp, I. C. (2007). Pinch Analysis and Process Integration: A User Guide on Process Integration for the Efficient Use of Energy. London, Butterworth-Heinemann.
- Kookos, I. K. and J. D. Perkins (2001). "An Algorithm for Simultaneous Process Design and Control." Industrial & Engineering Chemistry Research **40**(19): 4079-4088.
- Koolen, J. L. A. (2001). Design of Simple and Robust Process Plants. Weinheim, Germany, WILEY-VCH.
- Kotas, T. J. (1985). The exergy method of thermal plant analysis. London, Butterworths.
- Luyben, M. L. and C. A. Floudas (1994). "Analyzing the interaction of design and control--1. A multiobjective framework and application to binary distillation synthesis." Computers & Chemical Engineering **18**(10): 933-969.
- Luyben, M. L. and C. A. Floudas (1994). "Analyzing the interaction of design and control--2. reactor-separator-recycle system." Computers & Chemical Engineering **18**(10): 971-993.
- Luyben, W. L. (1993). "Dynamics and control of recycle systems. 1. Simple open-loop and closed-loop systems." Industrial & Engineering Chemistry Research **32**(3): 466-475.
- Luyben, W. L. (1993). "Dynamics and control of recycle systems. 2. Comparison of alternative process designs." Industrial & Engineering Chemistry Research **32**(3): 476-486.
- Luyben, W. L. (1993). "Dynamics and control of recycle systems. 3. Alternative process designs in a ternary system." Industrial & Engineering Chemistry Research **32**(6): 1142-1153.
- Luyben, W. L. (1994). "Snowball effects in reactor/separator processes with recycle." Industrial & Engineering Chemistry Research **33**(2): 299-305.
- Luyben, W. L., S. Panos and C. G. Michael (2004). Chapter A1 The need for simultaneous design education. Computer Aided Chemical Engineering, Elsevier. **Volume 17**: 10-41.
- Luyben, W. L., B. D. Tyreus. and M. L. Luyben. (1998). Plantwide Process Control. New York, McGraw-Hill.
- McAvoy, T. J. (1981). "Connection between relative gain and control loop stability and design." AIChE Journal **27**(4): 613-619.
- McAvoy, T. J. (1983). Interaction Analysis: Principles and Applications. Research Triangle Park, NC, Instrument Society of America.
- McAvoy, T. J., Y. Arkun, R. Chen, D. Robinson and P. D. Schnelle (2003). "A new approach to defining a dynamic relative gain." Control Engineering Practice **11**(8): 907-914.
- Meeuse, F. M. and A. E. M. Huesman (2002). "Analyzing Dynamic Interaction of Control Loops in the Time Domain." Industrial & Engineering Chemistry Research **41**(18): 4585-4590.
- Mizsey, P. and I. Kalmar (1996). "Effects of recycle on control of chemical processes." Computers & Chemical Engineering **20**(Supplement 2): S883-S888.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2007). "An exergy calculator tool for process simulation." Asia-Pacific Journal of Chemical Engineering **2**(5): 431-437.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2010). "The relative exergy array—a new measure for interactions in process design and control." The Canadian Journal of Chemical Engineering **89**(3): 545-549.

- Moran, M. J. and E. Sciubba (1994). "Exergy Analysis: Principles and Practice." Journal of Engineering for Gas Turbines and Power **116**(2): 285-290.
- Morari, M. and Z. Evangelhos (1989). Robust Process Control. Englewood Cliffs, NJ, Prentice Hall.
- Morud, J. and S. Skogestad (1994). "Effects of recycle on dynamics and control of chemical processing plants." Computers and Chemical Engineering **18**(SUPPL): S529-S534.
- Muangnoi, T., W. Asvapoositkul and S. Wongwises (2007). "An exergy analysis on the performance of a counterflow wet cooling tower." Applied Thermal Engineering **27**(5-6): 910-917.
- Munir, M. T., W. Yu and B. R. Young (2011). Analysis of control configuration changes with relative gain array and relative exergy array for units in plants with recycle. Chemeca 2011. Sydney, Australia.
- Munir, M. T., W. Yu and B. R. Young (2012). Determination of Plant-wide Control Loop Configuration and Eco-Efficiency, G.P. Rangaiah and V. Kariwala (Eds.). Plantwide Control: Recent Developments and Applications, John Wiley & Sons, ISBN:9780470980149.
- Munir, M. T., W. Yu and B. R. Young (2012). "Recycle effect on the relative exergy array." Chemical Engineering Research and Design **90**(1): 110-118.
- Niksiar, A. and A. Rahimi (2009). "Energy and exergy analysis for cocurrent gas spray cooling systems based on the results of mathematical modeling and simulation." Energy **34**(1): 14-21.
- Papadourakis, A., M. F. Doherty and J. M. Douglas (1987). "Relative gain array for units in plants with recycle." Industrial & Engineering Chemistry Research **26**(6): 1259-1262.
- Ricardez-Sandoval, L. A., H. M. Budman and P. L. Douglas (2009). "Integration of design and control for chemical processes: A review of the literature and some recent results." Annual Reviews in Control **33**(2): 158-171.
- Ruszkowski, M., V. Garcia-Osorio and B. E. Ydstie (2005). "Passivity based control of transport reaction systems." AIChE Journal **51**(12): 3147-3166.
- Seferlis, P. and M. C. Georgiadis (2004). The integration of process design and control- Summary and future directions. Computer Aided Chemical Engineering. **17**: 1-9.
- Seferlis, P. and E. M. C. Georgiadis (2004). The Integration of Process Design and Control. Computer-Aided Chemical Engineering. Amsterdam, Elsevier B. V.
- Seider, W. D., J. D. Seader., D. R. Lewin. and S. Widagdo. (2009). Product and Process Design Principles: Synthesis, Analysis, and Evaluation. New York, John Wiley.
- Sencan, A., K. A. Yakut and S. A. Kalogirou (2005). "Exergy analysis of lithium bromide/water absorption systems." Renewable Energy **30**(5): 645-657.
- Sinnot, R. K. (2005). Chemical Engineering Design. New York, Elsevier Butterworth-Heinemann.
- Smith J. M., H. C. V. Ness and M. M. Abbott. (2005). Introduction to Chemical Engineering Thermodynamics. New York, McGraw-Hill.
- Smith, R. (2005). Chemical Process Design and Integration. Chichester, England, John Wiley & Sons, Ltd.
- Sorin, M., A. Hammache and O. Diallo (2000). "Exergy based approach for process synthesis." Energy **25**(2): 105-129.

- Stephanopoulos, G. (1983). Chemical process control: An introduction to theory and practice. New Jersey, Prentice Hall.
- Svrcek, W. Y., D. P. Mahoney and B. R. Young (2006). A Real-Time Approach to Process Control. Chichester, John Wiley & Sons Ltd.
- Szargut, J., D. R. Morris. and F. R. Steward (1988). Exergy analysis of thermal, chemical, and metallurgical processes. New York, Hemisphere.
- Theodore, L., F. Ricci and T. Van Vliet (2009). Exergy: The concept of Quality energy. Thermodynamics for the Practicing Engineer. Hoboken, NJ, USA, John Wiley & Sons, Inc.: 377-390.
- Ulrich, G. D. and P. T. Vasudevan (2004). Chemical Engineering Process Design and Economics: A Practical Guide. Durham, New Hampshire, Process Publishing.
- Wall, G. (2003). "Exergy tools." Proceedings of the Institution of Mechanical Engineers, Part A: Journal of Power and Energy **217**(2): 125-136.
- Westphalen, D. L., B. R. Young and W. Y. Svrcek (2003). "A Controllability Index for Heat Exchanger Networks." Industrial & Engineering Chemistry Research **42**(20): 4659-4667.
- Xiong, Q., W.-J. Cai and M.-J. He (2005). "A practical loop pairing criterion for multivariable processes." Journal of Process Control **15**(7): 741-747.
- Ydstie, B. E. (2002). "Passivity based control via the second law." Computers & Chemical Engineering **26**(7-8): 1037-1048.
- Zeghal, S. and A. N. Palazoglu (1993). "Interaction measures and decentralized control of chemical plants." Computers & Chemical Engineering **17**(Supplement 1): 335-341.



## Chapter 3

---

### *Determination of Plant-wide control loop configuration and Eco-efficiency*

#### **Article # 1**

**Co-authors: Wei. Yu, Brent. R. Young**

*Industrial Information & Control Centre (I<sup>2</sup>C<sup>2</sup>), Department of Chemical &  
Materials Engineering, The University of Auckland, Auckland, New Zealand*

Munir, M. T., W. Yu and B. R. Young (2011). Determination of Plant-wide control loop configuration and Eco-efficiency, in G. P. Rangaiah and V. Kariwala (Eds.), Plant-wide control: Recent developments and Applications, John Wiley & Son, ISBN: 978-0-470-98014-9

## **Chapter 3. Determination of Plant-wide control loop configuration and Eco-efficiency**

This chapter presents the thermodynamic concept of exergy, exergy calculation procedures, the REA details, the visual basic exergy calculator and two case studies for the application of RGA and REA. It is emphasized in this chapter that RGA provides a quantitative comparison of interactions between control loops and REA compares the thermodynamic efficiency for differing control schemes. The intention is to show that the amalgamation of RGA and REA can provide the measure of controllability and eco-efficiency of a process under a certain design.

### **Abstract**

An eco-efficient process design is based on a deep understanding of all areas of chemical engineering, economics and consideration of sustainability. The thermodynamic concept of Exergy is used to analysis a process in terms of its efficiency. The Relative Exergy Array (REA) a new tool that measures the relative exergetic efficiency and controllability of a process is described. The REA can be used for the quick comparison between several process/control structure candidates. In this work, the origin of the properties of and the results obtained from the REA are presented for a process simulation case study.

### **3.1. Introduction**

The purpose of a process design is to convert raw materials into useful higher-value products economically without violating environmental rules and regulations. Environmental regulations have different forms in terms of intensity targets and emission limits. Process design is a complex task and has different stages. Each stage of process design has its own depth of knowledge and understanding. At the later stages, more detailed information of the process is required.

At the early design stage the process will be designed to fulfil the design criteria: maximizing production/profit while minimizing environmental impact. It is only in the final design stage that the process control scheme is developed since it will require a great amount of process information for activities such as dynamic modelling. Sometimes this design strategy can lead to the processes being uncontrollable or difficult to be controlled. Furthermore, if the

process needs to be modified (i.e. adding new equipment) it may make a large impact on the controllability and economic efficiency of the process/plant. To avoid these problems, an integrated approach of process design, control and economic efficiency in early process design stages is needed. Engineers can pick the best process configuration with consideration of control and economics by evaluating many control structure candidates simultaneously. This integrated approach results in better process design and process control in a cost effective manner.

Most industrial processes are naturally multi-input multi-output (MIMO) systems. These systems can be either controlled by a multivariable or centralized MIMO controller or by a set of single-input single-output (SISO) controllers. Since centralized multivariable controllers are complex and lack integrity, decentralized control systems have more advantages: (1) simple algorithms; (2) the ease of understanding by plant operating personnel; and (3) standard control designs have been developed for the common unit operations (Marlin 2000). Decentralized controllers are therefore more often selected for MIMO systems.

In a SISO system, one process variable or controlled variable (CV) is controlled by one manipulated variable (MV) which forms a control loop. When a manipulated variable controls the process variable of its control loop then, in MIMO processes, it also affects other process variables of other loops and causes loop interactions. These loop interactions can be large, small or zero.

A quantitative measure of interaction, which can guide the process design, is needed to determine the best decentralized control loop configuration. The most famous interaction measure is the relative gain array (RGA) developed by Bristol (1966). Since then, an extensive amount of research has been carried out in control loop configuration or input-output pairing selection such as the dynamic RGA (Witcher and McAvoy 1977; McAvoy et al. 2003) and effective relative gain array (ERGA) (Xiong et al. 2005). The RGA is still widely used in industry since it is a simple calculation which only requires simple open-loop step response tests; it is controller independent and scale invariant. RGA is, in a strict sense, not a controllability measure but a steady state interaction measure. It may indicate that there may be some controllability difficulties using decentralized control structure if the interactions are found to be large. But systems with large control loop interactions are not necessarily difficult to control.

For an eco-efficient process design, a deep understanding of all areas of chemical engineering, economics and consideration of sustainability is needed. Since the RGA only connects the control configuration to the process design, a new tool must be developed to integrate process design, process control and economics/sustainability. Exergy may play an important role in the new tool since it can be used for determining the exergetic efficiency and sustainability of a process (Dincer 2002). For example, environmental impacts can be minimized by reducing exergy losses and by efficient use of exergy (Rosen and Dincer 1997; Rosen and Dincer 1999). The relative exergy array (REA) was developed based on the exergy for the control configuration within the process design (Montelongo-Luna et al. 2010). The REA is the extension of RGA into the exergy domain. The REA is defined by placing the exergy thermodynamic property in the place of gain in the RGA analysis. The REA may provide a deeper insight into process control structure interactions and measurement of exergetic efficiency and can be used for quick comparison between several process/control structure candidates. The recycle effect on the REA analysis was studied by Munir et al. (2012).

This chapter is organized as follows. In Section 3.2, the concepts of RGA and REA are addressed. The thermodynamic concept of exergy and exergy calculation procedures are then discussed. A Visual Basic program and graphical user interface (GUI) integrated with the commercial simulator VMGSim are developed to calculate the REA values automatically. In Section 3.4, two case studies for the application of RGA and REA are used to illustrate the proposed methods. Finally, results are discussed and conclusions are made in the summary

## **3.2. RGA and REA**

### **3.2.1. RGA**

The RGA is defined as “The ratio of process gain in an isolated loop to apparent process gain in the same loop when all other control loops are closed”, according to Bristol (1966). It is a matrix composed of elements defined as the ratio of open-loop to closed-loop gains. One of its elements, relative gain,  $\lambda_{ij}$ , which relates the  $j^{th}$  input  $u_j$  and the  $i^{th}$  output  $y_i$  can be expressed by the equation:

$$\lambda_{ij} = \frac{\left( \frac{\partial y_i}{\partial u_j} \right)_{u_k = \text{const}, k \neq j}}{\left( \frac{\partial y_i}{\partial u_j} \right)_{y_k = \text{const}, k \neq i}} \quad 3-1$$

The relative gain  $\lambda_{ij}$  in Equation (3-1) is the ratio of change in the steady-state gain value of a control variable ( $y_i$ ) with respect to a manipulated variable ( $u_j$ ) when all loops are open to change in the steady-state value of gain of the control variable ( $y_i$ ) with respect to the manipulated variable ( $u_j$ ) when all other loops are closed and in ‘perfect control’. The phrase ‘perfect control’ refers to the condition of a control loop where no offset is present in the controlled variable at steady state (Svrcek et al. 2006). The assembly of the relative gains ( $\lambda_{ij}$ ) for all possible pairing combinations of multi-loop SISO systems is referred to as the RGA.

The RGA provides a quantitative comparison of interactions between control loops. It shows steady-state interactions between control loops. Although the RGA can be calculated by performing experiments for each possibility of control pairing using Equation (3-1), it is not usually possible to do so for an operating plant. An alternative method of RGA calculation is based on the availability of a process model. From the steady-state gain matrix,  $G$ , the RGA can be calculated directly (Bristol 1966).

$$\Lambda = G \otimes (G^{-1})^T \quad 3-2$$

Detailed interpretations of the RGA and the selection criteria of the control pairs can be found in Marlin (2000) and Svrcek et al.(2006).

Although the application of the RGA is empirical in nature, many of its properties have been theoretically proved (McAvoy 1983; McAvoy et al. 2003). The RGA was also extended to prove feasibility, closed-loop stability and robustness by using steady-state values (Grosdidier and Morari 1986). The dynamic and effective RGA has also been proposed for accounting for dynamic effects of the system (Xiong et al. 2005). Despite all the advantages of the RGA, it also has some limitations. Its values can change dramatically when a single unit is connected with other units in a plantwide layout through recycles. When recycles are also considered with a single unit, RGA values can change resulting in a different control configuration than initially selected based on the single unit without any recycles (Papadourakis et al. 1987; Monshizadeh-Naini et al. 2009). Sometimes RGA can give

contradictory results as it is based on steady-state information rather than response information (Skogestad et al. 1990).

### 3.2.2. REA

In every chemical process there are some materials coming in or going out. Similarly, every process needs some energy to perform its work and/or the process rejects energy to the surroundings. Material and energy balances of the process are generally used to evaluate the efficiency of the process at the process design stage. For energy balance calculations, chemical engineers mostly only focus on the first law of thermodynamics (Himmelblau and Riggs 2004). However, it may not fully reflect realistic energy efficiency. The second law of thermodynamics must be included to provide a more realistic understanding of energy usage and wastage (Denbigh 1956).

A general thermodynamic process is shown in Figure 3-1. The considered process has many arbitrary material streams coming from and going to the process boundary. The process has its own temperature  $T$ , pressure  $P$  and composition  $Z$ . The process is also being heated from different heating sources at different temperatures  $T_i$  and having different amounts of heat  $q_i$ . The process produces some shaft work  $W$  and delivers it to the environment with fixed values of temperature, pressure and composition ( $T_0$ ,  $P_0$  and  $Z_0$ ).

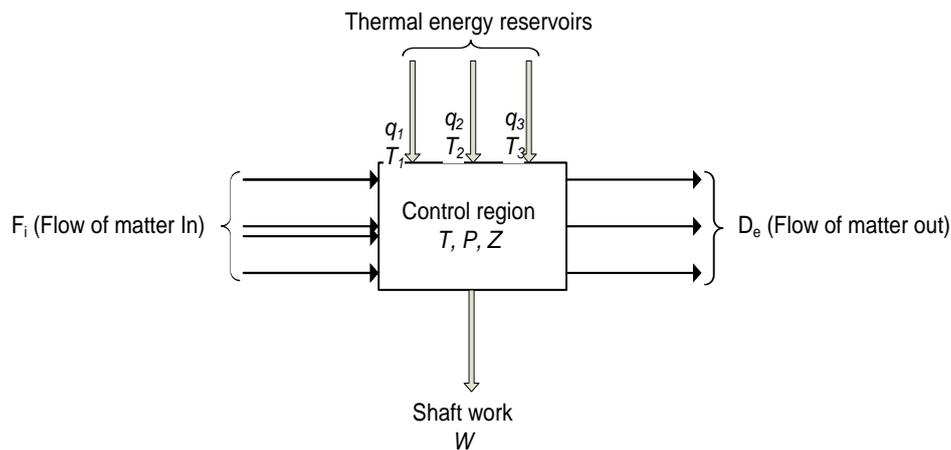


Figure 3-1. A general thermodynamic process

Change in internal energy  $\Delta U$  of the general thermodynamic system shown in Figure 3-1 is due to the addition of energies  $q_i$  and materials, flow of matter out and work done  $W$ . According to the first law of thermodynamics, internal energy change  $\Delta U$  can be expressed as:

$$\Delta U = -q_0 + \sum_i q_i - P_0 \Delta V + W \quad 3-3$$

where  $q_0$  is heat provided to the medium ,  $\sum_i q_i$  is all other heat effects,  $-P_0 \Delta V$  is work done in displacing the atmosphere at constant pressure, and  $W$  represents all other work terms.

According to the second law of thermodynamics, the total entropy created  $\sigma$  can be expressed as:

$$\Delta S + \Delta S_0 + \sum_i \Delta S_i = \sigma \geq 0 \quad 3-4$$

where  $S$  is entropy,  $\Delta S_0$  is the change in entropy outside the process and  $\Delta S_i$  is the change in entropy inside the process.

Recall that the heat medium is a heat reservoir at a constant temperature  $T_0$  and its change in entropy is  $\Delta S_0$ , i.e.

$$\Delta S_0 = \frac{q_0}{T_0} \quad 3-5$$

Evaluating  $q_0$  from Equations (3-4) and (3-5) then substituting that  $q_0$  value into Equation (3-3), we can obtain the following thermodynamic expression for the process in Figure 3-1:

$$W + \sum_i (q_i + T_0 \Delta S_i) = T_0 \sigma + \Delta U + P_0 \Delta V - T_0 \Delta S \quad 3-6$$

where  $W + \sum_i (q_i + T_0 \Delta S_i)$  denotes the total work performed on the process and  $T_0 \sigma$  denotes energy loss due to irreversibilities.

Exergy is the maximum possible amount of work which can be drawn from a material stream when it interacts only with the environment and changes from its initial state to the final dead state (Denbigh 1956; Kotas 1985). At the dead state, the material stream is in thermal, mechanical and chemical equilibrium with the environment. Since exergy accounts for the quality of energy, it can therefore be used as a measure to evaluate the eco-efficiency for a process design. A process is called an eco-efficient process if it uses a relatively small amount of energy or destruction of exergy is low. The calculation of the physical exergy change of the thermodynamic process in Figure 3-1 can be obtained from Equation (3-6) as:

$$\Delta B_{phys} = \Delta U + P_0 \Delta V - T_0 \Delta S \quad 3-7$$

Because the thermodynamic process composition  $Z$  in Figure 3-1 is designed for different work potentials, the total exergy of the material stream will also change. The total exergy,

including three main components (physical exergy, chemical exergy and exergy change due to mixing) is defined as (Hinderink et al. 1996):

$$B_{total} = B_{phys} + B_{chem} + \Delta_{mix} B \quad 3-8$$

The detailed definitions of chemical exergy  $B_{chem}$  and exergy change due to mixing  $\Delta_{mix} B$  are provided in Section 3.3. Based on an understanding of the total exergy of each material stream in and out of the thermodynamic process, it is possible that engineers can build an eco-efficient process which is ecological and economical.

The total exergy calculation in Equation (3-8) is simple and only needs easily obtainable thermodynamic data. This calculation requires data such as the Gibbs energy formation for the calculation of standard chemical exergies. The Gibbs energy formation data can be obtained from different sources such as thermodynamic databanks or process simulators, but special attention must be paid to the consistency of this data.

The RGA only accounts for the controllability of MIMO systems. The consideration of exergy is also an important factor and it should be included in the control design. The REA is a tool to utilize exergy in control design (Montelongo-Luna et al. 2010). The REA can be directly derived from the RGA concept in the exergy domain by placing the exergy thermodynamic property in place of gain. The REA for an  $n \times n$  MIMO system is defined analogously to RGA with relative exergy  $\gamma_{ij}$  defined:

$$\gamma_{ij} = \frac{\left( \frac{\Delta B(y_i)}{\Delta B(u_j)} \right)_{\text{all loops open}}}{\left( \frac{\Delta B(y_i)}{\Delta B(u_j)} \right)_{\text{all loops closed (in perfect control) except } u_j \text{ loop}}} \quad 3-9$$

The relative exergy  $\gamma_{ij}$  in Equation (3-9) is the ratio of gain change in the steady-state exergy of the material stream  $y_i$  with respect to that of the material/energy stream  $u_j$  when all loops are open to the gain change in the steady-state exergy of the material stream  $y_i$  with respect to that of the material/energy stream  $u_j$  when all other loops are closed and in ‘perfect control’. The numerator of Equation (3-9) shows the open-loop exergy gain change in a given control loop ( $u_j - y_i$ ). The denominator of Equation (3-9) shows the closed-loop exergy gain change when all other control loops are closed except the ( $u_j - y_i$ ) loop. If there is no interaction from other loops then the value of  $\gamma_{ij}$  is close to 1. This case ( $\gamma_{ij} \sim 1$ ) indicates that the thermodynamic efficiency of the control loop considered is less affected by interactions from

other loops. This would be a good pairing candidate from an exergy point of view as its thermodynamic efficiency is not affected by interactions from other control loops.

A value of relative exergy ( $\gamma_{ij}$ ) of less than 1 indicates that the exergy change increases due to loop interactions when all other loops are closed. In this case the exergy changes are less when all loops are open. When all other loops are closed, then interactions of these loops increase the exergy change in the control variable ( $y_i$ ) stream. A value of relative exergy  $\gamma_{ij}$  of more than 1 indicates that the exergy change decreases due to loop interactions when all other loops are closed. In this case, the exergy changes more when all loops are open.

Since exergy shows the maximum efficiency of a process, the REA can provide the process interactions in the sense of the energy use influenced by the control policy. The REA inherits many properties of the RGA, such as the summations of the rows and columns are equal to 1.

As the RGA can be calculated from the steady-state gain matrix, the REA can also be obtained from the steady-state exergy gain matrix defined as:

$$\bar{B} = \begin{bmatrix} \tau_{11} & \tau_{12} & \cdots & \tau_{1n} \\ \tau_{21} & \tau_{22} & \cdots & \tau_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \tau_{n1} & \tau_{n2} & \cdots & \tau_{nn} \end{bmatrix} \quad 3-10$$

where

$$\tau_{ij} = \left[ \frac{\Delta B(y_i)}{\Delta B(u_j)} \right]_{(u_{\sim j} = \text{Constant})} \quad 3-11$$

Let  $u_{\sim j}$  denotes all the manipulated variables except  $u_j$ . The exergy gain  $\tau_{ij}$  is the ratio of the exergy gain change in the controlled variable  $y_i$  to the exergy gain change in the manipulated variable  $u_j$ . The REA can be also calculated using the Hadamard product:

$$\Upsilon = \bar{B} \otimes (\bar{B}^{-1})^T \quad 3-12$$

The REA is a new controllability index which is the connector between the thermodynamic efficiency and process control. It can provide process engineers with an idea of the effects of loop interactions of a control structure on the thermodynamic efficiency of the process during the early stages of process control design. Thermodynamic efficiency can also be further related to economic efficiency. The REA can help to evaluate several control structure

candidates in terms of their thermodynamic efficiencies. This information can help in deciding the final control structure.

### 3.3. Exergy Calculation Procedure

The equations proposed by Hinderink et al.(1996) are used to calculate exergy discussed in Section 3.2.2. The standard chemical exergy of a reference species “ $i$ ”,  $B_{chem.ref,i}^0$ , is,

$$B_{chem.ref,i}^0 = RT_0 \ln \left( \frac{P_0}{P_{ref,i}} \right) \quad 3-13$$

The standard chemical exergy of any species  $i$  is,

$$B_{chem,i}^0 = \Delta_f G_i^0 - \sum_j \nu_j B_{chem,j}^0 \quad 3-14$$

where  $B_{chem,j}^0$  is the standard chemical exergy of the element  $j$  in species  $i$ ;  $\nu_j$  is the stoichiometric coefficient of element  $j$  in species  $i$ ;  $\Delta_f G_i^0$  is the standard Gibbs energy of formation;  $P_0$  is environment pressure; and  $P_{ref,i}$  is the reference pressure for component  $i$ .

If the system phases are different from the phases in the reference environment, the standard chemical exergy of a material stream with multiple components can be obtained from,

$$B_{chem,i}^{0\alpha} = B_{chem,i}^{0\beta} + \Delta_{\beta \rightarrow \alpha} G_i^0 \quad 3-15$$

$$\Delta_{\beta \rightarrow \alpha} G_i^0 = \Delta_f G_i^{0\alpha} - \Delta_f G_i^{0\beta} \quad 3-16$$

where  $B_{chem,i}^{0\alpha}$  is the standard chemical exergy of a species  $i$  in its phase  $\alpha$  and  $B_{chem,i}^{0\beta}$  is the standard chemical exergy of a species  $i$  in its phase  $\beta$ .

The chemical exergy of material streams can be calculated from,

$$B_{chem} = L_0 \sum_{i=1}^n x_{0,i} B_{chem,i}^{0L} + V_0 \sum_{i=1}^n y_{0,i} B_{chem,i}^{0V} \quad 3-17$$

where  $L_0$  denotes the liquid fraction;  $V_0$  denotes the vapour fraction;  $x_{0,i}$  denotes the mole fraction in liquid phase for the  $i$  component; and  $y_{0,i}$  denotes the mole fraction in vapour phase for the  $i$  component. The physical exergy calculation in Equation (3-18) must be used for multi-phase systems, as the calculation in Equation (3-7) is only for single-phase systems.

$$B_{phys} = \left[ L \left( \sum_{i=1}^n x_i H_i^L - T_0 \sum_{i=1}^n x_i S_i^L \right) + V \left( \sum_{i=1}^n y_i H_i^V - T_0 \sum_{i=1}^n y_i S_i^V \right) \right]_{T_0, P_0}^{T, P} \quad 3-18$$

Equation (3-19) is used to calculate the exergy change due to mixing:

$$\Delta_{mix}B = \Delta_{mix}H - T_0\Delta_{mix}S \quad 3-19$$

where  $\Delta_{mix}H$  is enthalpy change of mixing, and  $\Delta_{mix}S$  is entropy change of mixing.

The total exergy of a material stream is calculated by adding the three components as shown in Equation (3-8). The exergy calculation procedures with the related equations are also explained in Figure 3-2.

The automation of this exergy calculation was performed by using HYSYS and Sim42 (Montelongo-Luna et al. 2007). Exergy calculation using the commercial simulator VMGSim was performed by Munir et al. (2010).

In this integrated calculation procedure, the connections of thermodynamic properties, variables and constants in VMGSim are copied and linked into the Excel unit operation. The physical exergy, chemical exergy, mixing exergy and total exergy of material stream are then calculated using Equations (3-13) and (3-19).

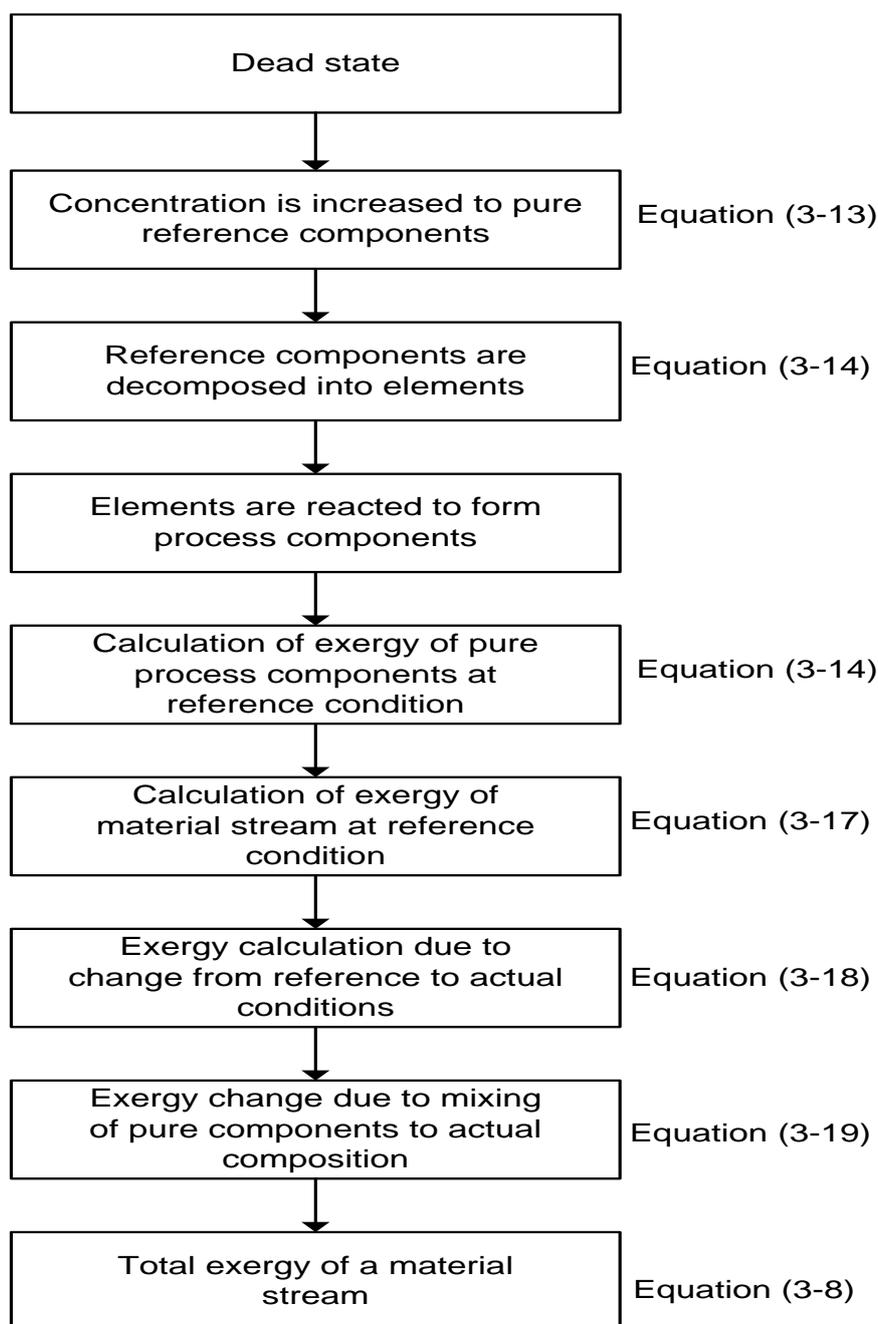


Figure 3-2. Steps involved in exergy calculation

This integrated calculation procedure with a commercial simulator allows the exergy calculation of a material stream with different components. It adds calculation of chemical exergy to physical exergy in the simulator. The exergy changes due to mixing are calculated separately from the physical and chemical exergies of a material stream. Separate calculation of exergy components can show which component is mainly responsible for the loss of exergy. The proposed calculation procedures extend the use of the simulator towards exergy analysis as a diagnostic tool during early stages of process development and design.

To illustrate these calculation procedures, a material stream discussed by Hinderink et al. (1996) is used to test the proposed tool. All required data and the results of the calculation are listed in Munir et al.(2012). Please note that some values are different from the original paper since the simulator (in this case VMGSim) has a different thermodynamic database (i.e.,  $B^0_{Chem, C}$  value). For calculation of chemical exergy, the reference environment in Szargut et al.(1988) is used.

The external data required for standard chemical exergy calculation of reference species is in the form of partial pressures of the reference species, while external data required for chemical exergy calculation is in the form of Gibbs energy of formation. Both of these external forms of data are used for the chemical exergy calculation of a material stream as shown in Equations (3-13) – (3-16). The exergy calculation shows the share of every exergy component in the total exergy of the material stream and enables us to determine the nature of process irreversibilities by monitoring exergy loss in a component. For this example it is clear that the chemical exergy component (3190 kW) has the main share of the total exergy of the material stream. The physical exergy component has a smaller share of the total exergy of the material stream. The mixing exergy has a negative sign because the exergy of pure components is higher when they are in their pure form than when they are mixed.

### **3.4. Case Studies**

#### **3.4.1. Case Study 1: Distillation Column**

A distillation column studied by Svrcek et al.(2006) is selected to illustrate the use of RGA and the new REA measure within process design. A schematic of this distillation column is shown in Figure 3-3. VMGSim with the non-random two-liquid (NRTL) activity thermodynamic model is used for the simulation. Table 3-1 summarizes the feed conditions and the distillation column specifications.

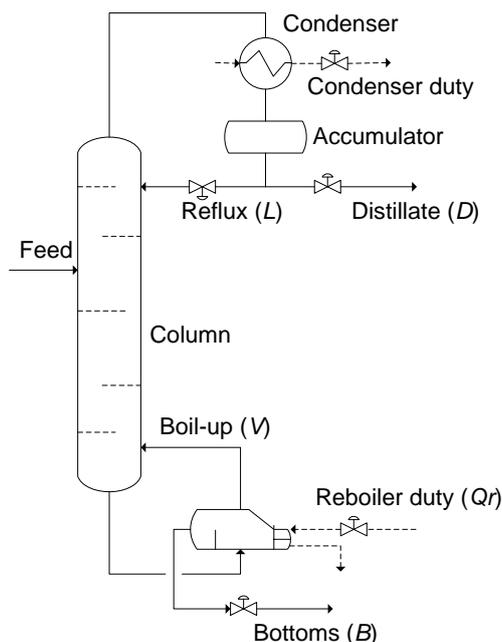


Figure 3-3. Distillation column schematic for case study 1

Table 3-1. Feed and distillation column specifications for case study 1

Feed		Column specifications		Feed specifications	
Flow (kmole/hr)	152.1	Total number of stages	10	E- oxide (Mole fraction)	0.014
Tray specifications		Feed stage	5 <sup>th</sup>	Water (Mole fraction)	0.31
Tray diameter (m)	1.5	Condenser type	Partial	E-glycol (Mole fraction)	0.676
Weir height (m)	0.5	Overhead pressure (kPa)	100	Pressure (kPa)	110
Weir length (m)	1.2	Reboiler pressure (kPa)	105	Temperature (°C)	65

The symbols of the MVs and CVs are listed in Table 3-2. The compositions at the top and bottom of the distillation column,  $x_D$  and  $x_B$ , are the controlled variables. For two-point composition control of a distillation column, three basic control configurations can be defined (*DV*, *LV* and *LB*).

Table 3-2. Control loop pairing nomenclature

Symbols		Description	Symbols		Description
	$L$	Reflux rate	MV	$D$	Distillate rate
MV	$V$	Boil-up rate		$x_D$	Distillate composition
	$B$	Bottom rate	CV	$x_B$	Bottom composition

Table 3-3. Variable pairing of different control configurations for case study 1

Configuration	$u_1$	$y_1$	$u_2$	$y_2$
$DV$	$D$	$x_D$	$V$	$x_B$
$LV$	$L$	$x_D$	$V$	$x_B$
$LB$	$L$	$x_D$	$B$	$x_B$

The summary of the manipulated and controlled variables for each of the proposed control configurations is listed in Table 3-3. For example, in the  $DV$  control configuration,  $D$  (distillate rate) is used to control the composition of top product and  $V$  (boil-up rate) is used to control the composition of bottom product. In this study, RGA and the REA are calculated from simulation experiments. The simulation experiment details are listed in Table 3-4.

Table 3-4. Configurations for step change experiments for case study 1

Pair	Loop mode	$u_1$	$y_1$	$u_2$	$y_2$
$u_1 - y_1$	Open	Step change	Observed	Constant	---
$u_2 - y_1$	Open	Constant	Observed	Step change	---
$u_1 - y_2$	Open	Step change	---	Constant	Observed
$u_2 - y_2$	Open	Constant	---	Step change	Observed
$u_1 - y_1$	Closed	Step change	Observed	---	Constant
$u_2 - y_2$	Closed	---	Constant	Step change	Observed

The RGA values for the three basic control configurations calculated from the gain matrix are

$$\Lambda_{LV} = \begin{bmatrix} 7.07 & -6.07 \\ -6.07 & 7.07 \end{bmatrix} \quad \Lambda_{DV} = \begin{bmatrix} -0.06 & 1.06 \\ 1.06 & -0.06 \end{bmatrix} \quad \Lambda_{LB} = \begin{bmatrix} 0.72 & 0.28 \\ 0.28 & 0.72 \end{bmatrix}$$

All three control configurations show loop interactions. According to RGA interpretation rules (Marlin 2000; Svrcek et al. 2006), the *LB* control configuration is better (has less loop interaction) than the other control configurations as its leading diagonal elements are close to 1. Another option is *LV* whose leading diagonal elements are 7.07. Since off-diagonal relative gains are negative, this control configuration may result in the system being unstable; special care must be taken when it is used. The *DV* control configuration is least desirable as its diagonal elements are far from 1. In this case the off-diagonal elements are close to 1, which is undesirable. The selection of off-diagonal elements would introduce a significant dead time in the control system, as paired manipulated and controlled variables will not be at the same end of the column.

Since two control configurations (*LB* and *LV*) can be selected, the next question could be: which is more eco-efficient? REA can give us the answer. The REA values of the distillation column for the three different control configurations in Table 3-3 are calculated as:

$$\Upsilon_{LV} = \begin{bmatrix} 0.84 & 0.16 \\ 0.16 & 0.84 \end{bmatrix}, \quad \Upsilon_{DV} = \begin{bmatrix} 0.01 & 0.99 \\ 0.99 & 0.01 \end{bmatrix}, \quad \Upsilon_{LB} = \begin{bmatrix} 1.02 & -0.02 \\ -0.02 & 1.02 \end{bmatrix}$$

A leading diagonal value of 0.84 for the *LV* control configuration REA shows that if reflux rate *L* and  $x_D$  are paired, then a step change in the exergy of reflux rate will have almost same impact on the exergy of the controlled variable stream in terms of both magnitude and direction. A leading diagonal value of 0.01 for the *DV* control configuration REA shows that if distillate rate *D* and  $x_D$  are paired, then a step change in the exergy of distillate will have a very small impact on the exergy of controlled variable  $x_D$  stream, both in magnitude and direction. For the *LB* control configuration, if *L* and  $x_D$  are paired then a step change in the exergy of reflux will have almost the same impact on the exergy of the controlled variable  $x_D$  stream in both magnitude and direction.

According to the REA results above, the *LV* and *LB* control configurations are better candidates; in those cases, exergetic efficiency is not affected by loop interactions. Since the *LB* control configuration is the best candidate according to the RGA analysis, the *LB* control

configuration will be the final selection for the process design, integrating control and eco-efficiency.

### 3.4.2. Case Study 2: Ethylene Glycol Production Plant

For this study, an ethylene glycol production plant with a recycle stream (Svrcek et al. 2006) is selected. The schematic of the ethylene glycol plant is shown in Figure 3-4.

This plant consists of a continuous stirred tank reactor (CSTR) and a distillation column. Water reacts with ethylene oxide in the CSTR to produce ethylene glycol. The liquid product stream of the CSTR is sent to a distillation column for the separation of ethylene glycol from the un-reacted water and ethylene oxide. The un-reacted feed is sent back to the CSTR via a recycle loop. VMGSim with the NRTL activity thermodynamic model is used for the simulation. The feed conditions and the distillation column specifications are listed in Table 3-5.

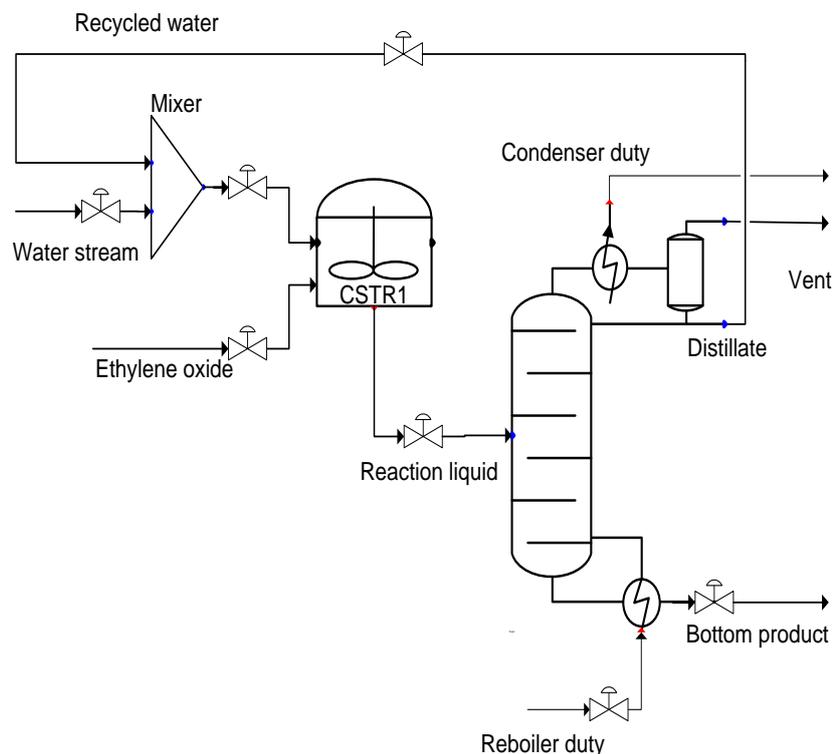


Figure 3-4. Ethylene glycol plant schematic for case study 2 (Svrcek et al. 2006)

Table 3-5. Feed, column and simulation model specifications for case study 2

<b>Feed specifications</b>			
<b>Water</b>		<b>Ethylene oxide</b>	
Temperature ( $^{\circ}\text{C}$ )	41	Temperature ( $^{\circ}\text{C}$ )	30
Pressure (kPa)	85	Pressure (kPa)	200
Molar flow (kmole/hr)	150	Molar flow (kmole/hr)	150
Reactor outlet temperature ( $^{\circ}\text{C}$ )	60		
<b>Column and simulation model specifications</b>			
Column theoretical stages	10	Condenser type	Partial
Feed stage	5 <sup>th</sup>	Reflux ratio	2.5
Column top pressure (kPa)	95	Vent rate (kmole/hr)	5
Column pressure drop (kPa)	5	Distillate rate (kmole/hr)	50
<b>Thermodynamic property package</b>			
Activity model	NRTL		

The same symbols as listed in Table 3-2 are adopted for this case study. Two new symbols are used for case study 2: (1) the coolant flow to reactor that controls the heat removal of exothermic reaction  $Q_R$  is a MV; and (2) the reactor temperature  $T$  is a CV. The compositions at the top and bottom of the distillation column ( $x_D$  and  $x_B$ , respectively) and the reactor temperature  $T$  are the controlled variables. These three controlled variables are controlled by distillate or reflux flow rate, bottom or boil-up flow rate and the coolant flow to the reactor, respectively. This system becomes a  $3 \times 3$  system when reactor temperature control is considered with two-point composition control of the distillation column. This system can be considered a  $4 \times 4$  system when the level control of the reactor is also considered; however, ‘perfect’ inventory control is assumed as a common situation in control scheme design e.g. (Svrcek et al. 2006).

Table 3-6 summarizes the manipulated and controlled variables for each of the proposed three control configurations:  $LVQ_R$ ,  $LBQ_R$  and  $DVQ_R$ .

Table 3-6. Control pairings of different control configurations for case study 2

Configurations	$u_1$	$y_1$	$u_2$	$y_2$	$u_3$	$y_3$
$LVQ_R$	$L$	$x_D$	$V$	$x_B$	$Q_R$	$T$
$LBQ_R$	$L$	$x_D$	$B$	$x_B$	$Q_R$	$T$
$DVQ_R$	$D$	$x_D$	$V$	$x_B$	$Q_R$	$T$

The steady-state gain matrix and the steady-state exergy gain matrix are obtained by step change experiments similar to case study 1. The RGA values for the three basic control configurations calculated from the gain matrix are:

$$\Lambda_{LVQ_R} = \begin{bmatrix} 0.80 & -1.09 & 1.29 \\ -4.60 & 5.75 & -0.15 \\ 4.81 & -3.66 & -0.14 \end{bmatrix},$$

$$\Lambda_{LBQ_R} = \begin{bmatrix} 1.06 & -0.02 & -0.04 \\ -0.06 & 0.92 & 0.14 \\ 0.00 & 0.10 & 0.90 \end{bmatrix} \quad \Lambda_{DVQ_R} = \begin{bmatrix} -0.004 & 1.13 & -0.13 \\ 0.82 & -0.13 & 0.31 \\ 0.19 & 0.00 & 0.81 \end{bmatrix}$$

For the  $LVQ_R$  control configuration, the leading diagonal and off-diagonal elements of RGA are (0.80, 5.75 and  $-0.14$ ) and (1.29, 5.75 and 4.81), respectively. This control configuration cannot be selected because most of the diagonal elements are far from 1 and one has a negative sign. When reflux rate is increased, this will increase the  $x_D$  as it returns more volatile components back to the column. The increase in  $L$  impacts on  $x_B$  to the same magnitude but opposite in direction due to the introduction of more volatile components in the column which would also increase the bottom flow.

The leading diagonal elements of the  $LBQ_R$  control configuration are (1.06, 0.92 and 0.90). It shows that the control variables must be paired with the manipulated variables of their control loop. In this control scheme there will be very small interactions among the loops. The RGA values of reflux rate with  $x_B$  and  $T$  are  $-0.02$  and  $-0.04$ . These small negative values show that reflux rate has a small impact in the opposite direction on these variables. A step change in reflux rate will reintroduce the more volatile component (water) rich stream into the

distillation column which will cause a positive increase in  $x_D$  (more volatile component), a decrease in  $x_B$  (low volatile component) and a decrease in reactor temperature, and vice versa.

The leading diagonal elements of  $DVQ_R$  control configuration are  $(-0.004, -0.13$  and  $0.81)$ . This shows that a step change in distillate rate  $D$  has a very small negative impact on  $x_D$  and  $x_B$  and a high positive impact on the temperature of the reactor. The reason for this is that when the distillate rate increases, this will increase the reflux rate which will impact negatively on the  $x_B$ . On the other hand, an increase in the distillate rate causes an increase in the recycle (which is mostly water). This increase in water will also increase the amount of ethylene oxide required for the reaction according to the stoichiometric balance. This will change the volume requirement for the conversion of reactants to products which is already fixed. The reaction would therefore not be complete and un-reacted components will exist in the exit stream of the reactor which will cause negative impacts on  $x_D$  and  $x_B$ .

Two control configurations ( $LBQ_R$  and  $DVQ_R$ ) show small loop interactions. According to RGA interpretation rules, the  $LBQ_R$  control configuration is better (has less loop interaction) than the other control configurations, as its leading diagonal elements are close to 1. While the  $DVQ_R$  control configuration has elements close to 1, they are not leading diagonal elements except for one element. The  $LVQ_R$  control configuration is the least desirable as its leading diagonal elements are far from 1 and one element is negative. In this case, manipulated variables have a small effect on the control variables. Its off-diagonal elements are positive and different from 1 and may introduce a significant dead time in the control system as paired manipulated and controlled variables will not be at the same end of the column.

Since two control configurations  $LBQ_R$  and  $DVQ_R$  can be selected, we will use REA to help us consider eco-efficiency. The REA values for the two selected control configurations are calculated using the proposed exergy procedure. The REA results are:

$$Y_{LBQ_R} = \begin{bmatrix} 0.07 & 1.54 & -0.61 \\ 0.93 & -0.32 & 0.39 \\ 0.00 & -0.23 & 1.23 \end{bmatrix} \quad Y_{DVQ_R} = \begin{bmatrix} 0.48 & 1.12 & -0.61 \\ 0.31 & -0.12 & 0.82 \\ 0.21 & 0.00 & 0.79 \end{bmatrix}$$

From the above REA results, it is not obvious which configuration is best. Consider the  $LBQ_R$  control configuration first. The pairs,  $y_1 - u_2$ ,  $y_2 - u_1$  and  $y_3 - u_3$  should be selected

according to the REA rules. Two pairs selected from the REA are contradicted by the pairing selections from the RGA. For the  $DVQ_R$  control configuration, only one pairing selection for the controlled variable,  $y_2$ , yields contradictory results from the RGA and REA analyses. Therefore the  $DVQ_R$  control configuration could be further considered for process design on the basis of eco-efficiency. This preliminary recommendation should be validated by further study involving dynamic plots or dynamic simulation. This case study illustrates the classical trade-off between control and exergy efficiency. The REA can help us consider options.

However, for the  $DVQ_R$  control configuration, the pairing must be  $x_D - V$  and  $x_B - D$  according to the RGA. These pairings are an off-diagonal pairings. It would therefore be unlikely that this configuration would provide adequate dynamic control performance. The only choice from a control quality point of view would seem to be the  $LBQ_R$  scheme, even though its REA values are far from 1. When the REA results contradict with the RGA results then the final selection of control scheme should be based on RGA results because controllability cannot be compromised. This suggestion also requires further validation from dynamic simulation.

### 3.5. Summary

The RGA provides a quantitative comparison of interactions between control loops. This tool integrates process control with process design. For eco-efficient process design, the REA is introduced to compare the thermodynamic efficiency for different control structures at the early process design stage. When the RGA and REA are used together, they can provide measures of controllability and eco-efficiency of the process under a certain process design. Although the final choice of the best control configuration may require more detailed analysis, that is, dynamic simulation, the combination of the RGA and REA will help guide the process designer to reach the optimal control design with low cost. When results from the RGA and REA contradict each other (e.g., in case study 2), dynamic simulation is required for validation purposes. Further investigation of the REA for a whole plant which includes recycle loops is explained in Chapter 4.

## References

- Bristol, E. (1966). "On a new measure of interaction for multivariable process control." Automatic Control, IEEE Transactions on **11**(1): 133-134.
- Denbigh, K. G. (1956). "The second-law efficiency of chemical processes." Chemical Engineering Science **6**(1): 1-9.
- Dincer, I. (2002). "The role of exergy in energy policy making." Energy Policy **30**(2): 137-149.
- Grosdidier, P. and M. Morari (1986). "Interaction measures for systems under decentralized control." Automatica **22**(3): 309-319.
- Himmelblau, D. M. and J. B. Riggs (2004). Basic Principles and Calculations in Chemical Engineering. Upper Saddle River, New Jersey, Prentice Hall.
- Hinderink, A. P., F. P. J. M. Kerkhof, A. B. K. Lie, J. De Swaan Arons and H. J. Van Der Kooi (1996). "Exergy analysis with a flowsheeting simulator - I. Theory; calculating exergies of material streams." Chemical Engineering Science **51**(20): 4693-4700.
- Kotas, T. J. (1985). The exergy method of thermal plant analysis. London, Butterworth-Heinemann Ltd.
- Marlin, T. E. (2000). Process control: design process and control system for dynamic performance. New York, McGraw Hill.
- McAvoy, T. J. (1983). Interaction Analysis: Principles and Applications. Research Triangle Park, NC, Instrument Society of America.
- McAvoy, T. J., Y. Arkun, R. Chen, D. Robinson and P. D. Schnelle (2003). "A new approach to defining a dynamic relative gain." Control Engineering Practice **11**(8): 907-914.
- Monshizadeh-Naini, N., A. Fatehi and A. Khaki-Sedigh (2009). "Input-Output Pairing Using Effective Relative Energy Array." Industrial & Engineering Chemistry Research **48**(15): 7137-7144.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2007). "An exergy calculator tool for process simulation." Asia-Pacific Journal of Chemical Engineering **2**(5): 431-437.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2010). "The relative exergy array—a new measure for interactions in process design and control." The Canadian Journal of Chemical Engineering **89**(3): 545-549.
- Munir, M. T., J. J. Chen and B. R. Young (2010). A computer program to calculate the stream exergy using the visual basic graphical interface. Chemeca 2010. Adelaide, Australia.
- Munir, M. T., W. Yu and B. R. Young (2012). Determination of Plant-wide Control Loop Configuration and Eco-Efficiency, G.P. Rangaiah and V. Kariwala (Eds.). Plantwide Control: Recent Developments and Applications, John Wiley & Sons, ISBN:9780470980149.
- Munir, M. T., W. Yu and B. R. Young (2012). "Recycle effect on the relative exergy array." Chemical Engineering Research and Design **90**(1): 110-118.
- Papadourakis, A., M. F. Doherty and J. M. Douglas (1987). "Relative gain array for units in plants with recycle." Industrial & Engineering Chemistry Research **26**(6): 1259-1262.

- Rosen, M. A. and I. Dincer (1997). "On exergy and environmental impact." International Journal of Energy Research **21**: 643-654.
- Rosen, M. A. and I. Dincer (1999). "Exergy analysis of waste emissions." International Journal of Energy Research **23**: 1153-1163.
- Skogestad, S., P. Lundström and E. W. Jacobsen (1990). "Selecting the best distillation control configuration." AIChE Journal **36**(5): 753-764.
- Svrcek, W. Y., D. P. Mahoney and B. R. Young (2006). A Real-Time Approach to Process Control. Chichester, John Wiley & Sons Ltd.
- Szargut, J., D. R. Morris. and F. R. Steward (1988). Exergy analysis of thermal, chemical, and metallurgical processes. New York, Hemisphere.
- Witcher, M. F. and T. J. McAvoy (1977). "Interacting control systems: steady state and dynamic measurement of interaction." ISA Trans. **16**(3): 35-41.
- Xiong, Q., W.-J. Cai and M.-J. He (2005). "A practical loop pairing criterion for multivariable processes." Journal of Process Control **15**(7): 741-747.



# Chapter 4

---

## *Recycle effect on the Relative Exergy Array*

### **Article # 2**

**Co-authors: Wei. Yu, Brent. R. Young**

*Industrial Information & Control Centre (I<sup>2</sup>C<sup>2</sup>), Department of Chemical & Materials Engineering, The University of Auckland, Auckland, New Zealand*

Munir, M. T., W. Yu and B. R. Young (2012). Recycle effect on the Relative Exergy Array. *Chemical Engineering Research and Design* **90**(1): 110 – 118.

## **Chapter 4. Recycle effect on the Relative Exergy Array**

This chapter presents the effect of recycles on the REA. As recycle systems are common in the process industry, it is necessary to study the effect of recycle loops on the REA results. Chapter 4 is a continuation of Chapter 3, mainly focusing on the unit or process with recycles in plant-wide layout. Two simulation case studies are also discussed in this chapter to explain the results.

### **Abstract**

Since the eco-efficiencies of all industrial processes/plants have become more and more important, engineers need to find a way to integrate process design, process control and measurements of eco-efficiency. The thermodynamic concept of Exergy can be used to analyse a process in terms of its efficiency. The Relative Exergy Array (REA) that measures both the relative exergetic efficiency and controllability of a process has been proposed (Montelongo-Luna et al. 2010). The REA can be used for quick comparison between several process/control structure candidates. It is very common that the industrial unit/process includes some recycle loops. The recycle effect on REA is investigated in this paper through two process case studies. Simulation results show that the REA without consideration of the recycle loop may mislead the selection of control configuration. Recycle loop should be considered for selection of control configuration.

Key words: Relative exergy array, Relative gain array, Recycle.

### **4.1. Introduction**

Since the environment is now of considerable importance internationally and energy is becoming more expensive, processes should not only convert raw materials into the higher value products economically but should also consider energy efficiency and environmental rules and regulations. Environmental regulations may have different forms in terms of such as intensity targets and emission limits. Process design is the design of processes for desired physical and/or chemical transformation of materials. It usually includes several stages and each stage has its own depth of knowledge and understanding. The later stage, the more detailed information of the process is required.

At the early design stage the process will be designed to fulfil the design criteria: maximizing production/profit while minimizing environmental impact. It is only in the final design stage that the process control scheme is developed since it requires great amount of process information for activities such as dynamic modelling. The processes may be uncontrollable or difficult to be controlled under this design strategy. Furthermore, if the process needs to be modified (i.e. adding new equipment) it may make a large impact on the controllability and economic efficiency of the process/plant. To avoid these problems, an integrated approach of process design, control and economic efficiency in early process design stages is needed. It can be achieved through well-developed simulation software, very powerful computation capacity and mature process dynamic information. Engineers/designers choose the best process configuration with consideration of control, economics and energy consumption by evaluating many control structure candidates simultaneously.

The pioneering method integrating process design and process control was the so called relative gain array (RGA) proposed by Bristol (1966). It provides a quantitative measure of interaction which can guide the process design to determine the best decentralized control loop configuration. Since then, an extensive amount of research has been done in control loop configuration or input – output pairing selection such as the dynamic RGA (Witcher and McAvoy 1977; McAvoy et al. 2003) and effective relative gain array (ERGA) (Xiong et al. 2005).

Extending the RGA idea to an eco-efficient process design, a new measure, relative exergy array (REA), was proposed by Montelongo-Luna et al.(2010). Since the REA can show a deep understanding of all areas of chemical engineering, economics and consideration of sustainability, it can be used to integrate process design, process control and economics/sustainability.

The Relative Exergy Array (REA) is based on the exergy for the control configuration within the process design (Montelongo-Luna et al. 2010). Exergy plays an important role in the new measurement REA, since it can be used for determining exergetic efficiency and sustainability of a process (Dincer 2002). For example, the environmental impacts can be minimised by reducing exergy losses and by efficient use of exergy (Rosen and Dincer 1997; Rosen and Dincer 1999). The REA adopts the same idea of RGA and is the extension of RGA into the exergy domain. The REA is defined by placing the exergy thermodynamic property in the place of gain in the RGA analysis. REA may provide a deeper insight into

process control structure interactions and measurement of exergetic efficiency and can be used for the quick comparison between several process/control structure candidates.

Recycling is frequently used in chemical plants and industrial processes since it can increase material usage and improve the energy efficiency. There are many investigations about recycling effects on controllability. For example, Papadourakis et al.(1987) proposed that the RGA for individual units are different than the RGA of the whole plant, as recycle changes the interactions in the plant. Luyben and Fluodas (1994) looked into the interaction between design and control using multi objective optimization. Luyben studied several recycle process (Luyben 1993; Luyben 1993; Luyben 1994), and as a remedy for the high gain in recycle flow he proposed to fix a flow in the recycle loop. Price and Georgakis (1993) looked at simulations of a large number of control structures, from which they makes general guide lines. Horvath et al.(2007) investigated the recycle effect on controllability for the ethyl benzene production system.

The REA has previously been implemented in systems without recycles (Montelongo-Luna et al. 2007; Montelongo-Luna et al. 2010). Since recycle systems are very popular in chemical plants and other industrial plants, it is necessary to study recycle effects on the REA. Recycle can increase equipment size and cost but cost is not considered in this work as this is usually considered separately in the design process. In this paper, through study of two typical chemical processes: ethyl benzene production and ethylene glycol production, we demonstrate that the presence of recycle loops in a process can have a significant effect on the REA. We show that the REA results from the process without including the recycles cannot be relied upon to design the control configuration for the process including the recycles. Controllability and eco-efficiency are the main foci in this work, not the process design.

This paper is organized as follows. In Section 4.2, the concepts of the relative gain array (RGA) and relative exergy array (REA) are addressed. Then, the thermodynamic concept of exergy and exergy calculation are discussed. In Section 4.4, two case studies are used to analyze the recycle effect on the REA. Finally, the major results are discussed and conclusion is addressed in the paper summary.

## 4.2. Relative Gain Array (RGA) and Relative Exergy Gain Array (REA)

### 4.2.1. Relative Gain Array (RGA)

RGA is defined as “The ratio of process gain in an isolated loop to apparent process gain in the same loop when all other control loops are closed”, (Bristol 1966). It is a matrix composed of elements defined as the ratio of open-loop to closed-loop gains. One of its elements, relative gain,  $\lambda_{ij}$ , which relates the  $j^{\text{th}}$  input  $u_j$  and the  $i^{\text{th}}$  output  $y_i$ , can be expressed by the following equation,

$$\lambda_{ij} = \frac{\left( \frac{\partial y_i}{\partial u_j} \right)_{u_k = \text{const}, k \neq j}}{\left( \frac{\partial y_i}{\partial u_j} \right)_{y_k = \text{const}, k \neq i}} \quad 4-1$$

The relative gain,  $\lambda_{ij}$ , in Equation (4-1) is the ratio of change in the steady state gain value of a control variable (CV),  $y_i$ , with respect to a manipulated variable (MV),  $u_j$ , when all loops are open, to change in the steady state value of gain of  $y_i$  with respect to  $u_j$  when all other loops are closed and in “perfect control”. The phrase “perfect control” refers to the condition of a control loop where no offset is present in the controlled variable at steady state.

The assembly of the relative gains ( $\lambda_{ij}$ ) for all possible pairing combinations of multi loop single input single output (SISO) systems is called the relative gain array (RGA), namely,

$$\Lambda = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \cdots & \lambda_{1n} \\ \lambda_{21} & \lambda_{22} & \cdots & \lambda_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \lambda_{n1} & \lambda_{n2} & \cdots & \lambda_{nn} \end{bmatrix} \quad 4-2$$

The RGA provides a quantitative comparison of interactions between control loops. It shows steady state interactions between control loops. Although the RGA can be calculated by performing experiments for each possibility of control pair using Equation (4-1), it is not usually possible to do so for an operating plant. An alternative method of RGA calculation is based on the availability of a process model, from the steady state gain matrix,  $G$ , the RGA can be calculated directly (Bristol 1966),

$$\Lambda = G \otimes (G^{-1})^T \quad 4-3$$

Detailed interpretations about the RGA and the selection criteria of the control pairs can be found in many text books (e.g. Marlin 2000; Svrcek et al. 2006).

#### 4.2.2. Exergy and Relative Exergy Array (REA)

##### 4.2.2.1. Exergy

In every chemical process there are some materials coming in or out. Similarly every process needs some energy to perform its work and/or the process rejects energy to the surroundings. So the material and energy balances of the process are generally used to evaluate the efficiency of the process at the process design stage. For energy balance calculations chemical engineers mostly only focus on the 1<sup>st</sup> Law of Thermodynamics (e.g. Himmelblau and Riggs 2004). However, this approach may not fully reflect energy efficiency in the realistic manner. The 2<sup>nd</sup> Law of the thermodynamics must be included to provide a more realistic understanding of energy usage and wastage (Denbigh 1956).

A general thermodynamic process is shown in Figure 4-1. The considered process has many arbitrary material streams coming from and going out of the process boundary. The process has its own temperature ( $T$ ), pressure ( $P$ ) and composition ( $Z$ ). The process is also being heated from different heating sources at different temperatures  $T_i$  and contributing different amounts of heat  $q_i$ . The process produces some shaft work ( $W$ ) and delivers it to the environment with fixed values of temperature, pressure and composition ( $T_0, P_0$  and  $Z_0$ ).

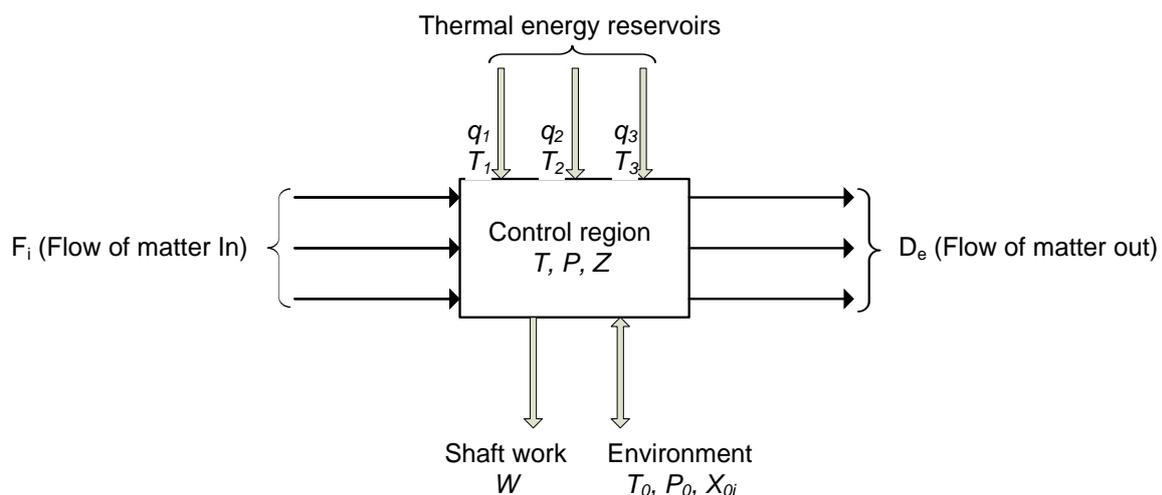


Figure 4-1. General thermodynamic process

The combination of the 1<sup>st</sup> and 2<sup>nd</sup> laws of thermodynamics for the thermodynamic process in Figure 4-1 can be expressed as,

$$W + \sum_i (q_i + T_0 \Delta S_i) = T_0 \sigma + \Delta U + P_0 \Delta V - T_0 \Delta S \quad 4-4$$

where  $W + \sum_i (q_i + T_0 \Delta S_i)$  denotes the total work performed on the process and  $T_0 \sigma$  denotes energy loss due to irreversibilities.

Exergy is the maximum possible amount of work which can be drawn from a material stream when it interacts only with the environment and it comes from its initial state to the final dead state (Denbigh 1956; Kotas 1985). At the dead state the material stream is in thermal, mechanical and chemical equilibrium with the environment. Since exergy accounts for the quality of energy, it can be used as a measure to evaluate eco-efficiency for process design. The calculation of the physical exergy of the thermodynamic process in Figure 4-1 can be obtained from Equation (4-4) as,

$$\Delta B_{phys} = \Delta U + P_0 \Delta V - T_0 \Delta S \quad 4-5$$

As the thermodynamic process composition  $Z$  and the environmental composition  $X_{0i}$  in Figure 4-1 are designed for different work potentials, the total exergy of the material stream will also change. The total exergy, including three main components: physical exergy, chemical exergy and exergy due to mixing, is defined as (Hinderink et al. 1996),

$$B_{total} = B_{phys} + B_{chem} + \Delta_{mix} B \quad 4-6$$

The detailed definitions of chemical exergy,  $B_{Chem}$ , and exergy change due to mixing,  $\Delta_{mix} B$ , are provided in Section 4.3 of this paper. Based on the total exergy of each material stream in and out of the thermodynamic process, it is possible that engineers can build an eco-efficient process which is highly ecological and economical.

The total exergy calculation in Equation (4-6) is simple and only needs easily obtainable thermodynamic data. This calculation requires data such as the Gibbs energy of formation for the calculation of standard chemical exergies. The Gibbs energy of formation data can be obtained from different sources like thermodynamic databanks or process simulators but special attention must be paid to the consistency of this data.

#### 4.2.2.2. Relative Exergy Array (REA)

RGA only accounts for the controllability of the MIMO systems. The consideration of exergy is also an important factor and it should be included in the control design. Relative Exergy Array (REA) is a tool to utilize control design and exergy (Montelongo-Luna et al. 2010). REA can be directly derived from the RGA concept in the exergy domain by placing the exergy thermodynamic property in place of gain. REA for an  $n \times n$  MIMO system is defined analogously to RGA as,

$$\Upsilon = \begin{bmatrix} \gamma_{11} & \gamma_{12} & \cdots & \gamma_{1n} \\ \gamma_{21} & \gamma_{22} & \cdots & \gamma_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \gamma_{n1} & \gamma_{n2} & \cdots & \gamma_{nn} \end{bmatrix} \quad 4-7$$

where

$$\gamma_{ij} = \frac{\left( \frac{\Delta B_{total}(y_i)}{\Delta B_{total}(u_j)} \right)_{\text{all loops open}}}{\left( \frac{\Delta B_{total}(y_i)}{\Delta B_{total}(u_j)} \right)_{\text{all loops closed (in perfect control) except } u_j \text{ loop}}} \quad 4-8$$

The relative exergy,  $\gamma_{ij}$ , in Equation (4-8) is the ratio of gain change in the steady state exergy of the material stream  $y_i$  with respect to that of the material/energy stream  $u_j$  when all loops are open to the gain change in the steady state exergy of the material stream  $y_i$  with respect to that of the material/energy stream  $u_j$  when all other loops are closed under “perfect control”. The relative exergy,  $\gamma_{ij}$  quantifies the amount of exergy change in the control variable ( $y_i$ ) stream due to exergy change introduced in the manipulated variable ( $u_j$ ) stream.

The relative exergy  $\gamma_{ij}$  indicates the change in effective exergy gain of one loop ( $u_j - y_i$ ) when all other loops are closed. It can provide the thermodynamic efficiency of a control loop considered when all other loops are closed. When the value of  $\gamma_{ij}$  is close to 1 then it indicates that the thermodynamic efficiency of the control loop considered is less affected by the other loops. This would be a good pairing candidate from an efficiency point of view as its thermodynamic efficiency is not affected by interactions of other control loops.

A value of relative exergy ( $\gamma_{ij}$ ) less than 1 indicates that the exergy changes increase due to loop interactions when all other loops are closed. In this case the exergy changes are less when all loops are open. The value of relative exergy ( $\gamma_{ij}$ ) more than 1 indicates that the

exergy change decreases due to loop interactions when all other loops are closed. In this case the exergy changes are more when all loops are open.

As RGA can be calculated from the steady state gain matrix, the REA can also be obtained from the steady state generic exergy gain matrix defined as,

$$\bar{B} = \begin{bmatrix} \tau_{11} & \tau_{12} & \cdots & \tau_{1n} \\ \tau_{21} & \tau_{22} & \cdots & \tau_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \tau_{n1} & \tau_{n2} & \cdots & \tau_{nn} \end{bmatrix} \quad 4-9$$

where

$$\tau_{ij} = \left[ \frac{\Delta B_{total}(y_i)}{\Delta B_{total}(u_j)} \right]_{(u_{\sim j} = \text{Constant})} \quad 4-10$$

Let  $u_{\sim j}$  denotes all the manipulated variables except  $u_j$ . The generic exergy gain  $\tau_{ij}$  is the ratio of the exergy gain change in the controlled variable,  $y_i$  to the exergy gain change in the manipulated variable  $u_j$ .

The steady state generic exergy gain,  $\tau_{ij}$  value can be positive or negative. A negative value of  $\tau_{ij}$  indicates that exergy of one stream increases and exergy of the other stream decreases. A positive value of  $\tau_{ij}$  indicates that the exergy changes of both streams have the same directions. The exergy of a stream can increase or decrease but the net exergy change of the process is zero or less than zero.

REA in Equation (4-7) can be also calculated by Hadamard product as,

$$\Upsilon = \bar{B} \otimes (\bar{B}^{-1})^T \quad 4-11$$

Since exergy shows the maximum efficiency of a process, REA can provide the process interactions in the sense of energy influenced by the control policy. The REA inherits many properties of RGA such as the summations of the rows and columns are equal to one. The interpretation of REA results is same as that of RGA. Also it is independent of scaling.

The REA is a new controllability index which is the connection between thermodynamic efficiency and process control.

REA can give some idea to process engineers about the effect loop interactions of a control structure will have on the thermodynamic efficiency of the process during early stages of process control design. REA can help to evaluate several control structure candidates in terms of their thermodynamic efficiencies. This information can help in deciding the final control structure. Thermodynamic efficiency can also be further related to economic efficiency. Although the final decision of best control configuration requires more detailed analysis i.e. dynamic simulation, the combination of RGA and REA will help guide the process designer to reach an optimal control design with low cost.

### 4.3. Exergy Calculation

The chemical exergy of a material stream,  $B_{Chem}$ , is the exergy content due to composition differences between pure components at reference conditions and the reference environment components in their environmental concentrations. The calculation of chemical exergy has two main steps. In the 1<sup>st</sup> step the standard chemical exergy of the pure reference environment components is calculated. These components are also called reference species. The calculation of standard chemical exergy of the reference species by assuming ideal gas behaviour can be written as (Moran 1982; Szargut et al. 1988),

$$B_{chem-ref,i}^0 = RT_0 \ln \left( \frac{P_0}{P_{ref,i}} \right) \quad 4-12$$

where,  $B_{chem-ref,i}^0$  = Standard chemical exergy of a reference species “ $i$ ”,  $P_{ref,i}$  = Partial pressure of reference species “ $i$ ”, and  $P_0$  = Reference overall pressure

In the 2<sup>nd</sup> step, standard chemical exergies of components which are not present in the environment (also called non reference species) are calculated from standard chemical exergies of reference species and Gibb’s energy of formation. The 2<sup>nd</sup> step is further divided into two parts: i) the standard chemical exergy of pure elements at reference conditions is calculated; and ii) the non-reference species are formed by formation reactions using pure elements and the exergy can be obtained from the following equation,

$$B_{chem,i}^0 = \Delta_f G_i^0 - \sum_j \nu_j B_{chem,j}^0 \quad 4-13$$

where,  $B_{chem,i}^0$  = Standard chemical exergy of any species “ $i$ ”, and  $B_{chem,j}^0$  = Standard chemical exergy of the element “ $j$ ” in species “ $i$ ”, and  $v_j$  = Stoichiometric coefficient of element “ $j$ ” in species “ $i$ ”,  $\Delta_f G_i^0$  = Standard Gibbs energy of formation.

Equations (4-12) and (4-13) can be used for the calculation of the standard chemical exergy of a system which has the same phase as the reference environment. If the system phases are different from the phases in the reference environment, the standard chemical exergy of a material stream with multiple components can be obtained from Equations (4-14) and (4-15).

$$B_{chem,i}^{0\alpha} = B_{chem,i}^{0\beta} + \Delta_{\beta \rightarrow \alpha} G_i^0 \quad 4-14$$

$$\Delta_{\beta \rightarrow \alpha} G_i^0 = \Delta_f G_i^{0\alpha} - \Delta_f G_i^{0\beta} \quad 4-15$$

where,  $B_{Chem,i}^{0\alpha}$  = Standard chemical exergy of a species “ $i$ ” in its phase “ $\alpha$ ”,  $B_{Chem,i}^{0\beta}$  = Standard chemical exergy of a species “ $i$ ” in its phase “ $\beta$ ”.

The chemical exergy of material streams can be calculated from,

$$B_{chem} = L_0 \sum_{i=1}^n x_{0,i} B_{chem,i}^{0L} + V_0 \sum_{i=1}^n y_{0,i} B_{chem,i}^{0V} \quad 4-16$$

where  $L_0$  denotes the liquid fraction,  $V_0$  denotes the vapour fraction,  $x_{0,i}$  denotes the mole fraction in liquid phase for the  $i$  component, and  $y_{0,i}$  denotes the mole fraction in vapour phase for the  $i$  component.

The physical exergy of a material stream is the exergy content due to the thermo-mechanical difference between pure components at process conditions and pure components at reference conditions. Equation (4-17) is used for calculation of the physical exergy of the material stream. The superscripts and subscripts in Equation (4-17) show the change from actual conditions ( $T, P$ ) to reference conditions ( $T_0, P_0$ ).

The physical exergy calculation in Equation (4-17) must be used for multi-phase systems, as the calculation in Equation (4-5) is only for single phase systems.

$$B_{phys} = \left[ L \left( \sum_{i=1}^n x_i H_i^L - T_0 \sum_{i=1}^n x_i S_i^L \right) + V \left( \sum_{i=1}^n y_i H_i^V - T_0 \sum_{i=1}^n y_i S_i^V \right) \right]_{T_0, P_0}^{T, P} \quad 4-17$$

where,  $L$ = Liquid fraction,  $x$ = mole fraction in liquid phase,  $H_i^L$  = molar enthalpy in liquid phase,  $T_0$ = Reference temperature,  $S_i^L$  = molar entropy in liquid phase,  $V$ = vapour fraction,  $y$ = mole fraction in vapour phase,  $H_i^V$  = molar enthalpy in vapour phase and  $S_i^V$  = molar entropy in vapour phase

The exergy change of mixing is due to mixing of pure components at process conditions to form the actual composition of the material stream. Equation (4-18) is used to calculate the exergy change due to mixing.

$$\Delta_{mix}B = \Delta_{mix}H - T_0\Delta_{mix}S \quad 4-18$$

where  $\Delta_{mix}H$ = Enthalpy change of mixing, and  $\Delta_{mix}S$  = Entropy change of mixing.

#### 4.3.1. Exergy Calculation Programme

The automation of the exergy calculation has been done previously by using HYSYS and Sim42 (Montelongo-Luna et al. 2007). Since VMGSim includes more up-to-date thermodynamic data from the National Institute of Standards and Technology (NIST) record (Virtual Materials Group Inc. 2010) and it reports physical exergy (Virtual Materials Group Inc. 2009), we propose exergy calculation using VMGSim as the simulator. Our exergy calculator consists of programming code and a Graphical user Interface (GUI). A GUI is used for the linkage of external manual data with programming code. Detailed information can be found in the paper Munir et al.(2010).

### 4.4. Case Studies

#### 4.4.1. Case Study 1: Ethyl Benzene Production

The Ethyl benzene process used for the case study is shown in Figure 4-2 and is adapted from Luyben (2002) . It has two reactors, two distillation columns and two recycle streams. In reaction section two CSTR reactors ( $200 \text{ m}^3$ ) are connected in series as shown in Figure 4-2. Fresh ethylene, fresh benzene and recycled benzene are fed to the first reactor ( $R_1$ ) where the main reaction occurs. This main reaction is exothermic in nature and heat is removed from this reactor. The effluent of the first reactor and recycled diethyl benzene are fed to the second reactor ( $R_2$ ) which operates adiabatically. The effluent of second reactor is fed to a distillation column ( $T_1$ ). Its overhead product mainly contains benzene which is recycled back to reactor 1 ( $R_1$ ), while an ethyl benzene/diethyl benzene mixture is out from the bottoms.

This bottom product is fed to the second distillation column ( $T_2$ ). Its overhead product contains mainly ethyl benzene, while its bottoms product is mainly diethyl benzene which is recycled back to reactor 2 ( $R_2$ ). Table 4-1 summarizes the feed conditions and the distillation column specifications.

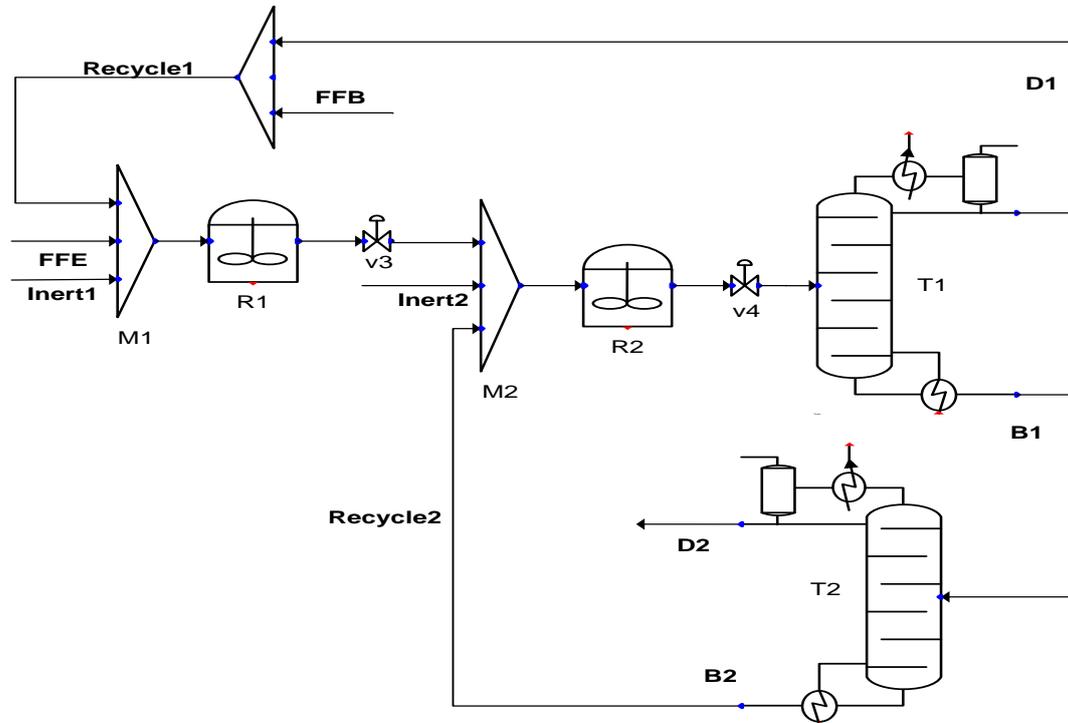


Figure 4-2. Case study 1 Ethyl benzene production schematic



The kinetic equations and data used for these reactions is given as,

$$R_1' = C_E C_B (1.528 \times 10^6) e^{\frac{-17000}{RT}} \quad 4-22$$

$$R_2' = C_E C_{EB} (2.778 \times 10^4) e^{\frac{-20000}{RT}} \quad 4-23$$

$$R_3^i = C_{DEB} C_B (0.4167) e^{\frac{-15000}{RT}} \quad 4-24$$

Table 4-1. Distillation columns details and specifications

Column 1 (T1)		Column 2 (T2)	
Feed Conditions		Feed Conditions	
Temperature ( $^{\circ}\text{C}$ )	163.4	Temperature ( $^{\circ}\text{C}$ )	202.4
Pressure (kPa)	470	Pressure (kPa)	350
Molar flow (kmol/hr)	1829	Molar flow (kmol/hr)	857.8
Composition (Mole fraction)		Composition (Mole fraction)	
Ethylene	0.00	Ethylene	0.00
Benzene	0.53	Benzene	0.00
E-Benzene	0.34	E-Benzene	0.730
12-E-Bz	0.13	12-E-Bz	0.270
Nitrogen	0.004	Nitrogen	0.00
Column Specifications		Column Specifications	
No of trays	24	No of trays	30
Feed tray	13 <sup>th</sup>	Feed tray	10 <sup>th</sup>
Overhead pressure (kPa)	450	Overhead pressure (kPa)	200
Bottom pressure (kPa)	460	Bottom pressure (kPa)	220
Condenser type	Partial	Condenser type	Total
Top product specification	0.001( <i>EB</i> )	Top product specification	0.001( <i>12-E-B</i> )
Bottom product specification	0.001( <i>EB</i> )	Bottom product specification	0.001( <i>EB</i> )

Table 4-2. Loop pairing nomenclature

	Symbols	Description		Symbols	Description
<b>MV</b>	<i>L</i>	Reflux rate	<b>CV</b>		
	<i>V</i>	Boil-up rate		$x_D$	Distillate composition
	<i>B</i>	Bottom rate		$x_B$	Bottom composition
	<i>D</i>	Distillate rate			

The symbols of the MVs and CVs are listed in Table 4-2. The compositions at the top and bottom of the distillation column,  $x_D$  and  $x_B$ , are the controlled variables. For two-point composition control of a distillation column three basic control configurations can be defined ( $DV$ ,  $LV$  and  $LB$ ).

Table 4-3 summarizes the manipulated and controlled variables for each of the proposed control configurations. For example, in  $DV$  control configuration,  $D$  (Distillate rate) is used to control the composition of top product and  $V$  (Boil-up rate) is used to control the composition of bottom product.

Table 4-3. Variable pairing of different control configurations for case study 1

Control configuration	$u_1$	$y_1$	$u_2$	$y_2$
$DV$	$D$	$x_D$	$V$	$x_B$
$LV$	$L$	$x_D$	$V$	$x_B$
$LB$	$L$	$x_D$	$B$	$x_B$

For testing the effects of recycles on the REA, the ethyl benzene process in Figure 4-2 is partitioned into four models for simulation listed in Table 4-4.

Table 4-4. Description of the 4 simulations performed for case study 1

Model	Description
1	Two CSTRs, $T_1$ and $T_2$ Columns connected in series
2	Two CSTRs, $T_1$ and $T_2$ Columns connected in series and with recycle 1
3	Two CSTRs, $T_1$ and $T_2$ Columns connected in series and with recycle 2
4	Two CSTRs, $T_1$ and $T_2$ Columns connected in series and with recycle 1 and 2

Model 4 includes both recycles 1 and 2. The RGA and REA results from this model will be used as the correct information. They will be used to compare the RGA and REA results from the other models. Through the differences, we can demonstrate the recycle effects on the RGA and REA. For each simulation process listed in Table 4-4, the RGA and REA values are calculated by doing simulation experiments, the experiment details are listed in Table 4-5.

Table 4-5. Configurations for step change experiments for case study 1

Pair	Loop mode	$u_1$	$y_1$	$u_2$	$y_2$
$u_1 - y_1$	Open	Step change	Observed	Constant	---
$u_2 - y_1$	Open	Constant	Observed	Step change	---
$u_1 - y_2$	Open	Step change	---	Constant	Observed
$u_2 - y_2$	Open	Constant	---	Step change	Observed
$u_1 - y_1$	Closed	Step change	Observed	---	Constant
$u_2 - y_2$	Closed	---	Constant	Step change	Observed

Table 4-6. RGA results for distillation column T1

Model	1	2	3	4
$LV$	$\begin{bmatrix} 1.2 & -0.2 \\ -0.2 & 1.2 \end{bmatrix}$	$\begin{bmatrix} 1.2 & -0.2 \\ -0.2 & 1.2 \end{bmatrix}$	$\begin{bmatrix} 1.2 & -0.2 \\ -0.2 & 1.2 \end{bmatrix}$	$\begin{bmatrix} 1.1 & -0.1 \\ -0.1 & 1.1 \end{bmatrix}$
$LB$	$\begin{bmatrix} 0.9 & 0.1 \\ 0.1 & 0.9 \end{bmatrix}$	$\begin{bmatrix} 0.9 & 0.1 \\ 0.1 & 0.9 \end{bmatrix}$	$\begin{bmatrix} 0.9 & 0.1 \\ 0.1 & 0.9 \end{bmatrix}$	$\begin{bmatrix} 0.9 & 0.1 \\ 0.1 & 0.9 \end{bmatrix}$
$DV$	$\begin{bmatrix} 0.9 & 0.1 \\ 0.1 & 0.9 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0.9 & 0.1 \\ 0.1 & 0.9 \end{bmatrix}$	$\begin{bmatrix} 0.1 & 0.9 \\ 0.9 & 0.1 \end{bmatrix}$

Since the controls of distillation columns  $T_1$  and  $T_2$  are quiet independent, we will select the control configurations for them separately. The RGA and REA results for the distillation column  $T_1$  with the three control configuration are list in Table 4-6 and Table 4-7.

Table 4-7. REA results for distillation column T1

Model	1	2	3	4
<i>LV</i>	$\begin{bmatrix} -6.4 & 7.4 \\ 7.4 & -6.4 \end{bmatrix}$	$\begin{bmatrix} -32 & 34 \\ 34 & -33 \end{bmatrix}$	$\begin{bmatrix} -187 & 188 \\ 188 & -187 \end{bmatrix}$	$\begin{bmatrix} 7 & -6 \\ -6 & 7 \end{bmatrix}$
<i>LB</i>	$\begin{bmatrix} 0.3 & 0.7 \\ 0.7 & 0.3 \end{bmatrix}$	$\begin{bmatrix} 1.1 & -0.1 \\ -0.1 & 1.1 \end{bmatrix}$	$\begin{bmatrix} -0.4 & 1.4 \\ 1.4 & -0.4 \end{bmatrix}$	$\begin{bmatrix} -1 & 2 \\ 2 & -1 \end{bmatrix}$
<i>DV</i>	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} -0.2 & 1.2 \\ 1.2 & -0.2 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Let us look at the RGA and REA values for the model 4, using the criteria of the RGA in the books by Marlin (2000) and Svrcek et al.(2006). We can conclude that for the distillation column  $T_1$ , three control configurations, *LV* and *LB* can be used for process control (see the right column in Table 4-6). If we select the control configuration *DV*, we must use the off-diagonal control pairs which are not recommended. Since we have two choices for the RGA analysis for the column 1 control configuration, we need to use the REA to help us select the more eco-efficient control configuration. Looking at the right column in Table 4-7, the REA values for the *LB* configuration suggest to select the off-diagonal control pairs, which is contradictory to the RGA analysis. So *LB* control configuration will be not eco-efficient. The REA values for the *LV* control configuration suggest the same diagonal control pair selection. *LV* control configuration with the diagonal control pairs will be the best control choice for both controllability and eco-efficiency for the distillation column 1. The control configuration selections based on the RGA and REA from models 1, 2, 3 and 4 are list in Table 4-8.

Although the selection of control configuration from the RGA and REA from the model 2 is *LB*, and the RGA and REA results show that this selection is controllable and eco-efficient, if we use this control configuration on the process with recycle like model 4, eco-efficient performance cannot be achieved. The correct control configuration from the model 4 is *LV*, and the REA values from model 4 indicate that the diagonal control pairs of *LB* control cannot be eco-efficient. The REA values from model 1 and 2 will not help us to select any control configuration to be eco-efficient, they will provide misleading information.

Table 4-8. Selection of control configuration for column T1 based on the RGA and REA values from models 1-4

	Model 1	Model 2	Model 3	Model 4
Control selection	<i>LV or LB or DV</i>	<i>LB</i>	<i>LV or LB</i>	<i>LV</i>
Controllability	√	√	√	√
Eco-efficiency	x	√	x	√

Similarly, the RGA and REA values for distillation column T2 are listed in Table 4-9 and Table 4-10.

Table 4-9. RGA results for distillation column T2

Model	1	2	3	4
<i>LV</i>	$\begin{bmatrix} 0.9 & 0.1 \\ 0.1 & 0.9 \end{bmatrix}$	$\begin{bmatrix} 1.6 & -0.4 \\ -0.4 & 1.6 \end{bmatrix}$	$\begin{bmatrix} 1.5 & -0.5 \\ -0.5 & 1.5 \end{bmatrix}$	$\begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{bmatrix}$
<i>LB</i>	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
<i>DV</i>	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

The control configuration selections for the column  $T_2$  based on the RGA and REA from models 1- 4 are listed in Table 4-11.

*LB* control will be the best control configuration for the process since the RGA and REA values from model 4 indicate that this control configuration is controllable and eco-efficient. From the RGA and REA values from model 3, *LB* control should be selected and is controllable and eco-efficient. From the RGA and REA from models 1 and 2, we only can conclude that there is no eco-efficient control configuration. This is contradictory to the conclusions from model 3 and 4. It indicates that the recycle 2 is the most important part of the process for control configuration selection for distillation column  $T_2$ . Without consideration of recycle 2, the control configuration selection will be biased.

Table 4-10. REA results for distillation column T2

Model	1	2	3	4
<i>LV</i>	$\begin{bmatrix} 26 & -25 \\ -25 & 26 \end{bmatrix}$	$\begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{bmatrix}$	$\begin{bmatrix} -27 & 28 \\ 28 & -27 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
<i>LB</i>	$\begin{bmatrix} -0.8 & 1.8 \\ 1.8 & -0.8 \end{bmatrix}$	$\begin{bmatrix} -0.5 & 1.5 \\ 1.5 & -0.5 \end{bmatrix}$	$\begin{bmatrix} 1.3 & -0.3 \\ -0.3 & 1.3 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
<i>DV</i>	$\begin{bmatrix} 0.4 & 0.6 \\ 0.6 & 0.4 \end{bmatrix}$	$\begin{bmatrix} 2.1 & -1.1 \\ -1.1 & 2.1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

Table 4-11. Selection of control configuration for column T2 based on the RGA and REA values from models 1-4

	Model 1	Model 2	Model 3	Model 4
Control selection	<i>LV or LB</i>	<i>LV or LB</i>	<i>LB</i>	<i>LB</i>
Controllability	√	√	√	√
Eco-efficiency	x	x	√	√

#### 4.4.2. Case Study 2: Ethylene Glycol Production

For this study, an ethylene glycol production plant with a recycle stream (Svrcek et al. 2006) is selected. The schematic of ethylene glycol plant is shown in Figure 4-3. Table 4-12 summarizes the feed conditions and the distillation column specifications.

This plant consists of a CSTR and a distillation column. Water reacts with ethylene oxide in the CSTR to produce ethylene glycol. The liquid product stream of the CSTR is sent to a distillation column for the separation of ethylene glycol from the un-reacted water and ethylene. The un-reacted feed is sent back to the CSTR via a recycle loop. VMGSim with the NRTL activity thermodynamic model is used for the simulation.

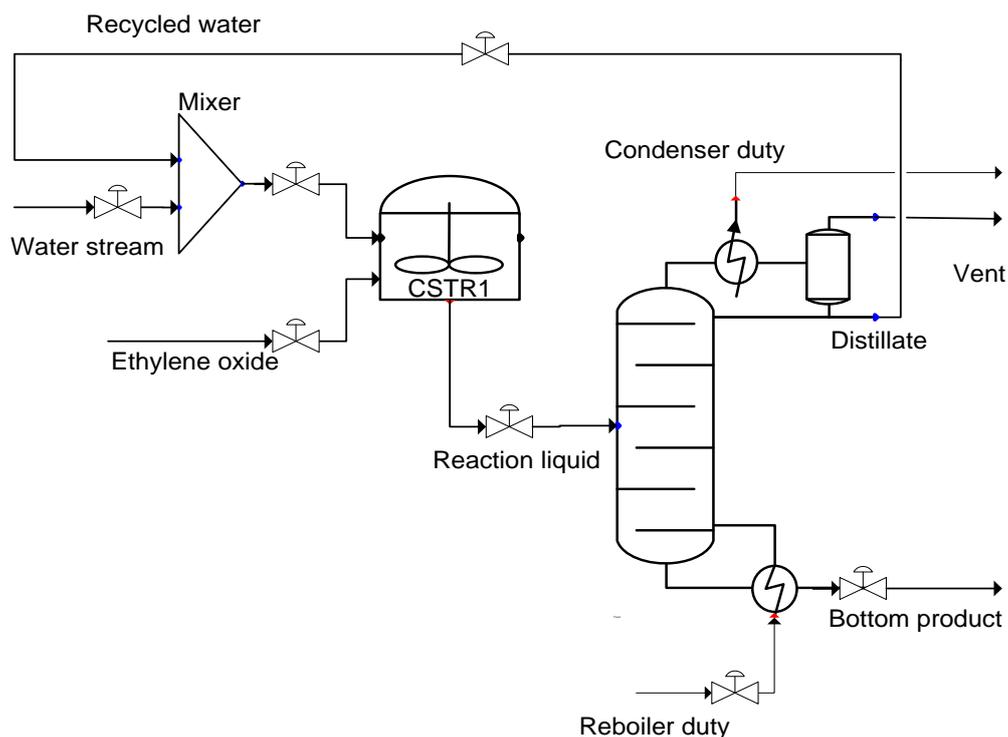


Figure 4-3. Case study 2 Ethylene glycol production schematic

Table 4-12. Feed, column and simulation model specifications for case study 2

<b>Feed specifications</b>			
Water		Ethylene oxide	
Temperature ( $^{\circ}\text{C}$ )	41	Temperature ( $^{\circ}\text{C}$ )	30
Pressure (kPa)	85	Pressure (kPa)	200
Molar flow (kmole/hr)	150	Molar flow (kmole/hr)	150
Reactor outlet temperature ( $^{\circ}\text{C}$ )	60		
<b>Column and simulation model specifications</b>			
Column theoretical stages	10	Condenser type	Partial
Feed stage	5 <sup>th</sup>	Reflux ratio	2.5
Column top pressure (kPa)	95	Vent rate (kmole/hr)	5
Column pressure drop (kPa)	5	Distillate rate (kmole/hr)	50
<b>Thermodynamic property package</b>			
Activity model	NRTL		

The same symbols listed in Table 4-2 are inherited for this case study. Two new symbols are used for the case study 2, i) the coolant flow to reactor that controls the heat removal of exothermic reaction,  $Q_R$ , is a MV; and ii) the reactor temperature,  $T$ , is a CV. The compositions at the top and bottom of the distillation column are  $x_D$  and  $x_B$  respectively, and the reactor temperature,  $T$ , are the controlled variables. These three controlled variables are controlled by distillate or reflux flow rate, bottom or boil-up flow rate and the coolant flow to the reactor respectively. This becomes a 3x3 system when reactor temperature control is considered with two point composition control of the distillation column. The control problem can transform into a 4x4 system when the level control of the reactor is also considered, however “perfect” inventory control is assumed as a common situation in control scheme design e.g. (Svrcek et al. 2006).

For this case study three basic control configurations are defined ( $LVQ_R$ ,  $LBQ_R$  and  $DVQ_R$ ). Any configuration has three variables to control, top composition, bottom composition and temperature control of the reactor. For example, in  $DVQ_R$  control configuration,  $D$  (Distillate rate) is used to control the composition of top product,  $V$  (Boil-up rate) is used to control the composition of bottom product and  $Q_R$  (reaction heat) is used to control the temperature of the reactor. Table 4-13 summarizes the manipulated and controlled variables for each of the proposed control configurations for the 3x3 system.

Table 4-13. Control pairings of different control configurations for case study 2

Configurations	$u_1$	$y_1$	$u_2$	$y_2$	$u_3$	$y_3$
$LVQ_R$	$L$	$x_D$	$V$	$x_B$	$Q_R$	$T$
$LBQ_R$	$L$	$x_D$	$B$	$x_B$	$Q_R$	$T$
$DVQ_R$	$D$	$x_D$	$V$	$x_B$	$Q_R$	$T$

The RGA and REA values for the Ethylene glycol process with and without recycle consideration are listed in Tables 4-14 and 4-15.

Table 4-14. RGA results for the study case 2

Control Configurations	$LVQ_R$	$LBQ_R$	$DVQ_R$
Without recycle	$\begin{bmatrix} 8.96 & -7.96 & 0 \\ -7.96 & 8.96 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1.24 & -0.24 & 0 \\ -0.24 & 1.24 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -0.07 & 1.07 & 0 \\ 1.07 & -0.07 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
With recycle	$\begin{bmatrix} 0.79 & -1.09 & 1.29 \\ -4.60 & 5.75 & -0.15 \\ 4.80 & -3.66 & -0.14 \end{bmatrix}$	$\begin{bmatrix} 1.06 & -0.02 & -0.04 \\ -0.06 & 0.92 & 0.14 \\ 0 & 0.1 & 0.9 \end{bmatrix}$	$\begin{bmatrix} -0.01 & 1.13 & -0.13 \\ 0.82 & -0.13 & 0.31 \\ 0.187 & 0 & 0.81 \end{bmatrix}$

Table 4-15. REA results for the study case 2

Control Configurations	$LVQ_R$	$LBQ_R$	$DVQ_R$
Without recycle	$\begin{bmatrix} 6.75 & -5.75 & 0 \\ -5.75 & 6.75 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1.22 & -0.22 & 0 \\ -0.22 & 1.22 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1.14 & -0.14 & 0 \\ -0.14 & 1.14 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
With recycle	$\begin{bmatrix} 0.12 & 1.12 & -0.24 \\ 1.02 & -0.11 & 0.09 \\ -0.14 & -0.01 & 1.15 \end{bmatrix}$	$\begin{bmatrix} 0.07 & 1.54 & -0.61 \\ 0.93 & -0.32 & 0.39 \\ 0 & -0.23 & 1.23 \end{bmatrix}$	$\begin{bmatrix} 0.48 & 1.13 & -0.61 \\ 0.31 & -0.13 & 0.82 \\ 0.21 & 0 & 0.79 \end{bmatrix}$

The RGA and REA values for the simulation without recycle do not show any interactions between CSTR and distillation, however these interactions can be observed from the RGA and REA values for the simulation with recycle. This difference will automatically provide a different conclusion. From the simulation without recycle, we would select the  $LBQ_R$  control configuration and it would be eco-efficient. However, if we look at the REA values from the simulation with recycle, two control configurations,  $LBQ_R$  and  $DVQ_R$  can be selected. It is not obvious to decide which configuration is better than the other configuration. Let us look at the  $LBQ_R$  control configuration first. The pairs,  $y_1-u_2$ ,  $y_2-u_1$  and  $y_3-u_3$  should be selected

according to the REA rules. Two pairs selected from the REA are contradicted by the pairing selections from the RGA. For the  $DVQ_R$  control configuration, only one pairing selection for the controlled variable,  $y_2$ , from the RGA and REA contradicted each other. We would therefore recommend the  $DVQ_R$  control configuration be further considered for process design. From this case study, we also observe that the wrong control configuration selection can be obtained if REA values are obtained without the recycle loop.

#### **4.5. Summary**

For eco-efficient process design, the REA can be used to compare the thermodynamic efficiency for different control structures at the early process design stage. When the RGA and REA are used together, they can provide the measures of controllability and eco-efficiency of the process under a certain process design. However, if a process includes one or more recycles, the RGA and REA calculations without consideration of the recycle loops will provide biased information which may cause the designer to select the wrong control configurations. The REA is a simple tool, only measuring the eco-efficiency within the scope of control loops. For the eco-efficiency analysis of the whole process, a new measure of eco-efficiency (EEF) was developed, as explained in Chapter 5.

## References

- Bristol, E. (1966). "On a new measure of interaction for multivariable process control." Automatic Control, IEEE Transactions on **11**(1): 133-134.
- Denbigh, K. G. (1956). "The second-law efficiency of chemical processes." Chemical Engineering Science **6**(1): 1-9.
- Dincer, I. (2002). "The role of exergy in energy policy making." Energy Policy **30**(2): 137-149.
- Himmelblau, D. M. and J. B. Riggs (2004). Basic principles and calculations in chemical engineering. Upper Saddle River, New Jersey, Prentice Hall.
- Hinderink, A. P., F. P. J. M. Kerckhof and A. B. K. Lie (1996). " Exergy analysis with a flowsheeting simulator--I. Theory; calculating exergies of material streams." Chemical Engineering Science **51**(20): 4693-4700
- Horvath, M., Z. Szitkai and P. Mizsey (2007). "Investigation of controllability of systems with recycle - A case-study." Periodica Polytechnica: Chemical Engineering **51**(2): 37-44.
- Kotas, T. J. (1985). The exergy method of thermal plant analysis. London, Butterworth-Heinemann Ltd.
- Luyben, M. L. and C. A. Fluodas (1994). "Analyzing the interaction of design and control--2. reactor-separator-recycle system." Computers & Chemical Engineering **18**(10): 971-993.
- Luyben, W. L. (1993a). "Dynamics and control of recycle systems. 1. Simple open-loop and closed-loop systems." Industrial & Engineering Chemistry Research **32**(3): 466-475.
- Luyben, W. L. (1993b). "Dynamics and control of recycle systems. 2. Comparison of alternative process designs." Industrial & Engineering Chemistry Research **32**(3): 476-486.
- Luyben, W. L. (1994). "Snowball effects in reactor/separators processes with recycle." Industrial & Engineering Chemistry Research **33**(2): 299-305.
- Luyben, W. L. (2002). Plantwide dynamic simulators in chemical processing and control. New York, Marcel Dekker Inc.
- Marlin, T. E. (2000). Process control: design process and control system for dynamic performance. New York, McGraw Hill.
- Marlin, T. E. (2000). Process control: design process and control system for dynamic performance. New York, McGraw Hill.
- McAvoy, T. J., Y. Arkun, R. Chen, D. Robinson and P. D. Schnelle (2003). "A new approach to defining a dynamic relative gain." Control Engineering Practice **11**(8): 907-914.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2007). "An exergy calculator tool for process simulation." Asia-Pacific Journal of Chemical Engineering **2**(5): 431-437.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2010). "The relative exergy array—a new measure for interactions in process design and control." The Canadian Journal of Chemical Engineering **89**(3): 545-549.

- Moran, M. J. (1982). Availability analysis: A guide to efficient energy use. Englewood Cliffs New Jersey, Prentice-Hall.
- Munir, M. T., J. J. Chen and B. R. Young (2010). A computer program to calculate the stream exergy using the visual basic graphical interface. Chemeca 2010. Adelaide, Australia.
- Papadourakis, A., M. F. Doherty and J. M. Douglas (1987). "Relative gain array for units in plants with recycle." Industrial & Engineering Chemistry Research **26**(6): 1259-1262.
- Price, R. M. and C. Georgakis (1993). "Plantwide regulatory control design procedure using a tiered framework." Industrial & Engineering Chemistry Research **32**(11): 2693-2705.
- Rosen, M. A. and I. Dincer (1997). "On exergy and environmental impact." International Journal of Energy Research **21**: 643-654.
- Rosen, M. A. and I. Dincer (1999). "Exergy analysis of waste emissions." International Journal of Energy Research **23**: 1153-1163.
- Svrcek, W. Y., D. P. Mahoney and B. R. Young (2006). A Real-Time Approach to Process Control. Chichester, John Wiley & Sons Ltd.
- Szargut, J., D. R. Morris. and F. R. Steward (1988). Exergy analysis of thermal, chemical, and metallurgical processes. New York, Hemisphere.
- Virtual Materials Group Inc. (2009). "VMGSim V5.0 User's Manual."
- Virtual Materials Group Inc. (2010). from <http://www.virtualmaterials.com/vmgsim>.
- Witcher, M. F. and T. J. McAvoy (1977). "Interacting control systems: steady state and dynamic measurement of interaction." ISA Trans. **16**(3): 35-41.
- Xiong, Q., W.-J. Cai and M.-J. He (2005). "A practical loop pairing criterion for multivariable processes." Journal of Process Control **15**(7): 741-747.



# Chapter 5

---

*Plant-wide control: Eco-efficiency and control loop configuration*

**Article # 3**

**Co-authors: Wei. Yu, Brent. R. Young**

*Industrial Information & Control Centre (I<sup>2</sup>C<sup>2</sup>), Department of Chemical & Materials Engineering, The University of Auckland, Auckland, New Zealand*

Munir, M. T., W. Yu and B. R. Young (2012). Plantwide control: Eco-efficiency and control loop configuration. *Industrial & Engineering Chemistry Research Journal*. (Submitted).

## **Chapter 5. Plant-wide control: Eco-efficiency and control loop configuration**

This chapter presents the extension of the eco-efficiency of the control scheme (configuration) to the whole process. In this chapter, a new measure of eco-efficiency, the Exergy Eco-efficiency Factor, EEF, is proposed, explained and implemented for a simulation case study. The implementation of EEF was necessary for the further development of the REA, discussed in chapter 3 and chapter 4, since the REA measures only the eco-efficiency within the scope of control loops. The results of the simulation show that the EEF can provide a qualitative and quantitative measure for the selection of the most eco-efficient control scheme.

### **Abstract**

Since the eco-efficiency of all industrial processes/plants has become increasingly important, engineers need to find a way to integrate the control loop configuration and the measurements of eco-efficiency. A new measure of eco-efficiency, the exergy efficiency factor, for control loop configuration, is proposed in this paper. The exergy efficiency factor is based on the thermodynamic concept of exergy which can be used to analyze a process in terms of its efficiency associated with the control configuration. The combination of control pairing configuration techniques (such as the Relative Gain Array, RGA and Niederlinski Index, NI) and the proposed exergy efficiency factor will guide the process designer to reach the optimal control design with low operational cost (i.e. energy consumption). The exergy efficiency factor is implemented in three process simulation case studies and the reliability of the proposed method is validated by dynamic simulation results.

Key words: Control loop configuration; Eco-efficiency; Dynamic exergy efficiency.

### **5.1. Introduction**

Plant-wide control refers to the control of an entire plant, usually consisting of many interconnected unit operations. The design of a plant-wide control system is a complex task, including a large number of choices are available for measurement, control structure and controller type. A literature review of plant-wide control can be found in the paper by Larsson and Skogestad (2000) and Rangaiah and Kariwala (2011). The most important issue

in regard to plant-wide control is to determine the control structure or control loop configuration. But this is not always necessarily true. In many cases multiple multivariable controllers may be used. For example, one MIMO controller is used to control one MIMO process units. These controllers may or may not communicate with each other, as in distributed control or decentralized plantwide control respectively. In this case, it is the interactions between process units rather than control loops that are most important. In this paper, this issue (determining control loop configuration) will be integrated with the concept of eco-efficiency.

Control loop configuration, or control pair selection, focuses on the selection of the best control scheme for pairing manipulated and controlled variables. Several common techniques, like Relative Gain Array (RGA), Niederlinski Index (NI), Singular Value Decomposition (SVD), Condition Number (CN), and the Morari Resiliency index (MRI), have been developed for control loop configuration, Detailed information can be found in books written by Seborg et al.(1989) and Svrcek et al. (2006). Many researchers have since developed more comprehensive techniques based on these commonly-recognised techniques for assigning control loops in more complex processes. For example, a controllability index for heat exchange networks (Westphalen et al. 2003), a decomposed relative interaction array (He and Cai 2004), a dynamic relative gain (McAvoy et al. 2003), an effective relative gain array (Xiong et al. 2005), and the comprehensive criteria for performance assessment of plant-wide control systems (Vasudevan and Rangaiah 2010). Although these techniques provide reliable support for industry to guarantee the quality of products, there is little consideration of the energy cost among these techniques. In this paper, we wish to develop a new approach which is able to integrate current control loop configuration techniques with energy cost.

Nowadays, in the wake of the energy crisis and global climate change, control loop configuration cannot focus on control loop analysis techniques, alone, such as control loop stability analysis and the consideration of the quality of the controller variable; it, also needs to include energy cost and environmental impact. A new tool must be developed to integrate the above two aspects for process control and economic/sustainability. In most control loops, exergy can play an important role in this new tool since it can be used for determining the efficiency and sustainability of a process (Dincer 2002). For example, environmental impacts

can be minimized by reducing exergy losses and by efficient use of exergy (Rosen and Dincer 1997; Rosen and Dincer 1999; Rosen and Dincer 2001).

Thermodynamic properties, such as exergy, have been used previously for the development of process control structures. For example, Luyben et al. (1998) added an appendix to their book which acts as a basic framework for the development of a dynamic exergy balance for process control evaluation.

The Relative Exergy Array (REA) was developed based on analyzing the exergy for the control configuration within the process design (Montelongo-Luna et al. 2009; 2010; Munir et al. 2012). REA is defined analogously to the RGA. The REA inherits many properties of RGA such as the summation of the rows or columns being equal to 1 and it is scale independent. During early stages of process control design, the REA can give some indication to process engineers concerning the effect of control loop interactions on the thermodynamic (exergetic) efficiency of the control loops. The REA can help to evaluate several control structure candidates in terms of their thermodynamic efficiencies. This information can help in deciding on the final control structure. Thermodynamic efficiency can also be further related to economic efficiency. An REA calculation using a commercial simulator (VMGSim) has also been developed (Munir et al. 2010; 2012). The effect of recycle on the REA analysis was studied by (Munir et al. 2012).

The REA has a limitation of evaluating the eco-efficiency only within the scope of the control loops studied; it cannot provide the eco-efficiency of the whole unit or plant. In this paper, we will extend the eco-efficiency of the control loop configuration into the whole process or even plant. A new measure of eco-efficiency, exergy eco-efficiency factor (EEF), is proposed.

For a general multi-input-multi-output (MIMO) process, a certain amount of exergy consumption/generation is needed to change a controlled variable (CV) by using a manipulated variable (MV). The EEF is designed to measure this amount of exergy for different control pairings. The control pair which needs the least exergy to fulfil the control targets will be the most eco-efficient control pair. By combining the analysis from control loop configuration methods such as RGA, NI and SVD with the proposed new measure, EEF, control engineers can select the best control configuration for both controllability and eco-efficiency.

As exergy accounts for the quality of energy, therefore energy has quality as well as quantity. The exergy destruction is directly proportional to the entropy production. Actual processes normally occur in the direction of decreasing quality (Exergy) of energy or increasing entropy (Dincer and Cengel 2001). Some research has also been done on plant-wide control using the entropy concept (Alonso et al. 2002; Ydstie 2002; Ruszkowski et al. 2005; Antelo et al. 2007).

This manuscript is organized as follows. In Section 5.2, the concept of eco-efficiency is introduced, the relevant exergy definitions are discussed and the exergy efficiency factor is proposed. In Section 5.3, the proposed method is implemented for the simulation example. The discussion, summary and conclusions are in sections 5.3, 5.4 and 5.5 respectively.

## **5.2. Control loop configuration**

Three basic techniques of the control loop configuration: RGA, NI and SVD are used to select the control pairs in this paper. Based on the results for these 3 techniques, the proposed EEF is used to determine the most eco-efficient control pairs. The EEF can also be integrated with any comprehensive/advanced control loop configuration technique or set of techniques.

### **5.2.1. Methods based on controllability**

The RGA is a popular tool used to check the controllability of a process or for the selection of control loop pairings. The use of RGA started in the 1960s after the work of Bristol (Bristol 1966). Since then, an extensive amount of research has been done in control loop configuration or input – output pairing selection such as the selection of the best control configuration for a distillation column (Skogestad et al. 1990), the dynamic RGA (Witcher and McAvoy 1977; McAvoy et al. 2003), the effective relative gain array (ERGA) (Xiong et al. 2005) and the normalized RGA (NRGA) (Fatehi and Shariati 2007). Despite some restrictions: i) applicable to linear systems; ii) based on steady state information, the RGA is still widely used in industry since it is a simple calculation which only requires simple open loop step response tests; it is also controller independent and scale invariant.

The Niederlinski Index (NI) is used for testing the stability of an RGA selected control loop pairing (Niederlinski 1971). Its use is more applicable for lower order systems (2x2). For higher order systems it can only provide information concerning the instability of the loop. A system having negative NI value will definitely be unstable. Systems having positive NI

values should be given further consideration by employing dynamic simulation to check stability. NI cannot be used for systems having dead time. A detailed procedure is required to be followed for using the NI for systems having dead time (Grosdidier et al. 1985). The NI has not only been used as a stability criteria but also as an interaction measure itself (Zhu and Jutan 1993).

Singular Value Decomposition (SVD) is a useful tool to check whether the control loop interactions are sensitive to small errors in process gains. The SVD also indicates whether the control loops may be decoupled. The problem is ill conditioned in the presence of a set of steady state gain matrix singular equations. In this situation it may not be possible to decouple control loop interactions (McAvoy 1983; Ogunnaiké and Ray 1994; Goldberg and Potter 1998; Svrcek et al. 2006). SVD is applicable to the steady state gain matrix which is decomposed into the product of three matrices: two are eigenvectors and one is a diagonal matrix of eigenvalues. The condition number (CN) is the ratio of the largest to the smallest singular values of the diagonal matrix of eigenvalues. The value of this ratio is very important in determining whether decoupling is feasible or not. A CN of 100 indicates that one manipulated variable is a hundred times more effective for the system than the other manipulated variable. It is difficult to decouple systems that have higher CN values. If the CN is equal or greater than 50 then the system considered is nearly singular and for such a system, decoupling is not possible (McAvoy 1983). If the CN is infinite then that matrix is singular and ill-conditioned.

### **5.2.2. Methods based on eco-efficiency**

According to the definition of the World Business Council for Sustainable Development (WBCSD), eco-efficiency is achieved through the delivery of "competitively priced goods and services that satisfy human needs and bring quality of life while progressively reducing environmental impacts of goods and resource intensity throughout the entire life-cycle to a level at least in line with the Earth's estimated carrying capacity." This concept describes a vision for the production of economically valuable goods and services while reducing the ecological impacts of production. In other words eco-efficiency means producing more with less.

When applying the concept of eco-efficiency to control loop configuration, a method needs to be developed which can help engineers to select the manipulated variables which achieve the

best products with the lowest energy cost. Exergy is a suitable concept which can be used to evaluate the eco-efficiency of a controlled process.

Thermodynamic laws (1<sup>st</sup> and 2<sup>nd</sup>) may give an idea about process efficiency, energy loss, work done, required work and entropy production. For the calculation of the energy efficiency of a process, inputs, outputs and losses are defined in terms of energy (Smith and Ness 2005). The combination of the 1<sup>st</sup> and 2<sup>nd</sup> laws of thermodynamics gives rise to the concept of exergy which is the basic measure of eco-efficiency. Exergy is the maximum possible amount of work which can be drawn from a material stream when it interacts only with the environment as it goes from its initial state to the final dead state (Denbigh 1956; Kotas 1985).

### 5.2.2.1. Exergy

A general thermodynamic process is shown in Figure 5-1. The process has many arbitrary material streams coming from and going out of the process boundary. The process has its own temperature ( $T$ ), pressure ( $P$ ) and composition ( $Z$ ). The process is also heated from different heating sources at different temperatures  $T_i$  delivering different amounts of heat  $q_i$ . The process produces some shaft work ( $W$ ) and delivers it to the environment with fixed values of temperature, pressure and composition ( $T_0, P_0$  and  $Z_0$ ).

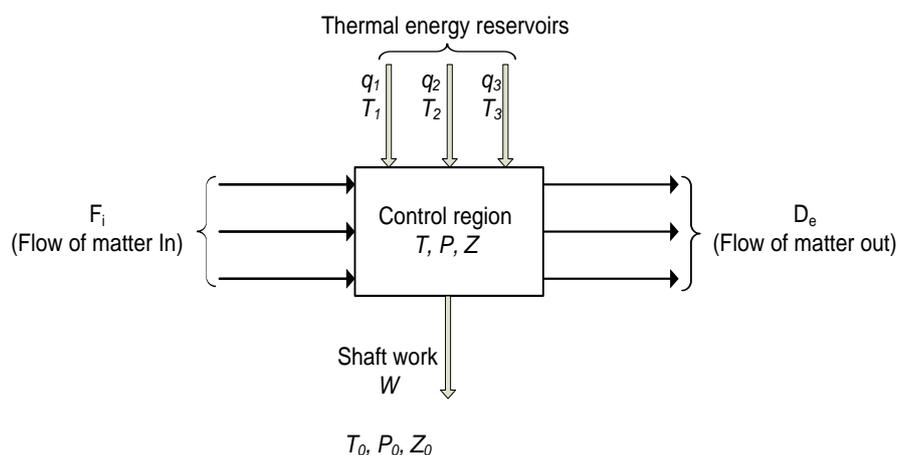


Figure 5-1. A general thermodynamic process

The calculation of the physical exergy change of the thermodynamic process in Figure 5-1 can be obtained by,

$$\Delta B_{phys} = \Delta U + P_0 \Delta V - T_0 \Delta S \quad 5-1$$

$$W + \sum_i (q_i + T_0 \Delta S_i) = T_0 \sigma + \Delta U + P_0 \Delta V - T_0 \Delta S \quad 5-2$$

where  $W + \sum (q_i + T_0 \Delta S_i)$  denotes the total work performed on the process and  $T_0 \sigma$  denotes energy loss due to irreversibilities. The change in internal energy ( $\Delta U$ ) of the general thermodynamic system shown in Figure 5-1 is due to the addition of energy inputs ( $q_i$ ) and work done ( $W$ ).  $\Delta S_i$  is the change in entropy inside the process.

Because the process composition  $Z$  and the environmental composition  $Z_0$  in Figure 5-1 are designed for a variety of work potentials, the total exergy of the material stream will also change. The total exergy, including the three components: physical exergy, chemical exergy and exergy due to mixing, is defined as (Hinderink et al. 1996).

$$B_{total} = B_{phys} + B_{chem} + \Delta_{mix} B \quad 5-3$$

The detailed definitions of chemical exergy,  $B_{chem}$ , and exergy change due to mixing,  $\Delta_{mix} B$ , are provided in (Hinderink et al. 1996).

The total exergy calculation in Equation (5-3) is relatively simple and only needs thermodynamic data, which is easily obtainable. This calculation requires data such as the Gibbs energy of formation for the calculation of standard chemical exergies. Gibbs energy of formation data can be obtained from various sources such as thermodynamic databanks, or process simulators, but special attention must be paid to the consistency of this data.

An automation of exergy calculation has also been undertaken with the use of an open source simulator (Sim42) and a commercial simulator (Aspen HYSYS) (Montelongo-Luna et al. 2007). An integrated Visual Basic (VB) program and Graphical User Interface (GUI) has recently been developed for exergy calculation (Munir et al. 2010).

#### 5.2.2.2. Exergy eco-efficiency factor (EEF)

Exergy is the maximum possible amount of work which can be drawn from a material stream when it interacts only with the environment and it comes from its initial state to the final dead state (Denbigh 1956; Kotas 1985). In its dead state, the material stream is in thermal, mechanical and chemical equilibrium with the environment. Since exergy accounts for the quality of energy, thus it can be used as a measure to evaluate the eco-efficiency for a process

design. A process is called eco-efficient if it uses a relatively small amount of energy or the destruction of exergy is low.

Based on an understanding of the total exergy of each material stream in and out of the thermodynamic process, it is possible for engineers to build an eco-efficient process which is ecological and economical.

In the above section, we introduced the idea that exergy can be used to measure the energy changes of one process/unit/plant. For a general process, as shown in Figure 5-2, exergetic efficiency is defined as the ratio of the exergy going out to the exergy coming in, namely, (Szargut et al. 1988).

$$\eta = B_{Out} / B_{In} \quad 5-4$$

where,  $\eta$  = exergetic efficiency,  $B_{Out}$  = total exergy going out of a process and  $B_{In}$  = total exergy coming in to a process.



Figure 5-2. Exergy flows for a general process

The ratio, Equation (5-4) is the exergetic efficiency of this process which is a measure of eco-efficiency. This general process is a portion of the control loop between the manipulated and the control variables. However it does not provide any information about how the control loop configuration affects this exergetic efficiency. In this paper we propose a new measure, the exergy eco-efficiency factor (EEF), which connects the control loop configuration to the eco-efficiency. The exergy eco-efficiency factor for a control pair  $(u_j, y_i)$ , is defined as,

$$\tau_{ij} = (\Delta B_{out} - \Delta B_{in}) \frac{\Delta u_j}{\Delta y_i} \quad 5-5$$

where  $\Delta u_j$  denotes a step change of the *MV*,  $u_j$ ,  $\Delta y_i$  denotes a response in the *CV*,  $y_i$ , caused by the step change of  $u_j$ , and  $\Delta B_{out}$  and  $\Delta B_{in}$  represent the exergy differences caused by the *MV* step change for exergy out and exergy in, respectively. The units of EEF would be kW.kmole/hr or kW.kJ/hr in this paper.

The EEF shows how much exergy will be destroyed by using different MV to control the same amount of CV change. It can provide a quantitative measurement of the exergy consumption. By comparing the sum of EEF of one control configuration with another, the approximate amount of exergy to be saved can be obtained. This will be very useful in some situations, for example, when control configuration A makes an exergy saving of 10%, compared to control configuration B, the implementation of control configuration B is more expensive than it is for control configuration A, Thus, on this basis, control configuration A may be selected. When the EEF results contradict with the RGA results then the final selection of control scheme should be based on the RGA results because controllability cannot be compromised.

For a 2x2 example, if  $\tau_{21}$  is less than  $\tau_{22}$ , it means that for the same amount of CV change,  $\Delta y_2$  using MV  $u_1$ , will cause less exergy change/loss than will using MV  $u_2$ . The final interpretation is that control pair  $(u_1, y_2)$  is more eco-efficient than pair  $(u_2, y_2)$ .

Control loop configurations can be determined by techniques such as RGA, NI and SVD, it is usual that several candidate control loop configurations can be implemented. In regard to eco-efficiency, the new EEF can be used to select the best control loop configuration from among the candidates.

### 5.2.2.3. Validation of EEF

Dynamic simulation is the best way to validate the proposed eco-efficiency factor. By recording the exergy consumptions of several control configurations, the most eco-efficient control configuration can be identified and dynamic results compared to the results from the eco-efficiency factor.

Dynamic exergy versus time can be approximated by several exergy calculations at different conditions during the dynamic response of a process. The exergy values of the process dynamic response at different time intervals are calculated. As chemical simulators still do not have the ability to directly calculate and display the total exergy of a material stream, these simulators cannot automatically calculate exergy versus time at every point. Simulators such as the HYSYS and the VMGSim can only calculate steady state exergy values at given process conditions. For dynamic exergy versus time, different process condition points are selected during the process dynamic response due to step input disturbances. The selection of calculation points depends on the dynamic response of the process. In order to get the

maximum information in regard to dynamic response, if the variation in the process conditions with time is large, then the time interval between the selected points is decreased. With less variation in the process conditions, the time interval between the selected points is increased. Then the exergy values are calculated on these selected points during the dynamic process response. Exergy values at different points are calculated with the procedure developed in (Munir et al. 2010). Then those exergy points are used to approximate the dynamic exergy response versus time.

### 5.3. Case study – MCB separation plant

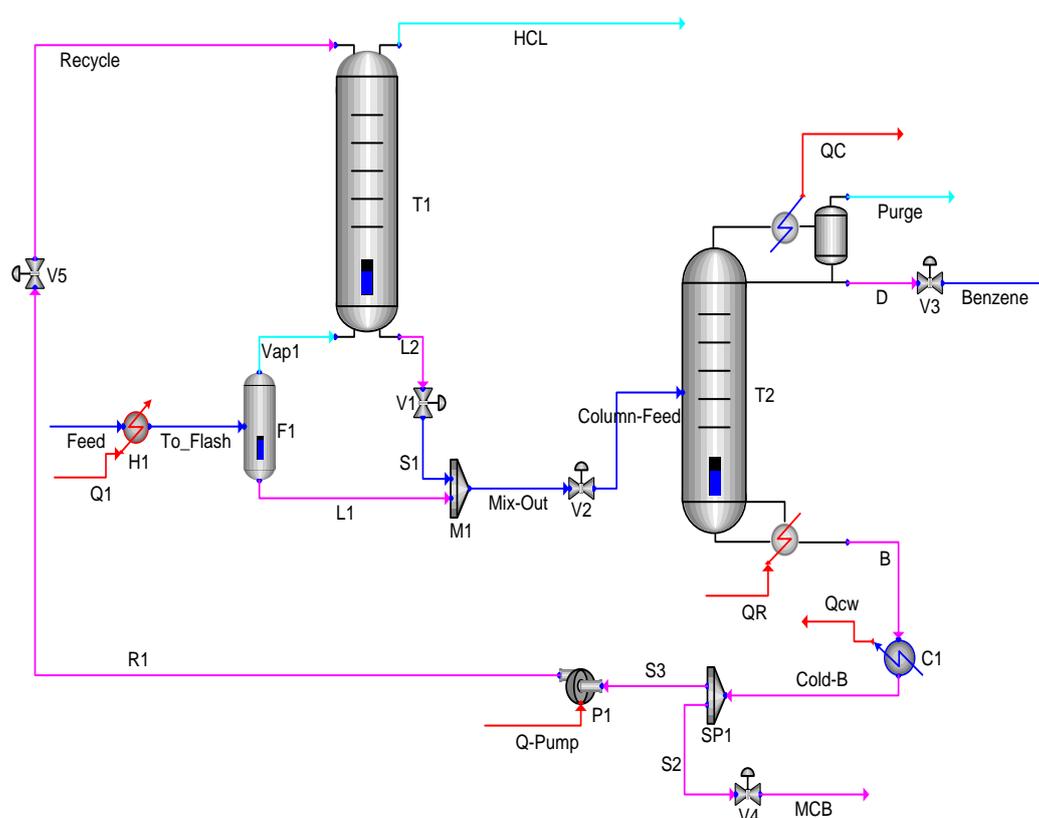


Figure 5-3. MCB separation process schematic

A monochlorobenzene (MCB) separation process is selected for this case study, and is used to show how the EEF provides information regarding the best control loop configuration among the candidates in the sense of eco-efficiency. MCB plant consists of three main units: a flash vessel (F1), an absorption column (T1) and a distillation column (T2), as shown in Figure 5-3. VMGSim (process simulator) with the NRTL activity thermodynamic model was

used for the simulation of the MCB separation process. The detailed information regarding feed conditions and column specification can be found in (Seider et al. 2004).

### 5.3.1. Process description

A mixture of benzene, monochlorobenzene (MCB), and HCl is present in the feed of this MCB separation process. The vapour stream coming out of the flash tank is fed into the absorber where it is put into contact with recycled MCB. Most of the HCl product comes out of the absorber as vapour. The liquid product (L2) coming out of the absorber is mixed with liquid product (L1) from the flash vessel (F1) in a mixer (M1). The mixture coming out of the mixer (M1) is then fed into the distillation column (T2). In this column a fixed amount (1% of inlet feed to the plant) is purged from the process to avoid HCl build-up in the system. The distillate product ( $D$ ) contains most of the benzene and bottom product ( $B$ ) contains most of the MCB. A fraction of the bottom product stream is recycled back into the absorber (Seider et al. 2004).

Classical controllability techniques e.g. RGA, DRGA, NI and CN only guarantee the controllability or quality of products. In this paper, for consideration of the energy cost among these techniques, the EEF is proposed. The EEF is a new measure of eco-efficiency and can provide reliable support for industry to enable the selection of the best control loop configuration from the candidates, in the sense of its eco-efficiency (Munir et al. 2012).

For comparison, three basic control configurations can be defined for the dual composition control of the distillation column (T2) and composition of HCl ( $x_{HCl}$ ) leaving in the vapour stream of the absorber, namely  $LVQ_{cw}$ ,  $LBQ_{cw}$  and  $DVQ_{cw}$ . Each configuration is comprised of three main composition control loops (name of each configuration). For example, in the  $LVQ_{cw}$  control configuration,  $L$  (*Reflux rate*) is used to control the composition of the top product ( $x_D$ ), boil-up rate ( $V$ ) is used to control the composition of the bottom product ( $x_B$ ), and cooler duty ( $Q_{cw}$ ) is used to control the composition of vapour stream leaving the absorber ( $x_{HCl}$ ). It behaves as a pseudo 3x3 system because; i) three inventory control loops of distillation column and other control loops of MCB plant are assumed to be under perfect control; and ii) Control loops other than the composition control are not interacting with the composition loops, therefore are not included in the analysis.

### 5.3.2. Results and Discussions

The simulation model shown in Figure 5-3 was used to do the required step tests. Step tests are performed to obtain the necessary information to calculate the RGA, DRGA, REA, NI and CN as shown in Table 5-1.

The RGA results indicate that all three control configurations have loop interactions, as shown in Table 5-1. From these RGA results,  $LVQ_{cw}$  control configuration seems to be the best candidate control scheme because its leading diagonal elements are positive and close to the value of 1.0. The  $LVQ_{cw}$  configuration can also be a viable, although its leading diagonal elements are quite large. The RGA results do not recommend  $DVQ_{cw}$  control configuration because its leading diagonal elements are far short of the value of 1.0 except for one element.

Table 5-1. The RGA, DRGA, REA, NI and CN results for the whole MCB plant

Configurations	RGA	DRGA	REA	NI	CN
$LVQ_{cw}$	$\begin{bmatrix} 6.30 & -4.76 & -0.54 \\ -5.80 & 6.50 & 0.35 \\ 0.52 & -0.70 & 1.20 \end{bmatrix}$	$\begin{bmatrix} 3.80 & -2.80 & 0.02 \\ -1.40 & 2.60 & -0.23 \\ -1.40 & 1.20 & 1.20 \end{bmatrix}$	$\begin{bmatrix} 0.006 & -0.25 & 1.25 \\ 1.21 & -0.23 & 0.02 \\ -0.21 & 1.48 & -0.27 \end{bmatrix}$	1.15	31.01
$LBQ_{cw}$	$\begin{bmatrix} 0.88 & 0.10 & 0.02 \\ 0.12 & 0.92 & -0.05 \\ 0.00 & -0.03 & 1.02 \end{bmatrix}$	$\begin{bmatrix} 0.84 & -1.60 & 1.76 \\ 0.18 & 0.38 & 0.43 \\ -0.03 & 2.20 & -1.19 \end{bmatrix}$	$\begin{bmatrix} 0.88 & 0.13 & -0.007 \\ 0.12 & 0.61 & 0.26 \\ -0.002 & 0.26 & 0.74 \end{bmatrix}$	-1.0	16.07
$DVQ_{cw}$	$\begin{bmatrix} 0.52 & 0.49 & -0.01 \\ 0.39 & 0.51 & 0.10 \\ 0.10 & 0.00 & 0.91 \end{bmatrix}$	$\begin{bmatrix} 0.91 & 0.03 & 0.06 \\ 0.03 & 1.02 & -0.05 \\ 0.06 & -0.05 & 0.99 \end{bmatrix}$	$\begin{bmatrix} 0.11 & 0.85 & 0.03 \\ 0.83 & 0.14 & 0.03 \\ 0.05 & 0.006 & 0.94 \end{bmatrix}$	0.97	23.62

The validation of the RGA results is done by DRGA because the RGA results are based on steady state information, which can be misleading as the RGA does not consider dynamics. The DRGA results, as shown in Table 5-1, confirm that leading diagonal elements of  $LVQ_{cw}$  configuration are positive and close to the value of 1.0. The DRGA results for the  $LBQ_{cw}$  and  $DVQ_{cw}$  control configurations are different to the results of the RGA analysis. From these DRGA results,  $LVQ_{cw}$  or  $DVQ_{cw}$  control configuration seems to be the best candidate control scheme for the reason that their leading diagonal elements are positive and close to the value of 1.0, shown in Table 5-1.

As the DRGA is used to overcome the limitations of steady state RGA, the DRGA analysis indicates the best candidate control scheme and it accurately determines the extent of interaction present. The NI and CN analyses are further employed to confirm the DRGA based control scheme selection. The NI and CN results of the  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are positive and less than 50, respectively, indicating that the  $LVQ_{cw}$  and  $DVQ_{cw}$  control loops are stable, can be decoupled and are not sensitive to small errors in process gain. The DRGA, NI and CN results do not recommend the further selection of  $LBQ_{cw}$  control configuration. So finally, the  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are further selected to ascertain the most eco-efficient control configuration ( $LVQ_{cw}$  or  $DVQ_{cw}$ ) by using the REA and EEF.

The REA results, as shown in Table 5-1, depict that all three control configurations ( $LVQ_{cw}$ ,  $LBQ_{cw}$  and  $DVQ_{cw}$ ) have exergy interactions and the thermodynamic (exergetic) efficiencies of the control loops are affected by these exergy interactions. For the  $LVQ_{cw}$  configuration, the REA results show that the exergy changes for open loop are smaller and opposite in direction to the exergy changes caused by loop interactions. For the  $LBQ_{cw}$  control configuration, the REA results show that exergy changes due to loop interactions are almost equal and larger than the exergy changes due to the open loop operation. For the  $DVQ_{cw}$  control configuration, the REA results show that exergy changes for open loop operation are much smaller and are in the same direction as the exergy changes caused in closed loop operation, except for one element.

According to the guidelines for interpreting the REA results, an element in REA close to the value of 1.0 indicates that thermodynamic (exergetic) efficiency and exergy changes of the control loop are not affected by other loops. The REA results, as shown in Table 5-1, show that leading diagonal elements of only the  $LBQ_{cw}$  control configuration are close to the value of 1.0 and that this would be a good candidate for selection because its thermodynamic (exergetic) efficiency and exergy changes are not affected by loop interactions.

The interpretation of the RGA, DRGA, NI, CN and REA results depict that a trade-off exists in this process between controllability, thermodynamic (exergetic) efficiency and exergy changes. The  $LBQ_{cw}$  control configuration is the best choice for selection, from the thermodynamic (exergetic) efficiency and exergy changes points of view, but it is the worst from the controllability point of view. When the results of the classical controllability

techniques (RGA, DRGA, NI and CN) and REA contradict each other (as in this case), then dynamic simulation for validation is required

As it is affected by control loop interactions, the REA provides a means for the analysis of the thermodynamic (exergetic) efficiency and exergy changes of a control loop. The REA does not provide any information concerning the eco-efficiency analysis of the whole process or plant. In this paper, the EEF is proposed for the eco-efficiency analysis of the whole process or plant. The EEF is developed in this work to minimize the limitations of the REA e.g. the REA measures eco-efficiency solely within the scope of control loops. The EEF determines the eco-efficiency of the whole plant because its calculation is based on the total exergy destroyed in a process, total exergy coming in and going out of a process. A higher EEF value indicates that selection of that control configuration will result in higher exergy destruction, and vice versa. As the EEF provides the means to determine the true eco-efficiency of the whole plant, EEF analysis is preferred over REA analysis.

There are some similarities and differences between the EEF and REA. For example: the EEF is affected by the recycling of materials and energy streams like REA (Munir et al. 2012; 2012); and unlike the REA, the EEF considers a single possible control scheme at a time for analysis (Munir et al. 2012).

Table 5-2. The EEFs for the MCB plant

Control pairs	$(L, x_D)$	$(D, x_D)$	$(V, x_B)$	$(B, x_B)$	$(Q_{cw}, x_{HCl})$
EEF (kW. kgmole/h) or (kW)	94.3	3.41	78.72	1.08 E3	1.28 E4

EEF results for whole MCB plant, as shown in Table 5-2, indicate that the control pair  $(Q_{cw}, x_{HCl})$  will use the most exergy and be the least eco-efficient control pair, and the control pair  $(D, x_D)$  is the most eco-efficient control pair. Since both control configurations  $(LVQ_{cw}$  and  $DVQ_{cw})$  include the same control pairs  $(V - x_B, Q_{cw} - x_{HCl})$ , we only need to compare the EEF for control pairs  $(L, x_D)$  and  $(D, x_D)$ . For controlling  $x_D$  if we use  $D$ , it will make an exergy saving  $\approx 2.0\%$  compared to use of  $L$ .

### 5.3.3. Validation of EEF Results

As EEF results based on steady state information, dynamic simulation and dynamic exergies are required to validate EEF results shown in Table 5-2. After building dynamic simulation

model of MCB plant, the total dynamic exergies in and out of MCB plant are approximated to validate the EEF results. To approximate dynamic exergies of MCB plant under selected control configurations ( $LVQ_{cw}$  and  $DVQ_{cw}$ ), the set points of  $CVs$   $x_D$ ,  $x_B$  and  $x_{HCl}$  are changed one at a time and by the same amount ( $\pm 5\%$ ) also shown in Figures 5-4 and 5-5.

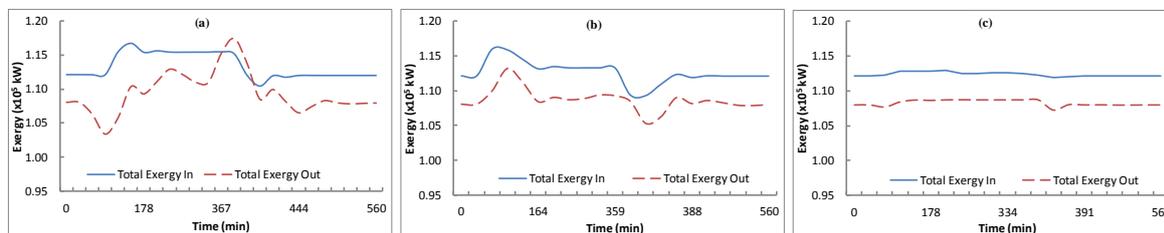


Figure 5-4. Variation of Exergy In and Out of MCB plant due to composition set point changes for the  $LVQ_{cw}$  configuration (a) Exergy variation due to step change in  $x_D$  (b) Exergy variation due to step change in  $x_B$  (c) Exergy variation due to step change in  $x_{HCl}$

After plotting the total dynamic exergies in and out of MCB plant, the total exergies in and out of MCB plant during the entire 560 min operation are calculated by area under the curves (Total exergy in and out). The total exergies (in and out of MCB plant) for the entire 560 min time period of the test are calculated and listed in Table 5-3.

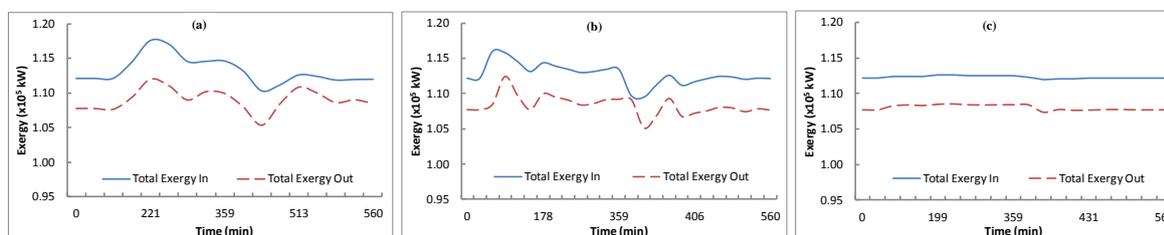


Figure 5-5. Variation of Exergy In and Out of MCB plant due to composition set point changes for the  $DVQ_{cw}$  configuration (a) Exergy variation due to step change in  $x_D$  (b) Exergy variation due to step change in  $x_B$  (c) Exergy variation due to step change in  $x_{HCl}$

Table 5-3. Total Exergy used by the whole MCB plant with the two control configurations

 $LVQ_{cw}$  and  $DVQ_{cw}$ 

Control Configuration		$LVQ_{cw}$	$DVQ_{cw}$
		Exergy( $\times 10^7$ kW)	
step change in $x_D$	Total exergy in	6.34	6.35
	Total exergy out	6.01	6.09
	Destroyed exergy	0.33	0.26
step change in $x_B$	Total exergy in	6.30	6.30
	Total exergy out	6.07	6.05
	Destroyed exergy	0.23	0.24
step change in $x_{HCl}$	Total exergy in	6.29	6.29
	Total exergy out	6.06	6.04
	Destroyed exergy	0.23	0.24
Total exergy destroyed		0.79	0.74

The total exergy destroyed, as shown in Table 5-3, for the whole MCB plant under the selected control configurations ( $LVQ_{cw}$  and  $DVQ_{cw}$ ) are approximated. Under the  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations, the exergies destroyed during the 560 min operation of the whole MCB plant are  $0.79 \times 10^7$  kW and  $0.74 \times 10^7$  kW respectively. Compared to  $LVQ_{cw}$  control,  $DVQ_{cw}$  control can save up to 6 % in exergy. This conclusion agrees with the result (save  $\approx 2.0$  % in exergy) from the EEF analysis.

#### 5.4. Summary

The best control scheme (easily controllable) selection is achieved with the help of a number of classical techniques such as the RGA, DRGA, NI and CN. To integrate controllability and eco-efficiency, the potential of the thermodynamic property exergy was used, which combines control structure selection and eco-efficiency. The EEF is a new tool that is proposed in this paper; it facilitates in the deciding of controllable and eco-efficient control schemes for the whole process. The further investigation of the EEF for a whole plant which includes recycle loops is explained in Chapter 6.

## 5.5. Conclusions

A new measure, an exergy eco-efficiency factor, for integrating the control loop configuration and eco-efficiency is proposed in this paper. The results of the simulation show that the eco-efficiency factor can provide a qualitative and quantitative measure to guide control engineers to select the most eco-efficient control configuration. The quantitative measure provides a reasonable estimate of the dynamic simulation result from the simulation studies.

The  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations were selected based on classical controllability techniques. Both the  $LVQ_{cw}$  and the  $DVQ_{cw}$  control configurations are equally controllable, but the  $DVQ_{cw}$  control configuration is preferred over the  $LVQ_{cw}$  because it causes less exergy destruction (eco-efficient) than the  $LVQ_{cw}$  control configuration.

## References

- Alonso, A. A., B. E. Ydstie and J. R. Banga (2002). "From irreversible thermodynamics to a robust control theory for distributed process systems." Journal of Process Control **12**(4): 507-517.
- Antelo, L. T., I. Otero-Muras, J. R. Banga and A. A. Alonso (2007). "A systematic approach to plant-wide control based on thermodynamics." Computers and Chemical Engineering **31**: 677-691.
- Bristol, E. (1966). "On a new measure of interaction for multivariable process control." Automatic Control, IEEE Transactions on **11**(1): 133-134.
- Denbigh, K. G. (1956). "The second-law efficiency of chemical processes." Chemical Engineering Science **6**(1): 1-9.
- Dincer, I. (2002). "The role of exergy in energy policy making." Energy Policy **30**(2): 137-149.
- Dincer, I. and Y. A. Cengel (2001). "Energy, entropy and exergy concepts and their roles in thermal engineering." Journal of entropy **3**(3): 116-149.
- Fatehi, A. and A. Shariati (2007). Automatic pairing of MIMO plants using normalized RGA. Mediterranean conference on control and automation. Athens Greece.
- Goldberg, J. and M. C. Potter (1998). Differential equations a systems approach. New Jersey, Prentice-Hall.
- Grosdidier, P., M. Morari and B. R. Holt (1985). "Closed-loop properties from steady-state gain information." Industrial & Engineering Chemistry Fundamentals **24**(2): 221-235.
- He, M. J. and W. J. Cai (2004). "New criterion for control-loop configuration of multivariable processes." Ind. Eng. Chem. Res.(43): 7057-7064.
- Hinderink, A. P., F. P. J. M. Kerkhof, A. B. K. Lie, J. De Swaan Arons and H. J. Van Der Kooi (1996). "Exergy analysis with a flowsheeting simulator--I. Theory; calculating exergies of material streams." Chemical Engineering Science **51**(20): 4693-4700.
- Kotas, T. J. (1985). The exergy method of thermal plant analysis. London, Butterworths.
- Larsson, T. and S. Skogestad (2000). "Plantwide control - A review and a new design procedure." Modeling, Identification and Control **21**(4): 209-240.
- Luyben, W. L., B. D. Tyreus. and M. L. Luyben (1998). Plantwide Process Control. New York, McGraw-Hill.
- McAvoy, T., Y. Arkun, R. Chen, D. Robinson and P. D. Schnelle (2003). "A new approach to defining a dynamic relative gain." Control Engineering Practice **11**(8): 907-914.
- McAvoy, T. J. (1983). Interaction Analysis: Principles and Applications. Research Triangle Park, NC, Instrument Society of America.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2007). "An exergy calculator tool for process simulation." Asia-Pacific Journal of Chemical Engineering **2**(5): 431-437.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2009). The Relative Exergy Array - A tool for integrated process design and control Chemeca 2009. Perth, Australia.

- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2010). "The relative exergy array—a new measure for interactions in process design and control." The Canadian Journal of Chemical Engineering **89**(3): 545-549.
- Munir, M. T., J. J. Chen and B. R. Young (2010). A computer program to calculate the stream exergy using the visual basic graphical interface. Chemeca 2010. Adelaide, Australia.
- Munir, M. T., W. Yu and B. R. Young (2012). Control loop configuration and eco-efficiency. FOCAPO/CPC-VIII. Savannah, Georgia, USA.
- Munir, M. T., W. Yu and B. R. Young (2012). Determination of Plant-wide Control Loop Configuration and Eco-Efficiency, G.P. Rangaiah and V. Kariwala (Eds.). Plantwide Control: Recent Developments and Applications, John Wiley & Sons, ISBN:9780470980149.
- Munir, M. T., W. Yu and B. R. Young (2012). Eco-efficiency and control loop configuration for recycle systems. American control conference. Montreal, Canada.
- Munir, M. T., W. Yu and B. R. Young (2012). "Recycle effect on the relative exergy array." Chemical Engineering Research and Design **90**(1): 110-118.
- Niederlinski, A. (1971). "A heuristic approach to the design of linear multivariable interacting control systems." Automatica **7**(6): 691-701.
- Ogunnaiké, B. and H. Ray (1994). Process dynamics, modeling and control, Oxford University Press.
- Rangaiah, G. P. and V. Kariwala, Eds. (2011). Plant-Wide Control: Recent Developments and Applications (in press), Wiley.
- Rosen, M. A. and I. Dincer (1997). "On Exergy and environmental impact." International Journal of Energy Research **21**(7): 643-654.
- Rosen, M. A. and I. Dincer (1999). "Exergy analysis of waste emissions." International Journal of Energy Research **23**(13): 1153-1163.
- Rosen, M. A. and I. Dincer (2001). "Exergy as the confluence of energy, environment and sustainable development." Exergy, An International Journal **1**(1): 3-13.
- Ruszkowski, M., V. Garcia-Osorio and B. E. Ydstie (2005). "Passivity based control of transport reaction systems." AIChE Journal **51**(12): 3147-3166.
- Seborg, D. E., T. F. Edgar and D. A. Mellichamp (1989). Process Dynamics and Control. New York, John Wiley & Sons.
- Seider, W. D., J. D. Seader. and D. R. Lewin. (2004). Product and Process Design Principles: Synthesis, Analysis, and Evaluation. New York, John Wiley.
- Skogestad, S., P. Lundström and E. W. Jacobsen (1990). "Selecting the best distillation control configuration." AIChE Journal **36**(5): 753-764.
- Smith, J. M. and H. C. V. Ness (2005). Introduction to Chemical Engineering Thermodynamics. New York, McGraw-Hill.
- Svrcek, W. Y., D. P. Mahoney and B. R. Young (2006). A Real-Time Approach to Process Control. Chichester, John Wiley & Sons Ltd.
- Szargut, J., D. R. Morris and F. R. Steward (1988). Exergy analysis of thermal chemical and metallurgical processes. New York, Hemisphere Publishing.
- Vasudevan, S. and G. P. Rangaiah (2010). "Criteria for performance assessment of plantwide control systems." Ind. Eng. Chem. Res. **49**: 9209-9221.

- Westphalen, D. L., B. R. Young and W. Y. Svrcek (2003). "A Controllability Index for Heat Exchanger Networks." Industrial & Engineering Chemistry Research **42**(20): 4659-4667.
- Witcher, M. F. and T. J. McAvoy (1977). "Interacting control systems: steady state and dynamic measurement of interaction." ISA Trans **16**(3): 35-41.
- Xiong, Q., W. J. Cai and M. J. He (2005). "A practical loop pairing criterion for multivariable processes." Journal of Process Control **15**(7): 741-747.
- Ydstie, B. E. (2002). "Passivity based control via the second law." Computers & Chemical Engineering **26**(7-8): 1037-1048.
- Zhu, Z.-X. and A. Jutan (1993). "A new variable pairing criterion based on the Niederlinski Index." Chemical Engineering Communications **121**(1): 235-250.



## Chapter 6

---

*Eco-efficiency and control loop configuration for recycle systems*

**Article # 4**

**Co-authors: Wei. Yu, Brent. R. Young**

*Industrial Information & Control Centre (I<sup>2</sup>C<sup>2</sup>), Department of Chemical & Materials Engineering, The University of Auckland, Auckland, New Zealand*

Munir, M. T., W. Yu and B. R. Young (2012). Eco-efficiency and control loop configuration for recycle systems. AIChE Journal (Submitted).

## **Chapter 6. Eco-efficiency and control loop configuration for recycle systems**

Chapter 6 is a continuation of Chapter 5, and is based on the effect of recycle loops on EEF results. The intention in this chapter is to show the further investigation of the EEF (proposed/discussed in Chapter 5) for the whole plant, which also includes recycles. It is necessary to study the effect of recycle loops on the EEF results because recycle loops are common in the process industry and consideration of recycle loops can have a significant effect on EEF results. The EEF value decreases due to recycle/reuse of material and energy.

### **Abstract**

To integrate measurements of Eco-efficiency with control loop configuration has become an important topic since all industrial processes/plants are requested to increase their eco-efficiency. The exergy eco-efficiency factor, a new measure of eco-efficiency for control loop configuration, has been developed recently (Munir et al. 2012). The exergy eco-efficiency factor is based on the thermodynamic concept of exergy which can be used to analyse a process in terms of its efficiency. The combination of the Relative Gain Array (RGA), NI, CN, dynamic RGA, and the exergy eco-efficiency factor will help guide the process designer to find the optimal control design with low operating cost/eco-efficiency. In this paper, we validate the proposed exergy eco-efficiency factor for processes with recycles which are very common industrially.

Key words: Eco-efficiency, Control loop configuration, Recycle

### **6.1. Introduction**

After designing a continuous process at steady state for given operating conditions, control system structure selection/control pair selection is an important part of process control. As control systems are common in the process industry due to their simplicity, therefore control structure selection mostly focuses on selecting the best decentralized control scheme for pairing manipulated (MV) and controlled variables (CV). There are many mathematical formulations and systematic strategies such as the relative gain array (RGA), the Niederlinski index (NI), singular value decomposition (SVD), the condition number (CN) and Morari's resiliency index (MRI) for selecting the best control configuration (Seborg et al. 1989; Svrcek

et al. 2006). During last decade, several attempts have been made to apply these common techniques to more complex processes. For example, the development of a controllability index for heat exchange networks (Westphalen et al. 2003), mathematical formulations of the decomposed relative interaction array, the dynamic relative gain array, the effective relative gain array, ERGA (McAvoy et al. 2003; He and Cai 2004; Xiong et al. 2005) and a comprehensive criteria for performance assessment of plant-wide control systems (Larsson and Skogestad 2000; Vasudevan and Rangaiah 2010).

In the present era, increasing energy demands and energy costs are exacerbating the energy crisis. As a poorly structured control algorithm can lose a lot of energy from the plant, control loop configuration should not only focus on control loop stability and quality of control, but should also include energy cost/energy usage and environmental impacts. The amalgamation of control quality and energy cost/energy usage/environmental impacts can be done by using the potential of thermodynamic properties like exergy. The concept of exergy indicates what is wasted in terms of energy or the eco-efficiency of the process/plant. More details on exergy are given by Szargut et al. (1988). Exergy analysis of a process/plant is used to locate its inefficient parts, which improves energy usage and decreases energy cost (Szargut et al. 1988; Moran and Sciubba 1994; Montelongo-Luna et al. 2007; Muangnoi et al. 2007). Exergy also plays an important role for sustainability and minimizing environmental impacts by efficient use of exergy (Rosen and Dincer 1997; Rosen and Dincer 1999; Rosen and Dincer 2001; Dincer 2002; Dincer et al. 2004; Dincer and Rosen 2007).

In recent decades, the utilization of exergy has spread to the process control spectrum. For example, a basic framework for the development of a dynamic exergy balance for process control evaluation (Luyben et al. 1998), development of the Relative Exergy Array (REA) based on analysing the exergy interactions for the control configuration (Montelongo-Luna et al. 2009; 2010; Munir et al. 2012) and development of the exergy eco-efficiency factor (EEF) a new measure of eco-efficiency (Munir et al. 2012). For REA calculation a simple algorithm/software package using VMGSim, a commercial simulator, has been developed (Munir et al. 2010; 2012). The effect of recycle on the REA analysis was also studied by Munir et al. (2012).

The REA is simple, easy to use and based on steady state exergy information but it evaluates the eco-efficiency only within the scope of the control loops studied; it cannot provide the eco-efficiency of the whole unit /plant. A new measure of eco-efficiency, EEF, was

developed to join together eco-efficiency and control loop configuration (Munir et al. 2012). To make eco-efficiency a useful indicator, it must be coupled with other indicators/tools like control quality. In this paper, we will continue investigating the EEF for the whole unit/process or plant which includes recycle loops. Measurements of eco-efficiency from EEF can be used to guide process designers or control engineers to achieve more eco-efficient control configurations.

For a multi-input-multi-output (MIMO) process, a definite amount of exergy is used due to certain change in a CV by using a MV. The EEF is designed to measure the amount of exergy used for different control pairing combinations. Out of different possible control pairing combinations, the control pair which fulfils its control target by utilizing the least exergy will be the most eco-efficient control pairing. Integration of control system structure analysis techniques such as RGA, NI and SVD with an eco-efficiency measure, EEF helps engineers to select the best control configuration for both controllability and eco-efficiency.

It is a common practice to recycle material and energy streams in the chemical process industry to reuse material and energy and improve the material usage and energy efficiency. However, recycling of material and energy from an individual unit like a distillation column can change the controllability and eco-efficiency of that unit significantly (Papadourakis et al. 1987). The EEF can be used to select the most eco-efficient control configuration for a process with recycle. The results for EEF are validated by dynamic simulation.

In this paper, our intention is to further investigate the EEF for a whole plant which includes recycle loops. Since recycle systems are very common in chemical plants and other industrial plants, it is necessary to study the effect of recycles on the EEF values. As the EEF values of a unit/plant are affected by the consideration of recycle loops, in this work the EEF also is employed to provide the exergy difference between the process with and without recycle.

This manuscript is organized as follows. After this general introduction, control loop configuration methods based on controllability and eco-efficiency are explained, then the concept of eco-efficiency is introduced, the EEF is defined and its validation is explained. Then, the proposed method is implemented for a simulation example. Finally, the results are discussed and conclusions are made in the summary.

## **6.2. Control loop configuration**

In this work three basic techniques of control structure selection: RGA, NI and SVD are used to select the control pairs. The selected control pairs based on the results of these three techniques are further considered to ascertain the most eco-efficient control pairs by using the EEF. The EEF can also be integrated with any other comprehensive/advanced control loop configuration technique or set of techniques, such as MRI, dynamic RGA, and ERGA.

### **6.2.1. Methods based on controllability**

The use of RGA started in 1960s after the work of Bristol (1966), and is a popular tool used to check the controllability of a process or for the selection of control loop pairings. Since then, an extensive amount of research has been done in this field. For example the selection of the best control configuration for a distillation column (Skogestad et al. 1990), the dynamic RGA (Witcher and McAvoy 1977; McAvoy et al. 2003), the effective relative gain array (ERGA) (Xiong et al. 2005) and the normalized RGA (NRGA) (Fatehi and Shariati 2007).

The Niederlinski Index (NI) is used for testing the stability of RGA selected control loop pairing (Niederlinski 1971). Its use is more applicable for lower order systems (2x2). For higher order systems it can only inform about the instability of the loop. The NI has also been used as an interaction measure itself as well as a stability criterion (Zhu and Jutan 1993).

Singular Value Decomposition (SVD) is a useful tool to check the sensitivity of the control loop interaction to small errors in process gains. SVD also informs the decoupling of the control loops. It may not be possible to decouple control loop interactions in the presence of a singular set of steady state gain matrix equations. In this case of singular steady state gain matrix equations, the problem is ill conditioned and control loop interactions may not be possible to decouple (McAvoy 1983; Ogunnaike and Ray 1994; Goldberg and Potter 1998; Svrcek et al. 2006).

### **6.2.2. Methods based on Eco-efficiency**

Eco-efficiency is analogous to the notion that increasing industrial and economic developments should be correlated with lowering of environmental impacts and optimized use of resources. Eco-efficiency analysis of a process harmonizes its economy and ecology.

The purpose of eco-efficiency analysis is to use as small amount of material/energy as possible with reduced wastes and emissions.

According to the World Business Council for Sustainable Development (WBCSD) definition, eco-efficiency is achieved through the delivery of "competitively priced goods and services that satisfy human needs and bring quality of life while progressively reducing environmental impacts of goods and resource intensity throughout the entire life-cycle to a level at least in line with the Earth's estimated carrying capacity." In other words eco-efficiency means producing more with less.

For control engineers to design/select control loop configurations, they need to convert the concept of eco-efficiency into a tool or method which can help them select the manipulated variables which achieve the best products with the lowest energy cost. Exergy is a suitable concept which can be used to evaluate the eco-efficiency of a controlled process. Exergy, the basic measure of eco-efficiency, is defined by combination of the 1<sup>st</sup> and 2<sup>nd</sup> laws of thermodynamics. The maximum possible amount of work which can be drawn from a material stream/process when it interacts only with the reference environment as it comes from its initial state to the final dead state is known as the exergy of that material stream/process (Denbigh 1956; Kotas 1985).

#### 6.2.2.1. Exergy

Since exergy accounts for the quality of energy, it can be used as a measure to evaluate the eco-efficiency for a process design. A process is called eco-efficient if it uses a relatively small amount of energy or destruction of exergy is low. The total exergy, which consists of three components (physical exergy, chemical exergy and exergy due to mixing) is defined as (Hinderink et al. 1996).

$$B_{total} = B_{phys} + B_{chem} + \Delta_{mix}B \quad 6-1$$

where,  $B_{total}$  = Total exergy,  $B_{phys}$  = Physical exergy,  $B_{chem}$  = Chemical exergy and  $\Delta_{mix}B$  = Exergy change due to mixing.

The physical exergy of a material stream/process is the amount of exergy due to the thermo-mechanical difference between pure components at process conditions and pure components at reference conditions. The chemical exergy of a stream/process is the amount of exergy due to the process components chemical potential difference at the process and reference

conditions. The exergy change upon mixing is due to the mixing of pure components at process conditions to form the actual composition of the material stream. The total exergy calculation in Equation (6-1) is relatively simple and only needs easily obtainable thermodynamic data. Detailed definitions and explanations of physical exergy,  $B_{phys}$ , chemical exergy,  $B_{chem}$ , and exergy change due to mixing,  $\Delta_{mix}B$ , are provided in (Hinderink et al. 1996).

For exergy calculations in this work, an integrated Visual Basic (VB) program and Graphical User Interface (GUI) was developed (Munir et al. 2010; 2012). The automation of exergy calculation has also been done by using process simulators. For example an open source simulator (Sim42) and a commercial simulator (Aspen HYSYS) has been used for automation of exergy calculation (Montelongo-Luna et al. 2007).

### 6.2.2.2. Exergy Eco-efficiency factor (EEF)

EEF is a new tool for analysing the eco-efficiency of a process. It is based on an understanding of the total exergy of each material stream in and out of the thermodynamic process. EEF helps engineers to build an eco-efficient process which is ecologically friendly and economical. In the above section, we discussed that exergy can be used to measure the energy changes of one process/unit/plant.

The exergetic efficiency of a process is equivalent to eco-efficiency. For a general process as shown in Figure 6-1, exergetic efficiency is defined as the ratio of the exergy going out, to the exergy coming in (Szargut et al. 1988), namely,

$$\eta = B_{out} / B_{in} \quad 6-2$$

where  $\eta$  = exergetic efficiency,  $B_{out}$  = total exergy going out of a process and  $B_{in}$  = total exergy coming in to a process.



Figure 6-1. Exergy flows for a general process

The exergetic efficiency for the whole process is shown in Equation (6-2); however it does not provide any information about how the control loop configuration affects this exergetic efficiency. The EEF was developed to estimate the effect of control loop configuration on

exergetic efficiency (Munir et al. 2012). The EEF connects control loop configuration to the eco-efficiency. The EEF for a control pair  $(u_j, y_i)$ , is defined as,

$$\tau_{ij} = (\Delta B_{out} - \Delta B_{in}) \frac{\Delta u_j}{\Delta y_i} \quad 6-3$$

where  $\Delta u_j$  denotes a step change of the *MV*,  $(u_j)$ ,  $\Delta y_i$  denotes a response in the *CV*,  $(y_i)$ , caused by a step change of the *MV*,  $(u_j)$ , and  $\Delta B_{out}$  and  $\Delta B_{in}$  represent the exergy differences caused by the *MV* step change for exergy out and exergy in, respectively. For example, for a 2x2 system, if  $\tau_{21}$  is less than  $\tau_{22}$ , it means that for the same amount of *CV* change,  $\Delta y_2$ , using *MV*  $u_1$ , will cause less exergy loss/change than using *MV*  $u_2$ . The final interpretation is that the control pairing  $(u_1, y_2)$  is more eco-efficient than the pairing  $(u_2, y_2)$ .

Techniques such as RGA, NI and SVD are used to determine control loop configurations. It is usual that several candidate control configurations can be implemented. EEF can be used to select the best control loop configuration among the candidates in the sense of eco-efficiency.

In plant-wide layouts the presence of recycle can also have a significant effect on the control configuration selection of a unit/process (Papadourakis et al. 1987). The final selection of a control configuration should be based on the plant-wide layout. After selection of a control configuration, the proposed method of EEF is applied and validated by dynamic simulation. The use of EEF is illustrated by a process simulation case study.

As the recycling of material and energy streams in a chemical process improves energy efficiency, it also has an impact on the EEF. The EEF decreases for a unit when it is considered with recycle and vice versa. Recycle of material and energy reuses energy, which decreases the destruction of exergy. In the EEF Equation (6-3), the term in brackets accounts for the exergy destruction. If exergy destruction is small then this term in brackets would be small, which means the EEF is small. A smaller value of EEF for units with recycles means a more eco-efficient process.

### 6.2.2.3. Validation of EEF

Dynamic simulation is used to validate the EEF results which are based on steady state information. During the dynamic response of a process, several exergy calculations at different conditions are performed to approximate the dynamic change of exergy with time, as explained below.

The latest simulators such as HYSYS and VMGSim still do not have the ability to directly calculate and display the total exergy of a material stream at every point versus time automatically. These simulators can only calculate steady state total exergy of a material stream via a customized calculation/external programme routine at given process conditions.

To approximate the dynamic change of exergy/dynamic exergy analysis, different points are selected during the process dynamic response due to step input disturbances. Selection of calculation points to reduce the computation depends on the process response. When the outputs changes are dramatic, the sampling interval is short; otherwise the sampling interval is large. Exergy values are then calculated at those selected points during the dynamic process response. The procedure developed by Munir et al. (2010) is used for the calculation of exergy values at those selected points. Then the dynamic exergy response is approximated by joining those exergy points.

#### **6.2.2.4. Plantwide EEF**

As the final selection of a control configuration should be based on plant-wide layout considerations, this paper is an exploration of the EEF for the whole process/plant which includes recycle loops, to select the best plant-wide control loop configuration in the sense of eco-efficiency among the good performing control configuration candidates obtained from controllability analysis. This work is performed with the aid of a case study (an MCB plant).

### 6.3. Case study – MCB separation plant

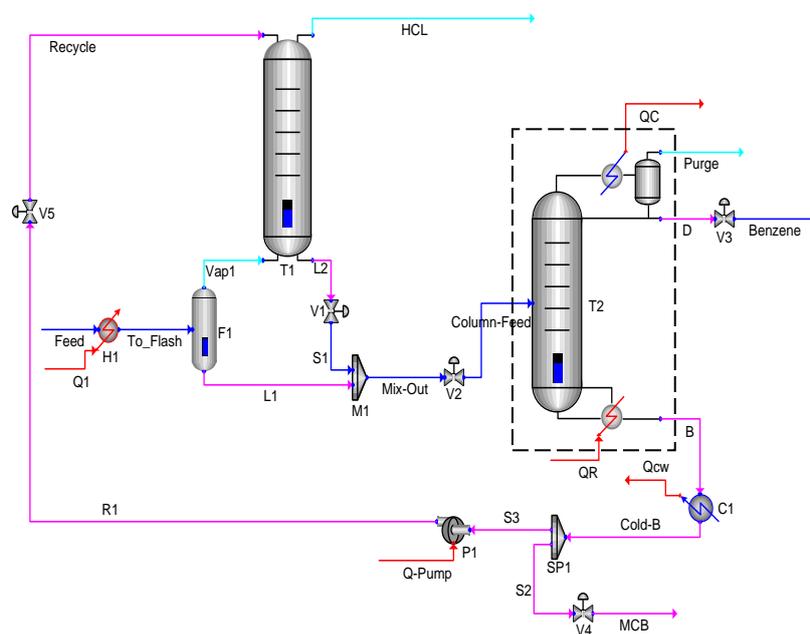


Figure 6-2. MCB separation process schematic

A monochlorobenzene (MCB) separation process is selected for this case study. It consists of three main units: a flash vessel (F1), an absorption column (T1) and a distillation column (T2) as shown in Figure 6-2. The detailed information of the feed conditions and column specification can be found in (Seider et al. 2004). VMGSim with the NRTL activity thermodynamic model is used for simulation of the MCB separation process.

The feed of this process consists of a mixture of monochlorobenzene (MCB), benzene and HCl. The vapour stream coming out of the flash tank is fed into the absorber where it is contacted with recycled MCB. Most of the HCl product comes out of the absorber as vapour. The liquid product (L2) coming out of the absorber is mixed with liquid product (L1) from the flash vessel (F1) in a mixer (M1). The mixture coming out of the mixer (M1) is then fed into the distillation column (T2). In this column a fixed amount (1% of inlet feed to the plant) is purged from the process to avoid HCl build-up in the system. The distillate product (D) contains most of the benzene and bottom product (B) contains most of the MCB. Some fraction of bottom product stream is recycled back into the absorber.

Although these techniques “classical” controllability techniques e.g. RGA, DRGA, NI and CN provide reliable support for industry to guarantee the quality of products, there is less consideration of the energy cost among these techniques. We consider this via the EEF in this

paper/study. We study four aspects in this case study: 1) An isolated distillation column; 2) a distillation column with recycle; 3) the whole plant with a distillation column but without recycle; and 4) the whole plant with a distillation column and recycle.

### 6.3.1. An Isolated distillation column

As the 1<sup>st</sup> step of the case study, the distillation column in a MCB plant is considered in isolation without any recycle, as shown by the dashed boundary in Figure 6-2. The results for controllability for different control loop configurations are shown in Table 6-1.

Table 6-1. The RGA, DRGA, NI and CN Results for the MCB distillation column alone (T2)

Configurations	RGA	DRGA	NI	CN
<i>LV</i>	$\begin{bmatrix} 0.11 & 0.89 \\ 0.89 & 0.11 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	-213.9	1.18
<i>LB</i>	$\begin{bmatrix} 0.97 & 0.03 \\ 0.03 & 0.97 \end{bmatrix}$	$\begin{bmatrix} 1.24 & -0.24 \\ -0.24 & 1.24 \end{bmatrix}$	1.02	71
<i>DV</i>	$\begin{bmatrix} 0.84 & 0.16 \\ 0.16 & 0.84 \end{bmatrix}$	$\begin{bmatrix} 0.86 & 0.14 \\ 0.14 & 0.86 \end{bmatrix}$	1.19	264

From Table 6-1, the RGA results show that the leading diagonal elements of the *LB* and *DV* control configurations are positive and close to 1. The RGA results are validated with the Dynamic Relative Gain Array (DRGA), which confirms that leading diagonal elements of the *LB* and *DV* control configurations are positive and close to 1.

The NI results of the *LB* and *DV* control configurations are positive and greater than 1 which is favourable. The CN of the *LB* control configuration is close to 50, so it indicates that *LB* is favourable. The CN of the *DV* control configuration is much greater than 50, but it may be still acceptable depending on how rigorously the heuristic of  $< 50$  is adhered to. The *LV* control configuration is not selected as its leading diagonal elements are significantly less than 1 which is not acceptable. Its off-diagonal elements are positive and close to 1, but the pairing of off-diagonal elements introduce a significant amount of dead time in the process. The DRGA also confirms that the off-diagonal elements of the *LV* control configuration are

positive and close to 1. The NI result for the  $LV$  control configuration is negative which means the system is unstable.

The results based on eco-efficiency analysis (EEF) for control loop configurations are shown in Table 6-2. From Table 6-2, the control pairing  $(V, x_B)$  will use the most exergy and be the least eco-efficient control pair, and the control pairing  $(D, x_D)$  is the most eco-efficient pairing. The sums of the EEFs for the  $LB$  and  $DV$  control configurations are  $3.57 \times 10^5$  kW.kmole/h and  $6.44 \times 10^5$  kW.kmole/h, respectively. So from Tables 6-1 and 6-2, both  $LB$  and  $DV$  control configurations are controllable but the process with the  $LB$  control configuration is more eco-efficient than the same process with the  $DV$  control configuration. The  $LB$  control configuration can save up to 44% more exergy compared to the  $DV$  control configuration as calculated from Table 6-2.

Table 6-2. The EEFs for the MCB column alone

Control pairs	$(L, x_D)$	$(D, x_D)$	$(V, x_B)$	$(B, x_B)$
EEF (kW. kmole/h)	3.28 E5	691.05	6.44 E5	2.91 E4

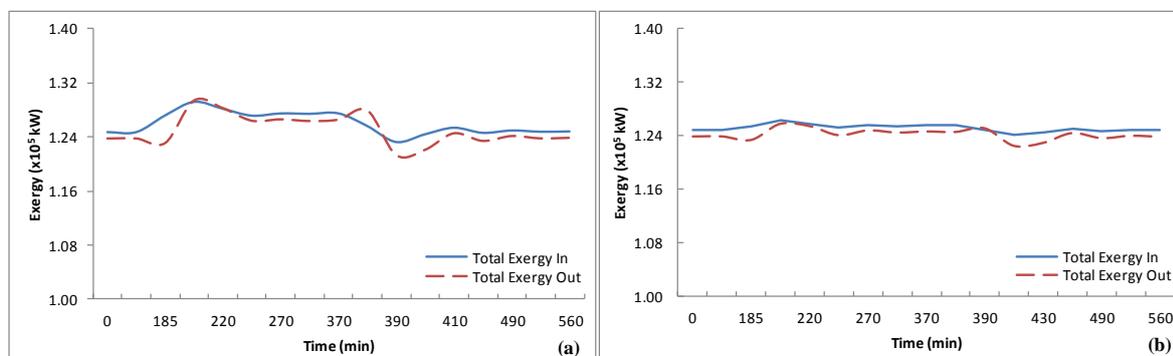


Figure 6-3. Variation of Exergy In and Out of the isolated MCB column due to composition set point changes for the  $LB$  configuration (a) Exergy variation due to step change in  $x_D$  (b) Exergy variation due to step change in  $x_B$

For the validation of the EEFs shown in Table 6-2, dynamic simulation of the isolated distillation column is used. Figures 6-3 and 6-4 show the total dynamic exergies in and out of the isolated distillation column for the two control configurations  $LB$  and  $DV$ , respectively. Figures 6-3 (a) and 6-3 (b) show the dynamic exergies in and out of the column under  $LB$  control due to a step change in the set points of  $CVs$   $x_D$  and  $x_B$ , respectively. Similarly, Figures 6-4 (a) and 6-4 (b) show the dynamic exergies of the column under  $DV$  control.

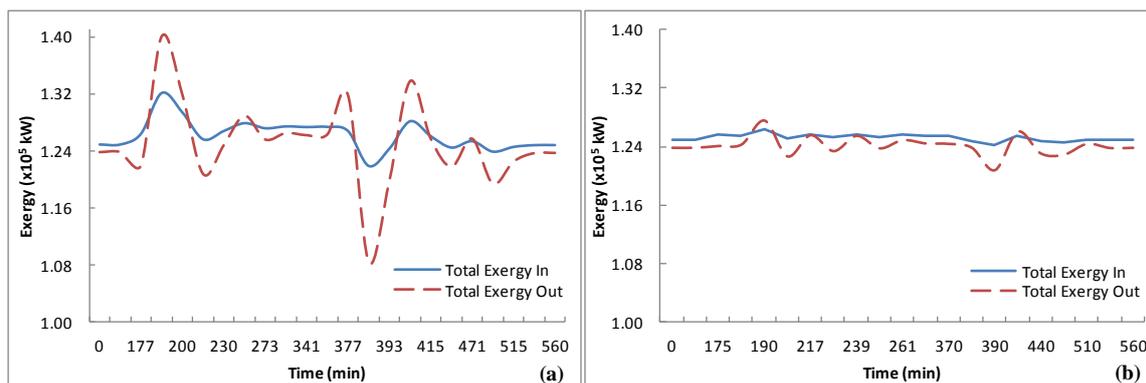


Figure 6-4. Variation of Exergy In and Out of the isolated MCB column due to composition set point changes for the *DV* configuration (a) Exergy variation due to step change in  $x_D$  (b) Exergy variation due to step change in  $x_B$

The total exergies of isolated column for the entire 560 min time period of the test are listed in Table 6-3. The total destroyed exergy for the whole column is  $1.12 \times 10^7$  kW under *LB* control. Compared to *DV* control, *LB* control can save up to 45% in exergy. This conclusion agrees with the result (save 44% in exergy) from the EEF analysis.

Table 6-3. Exergy used by the two control configurations *LB* and *DV* on the isolated MCB column

		Control Configuration	
		<i>LB</i>	<i>DV</i>
Exergy( $\times 10^7$ kW)			
step change in $x_D$	Total exergy in	7.13	7.16
	Total exergy out	6.07	5.15
	Destroyed exergy	1.06	2.01
step change in $x_B$	Total exergy in	7.03	7.03
	Total exergy out	6.97	6.98
	Destroyed exergy	0.06	0.05
Total exergy destroyed		1.12	2.06

### 6.3.2. MCB distillation column with recycle

In practice, control configurations are the same during start-up and steady state operational periods. Therefore chosen control configurations should work fine for both periods of

operation, which is a consideration for the final selection of a control configuration. As the distillation column is ultimately connected to other units and recycles in a plantwide layout therefore the final selection of a control configuration is based on RGA, DRGA, NI and CN for the column in plantwide layout. The results of studying an isolated distillation column are used only as a check that the selected control configuration based on plantwide layout can work fine during start-up period as well as during normal operational period of the plant which rules out the *LV* distillation column configuration.

In this part of the case study, the distillation column with a recycle in a plantwide layout is considered. In this part of the case study there are three composition control loops. The composition of HCl ( $x_{HCl}$ ) leaving in the vapour stream of the absorber is controlled by manipulating the cooler (*CI*) duty ( $Q_{cw}$ ). The compositions at the top and bottom of the distillation column,  $x_D$  and  $x_B$ , are the other two controlled variables. For this three-point composition control of the MCB separation plant, three basic control configurations:  $LVQ_{cw}$ ,  $LBQ_{cw}$  and  $DVQ_{cw}$  are considered. For example, in the  $LVQ_{cw}$  control configuration,  $L$  (*Reflux rate*) is used to control the composition of the top product ( $x_D$ ), boil-up rate ( $V$ ) is used to control the composition of the bottom product ( $x_B$ ), and cooler duty ( $Q_{cw}$ ) is used to control the composition of vapour stream leaving the absorber ( $x_{HCl}$ ) (Seider et al. 2004). The simulation results are listed in Table 6-4.

From Table 6-4, the RGA results show that the leading diagonal elements of the  $LVQ_{cw}$  and  $LBQ_{cw}$  control configurations are positive, although quite large for  $LVQ_{cw}$ . The RGA results of the  $DVQ_{cw}$  control configuration are far away from 1 except for one element. The Dynamic Relative Gain Array (DRGA) results are interesting, showing that the leading diagonal elements of the  $LVQ_{cw}$  control configuration are positive although quite large. The DRGA results for the  $LBQ_{cw}$  and  $DVQ_{cw}$  control configurations are also different to the results of the steady state RGA analysis. From Table 6-4, the DRGA results show that the leading diagonal elements of the  $DVQ_{cw}$  control configuration are positive and close to 1. The NI results of the  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are positive which is favourable. The CN of the  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are less than 50; this indicates that the  $LVQ_{cw}$  and  $DVQ_{cw}$  control loops can be decoupled and are not sensitive to small errors in process gains. The  $LBQ_{cw}$  control configuration is not further selected as its DRGA leading diagonal elements are significantly away from 1 which is not acceptable, and the NI result for the  $LBQ_{cw}$  control configuration is negative which indicates instability of the system. This is a different conclusion to the isolated distillation column case study.

Table 6-4.The RGA, DRGA, NI and CN Results for the whole MCB plant

Configurations	RGA	DRGA	NI	CN
$LVQ_{cw}$	$\begin{bmatrix} 6.3 & -4.76 & -0.54 \\ -5.8 & 6.5 & 0.35 \\ 0.52 & -0.7 & 1.2 \end{bmatrix}$	$\begin{bmatrix} 3.8 & -2.8 & 0.02 \\ -1.4 & 2.6 & -0.23 \\ -1.4 & 1.2 & 1.2 \end{bmatrix}$	1.15	31.01
$LBQ_{cw}$	$\begin{bmatrix} 0.88 & 0.1 & 0.02 \\ 0.12 & 0.92 & -0.05 \\ 0 & -0.03 & 1.02 \end{bmatrix}$	$\begin{bmatrix} 0.84 & -1.6 & 1.76 \\ 0.18 & 0.38 & 0.43 \\ -0.03 & 2.2 & -1.19 \end{bmatrix}$	-1.0	16.07
$DVQ_{cw}$	$\begin{bmatrix} 0.52 & 0.49 & -0.01 \\ 0.39 & 0.51 & 0.1 \\ 0.1 & 0 & 0.91 \end{bmatrix}$	$\begin{bmatrix} 0.91 & 0.03 & 0.06 \\ 0.03 & 1.02 & -0.05 \\ 0.06 & -0.05 & 0.99 \end{bmatrix}$	0.97	23.62

Exergy analysis of the MCB separation plant shows that most of exergy of this plant is destroyed in the distillation column (Montelongo-Luna 2010). To minimize this exergy destruction in the column, a suitable control configuration is required.

Based on the analysis from RGA, DRGA, NI and CN, either of the  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations can be used to control this MCB separation plant, with pros and cons for both schemes. Through comparing the exergy destruction using the EEF, we can determine the best control configuration in the sense of eco-efficiency which may help us choose between the two configurations. Here we are unlikely to choose  $LVQ_{cw}$  as the  $LV$  is uncontrollable i.e. for distillation column with no recycle. However, this is not necessarily always the case, so we will proceed with the analysis. The EEFs for the distillation column are calculated and are listed in Table 6-5. Exergy changes considered for this section are only included inside the distillation column inside the dashed boundary within the MCB separation plant schematic shown in Figure 6-2. For comparing the exergy changes for the distillation column alone and with a recycle, we also re-list the EEF results from section 6.3.1 in the right column of Table 6-5.

Table 6-5. EEFs for the MCB column in the plantwide layout

Control Pairs	EEF (kW.kmole/h) or (kW)	
	Without recycle	With recycle
$(L, x_D)$	3.28 E5	3.18 E4
$(D, x_D)$	691.05	652
$(V, x_B)$	6.44 E5	1.22 E5
$(B, x_B)$	2.91 E4	2.19 E4
$(Q_{cw}, x_{HCl})$	—	1.53 E4

From Table 6-5, the control pairing  $(V, x_B)$  will use the most exergy and be the least eco-efficient control pair, and the control pairing  $(D, x_D)$  is the most eco-efficient pairing. The sums of the EEFs for the  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are  $1.77 \times 10^5$  kW.kmole/h and  $1.44 \times 10^5$  kW.kmole/h, respectively. So both  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are controllable but the process with a  $DVQ_{cw}$  control configuration is more eco-efficient than the same process with an  $LVQ_{cw}$  control configuration. The  $DVQ_{cw}$  control configuration can save up to 19% of the exergy of the  $LVQ_{cw}$  control configuration. The exergy destruction involved in the control pairing  $(Q_{cw}, x_{HCl})$  is the same for both configurations ( $LVQ_{cw}$  and  $DVQ_{cw}$ ).

In the plant-wide layout, a bottoms product fraction is recycled back to the top of the absorber. Material and energy are reused due to the recycling of bottom product, which improves the exergy efficiency of the process. Improved exergy efficiency of the process decreases the amount of exergy destruction.

For the validation of EEFs, dynamic models for the MCB distillation column and MCB plant with recycle are built. We implemented PI controllers for the two ( $LVQ_{cw}$  and  $DVQ_{cw}$ ) control configurations in the column in the plantwide layout along with inventory controls. In the plant wide layout, feed flow control, heater ( $HI$ ) temperature control, flash tank ( $FI$ ) level control and recycle stream flow controls are also implemented. Trial and error was used to determine acceptable tuning for this simulation and the PI controller parameters are listed in Table 6-6.

Table 6-6. PI controllers for the MCB distillation column

Control loops	<i>LVQ<sub>cw</sub> configuration</i>		<i>DVQ<sub>cw</sub> configuration</i>	
	$K_c$	$T_i(min)$	$K_c$	$T_i(min)$
Feed flow control	2.6	2	3	2
Overhead pressure control	3.3	0.6	3	0.5
Condenser level control	2	26	2	20
Reboiler level control	2	30	2	30
$x_D$ Composition control	5	20	5	23
$x_B$ Composition control	6.3	10	7	10

For each control configuration, the set points of CVs  $x_D$  and  $x_B$  are changed one by one and by the same amount ( $\pm 5\%$ ). The dynamic exergies in and out of the process are approximated by the proposed method of section 6.2.2.3. Figures 6-5 and 6-6 show the total dynamic exergies in and out of the distillation column in the plantwide layout for the two control configurations  $LVQ_{cw}$  and  $DVQ_{cw}$ , respectively. Figures 6-5 (a) and 6-5 (b) show the dynamic exergies in and out of the column under  $LVQ_{cw}$  control due to a step change in the set points of CVs  $x_D$  and  $x_B$ , respectively. Similarly, Figures 6-6 (a) and 6-6 (b) show the dynamic exergies of the column under  $DVQ_{cw}$  control.

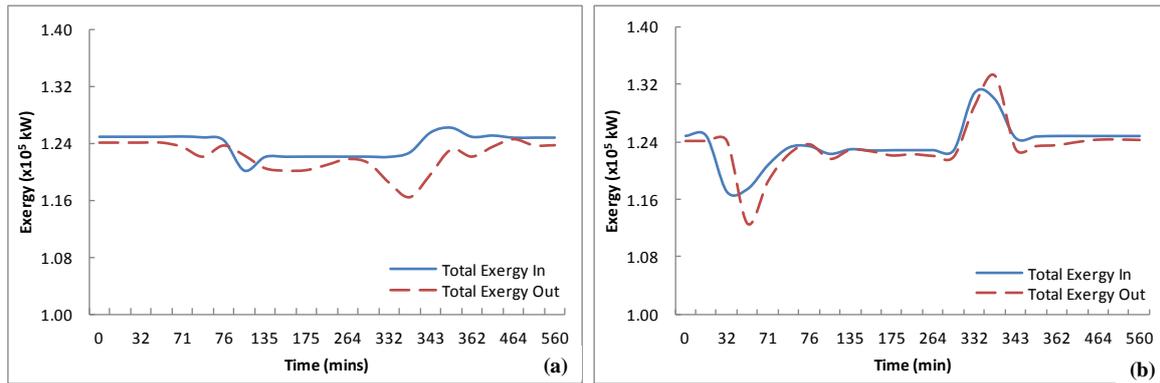


Figure 6-5. Variation of Exergy In and Out due to composition set point changes for the  $LVQ_{cw}$  configuration (a) Exergy variation due to step change in  $x_D$  (b) Exergy variation due to step change in  $x_B$

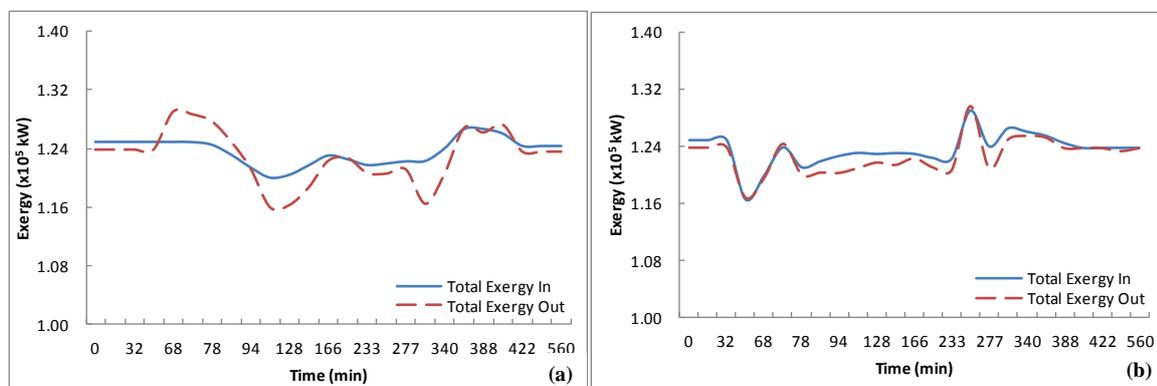


Figure 6-6. Variation of Exergy In and Out due to composition set point changes for the  $DVQ_{cw}$  configuration (a) Exergy variation due to step change in  $x_D$  (b) Exergy variation due to step change in  $x_B$

The total exergies for the entire 560 min time period of the test are listed in Table 6-7. From Table 6-7, the total destroyed exergy for the whole column is  $4.72 \times 10^7$  kW under  $DVQ_{cw}$  control. Compared to  $LVQ_{cw}$  control,  $DVQ_{cw}$  control can save up to 24% in exergy. This conclusion agrees with the result (save 19% in exergy) from the EEF analysis.

Table 6-7. Exergy used by the two control configurations  $LVQ_{cw}$  and  $DVQ_{cw}$  on the column within the MCB plantwide layout

Exergy( $\times 10^7$ kW)		Control Configuration	
		$LVQ_{cw}$	$DVQ_{cw}$
step change in $x_D$	Total exergy in	7.24	7.19
	Total exergy out	5.97	6.13
	Destroyed exergy	1.27	1.06
step change in $x_B$	Total exergy in	10.3	10.42
	Total exergy out	5.3	6.76
	Destroyed exergy	5.0	3.66
Total exergy destroyed		6.27	4.72

From the results discussed above, in the plantwide layout the distillation column is more eco-efficient under  $DVQ_{cw}$  control which contradicts the results from the eco-efficient control configuration  $LB$  control, for the same column in isolation. So the presence of recycle can have a significant impact on the control loop pair selection based on controllability and eco-efficiency. As the column has to be connected with other units of the plant in a plantwide layout, therefore the selection of controllable and eco-efficient control loop configuration should be based on plantwide layout.

Also from Table 6-5, significant EEF reduction is achieved by the control pair  $(V, x_B)$  from  $6.44 (\times 10^5 \text{ kW})$  to  $1.22 (\times 10^5 \text{ kW})$ . The most eco-efficient control configuration for the process design including a recycle is  $DVQ_{cw}$  control where the total EEF will be  $1.44 (\times 10^5 \text{ kW})$ . The most eco-efficient control configuration for the process design without a recycle is  $LB$  control. According to the analysis from Table 6-2, the total EEF is  $3.57 (\times 10^5 \text{ kW})$ . From comparing the values of EEF, we may conclude that the process design with recycle may save up to 60% exergy. Thus we may say that EEF can be used as an indicator to help evaluate different process designs.

However, the exergy saving with a recycle may not be significant for the whole plantwide layout. In the next section, we will evaluate the exergy changes account for the whole plantwide layout.

### 6.3.3. MCB plant with distillation column without recycle

Without consideration of the recycle, the control loop configuration selection ( $LB$  and  $DV$ ) remains the same as that of an isolated column. To study the effect of exergy destruction under different, well-performing control configurations ( $LB$  and  $DV$ ) on the whole MCB plant without a recycle, the effect on total exergy coming in and out of the plant due to step changes in composition controls ( $x_D$  and  $x_B$ ) is studied. The EEFs in Equation (6-3) for the MCB separation plant without recycle are listed in Table 6-8.

Table 6-8. EEFs for MCB plant with and without recycle

Control Pairs	EEF (kW.kmole/h) or (kW)	
	Without recycle	With recycle
$(L, x_D)$	115.2	94.3
$(D, x_D)$	5.87 E3	3.41
$(V, x_B)$	105.3	78.72
$(B, x_B)$	5.11 E3	1.08 E3
$(Q_{cw}, x_{HCl})$	—	1.28 E4

From Table 6-8, the control pairing ( $D, x_D$ ) will use the most exergy and be the least eco-efficient control pair, and the control pairing ( $V, x_B$ ) is the most eco-efficient pairing. The sums of the EEFs for the  $LB$  and  $DV$  control configurations are  $5.22 \times 10^5$  kW.kmole/h and  $5.98 \times 10^5$  kW.kmole/h, respectively. Both  $LB$  and  $DV$  control configurations are controllable but the process with an  $LB$  control configuration is more eco-efficient than the same process with a  $DV$  control configuration. The  $LB$  control configuration can save up to 12 % more exergy compared to the  $DV$  control configuration as calculated from Table 6-8.

For the validation of EEFs as shown in Table 6-8, dynamic simulation of the MCB plant without recycle is used. Figures 6-7 and 6-8 show the total dynamic exergies in and out of the MCB plant without recycle for the two control configurations  $LB$  and  $DV$ , respectively. Figures 6-7 (a) and 6-7 (b) show the dynamic exergies in and out of the MCB plant without recycle under  $LB$  control due to a step change in the set points of  $CVs$   $x_D$  and  $x_B$ , respectively.

Similarly, Figures 6-8 (a) and 6-8 (b) show the dynamic exergies of the MCB plant without recycle under *DV* control.

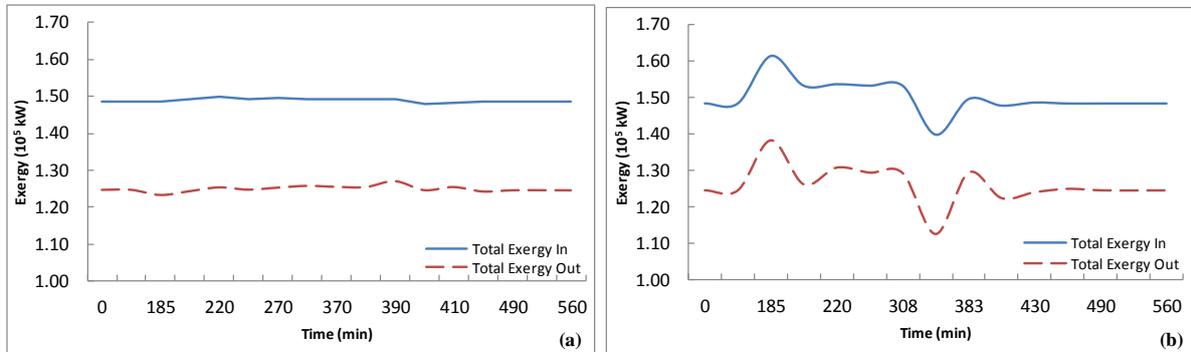


Figure 6-7. Variation of Exergy In and Out of MCB plant without recycle due to composition set point changes for the *LB* configuration (a) Exergy variation due to step change in  $x_D$  (b) Exergy variation due to step change in  $x_B$

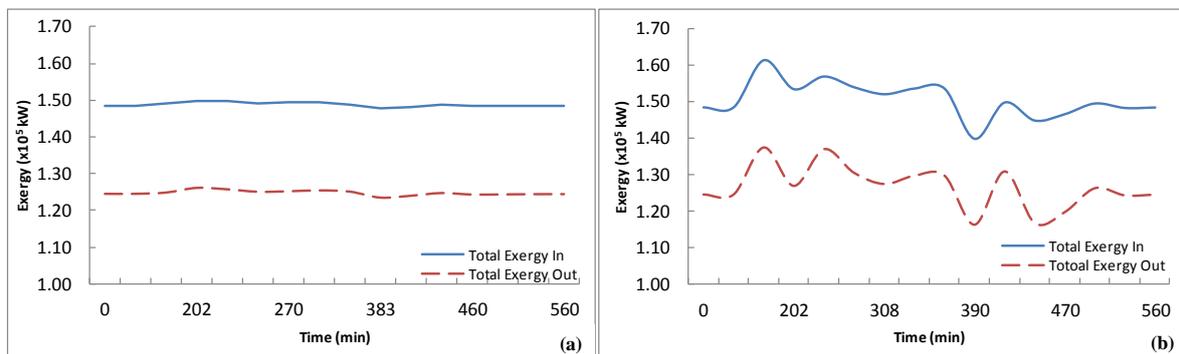


Figure 6-8. Variation of Exergy In and Out of MCB plant without recycle due to composition set point changes for the *DV* configuration (a) Exergy variation due to step change in  $x_D$  (b) Exergy variation due to step change in  $x_B$

Table 6-9. Exergy used by control configurations *LB* and *DV* in MCB plant without recycle

Exergy( $\times 10^7$ kW)		Control Configuration	
		<i>LB</i>	<i>DV</i>
step change in $x_D$	Total exergy in	8.36	8.36
	Total exergy out	6.98	7.02
	Destroyed exergy	1.38	1.34
step change in $x_B$	Total exergy in	8.59	8.67
	Total exergy out	7.22	7.19
	Destroyed exergy	1.37	1.48
Total exergy destroyed		2.75	2.84

The total exergies of the MCB plant without recycle for the entire 560 min time period of the test are listed in Table 6-9. The total exergy destroyed for the whole MCB plant without recycle is  $2.75 \times 10^7$  kW under *LB* control. Compared to *DV* control, *LB* control can save up to 3.1% in exergy.

#### 6.3.4. MCB plant with distillation column and recycle

To study the effect of exergy destruction under different, well-performing control configurations ( $LVQ_{cw}$  and  $DVQ_{cw}$ ) on the whole MCB plant, the effect on total exergy coming in and out of the plant due to step changes in composition controls ( $x_D$ ,  $x_B$ , and  $x_{HCl}$ ) is studied. Similar to previously, *LV* is still uncontrollable alone but we will study  $LVQ_{cw}$  for completeness. The EEFs for the whole MCB plant are shown in Table 6-8. From Table 6-8, the control pairing ( $B$ ,  $x_B$ ) will use the most exergy and be the least eco-efficient control pair, and the control pairing ( $D$ ,  $x_D$ ) is the most eco-efficient pairing. The sums of the EEFs for the  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are  $1.297(\times 10^4)$  kW.kmole/h) and  $1.28 (\times 10^4)$  kW.kmole/h), respectively. Both  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are controllable but the process with a  $DVQ_{cw}$  control configuration is more eco-efficient than the same process with a  $LVQ_{cw}$  control configuration. The  $DVQ_{cw}$  control configuration can save up to 1.3% more exergy compared to the  $LVQ_{cw}$  control configuration as calculated from Table 6-8.

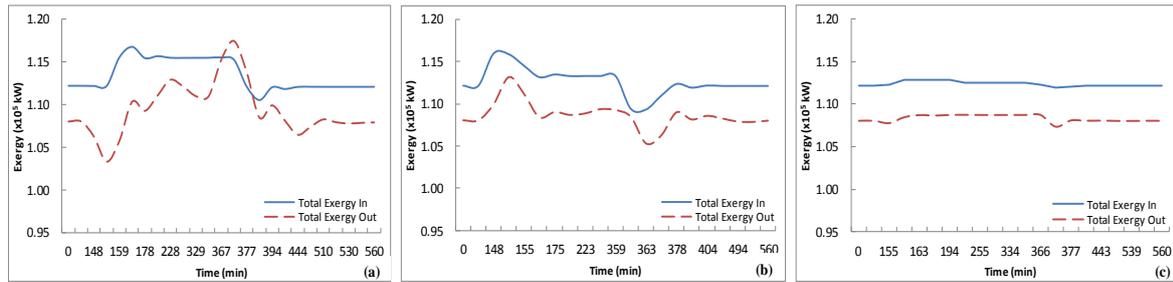


Figure 6-9. Variation of Exergy In and Out of MCB plant due to composition set point changes for the  $LVQ_{cw}$  configuration (a) Exergy variation due to step change in  $x_D$  (b) Exergy variation due to step change in  $x_B$  (c) Exergy variation due to step change in  $x_{HCl}$

These EEFs are validated by dynamic exergy plots after building a dynamic model of MCB plant. Figures 6-9 and 6-10 show the total dynamic exergies in and out of the whole MCB plant with the distillation column in the plantwide layout having two alternative control configurations  $LVQ_{cw}$  and  $DVQ_{cw}$ , respectively. Figures 6-9 (a), 6-9 (b) and 6-9 (c) show the dynamic exergies in and out of the MCB plant under  $LVQ_{cw}$  control due to a step change in the set points of  $CVs$   $x_D$ ,  $x_B$ , and  $x_{HCl}$ , respectively. Figures 6-10 (a), 6-10 (b) and 6-10 (c) show the dynamic exergies of the column under  $DVQ_{cw}$  control.

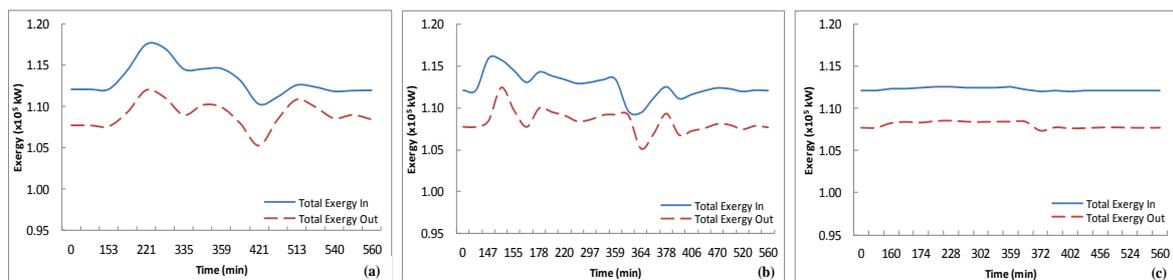


Figure 6-10. Variation of Exergy In and Out of MCB plant due to composition set point changes for the  $DVQ_{cw}$  configuration (a) Exergy variation due to step change in  $x_D$  (b) Exergy variation due to step change in  $x_B$  (c) Exergy variation due to step change in  $x_{HCl}$

Table 6-10. Total Exergy used by the whole MCB plant with the two control configurations

 $LVQ_{cw}$  and  $DVQ_{cw}$ 

Control Configuration		$LVQ_{cw}$	$DVQ_{cw}$
		Exergy( $\times 10^7$ kW)	
step change in $x_D$	Total exergy in	6.34	6.35
	Total exergy out	6.01	6.09
	Destroyed exergy	0.33	0.26
step change in $x_B$	Total exergy in	6.30	6.30
	Total exergy out	6.07	6.05
	Destroyed exergy	0.23	0.24
step change in $x_{HCl}$	Total exergy in	6.29	6.29
	Total exergy out	6.06	6.04
	Destroyed exergy	0.23	0.24
Total exergy destroyed		0.79	0.74

The total exergies of the MCB plant for the entire 560 min time period of the test are listed in Table 6-10. The exergy destroyed for the whole plant is  $0.74 \times 10^7$  kW under the  $DVQ_{cw}$  control configuration. Compared to  $LVQ_{cw}$  control,  $DVQ_{cw}$  control can save up to 6 % in exergy. Exergy destruction under both  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations due to step changes in  $x_B$  or  $x_{HCl}$  is similar. The major difference in exergy destruction between  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations is due to the step change in the top product composition control loop. So the selection of the manipulated variable for the top product composition control plays an important role in exergy destruction of the process during operation. It is not surprising that the exergy saved is much smaller for the whole plant than the individual distillation column (from 19% to 6%). The simple explanation is that the distillation column is only a portion of the whole plant.

We have used EEF to find that  $DVQ_{cw}$  control is the most eco-efficient control configuration in the whole plantwide sense. Now we would like to know how much exergy we can save for the process design with a recycle.

Compared to the exergy consumption of  $2.75 (\times 10^7 \text{kW})$  using *LB* control for the whole process without a recycle in Table 6-9, the exergy consumption using *DVQ<sub>cw</sub>* control is  $0.74 (\times 10^7 \text{kW})$  in Table 6-10, so we may save 73% of the exergy. This value is very close to the 60% saving which is calculated in section 6.3.2.

#### **6.4. Summary**

After selecting the best control scheme (one which is easily controllable) with the help of a number of classical techniques such as RGA, DRGA, NI and CN, EEF is used to decide the most eco-efficient control scheme for the whole process. The simulated case study results show that the presence of a recycle loop can have a significant impact on exergy destruction, thus affecting EEF results for an isolated unit. As, in practice, individual units are connected with other units of the plant through recycle loops, so the eco-efficiency (EEF) and controllability (RGA, DRGA, NI and CN) criterion should be based on plantwide layout with the consideration of recycle loops. A software algorithm/package for EEF calculation is explained in Chapter 7.

#### **6.5. Conclusions**

The selection of a control configuration can change significantly depending on whether it is considered alone or within a plantwide layout. The selection of control configuration for a unit should be based on results from when that unit is considered within the plantwide layout although it still needs to be controllable alone for start-up purposes, etc. EEF, a new measure, for integrating control loop configuration and eco-efficiency is described in this paper in detail. For plants with recycles the EEF decreases due to recycle of material and energy since recycling of material and energy decreases the exergy destruction within a process. The case study results show that the EEF can provide a qualitative and quantitative measure to guide engineers to select the most eco-efficient control configuration.

## References

- Bristol, E. (1966). "On a new measure of interaction for multivariable process control." Automatic Control, IEEE Transactions on **11**(1): 133-134.
- Denbigh, K. G. (1956). "The second-law efficiency of chemical processes." Chemical Engineering Science **6**(1): 1-9.
- Dincer, I. (2002). "The role of exergy in energy policy making." Energy Policy **30**(2): 137-149.
- Dincer, I., M. M. Hussain and I. Al-Zaharnah (2004). "Energy and exergy use in public and private sector of Saudi Arabia." Energy Policy **32**(14): 1615-1624.
- Dincer, I. and M. A. Rosen (2007). Exergy: Energy, Environment and Sustainable Development. Amsterdam, Elsevier.
- Fatehi, A. and A. Shariati (2007). Automatic pairing of MIMO plants using normalized RGA. Mediterranean conference on control and automation. Athens Greece
- Goldberg, J. and M. C. Potter (1998). Differential equations a systems approach. New Jersey, Prentice-Hall.
- He, M.-J. and W.-J. Cai (2004). "New Criterion for Control-Loop Configuration of Multivariable Processes." Industrial & Engineering Chemistry Research **43**(22): 7057-7064.
- Hinderink, A. P., F. P. J. M. Kerkhof, A. B. K. Lie, J. De Swaan Arons and H. J. Van Der Kooi (1996). "Exergy analysis with a flowsheeting simulator - I. Theory; calculating exergies of material streams." Chemical Engineering Science **51**(20): 4693-4700.
- Kotas, T. J. (1985). The exergy method of thermal plant analysis. London, Butterworths.
- Larsson, T. and S. Skogestad (2000). "Plantwide control - a review and a new design procedure." Modeling, Identification and Control **21**(4): 209-240.
- Luyben, W. L., B. D. Tyreus. and M. L. Luyben. (1998). Plantwide Process Control. New York, McGraw-Hill.
- McAvoy, T. J. (1983). Interaction Analysis: Principles and Applications. Research Triangle Park, NC, Instrument Society of America.
- McAvoy, T. J., Y. Arkun, R. Chen, D. Robinson and P. D. Schnelle (2003). "A new approach to defining a dynamic relative gain." Control Engineering Practice **11**(8): 907-914.
- Montelongo-Luna, J. M. (2010). Process design and control for eco-efficiency. Chemical and petroleum engineering. Calgary, Alberta, University of Calgary. **PhD**.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2007). "An exergy calculator tool for process simulation." Asia-Pacific Journal of Chemical Engineering **2**(5): 431-437.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2009). The Relative Exergy Array - A tool for integrated process design and control Chemeca 2009. Perth, Australia.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2010). "The relative exergy array—a new measure for interactions in process design and control." The Canadian Journal of Chemical Engineering **89**(3): 545-549.
- Moran, M. J. and E. Sciubba (1994). "Exergy Analysis: Principles and Practice." Journal of Engineering for Gas Turbines and Power **116**(2): 285-290.

- Muangnoi, T., W. Asvapoositkul and S. Wongwises (2007). "An exergy analysis on the performance of a counterflow wet cooling tower." Applied Thermal Engineering **27**(5-6): 910-917.
- Munir, M. T., J. J. Chen and B. R. Young (2010). A computer program to calculate the stream exergy using the visual basic graphical interface. Chemeca 2010. Adelaide, Australia.
- Munir, M. T., W. Yu and B. R. Young (2012). Control loop configuration and eco-efficiency. FOCAPO/CPC-VIII. Savannah, Georgia, USA.
- Munir, M. T., W. Yu and B. R. Young (2012). Determination of Plant-wide Control Loop Configuration and Eco-Efficiency, G.P. Rangaiah and V. Kariwala (Eds.). Plantwide Control: Recent Developments and Applications, John Wiley & Sons, ISBN:9780470980149.
- Munir, M. T., W. Yu and B. R. Young (2012). "Recycle effect on the relative exergy array." Chemical Engineering Research and Design **90**(1): 110-118.
- Niederlinski, A. (1971). "A heuristic approach to the design of linear multivariable interacting control systems." Automatica **7**(6): 691.
- Ogunnaike, B. A. and W. H. Ray (1994). Process dynamics, modelling and control, Oxford University press.
- Papadourakis, A., M. F. Doherty and J. M. Douglas (1987). "Relative gain array for units in plants with recycle." Industrial & Engineering Chemistry Research **26**(6): 1259-1262.
- Rosen, M. A. and I. Dincer (1997). "On exergy and environmental impact." International Journal of Energy Research **21**: 643-654.
- Rosen, M. A. and I. Dincer (1999). "Exergy analysis of waste emissions." International Journal of Energy Research **23**: 1153-1163.
- Rosen, M. A. and I. Dincer (2001). "Exergy as the confluence of energy, environment and sustainable development." Exergy, An International Journal **1**(1): 3-13.
- Seborg, D. E., T. F. Edgar and D. A. Mellichamp (1989). Process Dynamics and Control. New York, John Wiley & Sons.
- Seider, W. D., J. D. Seader. and D. R. Lewin. (2004). Product and Process Design Principles: Synthesis, Analysis, and Evaluation. New York, John Wiley.
- Skogestad, S., P. Lundström and E. W. Jacobsen (1990). "Selecting the best distillation control configuration." AIChE Journal **36**(5): 753-764.
- Svrcek, W. Y., D. P. Mahoney and B. R. Young (2006). A Real-Time Approach to Process Control. Chichester, John Wiley & Sons Ltd.
- Szargut, J., D. R. Morris and F. R. Steward (1988). Energy analysis of thermal, chemical, and metallurgical processes.
- Szargut, J., D. R. Morris. and F. R. Steward (1988). Exergy analysis of thermal, chemical, and metallurgical processes. New York, Hemisphere.
- Vasudevan, S. and G. P. Rangaiah (2010). "Criteria for Performance Assessment of Plantwide Control Systems." Industrial & Engineering Chemistry Research **49**(19): 9209-9221.
- Westphalen, D. L., B. R. Young and W. Y. Svrcek (2003). "A Controllability Index for Heat Exchanger Networks." Industrial & Engineering Chemistry Research **42**(20): 4659-4667.

- Witcher, M. F. and T. J. McAvoy (1977). "Interacting control systems: steady state and dynamic measurement of interaction." ISA Trans. **16**(3): 35-41.
- Xiong, Q., W.-J. Cai and M.-J. He (2005). "A practical loop pairing criterion for multivariable processes." Journal of Process Control **15**(7): 741-747.
- Zhu, Z.-X. and A. Jutan (1993). "A new variable pairing criterion based on the NIEDERLINSKI INDEX." Chemical Engineering Communications **121**(1): 235 - 250.

## Chapter 7

---

*A software algorithm/package for control loop configuration  
and eco-efficiency*

### **Article # 5**

**Co-authors: Wei. Yu, Brent. R. Young**

*Industrial Information & Control Centre (I<sup>2</sup>C<sup>2</sup>), Department of Chemical &  
Materials Engineering, The University of Auckland, Auckland, New Zealand*

Munir, M. T., W. Yu and B. R. Young (2012). A software algorithm/package for control loop configuration and eco-efficiency. IEEE transactions on industrial informatics. (Submitted).

## **Chapter 7. A software algorithm/package for control loop configuration and eco-efficiency**

This chapter is linked with Chapters 5 and 6, and presents all the details of an algorithm and software package (EEF calculator) for EEF calculation. The EEF calculator combines a commercial simulator, VMGSim, and Excel together for EEF calculation. EEF calculations are required in Chapters 5, 6, 7 and 8.

### **Abstract**

Software is a powerful tool to help us analyze industrial information and control processes. In this paper, we will show our recently development of a software algorithm/package which can help us select the more eco-efficient control configuration. Nowadays, the eco-efficiency of all industrial processes/plants has become more and more important; engineers need to find a way to integrate control loop configuration and measurements of eco-efficiency. The exergy eco-efficiency factor; a new measure of eco-efficiency for control loop configuration has been developed. This software algorithm/package will combine a commercial simulator, VMGSim, and Excel together to calculate the exergy eco-efficiency factor.

Key words: Software algorithm/package, process simulation, energy efficiency, eco-efficiency, exergy eco-efficiency factor.

### **7.1. Introduction**

The role of a process engineer has shifted from problem solving to new tool developments, planning, interpretations, new implementations and assessing processes for their relevance during last few decades. This shift of process engineer's role is due to the capabilities provided by modern age computers, software, solvers and process simulators e.g. complex/large data storage, easy/fast algorithm solution, complex data analysis, solving thousands of differential equations and logical decision making. It allows process engineers to solve/tackle quite complex problems rapidly which was not possible before (Peters and Timmerhaus 1991; Luyben 2002). A new role of process engineers and support of software for process engineering is explained in (Becker-Kornstaedt et al. 1999).

Most process simulators and solvers are based on numerical algorithms. A complex algorithm can also be a set of elementary algorithms of different types. The selection of algorithm for a

particular application depends on the nature of problem being solved and availability of additional information concerned with model equations (Tolsma et al. 2002).

There are many software programs solvers and commercial process simulators widely used in both industry and universities like Aspen HYSYS, VMGSim and Aspen Plus to analyze the steady state and dynamic behaviors of chemical processes. These simulators can also be used for customized functions/calculations, tools development for process design/process control/thermodynamics, steady state economics and dynamic controllability (Luyben 2002; Montelongo-Luna et al. 2007; Munir et al. 2010). These simulators are also used to test, optimize and integrate process plants with the design of industrial ecosystems (Casavant and Cote).

Process engineers have developed many mathematical and heuristic tools to facilitate the complex process of process design, process control, thermodynamic analysis, Eco-efficiency and integration of these fields (Koolen 2001; Wall 2003; Seferlis and Georgiadis 2004; Montelongo-Luna et al. 2007; Montelongo-Luna et al. 2010; Munir et al. 2012). For example, to integrate control loop configuration and measurement of eco-efficiency, we developed a new tool: the Exergy eco-efficiency factor (EEF) (Munir et al. 2012). Because of the complexity of the industrial processes, we cannot obtain the EEF values analytically. We have to use process simulators like Aspen HYSYS/VMGSim which are common in the development/calculation of these tools and which facilitate complex mathematical calculations (Montelongo-Luna et al. 2010; Munir et al. 2012).

In this paper, our intention is to show the potential help obtainable in EEF development/calculation by using the commercial process simulator VMGSim. EEF is based on the concept of exergy which is reusable energy; exergy can be used as a measure of eco-efficiency. For a general multi-input multi-output (MIMO) process, a certain amount of exergy consumption/generation is needed to change one controlled variable (CV) by using one manipulated variable (MV). The EEF is designed to measure this amount of exergy for different control pairings. The control pairing which needs the least exergy to fulfill its control targets will be most eco-efficient control pairing. EEF helps engineers to select the best control configuration for eco-efficiency.

Similarly, thermodynamic properties like exergy have the potential to be used for the development of process control structures, which involves integration of thermodynamics and process control. A basic framework for the development of a dynamic exergy balance for

process control evaluation has been proposed (Luyben et al. 1998). Some research has also been done on process control effects on entropy production (Alonso et al. 2002; Ydstie 2002; Antelo et al. 2007). The Relative Exergy Array (REA) was subsequently developed based on analyzing the exergy interactions for the control configuration within the process design (Montelongo-Luna et al. 2009; 2010; Munir et al. 2012). REA calculation using a commercial simulator (VMGSim) has been developed (Munir et al. 2010; 2012). The effect of recycle on the REA analysis was studied by (Munir et al. 2012). In analyzing most control loops, exergy can play an important role since it can be used for determining the exergetic efficiency and sustainability of a process (Dincer 2002). For example, environmental impacts can be minimized by reducing exergy losses and by the efficient use of exergy (Rosen and Dincer 1997; 1999; Rosen and Dincer 2001; Dincer et al. 2004).

In this work we used a commercial process simulator VMGSim for the development/calculation of EEF. VMGSim is one of the latest commercial process simulators. VMGSim has the most recent and updated thermodynamics for the prediction of thermodynamic data like Gibbs energy of formation used in exergy calculation. Therefore the use of process simulator/VMGSim helps in calculating the correct material exergy values.

This manuscript is organized as follows. After this general introduction, the concepts of eco-efficiency and EEF are explained. Then the software package/algorithm for the EEF calculation is explained. It follows the implementation of the proposed method for a simulation example. Finally, the results are discussed and conclusions drawn.

## **7.2. Eco-efficiency and Exergy Eco-efficiency factor (EEF)**

### **7.2.1. Eco-efficiency**

An Eco-efficient process is ecologically friendly and economically viable. Ecological friendly means the process has less consumption of energy or destruction of exergy.

According to the World Business Council for Sustainable Development (WBCSD) definition, eco-efficiency is achieved through the delivery of “competitively priced goods and services that satisfy human needs and bring quality of life while progressively reducing environmental impacts of goods and resource intensity throughout the entire life-cycle to a level at least in line with the Earth's estimated carrying capacity.” This concept describes a vision for the

production of economically valuable goods and services while reducing the ecological impacts of production. In other words eco-efficiency means producing more with less.

When applying the concept of eco-efficiency to control loop configuration, we developed a method which can help engineers select the manipulated variables which achieve the best products with the lowest energy cost. To achieve this aim, the EEF was developed (Munir et al. 2012).

### 7.2.2. Exergy eco-efficiency factor (EEF)

Exergy, and calculations involving it and its different components are explained in (Hinderink et al. 1996; Munir et al. 2012). Exergetic efficiency,  $\eta$ , is defined as the ratio of the exergy going out from, to the exergy going into a process (Szargut et al. 1988),

$$\eta = B_{out} / B_{in} \quad 7-1$$

where  $\eta$  = Exergetic efficiency,  $B_{out}$  = Total exergy going out of a process and  $B_{in}$  = Total exergy coming in to a process.



Figure 7-1. Exergy flows for a general process

The ratio can be used to measure the exergy efficiency of a process which is equivalent to eco-efficiency. A general process for exergetic efficiency calculation is shown in Figure 7-1. The definition of total exergy and detailed exergy calculation procedures using the simulator software VMGSim can be found in (Munir et al. 2010; Munir et al. 2012).

Equation (7-1) includes the exergy efficiency for the whole process; however it does not provide any information about how the control loop configuration affects this exergy efficiency. A new measure, EEF, which connects the control loop configuration to the eco-efficiency has been developed (Munir et al. 2012). The EEF for a control pair  $(u_j, y_i)$ , is defined as,

$$\tau_{ij} = (\Delta B_{out} - \Delta B_{in}) \frac{\Delta u_j}{\Delta y_i} \quad 7-2$$

where  $\Delta u_j$  denotes a step change of the *MV*,  $u_j$ ,  $\Delta y_i$  denotes a response in the *CV*,  $y_i$ , caused by a step change of the *MV*,  $u_j$ , and  $\Delta B_{out}$  and  $\Delta B_{in}$  represent the exergy differences caused by the *MV* step change for exergy out and exergy in, respectively. For example, if  $\tau_{21}$  is less than  $\tau_{22}$ , it means that for the same amount of *CV* change,  $\Delta y_2$ , using *MV*,  $u_1$ , will cause less exergy loss than using *MV*,  $u_2$ . The final interpretation is that the control pairing  $(u_1, y_2)$  is more eco-efficient than the pairing  $(u_2, y_2)$ .

### 7.3. Software algorithm/package for EEF calculation

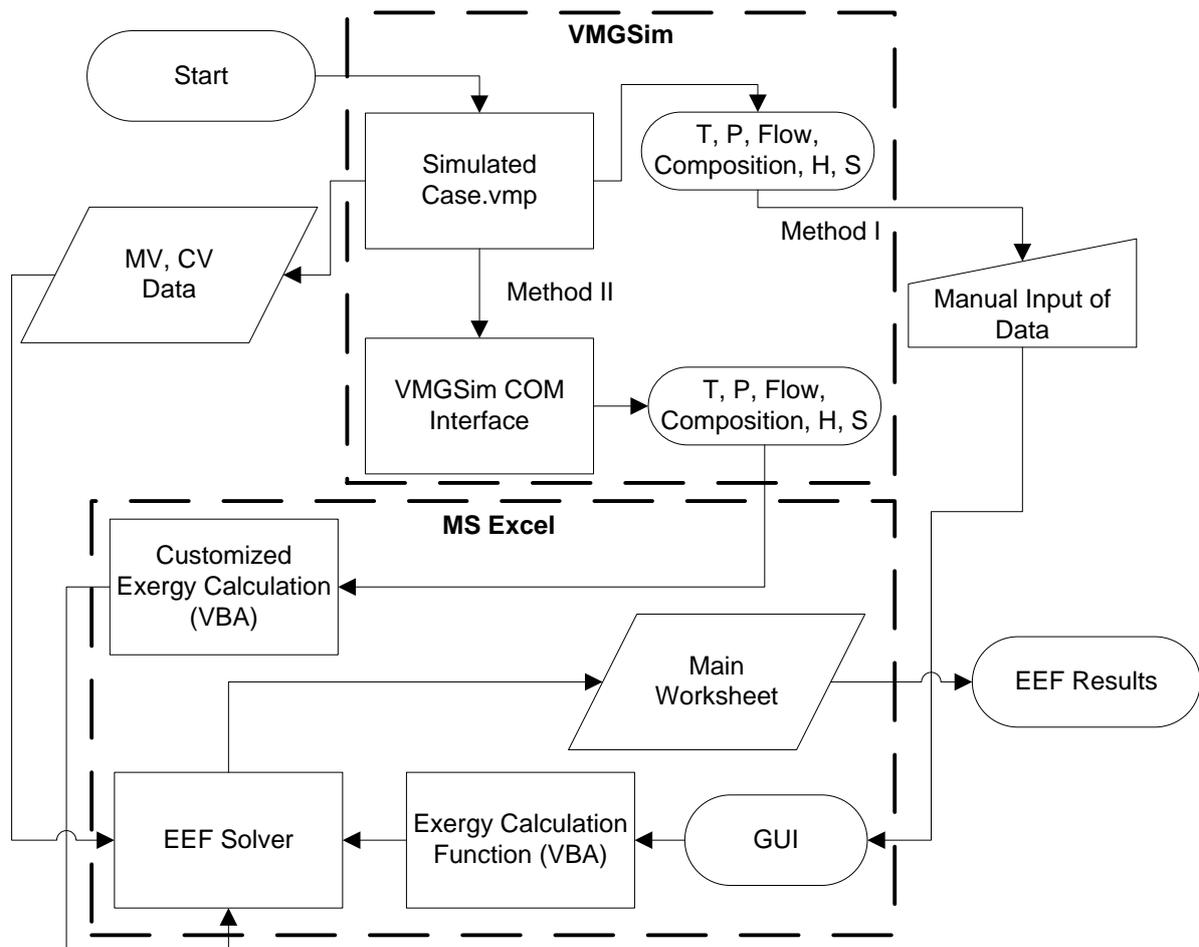


Figure 7-2. A generalized EEF calculation algorithm

A general algorithm for the calculation of EEF is shown in Figure 7-2. It consists of two integrated parts of VMGSim and MS Excel for EEF calculation. The EEF calculation algorithm starts with simulation of a given case study using process simulator (.vmp). The data of *MV*, *CV*, temperature (*T*), pressure (*P*), molar flow, composition, molar entropy (*S*) and molar enthalpy (*H*) of all material/energy streams are obtained from a simulated case.

These required data are obtained from the simulated case manually or by using the VMGSim COM interface. More details of the VMGSim COM (Component object modular) interface are explained in (Virtual Materials Group Inc. 2009). Based on the method (manual & VMGSim COM interface) selected for extracting data from simulated case, there are two types of exergy calculation paths/methods (Method I and Method II) as shown in Figure 7-2.

In method I, manual inputs of data in the GUI (Graphical user interface) are used for exergy calculation. More details of this method of exergy calculation are explained in (Munir et al. 2010). Method II is based on information extracted from the simulated case by using the VMGSim COM interface. In method II, a VBA (Visual Basics for applications) exergy calculation computer program needs customization. In this work we used Method I for exergy calculation. The information of exergies, MV and CV is given to the EEF solver which is based on Equation (7-2). Finally all the results from the EEF solver are arranged in main worksheet for analysis.

A more detailed general scheme for the calculation of EEF for a 3x3 system (three point composition control system) is shown in Figure 7-3. Figure 7-3 depicts a detailed version of the algorithm shown in Figure 7-2 for the EEF calculation of a three point composition control system e.g. a MCB plant. The EEF calculation scheme is divided into three main sections: i) VMGSim simulation, ii) Exergy calculation, and iii) EEF calculation as shown by dotted boundaries in Figure 7-3.

In process simulator /VMGSim simulation, following three basic steps are involved in order to get the information required for the exergy and EEF calculation as shown in Figure 7-3.

- 1) A Steady state base case is simulated by using process simulator to get the  $T$ ,  $P$ , molar flow, composition,  $S$  and  $H$  data of all material/energy streams.
- 2) Steady state cases with compositions AC1( $x_D$ ), AC2 ( $x_B$ ) and AC3 ( $x_{HCl}$ ) step changes are simulated using process simulator to get the  $T$ ,  $P$ , molar flow, composition,  $S$  and  $H$  data of all material/energy streams.
- 3) Manipulated and control variables (MV & CV) data is extracted from the simulated case study steady state base case and cases with AC1/AC2/AC3 step changes.

Exergy calculation requires the  $T$ ,  $P$ , molar flow, composition,  $S$  and  $H$  data of all material/energy streams from VMGSim simulation for the exergy calculation as shown in Figure 7-3. An integrated Visual Basic (VB) program and GUI was recently developed for this exergy calculation (Munir et al. 2010; 2012). The automation of exergy calculation has

also been done by using an open source simulator (Sim42) and a commercial simulator (Aspen HYSYS) (Montelongo-Luna et al. 2007). The total exergy of a material stream, including the three components: physical exergy, chemical exergy and exergy due to mixing, is defined and explained in (Hinderink et al. 1996).

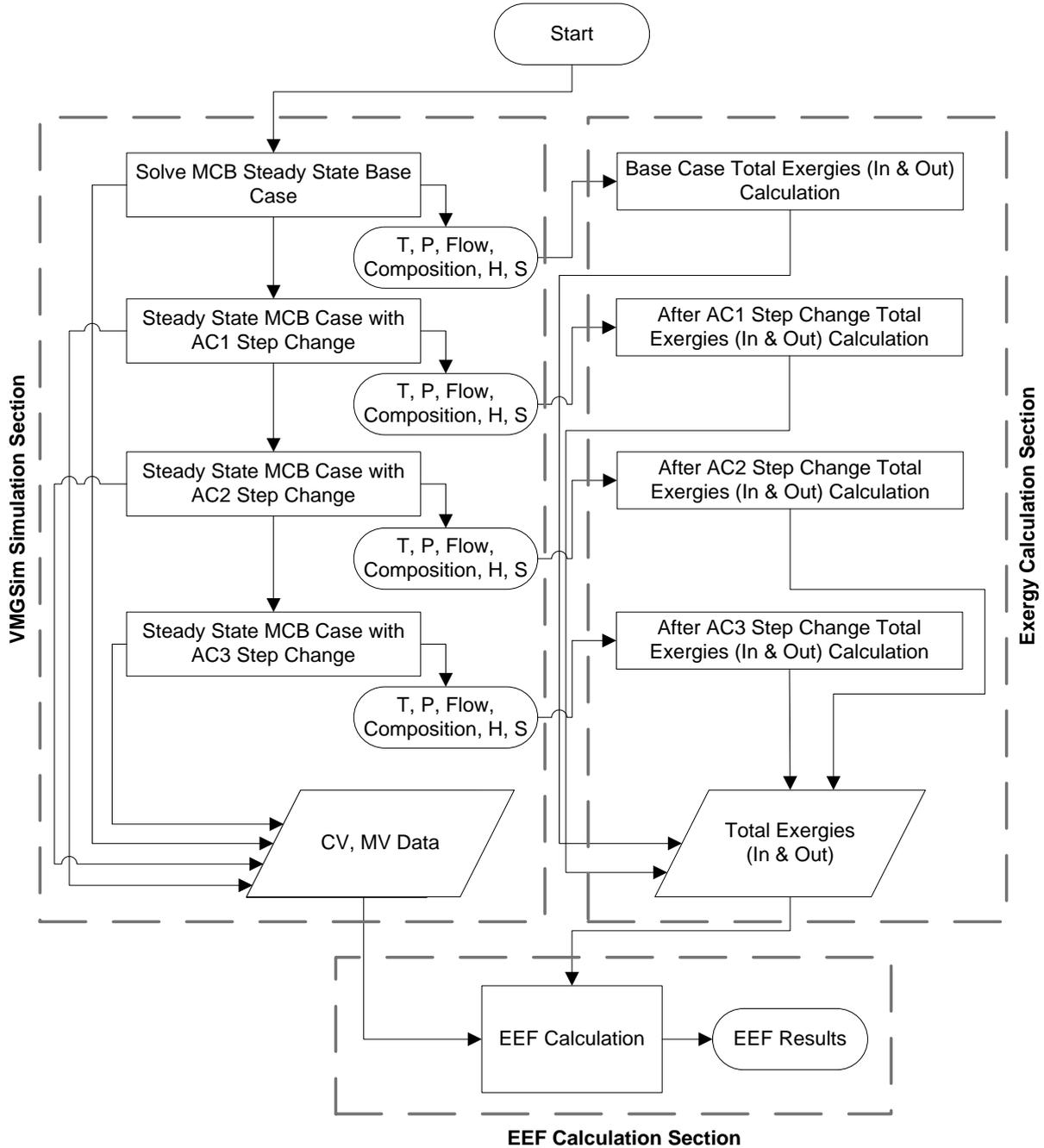


Figure 7-3. EEf calculation algorithm for 3x3 system

EEf calculation is based on MV, CV, total exergy in and exergy out data. MV, CV, total exergy in and exergy out data for EEf calculation is obtained from process

simulator/VMGSim simulation and exergy calculation as shown in Figure 7-3. EEF is calculated by using Equation (7-2), which correlates the MV, CV, and total exergies in and out of a process.

The integrated setup of the process simulator calculation, exergy calculation and EEF calculation sections is shown in Figure 7-3. VMGSim for simulation, MS Excel for exergy and EEF calculations are used as shown in Figures 7-2 and 7-3. The EEF calculation algorithm is applied below on an illustrative example (simple reactor, R1), for more explanation and understanding of algorithms in Figures 7-2 and 7-3.

For the explanation of EEF calculation using the algorithm shown in Figure 7-3, a simple reactor (R1) is used with hypothetical components as shown in Figure 7-4. The information about the hypothetical components and reaction is given Table 7-1.

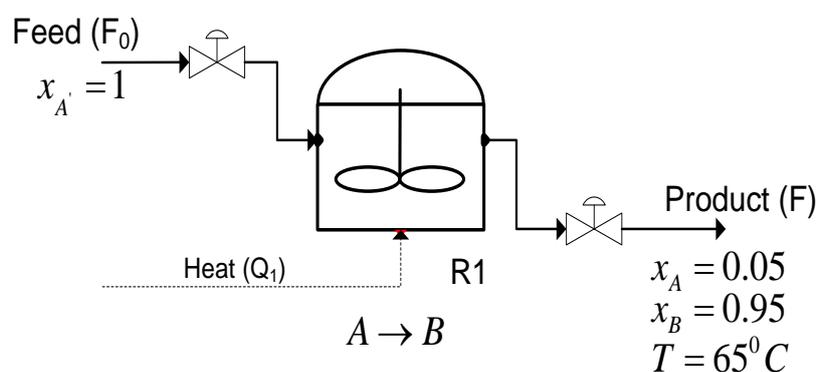


Figure 7-4. A simple CSTR with a hypothetical reaction,  $A \rightarrow B$

where  $F_0$  denotes the fresh feed flow rate having pure A,  $x_A$  denotes the mole fraction of A,  $x_B$  denotes the mole fraction of B, and  $F$  denotes the product flow rate of the mixture of A & B.

Table 7-1. Hypothetical components and reaction information

Hypothetical components details				Reaction Information
Component - A		Component - B		$r = k * x_A$
NBP (°C)	80	NBP (°C)	110	$k = A * \exp(-E / RT)$
Molecular weight	78	Molecular weight	96	$A = 6 * 10^8 \text{ kmol} / \text{m}^3 / \text{s}$ $E = 69,780 \text{ kJ} / \text{kmol}$

In this process, there are two controlled variables: component  $B$  composition,  $x_B$  and the temperature,  $T$  of the product. The composition and temperature of the product are affected by the feed flow rate or heat flow to the reactor. After selecting two control loops (composition and temperature control) the EEF is calculated by using the EEF algorithm as shown in Figure 7-3.

For EEF calculation of this reactor, steady state base case, steady state cases with component  $B$  composition,  $x_B$  and temperature,  $T$  step changes in the reactor were simulated in process simulator as per the algorithm shown in the VMGSim simulation section of Figure 7-3. The  $T$ ,  $P$ , molar flow, composition,  $S$  and  $H$  data of material/energy streams coming in ( $F_0$  and  $Q_I$ ) and going out ( $F$ ) of the reactor was extracted and used in exergy calculation as per the algorithm shown in the exergy calculation section of Figure 7-3. Finally, MV ( $F_0$  and  $Q_I$ ), CV ( $x_B$  and  $T$ ) and total exergy (in and out of reactor) data were used for EEF calculation as per the algorithm shown in the EEF calculation section of Figure 7-3. EEF is used to evaluate the effect of each control pair on the overall exergetic efficiency of the process. The calculated EEF results are listed in Table 7-2.

Table 7-2. EEFs for reactor, R1

Control loop pairs	$(F_0, x_B)$	$(Q, x_B)$	$(F_0, T)$	$(Q, T)$
EEF	2.77 E3	1.24 E4	14.71	27.30

From Table 7-2, the control pair  $(F_0, x_B)$  will use less exergy than control pair  $(Q, x_B)$  for controlling the product stream composition ( $x_B$ ). The control pair  $(F_0, T)$  uses slightly less exergy than the control pair  $(Q, T)$ . In the sense of eco-efficiency, the best control pair selections for this process should be  $(F_0, x_B)$  and  $(Q, T)$ .

For further explanation of the EEF calculation using the algorithm shown in Figure 7-3, a practical example of a MCB plant as shown in Figure 7-5 is used.

#### 7.4. Case study

For this case study a monochlorobenzene (MCB) separation process is selected from (Seider et al. 2004). It consists of three main parts: a flash vessel (F1), an absorption column (T1) and a distillation column (T2) as shown in Figure 7-5.

The feed of this process consists of a mixture of monochlorobenzene (MCB), benzene and hydrochloric acid (HCl). The vapor stream coming out of the flash tank is fed into the absorber where it is contacted with recycled MCB. Most HCl product comes out of the absorber as vapor. The liquid product (L2) coming out of the absorber is mixed with liquid product (L1) of the flash vessel in a mixer (M1). The mixture coming out of the mixer (M1) is then fed into the distillation column (T2). In this column a fixed amount (1% of inlet feed to the plant) is purged from the process to avoid HCl build-up in the system. The distillate product (*D*) contains most of the benzene and the bottom product (*B*) contains most of the MCB. A fraction of the bottom product stream is recycled back into the absorber.

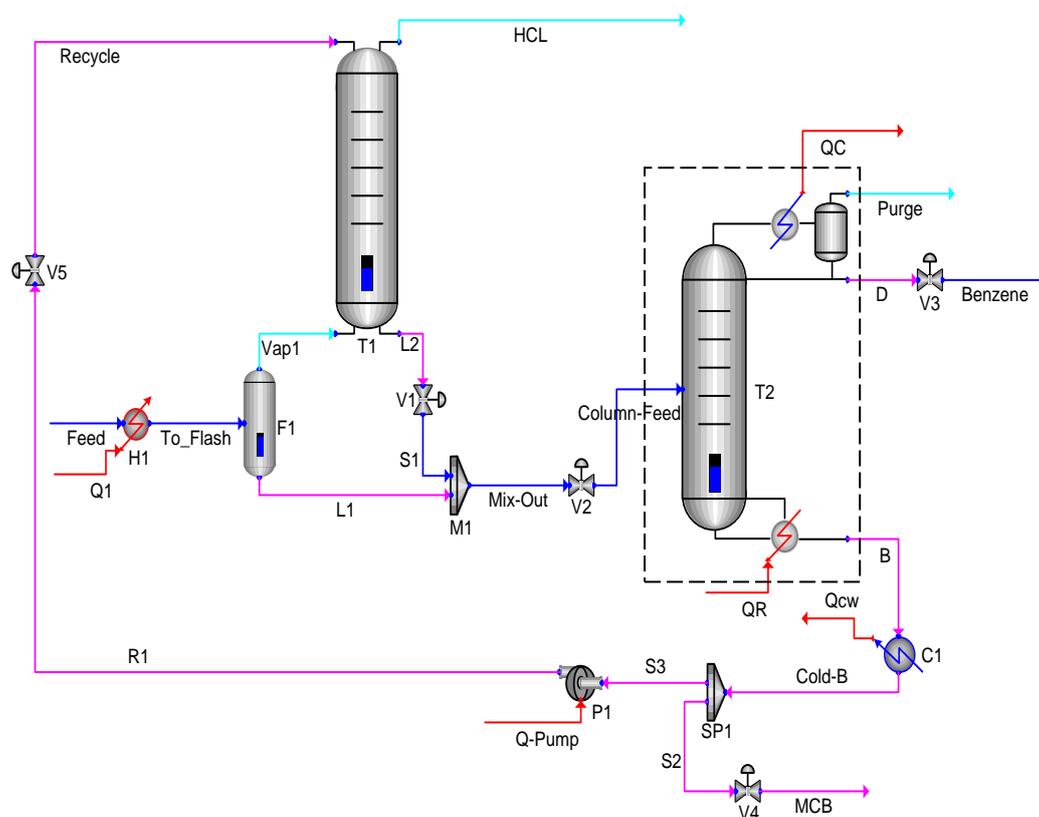


Figure 7-5. MCB separation process schematic

Process simulator/VMGSim with the NRTL activity thermodynamic model is used for this simulation of the MCB separation process. The detailed information of the feed conditions and column specifications can be found in (Seider et al. 2004). There are two further classifications of this case study: 1) an isolated distillation column and 2) MCB plant with distillation column and recycle.

In this case study, there are three composition control loops. The composition of HCl ( $x_{HCl}$ ) leaving in the vapor stream of the absorber is controlled by manipulating the cooler ( $CI$ ) duty ( $Q_{cw}$ ). The compositions at the top and bottom of the distillation column,  $x_D$  and  $x_B$ , are the other two controlled variables with  $x_{HCl}$  composition. For this three-point composition control of the MCB separation plant, three basic control configurations:  $LVQ_{cw}$ ,  $LBQ_{cw}$  and  $DVQ_{cw}$  are considered. For example, in the  $LVQ_{cw}$  control configuration,  $L$  (*Reflux rate*) is used to control the composition of the top product,  $x_D$ , boil-up rate ( $V$ ) is used to control the composition of the bottom product,  $x_B$ , and cooler duty ( $Q_{cw}$ ) is used to control the composition of vapor stream leaving the absorber (Seider et al. 2004).

### 7.5. EEF calculation software algorithm/package

A schematic of the integrated EEF calculation software algorithm/package is shown in Figure 7-6. It shows the integrated and combined working of a commercial process simulator and MS Excel to calculate the EEF in detail. It follows the same patterns of the generalized EEF calculation algorithm in Figure 7-2 and the EEF calculation algorithm for a 3x3 system in Figure 7-3.

In the process simulator/VMGSim simulation section, the MCB plant is simulated to extract the  $T$ ,  $P$ , molar flow, composition,  $S$  and  $H$  data of all material/energy streams. VMGSim is a flexible simulator as it can be integrated with Microsoft Excel by using the Excel unit operation in VMGSim. The MS Excel unit operation is used to extract this data. All the required data ( $T$ ,  $P$ , molar flow, composition,  $S$  and  $H$ ) of the material streams are fed into the exergy calculation section for exergy calculation of material streams.

The Exergy calculation section is based on data extracted from the process simulator simulation section as shown in Figure 7-6. In this section the three main parts of exergy: physical exergy, chemical exergy and exergy change due to mixing are calculated separately. An exergy calculation GUI is developed based on MS Excel VBA. More details of this exergy calculation GUI are given in (Munir et al. 2010; Munir et al. 2012).

The Exergy calculation GUI consists of four command buttons: “Physical Exergy”, “Chemical Exergy”, “Mixing Exergy” and “Total Exergy”. Each command button is assigned /based on VBA macros. These macros are developed by using the equations for calculation of these exergy components. The different exergy component results are also shown in the exergy calculation GUI as shown in Figure 7-6.

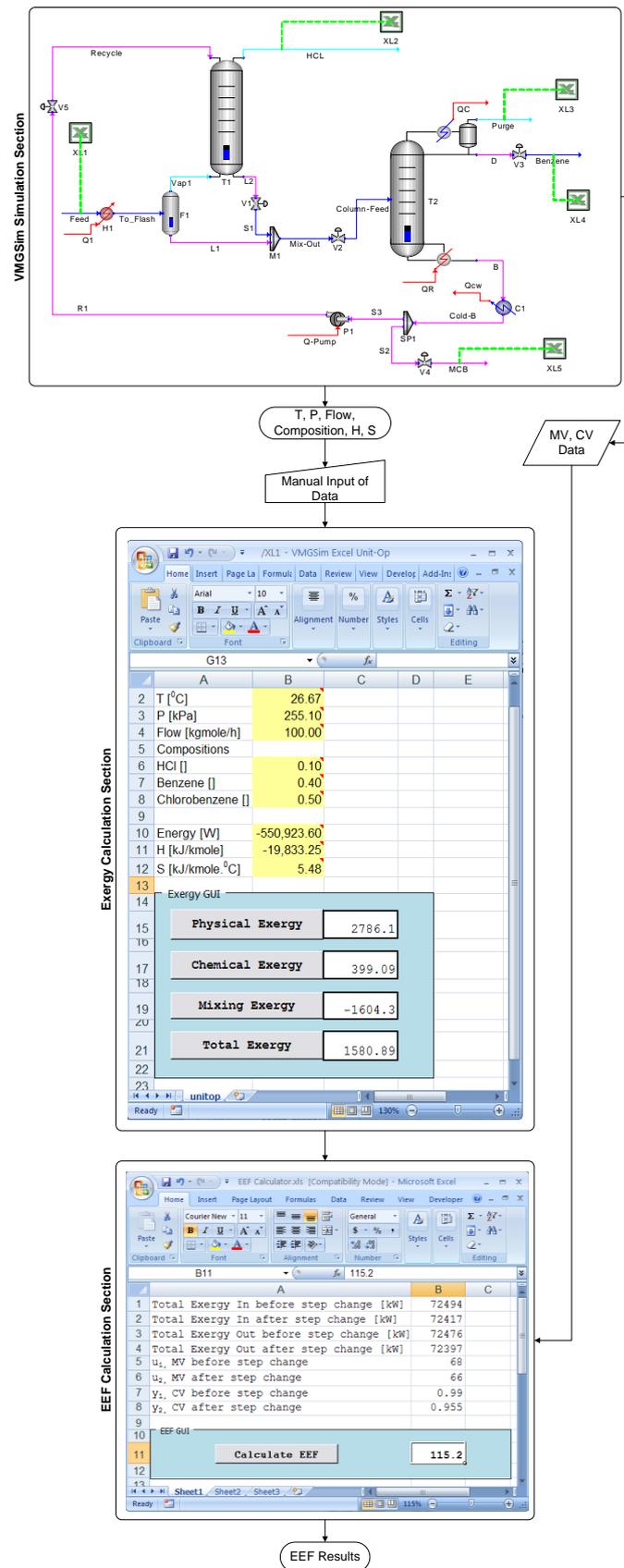


Figure 7-6. Schematic of EEF calculation software algorithm/package

The EEF calculation section is based on data extracted from the process simulator simulation and exergy calculation sections as shown in Figure 7-6.

Exergy values of material streams; before and after the step changes are calculated in the exergy calculation section and fed into the EEF calculation section. The MV and CV data are extracted from the simulated case study in the process simulator simulation section.

The EEF calculation GUI includes one command button “Calculate EEF”, which is on VBA macro for EEF calculation, based on Equation (7-2). All the information of total exergies in, out, MV and CV is entered manually in the EEF calculation section. The EEF result is also shown in the EEF calculation GUI as shown in Figure 7-6.

In this software package there is some data which needs to be entered manually, like  $T$ ,  $P$ , molar flow, composition,  $S$  and  $H$  of all material/energy streams in the exergy calculation section and total exergies in, out, MV and CV in the EEF calculation section. This software package can be further improved to avoid manual input by using VMGSim COM (Component object modular) automation. VMGSim COM automation is a programming interface to interact directly with the process simulator (VMGSim) without using process simulator’s graphical user interface.

The Exergy calculation section in Figure 7-6 shows the values of the three exergy components (physical; 2786.1kW, chemical; 399.09kW and mixing; -1604.3kW) and the total exergy (1580.89) of feed material stream coming into the MCB plant. The EEF calculation section in Figure 7-6 also shows the value of  $(L, x_D)$ , EEF calculation (115.2).

For EEF calculation of an isolated distillation column in the MCB plant as shown in the dotted boundary in Figure 7-5; a steady state base case and steady state cases with AC1 ( $x_D$ ) and AC2 ( $x_B$ ) step changes to the distillation column were simulated in process simulator as per the algorithm shown in VMGSim simulation section of Figure 7-3. The  $T$ ,  $P$ , molar flow, composition,  $S$  and  $H$  data of material/energy streams coming in (Column feed and  $Q_R$ ) and going out ( $Q_C$ , Purge, Benzene and  $B$ ) of the MCB column were extracted and used in exergy calculation as per the algorithm shown in the exergy calculation section of Figure 7-3. Finally, MV ( $LV / LB / DV$ ), CV ( $x_D$  and  $x_B$ ) and total exergies (in and out) of column data were used for EEF calculation as per the algorithm shown in the EEF calculation section of Figure 7-3.

For EEF calculation for the MCB plant, the steady state base case and steady state cases with

AC1( $x_D$ ), AC2 ( $x_B$ ) and AC3 ( $x_{HCl}$ ) step changes were simulated in process simulator as per the algorithm shown in the VMGSim simulation section of Figure 7-3. The  $T$ ,  $P$ , molar flow, composition,  $S$  and  $H$  data of material/energy streams coming in (Feed,  $Q_I$ ,  $Q_{Pump}$  and  $Q_R$ ) and going out ( $HCl$ ,  $Q_C$ , Purge, Benzene, MCB and  $Q_{CW}$ ) of the MCB plant were extracted and used in exergy calculation as per the algorithm shown in the exergy calculation section of Figure 7-3. Finally, MV ( $LVQ_{cw}/LBQ_{cw}/DVQ_{cw}$ ), CV ( $x_D$ ,  $x_B$  and  $x_{HCl}$ ) and total exergies (in and out of plant) data were used for EEF calculation as per the algorithm shown in the EEF calculation section of Figure 7-3. EEF is used to evaluate the effect of each control pair on the overall exergetic efficiency of the process.

Table 7-3. EEFs for MCB plant with and without recycle

Control Pairs	EEF (kW.kmole/h) or (kW)	
	Without	With recycle
( $L$ , $x_D$ )	115.2	94.3
( $D$ , $x_D$ )	5.87 E3	3.41
( $V$ , $x_B$ )	105.3	78.72
( $B$ , $x_B$ )	5.11 E3	1.08 E3
( $Q_{cw}$ , $x_{HCl}$ )	—	1.28 E4

The EEFs in Equation (7-2) for an isolated column without recycle are listed in Table 7-2. From Table 7-3, the control pairing ( $D$ ,  $x_D$ ) will use the most exergy and be the least eco-efficient control pair, and the control pairing ( $V$ ,  $x_B$ ) is the most eco-efficient pairing. The sums of the EEFs for the  $LB$  and  $DV$  control configurations are 5.22 and 5.98 ( $\times 10^5$  kW) respectively. Both  $LB$  and  $DV$  control configurations are controllable but the process with an  $LB$  control configuration is more eco-efficient than the same process with a  $DV$  control configuration. The  $LB$  control configuration can save up to 12 % more exergy compared to the  $DV$  control configuration as calculated from Table 7-3.

The EEFs for the whole MCB plant are shown in Table 7-3. From Table 7-3, the control pairing ( $B$ ,  $x_B$ ) will use the most exergy and be the least eco-efficient, and the control pairing ( $D$ ,  $x_D$ ) is the most eco-efficient. The sums of the EEFs for the  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are  $1.30 \times 10^4$  kW and  $1.28 \times 10^4$  kW, respectively. Both  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are controllable but the process with a  $DVQ_{cw}$  control configuration is slightly more eco-efficient than the same process with an  $LVQ_{cw}$  control configuration. The

$DVQ_{cw}$  control configuration can save 1.3% more exergy compared to the  $LVQ_{cw}$  control configuration as calculated from Table 7-3.

## 7.6. Summary

EEF integrates the control loop configuration and eco-efficiency of a process. EEF is calculated by using a software package/algorithm, developed and explained in this chapter, where we showed the potential help obtainable in EEF calculation by using a commercial simulator VMGSim. VMGSim works together with MS Excel to calculate EEF. All the data ( $T$ ,  $P$ , molar flow, composition,  $S$ ,  $H$ ,  $MV$  and  $CV$ ) of material/energy streams coming in and going out of the process is fed into exergy and EEF calculators for EEF calculation of all control pair combinations. EEF results are arranged in a main worksheet to compare/evaluate the effect of each control pair on the overall exergetic efficiency of the process.

## 7.7. Conclusions

Commercial simulators like VMGSim have a great potential to help in tools development/calculation for process design, control and thermodynamics like EEF. VMGSim has ability to facilitate complex mathematical calculations involved in EEF calculation. EEF calculated with process simulator/VMGSim helps engineers to select the best control configuration for eco-efficiency within a short period of time and in a cost effective manner during the early process design stages. This software package can be further improved and avoid manual inputs by using process simulator COM automation.

## References

- Alonso, A. A., B. E. Ydstie and J. R. Banga (2002). "From irreversible thermodynamics to a robust control theory for distributed process systems." Journal of Process Control **12**(4): 507-517.
- Antelo, L. T., I. Otero-Muras, J. R. Banga and A. A. Alonso (2007). "A systematic approach to plant-wide control based on thermodynamics." Computers & Chemical Engineering **31**(5-6): 677-691.
- Becker-Kornstaedt, U., D. Hamann, R. Kempkens, P. Rosch, M. Verlage, R. Webby, J. Zettel, M. Jarke and A. Oberweis (1999). Support for the Process Engineer: The Spearmint Approach to Software Process Definition and Process Guidance Advanced Information Systems Engineering, Springer Berlin / Heidelberg. **1626**: 119-133.
- Casavant, T. E. and R. P. Cote "Using chemical process simulation to design industrial ecosystems." Journal of Cleaner Production **12**(8-10): 901-908.
- Dincer, I. (2002). "The role of exergy in energy policy making." Energy Policy **30**(2): 137-149.
- Dincer, I., M. M. Hussain and I. Al-Zaharnah (2004). "Energy and exergy use in public and private sector of Saudi Arabia." Energy Policy **32**(14): 1615-1624.
- Hinderink, A. P., F. P. J. M. Kerkhof, A. B. K. Lie, J. De Swaan Arons and H. J. Van Der Kooi (1996). "Exergy analysis with a flowsheeting simulator - I. Theory; calculating exergies of material streams." Chemical Engineering Science **51**(20): 4693-4700.
- Koolen, J. L. A. (2001). Design of Simple and Robust Process Plants. Weinheim, Germany, WILEY-VCH.
- Luyben, W. L. (2002). Plantwide dynamic simulators in chemical processing and control. New York, Marcel Dekker, Inc.
- Luyben, W. L., B. D. Tyreus. and M. L. Luyben. (1998). Plantwide Process Control. New York, McGraw-Hill.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2007). "An exergy calculator tool for process simulation." Asia-Pacific Journal of Chemical Engineering **2**(5): 431-437.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2009). The Relative Exergy Array - A tool for integrated process design and control Chemeca 2009. Perth, Australia.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2010). "The relative exergy array—a new measure for interactions in process design and control." The Canadian Journal of Chemical Engineering **89**(3): 545-549.
- Munir, M. T., J. J. Chen and B. R. Young (2010). A computer program to calculate the stream exergy using the visual basic graphical interface. Chemeca 2010. Adelaide, Australia.
- Munir, M. T., W. Yu and B. R. Young (2012). Control loop configuration and eco-efficiency. FOCAPO/CPC-VIII. Savannah, Georgia, USA.
- Munir, M. T., W. Yu and B. R. Young (2012). Determination of Plant-wide Control Loop Configuration and Eco-Efficiency, G.P. Rangaiah and V. Kariwala (Eds.). Plantwide

- Control: Recent Developments and Applications, John Wiley & Sons, ISBN:9780470980149.
- Munir, M. T., W. Yu and B. R. Young (2012). "Recycle effect on the relative exergy array." Chemical Engineering Research and Design **90**(1): 110-118.
- Peters, M. S. and K. D. Timmerhaus (1991). Plant Design and Economics for Chemical Engineers. New York, McGraw-Hill.
- Rosen, M. A. and I. Dincer (1997). "On exergy and environmental impact." International Journal of Energy Research **21**: 643-654.
- Rosen, M. A. and I. Dincer (1999). "Exergy analysis of waste emissions." International Journal of Energy Research **23**: 1153-1163.
- Rosen, M. A. and I. Dincer (2001). "Exergy as the confluence of energy, environment and sustainable development." Exergy, An International Journal **1**(1): 3-13.
- Seferlis, P. and M. C. Georgiadis (2004). The integration of process design and control-Summary and future directions. Computer Aided Chemical Engineering. **17**: 1-9.
- Seider, W. D., J. D. Seader. and D. R. Lewin. (2004). Product and Process Design Principles: Synthesis, Analysis, and Evaluation. New York, John Wiley.
- Szargut, J., D. R. Morris. and F. R. Steward (1988). Exergy analysis of thermal, chemical, and metallurgical processes. New York, Hemisphere.
- Tolsma, J. E., P. I. Barton, B. Bertrand and G. Rafiqul (2002). Chapter 3.2 Numerical solvers. Computer Aided Chemical Engineering, Elsevier. **Volume 11**: 127-164.
- Virtual Materials Group Inc. (2009). "VMGSim V5.0 User's Manual."
- Wall, G. (2003). "Exergy tools." Proceedings of the Institution of Mechanical Engineers, Part A: Journal of Power and Energy **217**(2): 125-136.
- Ydstie, B. E. (2002). "Passivity based control via the second law." Computers & Chemical Engineering **26**(7-8): 1037-1048.

## Chapter 8

---

*The relative exergy destroyed: A new tool for process design  
and control*

**Article # 6**

**Co-authors: Wei. Yu, Brent. R. Young**

*Industrial Information & Control Centre (I<sup>2</sup>C<sup>2</sup>), Department of Chemical &  
Materials Engineering, The University of Auckland, Auckland, New Zealand*

Munir, M. T., W. Yu and B. R. Young (2012). The relative exergy destroyed: A new tool for process design and control. The Canadian Journal of Chemical Engineering. (Submitted)

## **Chapter 8. The Relative exergy-destroyed array: A new tool for process design and control**

This chapter presents a new tool, the relative exergy-destroyed array or REDA, for process design and control, and guidelines for interpreting its results. The REDA provides a means to compare the eco-efficiency of MIMO processes for various combinations of control schemes. This chapter is a continuation of chapters 5, 6, and 7 and also demonstrates the implementation of REDA in various simulation case studies.

### **Abstract**

Due to increasing energy demands, energy crises and strict environmental regulations, the eco-efficiency of all industrial processes and plants has become vitally important. Control loop configuration or control system structure is a major and vitally important activity in the complex task of process control because a poorly structured control strategy can lose a lot of energy from the process or plant. To save the loss of energy due to a poorly structured control strategy, engineers need to find a way to integrate control loop configuration and measurements of eco-efficiency. In this paper, we present the relative exergy-destroyed array (REDA), a new tool to measure the relative eco-efficiency of a process. The REDA is a means to compare eco-efficiency of multi-input multi-output processes for different combinations of control structures. Although based on steady state information, it is a simple tool for comparing eco-efficiency. The results obtained from the REDA are interpreted and explained with the help of simple case studies. The REDA will help guide the process designer to quickly find an optimal control design with low operating costs and high eco-efficiency.

Key words: Relative exergy-destroyed array (REDA), Exergy eco-efficiency factor (EEF), Relative Gain Array (RGA), Control configuration, Process design.

### **8.1. Introduction**

Process control is a complex task. It can be divided into five main parts: 1) process design, 2) control system structure, 3) controller algorithm/configuration, 4) controller tuning, and 5) control hardware/infrastructure. Process design is the design of the process that can be controlled easily. It is the first step in this complex task of process control. Control system

structure deals with control loop configuration or control pair selection. Controller algorithm/configuration decides the type of controller, i.e. P only, PI or PID control. The next part of this task deals with tuning of controllers and determining the tuning constants. The last part involves the selection of control hardware, i.e. control valves, sensors and final control elements (Luyben et al. 1998; Marlin 2000).

Control system structure selection is the second step in the process control task after process design, and is based on the type of control used for the process. The process can be either controlled by a centralized multi-input multi-output (MIMO) controller or by a set of single-input single-output (SISO) controllers, also called decentralized controllers. Decentralized control systems are more common in industry and have several attractive advantages: 1) simple algorithms, 2) easy to understand, 3) hardware simplicity, and 4) design simplicity (Morari and Evangelos 1989; Marlin 2000).

Control system structure determination for a decentralized control system focuses on deciding the best control scheme for pairing manipulated variables (MV) and controlled variables (CV). Effective control system structure selection is vital because a poor control structure will result in poor performance. For selecting the best control configuration, there are several common techniques in use, such as the relative gain array (RGA), the Niederlinski index (NI), singular value decomposition (SVD), the condition number (CN), and Morari's resiliency index (MRI) (Seborg et al. 1989; Svrcek et al. 2006). However, all of these techniques only consider the controllability and do not provide any information about the eco-efficiency of the different control configurations.

In this modern age of decreasing energy resources, energy crises and increasing energy costs, control loop configuration must not only focus on control loop analysis and consideration of the quality of control, but should also consider energy usage, energy costs, and environmental impact. Eco-efficiency is achieved through the pursuit of three objectives: to improve energy usage, reduce energy costs, and minimize environmental impact.

Thermodynamic properties like exergy have the potential to be used to improve the energy usage, reduce energy costs, and minimize environmental impacts. The concept of exergy unequivocally indicates what is wasted in terms of energy. More details of exergy are given by Szargut et al. (1988). The concept of exergy improves the energy usage and reduces the cost by providing a means of finding the inefficient parts of a process (Szargut et al. 1988; Moran and Sciubba 1994; Montelongo-Luna et al. 2007; Muangnoi et al. 2007). Exergy can

also play an important role in controlling environmental impacts by reducing exergy losses and by the efficient use of exergy (Rosen and Dincer 1997; Rosen and Dincer 1999; Dincer et al. 2004; Dincer and Rosen 2007).

Exergy also has the potential to be used for the development of process control structures to integrate control loop configuration and eco-efficiency. A basic framework for the development of a dynamic exergy balance for process control evaluation has been proposed by Luyben et al. (1998). The Relative Exergy Array (REA) was developed based on analysing the exergy interactions for the control configuration within the process design (Montelongo-Luna et al. 2009; 2010). But the REA measures the eco-efficiency only within the scope of the individually selected control loops. A new measure of eco-efficiency, the exergy eco-efficiency factor (EEF), has also been proposed for the eco-efficiency analysis of the whole unit, process or even plant (Munir et al. 2012). Some research has also been done on the process control effects on entropy production (Alonso et al. 2002; Ydstie 2002).

The use of EEFs integrates control loop configuration and eco-efficiency analysis of the whole process. For a general MIMO process, a certain amount of exergy consumption/generation is needed to change one CV by using one MV. The EEF is designed to measure this amount of exergy for different control pairings. The control pairing which needs the least exergy to fulfil its control targets will be most eco-efficient control pairing. The EEF helps engineers to select the best control configuration for eco-efficiency. This measure only considers the steady state situation and ignores the exergy interaction. More details on the EEF are given by Munir et al. (2012).

The relative exergy eco-efficiency factor array (REEFA) for an  $n \times n$  MIMO process is defined analogously to the RGA. A REEFA is an array of EEFs for all possible pairing combinations of a MIMO process. The combination of the REEFA and the RGA helps to develop a new tool called the Relative exergy-destroyed array (REDA). The application of the REDA is a two-step process in which the controllability is fixed before addressing the results of REEFA (i.e. RGA results are selected before comparing REEFA results). The REDA is a new tool to compare relative eco-efficiency of a MIMO process with different possible control schemes simultaneously.

In this paper, the development of a new tool, the relative exergy destroyed array (REDA), is proposed to measure the relative eco-efficiency of a MIMO process for different combinations of control structures. The REDA compares the eco-efficiency of a process

under different control structures including the exergy interaction. As the REDA is the product of the RGA and the REEFA, REDA combines the properties of RGA, REA and EEF (controllability and eco-efficiency). In other words, the REDA arranges destroyed exergy during a step input in an array under different possible control schemes. This array of the destroyed exergies for a MIMO process with different possible control schemes compares destroyed exergies qualitatively during a step input disturbance simultaneously and helps to select a control scheme which destroys the least exergy among all possible control schemes - also called the most eco-efficient control scheme.

This chapter is organized as follows. After this general introduction, the concepts of eco-efficiency, the EEF and the RGA are explained in section 8.2. The REDA is then proposed and guidelines for interpreting its results are presented and explained in section 8.3. Then the proposed method is implemented for simulation examples in section 8.4. Finally, in sections 8.5 and 8.6, the results are discussed and conclusions are made.

## **8.2. Eco-efficiency, Exergy eco-efficiency factor (EEF) and RGA**

### **8.2.1. Eco-efficiency**

Eco-efficiency is a strategy of doing more with less. Eco-efficiency is achieved through the pursuit of three main tasks: optimizing use of resources, reducing environmental impacts, and increasing product or service value. Eco-efficiency reduces the material and energy intensity of products and increases product durability; this results in cost saving and sustainability. Eco-efficiency also optimizes the use of materials and resources and minimizes waste (DeSimone and Popoff 1998).

An ecologically friendly process is one that consumes less energy or destroys less exergy. Because an eco-efficient process minimizes waste emissions, increases cost savings, and improves sustainability, it is, therefore, both ecologically friendly and economically viable.

When applying the concept of eco-efficiency to control loop configuration, the researchers developed a method that can help engineers select the manipulated variables that achieve the best products with the lowest energy cost. The EEF was developed to achieve this aim.

### 8.2.2. Exergy eco-efficiency factor (EEF)

The concept of EEF is based on exergy. The details of exergy, its calculations and its different components are explained by (Hinderink et al. 1996; Munir et al. 2012). Exergetic efficiency,  $\eta$ , is defined as the ratio of the exergy going out to the exergy going into a process (Szargut et al. 1988),

$$\eta = B_{Out} / B_{In} \quad 8-1$$

where  $\eta$  = exergetic efficiency,  $B_{Out}$  = total exergy going out of a process and  $B_{In}$  = total exergy coming in to a process.

The above ratio can be used to measure the exergy efficiency of a process (Figure 8-1), which is equivalent to eco-efficiency. The definition of total exergy and the detailed exergy calculation procedures using the simulator software VMGSim can be found in (Munir et al. 2010; 2012).

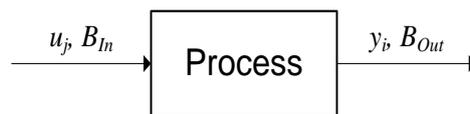


Figure 8-1. Exergy flows for a general process

Equation (8-1) includes the exergy efficiency for the whole process; however, it does not provide any information about how the control loop configuration affects this exergy efficiency. Thus, a new measure has been developed, the EEF, which connects the control loop configuration to the eco-efficiency (Munir et al. 2012). The EEF for a control pair ( $u_j$ ,  $y_i$ ), is defined as:

$$\tau_{ij} = (\Delta B_{out} - \Delta B_{in}) \frac{\Delta u_j}{\Delta y_i} \quad 8-2$$

where  $\Delta u_j$  denotes a step change of the *MV*,  $u_j$ ;  $\Delta y_i$  denotes a response in the *CV*,  $y_i$ , caused by a step change of the *MV*,  $u_j$ ; and  $\Delta B_{out}$  and  $\Delta B_{in}$  represent the exergy differences caused by the *MV* step change for exergy out and exergy in, respectively. For example, if  $\tau_{21}$  is less than  $\tau_{22}$ , it means that for the same amount of *CV* change,  $\Delta y_2$ , using *MV*,  $u_1$ , will cause less exergy destruction than using *MV*,  $u_2$ . The final interpretation is that the control pairing ( $u_1$ ,  $y_2$ ) is more eco-efficient than the pairing ( $u_2$ ,  $y_2$ ).

### 8.2.3. The Relative Gain Array (RGA)

The RGA is an array of relative gains ( $\lambda_{ij}$ ) for all possible pairing combinations of a multi loop single-input single-output (SISO) system, as shown in Equation (8-3) (Bristol 1966).

$$\Lambda = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \cdots & \lambda_{1n} \\ \lambda_{21} & \lambda_{22} & \cdots & \lambda_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \lambda_{n1} & \lambda_{n2} & \cdots & \lambda_{nn} \end{bmatrix} \quad 8-3$$

where  $\Lambda$  = Relative gain array and  $\lambda_{ij}$  = relative gain for a control pair ( $u_j, y_i$ )

The relative gain,  $\lambda_{ij}$ , which relates the  $j^{\text{th}}$  input,  $u_j$ , and  $i^{\text{th}}$  output,  $y_i$ , can be expressed by the following equation:

$$\lambda_{ij} = \frac{\left( \frac{\Delta y_i}{\Delta u_j} \right)_{u_k = \text{const}, k \neq j}}{\left( \frac{\Delta y_i}{\Delta u_j} \right)_{y_k = \text{const}, k \neq i}} \quad 8-4$$

Relative gain is defined as the ratio of open loop process gain in an isolated loop to apparent process gain in the same loop when all other control loops are closed and are in perfect control. The open loop process gain is defined as:

$$k_{ij} = \left( \frac{\Delta y_i}{\Delta u_j} \right)_{u_k = \text{const}, k \neq j} \quad 8-5$$

where  $k_{ij}$  = dimensionless open loop gain for a control pair ( $u_j, y_i$ )

The RGA provides a quantitative comparison of interactions between different possible pairing combinations of control loops. The RGA illustrates the steady state interactions between possible paired control loops. Guidelines for interpreting the RGA results and details are also given by (McAvoy 1983; Svrcek et al. 2006).

## 8.3. Relative Exergy Destroyed Array (REDA) – A new tool

### 8.3.1. REDA definition

The EEF in Equation (8-2) can be re-arranged with basic definitions of steady state gain and destroyed exergy during a step input. The re-arrangement gives:

$$\tau_{ij} = \frac{\Delta B_D}{k_{ij}} \quad 8-6$$

where  $k_{ij}$  = steady state gain for a control pair ( $u_j, y_i$ ) and  $\Delta B_D = \Delta B_{Out} - \Delta B_{In}$  = exergy destroyed in a process during a step input.

The relative EEF (REEF) is defined as:

$$v_{ij} = \frac{(\tau_{ij})_{u_k=const, k \neq j}}{(\tau_{ij})_{y_k=const, k \neq i}} \quad 8-7$$

The REEF Array (REEFA) is an array of REEF ( $v_{ij}$ ) for all possible pairing combinations.

$$V = \begin{bmatrix} v_{11} & v_{12} & \cdots & v_{1n} \\ v_{21} & v_{22} & \cdots & v_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nn} \end{bmatrix} \quad 8-8$$

Mathematically, the relative exergy destroyed (RED) is derived from basic definitions of steady state gain, exergy destroyed during a step input, and the definition of EEF in Equations (8-5), (8-6) and (8-2) respectively. The exergy destroyed in a process during a step input is equal to the product of the steady state gain and the EEF for a control pair ( $u_j, y_i$ ) as shown in Equation (8-6). The relative exergy destroyed ( $\zeta_{ij}$ ) is defined from Equation (8-6) as:

$$\zeta_{ij} = \frac{\left( \frac{\Delta B_D}{\Delta u_j} \right)_{u_k=const, k \neq j}}{\left( \frac{\Delta B_D}{\Delta u_j} \right)_{y_k=const, k \neq i}} = \frac{\left( k_{ij} \tau_{ij} / \Delta u_j \right)_{u_k=const, k \neq j}}{\left( k_{ij} \tau_{ij} / \Delta u_j \right)_{y_k=const, k \neq i}} \quad 8-9$$

$$\zeta_{ij} = \frac{(k_{ij})_{u_k=const, k \neq j}}{(k_{ij})_{y_k=const, k \neq i}} * \frac{(\tau_{ij})_{u_k=const, k \neq j}}{(\tau_{ij})_{y_k=const, k \neq i}} = \lambda_{ij} * v_{ij} \quad 8-10$$

where  $k_{ij}$  = steady state gain for a control pair ( $u_j, y_i$ ),  $\tau_{ij}$  = EEF for a control pair ( $u_j, y_i$ ),  $\lambda_{ij}$  = relative gain for a control pair ( $u_j, y_i$ ),  $v_{ij}$  = REEF for a control pair ( $u_j, y_i$ ) and  $u_j$  = step input.

The relative exergy destroyed is defined analogously to the original relative gain ( $\lambda_{ij}$ ) of RGA. The relative exergy destroyed is the ratio of the total exergy destroyed in a process due to a step input ( $u_j$ ) when all loops are open to the total exergy destroyed in a process due to a

step input ( $u_j$ ) when all other loops are closed and in “perfect” control, as shown in Equations (8-8) and (8-9).

After we put the relative exergy destroyed in Equation (8-9) into a matrix form, we obtain the relative exergy destroyed array (REDA) in Equation (8-10). The REDA can be directly obtained through a Hadamard product of RGA and REEFA matrices as:

$$\mathbf{Z} = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \cdots & \lambda_{1n} \\ \lambda_{21} & \lambda_{22} & \cdots & \lambda_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \lambda_{n1} & \lambda_{n2} & \cdots & \lambda_{nn} \end{bmatrix} \begin{bmatrix} v_{11} & v_{12} & \cdots & v_{1n} \\ v_{21} & v_{22} & \cdots & v_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nn} \end{bmatrix} \quad 8-11$$

$$\mathbf{Z} = \Lambda \otimes \Upsilon \quad 8-12$$

where  $Z$  = relative exergy destroyed array (REDA),  $\zeta_{ij}$  = RED for a control pair ( $u_j$ ,  $y_i$ ) and  $v_{ij}$  = REEF for a control pair ( $u_j$ ,  $y_i$ ).

### 8.3.2. Interpretation of the REDA

The REDA is a new and useful tool, even though it is based only steady state information. This new tool can be applied to a process after selecting control pairing from the RGA. The REDA compares the eco-efficiency of a process under different control structures. To understand the significance of the REDA, guidelines for interpreting the REDA results are explained below and should be understood.

The sum of the elements of any row or column of the REDA is unity.

$\zeta_{ij}$  is dimensionless and independent of scaling.

If  $\zeta_{ij} = 0$ , then the manipulated variable  $u_j$  has no effect on the eco-efficiency of that process. In this situation a step input in  $u_j$  does not increase exergy destruction. If the diagonal elements of the REDA  $\zeta_{ij} = 0$ , then pair  $u_j$  with  $y_i$ .

If  $\zeta_{ij} = 1$ , then this implies that the manipulated variable  $u_j$  is the only variable responsible for the exergy destruction of the process. If the diagonal elements of the REDA  $\zeta_{ij} = 1$ , then avoid pairing  $u_j$  with  $y_i$ .

If  $0 < \zeta_{ij} < 1$ , then this implies that the manipulated variable  $u_j$  is not the only variable responsible for the exergy destruction of the process, i.e. other manipulated variables are also responsible for the exergy destruction of the process.

If  $\zeta_{ij} = 0.5$ , then this implies that the all manipulated variable have same effect on the eco-efficiency of the process. In this situation the final selection of control loop pairing should be based on RGA results.  $\zeta_{ij}$  value should be close to unity.

$\zeta_{ij} > 1$ , then this implies that the open loop EEF is higher than closed loop EEF. This implies that closing the control loops causes decrease in exergy destruction.  $\zeta_{ij} \gg 1$  is not favourable due to more exergy destruction during a step input in the process.  $\zeta_{ij}$  value should be close to unity.

If  $\zeta_{ij} < 1$ , then this implies that the open loop EEF is lower than the closed loop EEF. This implies that closing the control loops causes an increase in exergy destruction.  $\zeta_{ij} \ll 1$  is not favourable due to more exergy destruction during a step input in the process.  $\zeta_{ij}$  value should be close to unity.

The off-diagonal elements of the REDA being close to unity or the diagonal elements of the REDA being close to zero are recommended.

### 8.3.3. Rank based on the REDA

In Table 8-1, if the diagonal elements in both the RGA and REEFA are close to one, then we use “diagonal” to denote this situation. At the same way, we use “off-diagonal” to denote that the off-diagonal elements in both the RGA and REEFA are close to one.

Base on the structure (diagonal or off-diagonal) of the RGA and REEFA matrices, a rank of options can be developed between best and worst, as shown in Table 8-1. The best choice is the control pair whose diagonal elements in the RGA and off-diagonal elements in the REEFA are close to 1 because this pairing is both controllable and eco-efficient.

Table 8-1. REDA ranks for selecting control configuration

Configuration (RGA*REEFA) Matrices	Results	REDA
Diagonal–Diagonal	controllable, not eco-efficient	OK
Diagonal–Off-diagonal	controllable, eco-efficient	best
Off-diagonal–Diagonal	uncontrollable, not eco-efficient	worst
Off-diagonal–Off-diagonal	uncontrollable, eco-efficient	bad

### 8.3.4. An illustrative example

To illustrate how the REDA works, a simple reactor (R1) is used with hypothetical components, as shown in Figure 8-2.

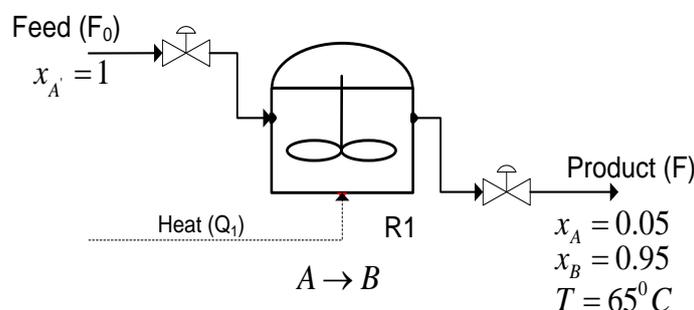


Figure 8-2. A simple CSTR with a hypothetical reaction,  $A \rightarrow B$

In the reactor, component  $A$  is converted into component  $B$  via a simple ( $A \rightarrow B$ ) 1<sup>st</sup> order reaction. The information about the hypothetical components and reaction is given in Table 8-2.  $F_0$  denotes the fresh feed flow rate having pure  $A$ ,  $x_A$  denotes the mole fraction of  $A$ ,  $x_B$  denotes the mole fraction of  $B$ , and  $F$  denotes the product flow rate of the mixture of  $A$  and  $B$ .

Table 8-2. Hypothetical components and reaction information

Hypothetical components details				Reaction Information
Component - $A$		Component - $B$		$r = k * x_A$
NBP ( $^{\circ}\text{C}$ )	80	NBP ( $^{\circ}\text{C}$ )	110	$k = \alpha * \exp(-E / RT)$
Molecular weight	78	Molecular weight	96	$\alpha = 6 * 10^8 \text{ kmol} / \text{m}^3 / \text{s}$ $E = 69,780 \text{ kJ} / \text{kmol}$

In this process, there are two controlled variables: component  $B$  composition,  $x_B$ , and the temperature,  $T$ , of the product. The composition and temperature of the product are affected by the feed flow rate or heat flow into the reactor.

#### 8.3.4.1. Results

After selecting two control loops (composition and temperature control), the EEF is used to evaluate the effect of each control pair on the overall exergetic efficiency of the process. The results are listed in Table 8-3.

Table 8-3. The EEFs for an illustrative example

Control loop pairs	$(F_0, x_B)$	$(Q, x_B)$	$(F_0, T)$	$(Q, T)$
EEF	2.77 E3	1.24 E4	14.71	27.30

From Table 8-3, the control pair  $(F_0, x_B)$  will use less exergy than control pair  $(Q, x_B)$  for controlling the product stream composition ( $x_B$ ), and the control pair  $(F_0, T)$  uses slightly less exergy than the control pair  $(Q, T)$ . In the sense of eco-efficiency, the best control pair selections for this process should be  $(F_0, x_B)$  and  $(Q, T)$ .

Table 8-4. The RGA, REEFA and REDA results for an illustrative example

RGA	REEFA	REDA
$\begin{bmatrix} 0.92 & 0.08 \\ 0.08 & 0.92 \end{bmatrix}$	$\begin{bmatrix} -0.70 & 1.70 \\ 1.70 & -0.70 \end{bmatrix}$	$\begin{bmatrix} -0.51 & 1.51 \\ 1.51 & -0.51 \end{bmatrix}$

Table 8-4 shows the RGA, REEFA and REDA results for this illustrative example. The RGA result indicates both control loops have small interactions. From this RGA result, pairing diagonal elements ( $(F_0, x_B)$  and  $(Q, T)$ ) seems to be the best option for pairing because the diagonal elements approach the value of 1 without exceeding it.

The REEFA result indicates that both manipulated variables ( $F_0$  and  $Q$ ) affect the destruction of exergy in this process. As the off-diagonal elements are close to 1, pairing the diagonal elements ( $(F_0, x_B)$  and  $(Q, T)$ ) is thus more eco-efficient than pairing the off-diagonal elements ( $(F_0, T)$  and  $(Q, x_B)$ ) as shown in Table 8-4.

The REDA results show that pairing the diagonal elements ( $(F_0, x_B)$  and  $(Q, T)$ ) gives a relative exergy-destroyed value closer to 0, as shown in Table 8-4. A smaller diagonal relative exergy-destroyed value of the REDA implies that a process with diagonal elements pairing is more eco-efficient than the same process with off-diagonal elements pairing.

Thus the REDA ranks diagonal RGA and off-diagonal REEFA as the best option. In this situation, the process with pairing diagonal elements ( $(F_0, x_B)$  and  $(Q, T)$ ) is easily controllable and eco-efficient. Conversely, the REDA ranks pairing diagonal elements ( $(F_0, x_B)$  and  $(Q, T)$ ) RGA and diagonal REEFA as controllable but not eco-efficient.

In this illustrative example, as the off-diagonal REDA values are close to 1, then the pairing of diagonal elements  $((F_0, x_B)$  and  $(Q, T))$  is easily controllable and eco-efficient. The REDA is an off-diagonal matrix if the RGA is a diagonal matrix and the REEFA is an off-diagonal matrix. A diagonal matrix of a RGA implies that most of the interaction lies between the diagonal elements  $((F_0, x_B)$  and  $(Q, T))$ , and the off-diagonal elements are not much affected. An off-diagonal matrix of a REEFA implies that the EEf values of the diagonal elements  $((F_0, x_B)$  and  $(Q, T))$  are smaller, meaning that these elements cause less exergy destruction than do the off-diagonal elements  $((F_0, T)$  and  $(Q, x_B))$ . A REDA with off-diagonal elements close to 1 is recommended if the RGA recommends pairing diagonal elements, and vice versa.

## **8.4. Case studies**

In this section, several case studies are described to illustrate how the REDA works.

### **8.4.1. MCB separation process description**

A monochlorobenzene (MCB) separation process is selected for this case study. It consists of three main parts: a flash vessel (F1), an absorption column (T1) and a distillation column (T2), as shown in Figure 8-3. The detailed information of the feed conditions and column specification can be found in (Seider et al. 2004). VMGSim with the NRTL activity thermodynamic model is used for this simulation of the MCB separation process.

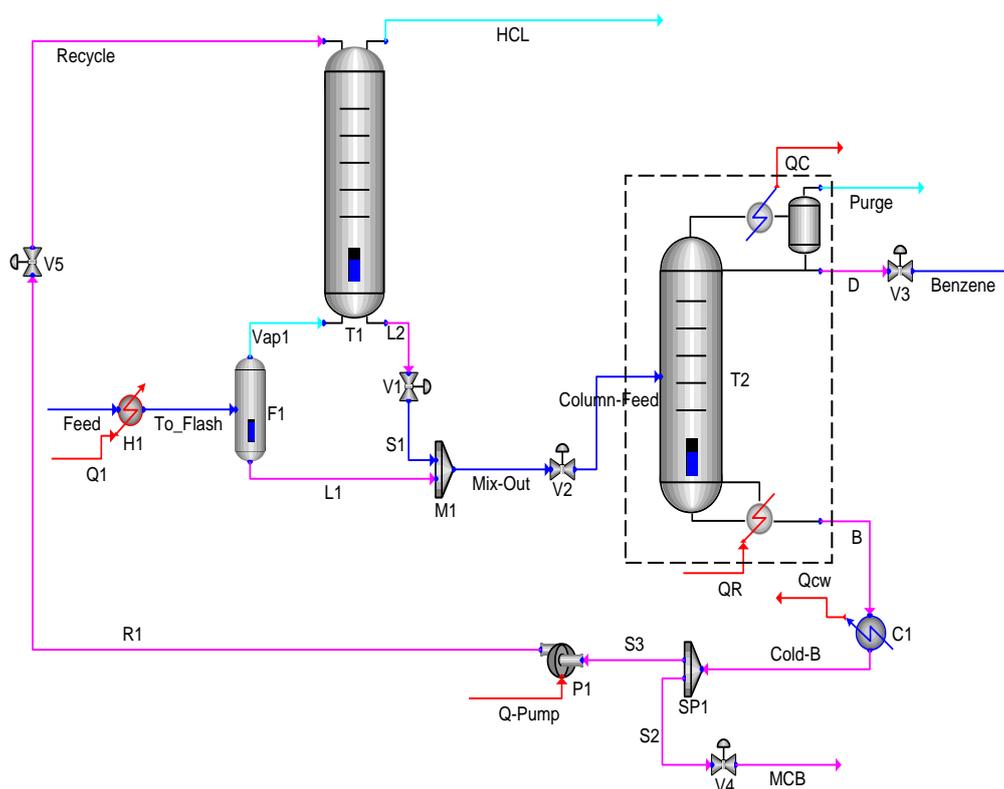


Figure 8-3. Schematic of MCB separation process

The feed of this process consists of a mixture of monochlorobenzene (MCB), benzene and hydrochloric acid (HCl). The vapour stream coming out of the flash tank is fed into the absorber where it comes in contact with recycled MCB. Most of HCl product comes out of the absorber as vapour. The liquid product (L2) coming out of the absorber is mixed with liquid product (L1) from the flash vessel (F1) in a mixer (M1). The mixture coming out of the mixer (M1) is then fed into the distillation column (T2). In this column a fixed amount (1% of inlet feed to the plant) is purged from the process to avoid HCl build-up in the system. The distillate product (D) contains most of the benzene and the bottom product (B) contains most of the MCB. Some fraction of bottom product stream is recycled back into the absorber.

Although “classical” controllability techniques such as RGA, DRGA, NI and CN provide reliable support for industry to guarantee the quality of products, there is less consideration of the energy cost among these techniques. There are two classifications of this case study: 1) an isolated distillation column and 2) a MCB plant with a distillation column and recycle loop.

### 8.4.2. MCB distillation column

In this case study, the distillation column in the MCB plant is considered in isolation without any recycling, as shown by the dashed boundary in Figure 8-3. The compositions at the top and bottom of the distillation column,  $x_D$  and  $x_B$ , are the controlled variables. Three basic control configurations,  $DV$ ,  $LV$  and  $LB$ , are the possible control candidates for a two-point composition control of this distillation column. For example, in the  $LV$  control configuration,  $L$  (reflux rate) is used to control the composition of the top product,  $x_D$ , and  $V$  (boil-up rate) is used to control the composition of the bottom product,  $x_B$ . The configuration behaves as a 2 x 2 square system in which the number of manipulated and control variables are equal and two in number. In reality this system is higher order, but it can be considered 2 x 2 if the assumption of near perfect inventory control holds.

Table 8-5. The EEFs for the MCB distillation column

Diagonal pairs	$(L, x_D)$	$(D, x_D)$	$(V, x_B)$	$(B, x_B)$
EEF	3.28 E5	691.05	6.44 E5	2.91 E4
Off-Diagonal pairs	$(L, x_B)$	$(D, x_B)$	$(V, x_D)$	$(B, x_D)$
EEF	8.33 E4	3.74 E3	2.32 E7	9.72 E5

EEFs for different diagonal and off-diagonal control loop pairs are shown in Table 8-5. From Table 8-5, the control pairing  $(V, x_B)$  will use the most exergy and be the least eco-efficient control pair, and the control pairing  $(D, x_D)$  is the most eco-efficient pairing. The sums of the EEFs for the  $LB$  and  $DV$  control configurations are 3.57 and 6.44 ( $\times 10^5$  kW) respectively.

Table 8-6. The RGA, REEFA and REDA results for the MCB distillation column

Configuration	RGA	REEFA	REDA
$LV$	$\begin{bmatrix} 0.11 & 0.89 \\ 0.89 & 0.11 \end{bmatrix}$	$\begin{bmatrix} -0.12 & 1.12 \\ 1.12 & -0.12 \end{bmatrix}$	$\begin{bmatrix} 0.98 & 0.02 \\ 0.02 & 0.98 \end{bmatrix}$
$LB$	$\begin{bmatrix} 0.97 & 0.03 \\ 0.03 & 0.97 \end{bmatrix}$	$\begin{bmatrix} -0.13 & 1.13 \\ 1.13 & -0.13 \end{bmatrix}$	$\begin{bmatrix} -0.09 & 1.09 \\ 1.09 & -0.09 \end{bmatrix}$
$DV$	$\begin{bmatrix} 0.84 & 0.16 \\ 0.16 & 0.84 \end{bmatrix}$	$\begin{bmatrix} 0.01 & 1.01 \\ 1.01 & 0.01 \end{bmatrix}$	$\begin{bmatrix} 0.15 & 0.85 \\ 0.85 & 0.15 \end{bmatrix}$

Table 8-6 shows the RGA, REEFA and REDA results for the MCB distillation column. The RGA results indicate that the leading diagonal elements of the *LB* and *DV* control configurations are positive and close to 1. *LB* and *DV* control configurations are further selected to check for their eco-efficiency; the *LV* control configuration is not further selected for eco-efficiency as its RGA leading diagonal elements are away from 1, which is not acceptable. The off-diagonal elements in the *LV* control configuration are positive and close to 1, but the pairing of off-diagonal elements introduce a significant amount of dead time in the process.

So from Tables 8-5 and 8-6, both *LB* and *DV* control configurations are controllable but the process with a *LB* control configuration is more eco-efficient than the same process with a *DV* control configuration. The *LB* control configuration ( $EEF = 3.57 \times 10^5$  kW) can save up to 44% more exergy compared with the *DV* control configuration ( $EEF = 6.44 \times 10^5$  kW), as calculated from Table 8-5.

The REEFA results of *LV*, *LB* and *DV* show that their leading diagonal elements are away from 1. As their off-diagonal elements are close to 1, pairing diagonal elements of *LV*, *LB* and *DV* control configurations is thus more eco-efficient than pairing off-diagonal elements, as shown in Table 8-6.

The REDA results from Tables 8-1 and 8-6 show that MCB distillation column under *LV* control configuration has off-diagonal–off-diagonal configuration matrices, i.e. this pairing is eco-efficient but not controllable, and so is a bad option. Conversely, the column under *LB* and *DV* control configurations has diagonal–off-diagonal configuration matrices, i.e. this pairing is both controllable and eco-efficient, and so is the best option. The REDA results in Table 8-6 also show that the column under *LB* control configuration has leading diagonal elements (-0.09) closer to 0 than when the column is under *DV* control configuration (0.15); this means the column under *LB* control configuration is more eco-efficient than when it is under *DV* control configuration. This result also agrees with the result based on summation of the EEFs in Table 8-5.

A smaller diagonal relative exergy-destroyed value of REDA implies that the process with diagonal elements pairing is more eco-efficient than the same process with off-diagonal elements pairing.

### 8.4.3. Heat exchanger networks (HEN)

In this case study, a HEN cools hot stream (H1) from 500 °F to 300 °F using two cold streams (C1 and C4) with temperatures of 200 °F and 300 °F, as shown in Figure 8-4. This case was studied and explained by (Seider et al. 2004).

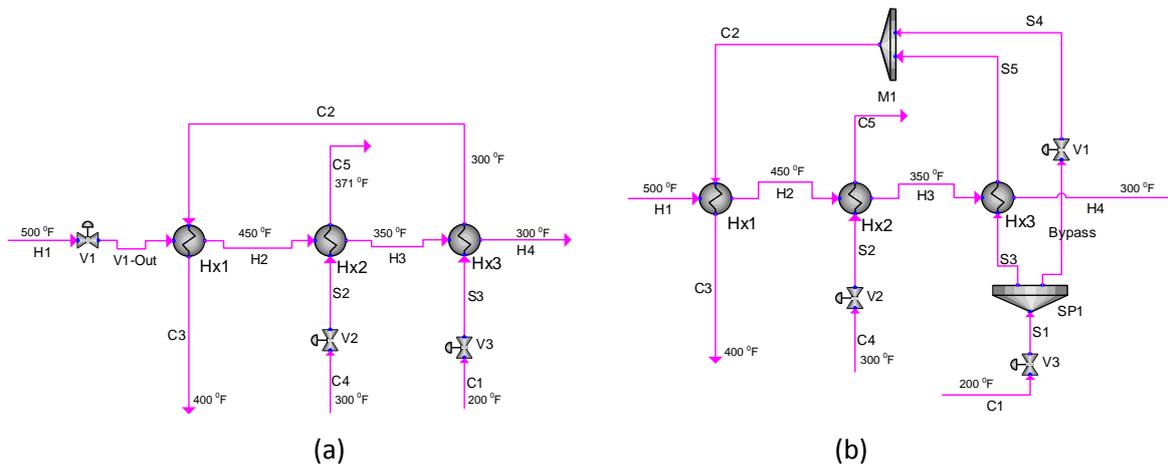


Figure 8-4. Heat exchanger networks (a) original configuration and (b) modified configuration with bypass

In this case study there are three temperature controls with CV temperatures:  $C5(T)$ ,  $C3(T)$  and  $H4(T)$ . These three CVs are controlled by manipulating the flow rates of the two cold streams ( $C1$  and  $C4$ ) and the hot stream ( $H1$ ), as shown by the control valves in Figure 8-4 (a). In an alternate configuration, a bypass around heat exchanger (Hx3) is involved instead of hot steam ( $H1$ ) manipulation. In this modified configuration, three temperatures ( $C5(T)$ ,  $C3(T)$  and  $H4(T)$ ) are controlled by manipulating the flow rates of the two cold streams ( $C1$  and  $C4$ ) and bypass flow fraction ( $S4$ ), as shown in Figure 8-4 (b). This configuration behaves as a 3 x 3 square system in which the number of manipulated and control variables are equal and three in number. The steady state gain matrix derived/defined for HEN with original and modified configurations are shown in Equations (8-13) and (8-14) respectively.

$$\begin{bmatrix} C5(T) \\ C3(T) \\ H4(T) \end{bmatrix} = \begin{bmatrix} \frac{\partial C5(T)}{\partial C4} & \frac{\partial C5(T)}{\partial C1} & \frac{\partial C5(T)}{\partial H1} \\ \frac{\partial C3(T)}{\partial C4} & \frac{\partial C3(T)}{\partial C1} & \frac{\partial C3(T)}{\partial H1} \\ \frac{\partial H4(T)}{\partial C4} & \frac{\partial H4(T)}{\partial C1} & \frac{\partial H4(T)}{\partial H1} \end{bmatrix} \begin{bmatrix} C4 \\ C1 \\ H1 \end{bmatrix} \quad 8-13$$

$$\begin{bmatrix} C5(T) \\ C3(T) \\ H4(T) \end{bmatrix} = \begin{bmatrix} \frac{\partial C5(T)}{\partial C4} & \frac{\partial C5(T)}{\partial C1} & \frac{\partial C5(T)}{\partial S4} \\ \frac{\partial C3(T)}{\partial C4} & \frac{\partial C3(T)}{\partial C1} & \frac{\partial C3(T)}{\partial S4} \\ \frac{\partial H4(T)}{\partial C4} & \frac{\partial H4(T)}{\partial C1} & \frac{\partial H4(T)}{\partial S4} \end{bmatrix} \begin{bmatrix} C4 \\ C1 \\ S4 \end{bmatrix} \quad 8-14$$

Table 8-7. The RGA, REEFA and REDA results for the HEN

<i>Configuration</i>	<i>RGA</i>	<i>REEFA</i>	<i>REDA</i>
<i>Original</i>	$\begin{bmatrix} 1.0 & 0.0 & 0.0 \\ 0.0 & 0.65 & 0.35 \\ 0.0 & 0.35 & 0.65 \end{bmatrix}$	$\begin{bmatrix} 0.0 & 2.42 & -1.42 \\ 1.04 & 0.0 & -0.04 \\ -0.05 & -1.43 & -2.48 \end{bmatrix}$	$\begin{bmatrix} 0.0 & 1.07 & -0.07 \\ 1.04 & -0.01 & -0.03 \\ -0.05 & -0.06 & 1.10 \end{bmatrix}$
<i>Modified</i>	$\begin{bmatrix} 1.19 & 0.01 & -0.20 \\ 0.0 & 1.14 & -0.14 \\ -0.19 & -0.15 & 1.34 \end{bmatrix}$	$\begin{bmatrix} 0.0 & -0.01 & 1.01 \\ 1.08 & -0.08 & 0.0 \\ -0.08 & 1.09 & -0.01 \end{bmatrix}$	$\begin{bmatrix} 0.07 & -0.23 & 1.24 \\ 1.24 & -0.24 & 0.0 \\ -0.27 & 1.47 & -0.20 \end{bmatrix}$

Table 8-7 shows the RGA, REEFA and REDA results for the HEN. The RGA results indicate that the leading diagonal elements of the original and modified control configurations are positive and close to 1. The RGA recommends (*C5 (T)-C4*, *C3 (T)-C1* and *H4 (T)-H1*) pairings for the original configuration and (*C5 (T)-C4*, *C3 (T)-C1* and *H4 (T)-S4*) pairings for the modified configuration. Both original and modified control configurations are further selected to check for their eco-efficiency.

The EEFs for different diagonal, off-diagonal and other pairs (other than diagonal and off-diagonal pairs) control loop pairs are shown in Table 8-8. With the original configuration, the control pairing (*C4*, *C3(T)*) will use the most exergy and be the least eco-efficient control pair, and the control pairing (*C1*, *C3(T)*) is the most eco-efficient pairing. The sum of the EEFs for the original configuration diagonal pairing (*C5(T)-C4*, *C3(T)-C1* and *H4(T)-H1*) is 630 kW. With the modified configuration (i.e. the bypass), the control pairing (*S4*, *C3(T)*) is the most eco-efficient pairing. The sum of the EEFs for the modified configuration diagonal pairing (*C5(T)-C4*, *C3(T)-C1* and *H4(T)-S4*) is 322 kW. As the sum of the EEFs for the

modified configuration diagonal elements (322 kW) is less than the sum of the original configuration diagonal elements (630 kW), the HEN with the modified configuration is thus more eco-efficient than the same process with the original configuration. Specially, the modified configuration (EEF = 322 kW) can save 48% more exergy compared with the original configuration (EEF = 630kW), as calculated from Table 8-8.

Table 8-8. The EEFs for the HEN

	Original Configuration			Modified Configuration		
Diagonal pairs	$(C4, C5(T))$	$(C1, C3(T))$	$(H1, H4(T))$	$(C4, C5(T))$	$(C1, C3(T))$	$(S4, H4(T))$
EEF	184	101.59	343.54	184	99	39.11
Off-Diagonal pairs	$(H1, C5(T))$	$(C4, H4(T))$	$(H1, C3(T))$	$(S4, C5(T))$	$(C4, H4(T))$	$(S4, C3(T))$
EEF	874.54	460	2.63 E3	3.85 E3	920	26.01
Other pairs	$(C4, C3(T))$	$(C1, C5(T))$	$(C1, H4(T))$	$(C4, C3(T))$	$(C1, C5(T))$	$(C1, H4(T))$
EEF	1.84 E5	828	188.28	6.13 E3	227.7	189.75

The REEFA results of the original and modified configurations show that their leading diagonal elements  $(C5(T)-C4, C3(T)-C1$  and  $H4(T)-H1)/(C5(T)-C4, C3(T)-C1$  and  $H4(T)-S4)$  are away from 1 and close to 0. This means that, pairing diagonal elements for both the original and modified control configurations is more eco-efficient than pairing off-diagonal or other elements, as shown in Table 8-7.

The REDA is calculated by the product of the RGA and REEFA matrices. The REDA results show that the leading diagonal elements of the HEN are closer to 0 (0.07, -0.24 and -0.20) under the modified control configuration than when the process is under the original control configuration (0.0, -0.01 and 1.10). This means that the HEN is more eco-efficient under the modified control configuration than under the original control configuration, as shown in Table 8-7. This result agrees with the result based on summation of the EEFs in Table 8-8.

#### 8.4.4. MCB whole plant

In this case study, a whole MCB plant with distillation column and recycle is considered. As shown in Figure 8-3, there are three composition control loops. The composition of HCl ( $x_{HCl}$ ) leaving in the vapour stream of the absorber is controlled by manipulating the cooler ( $CI$ ) duty ( $Q_{cw}$ ). The compositions at the top and bottom of the distillation column,  $x_D$  and  $x_B$ , are the other two controlled variables. For this three-point composition control of the MCB separation plant, three basic control configurations,  $LVQ_{cw}$ ,  $LBQ_{cw}$  and  $DVQ_{cw}$  are considered. For example, in the  $LVQ_{cw}$  control configuration,  $L$  (reflux rate) is used to control the composition of the top product ( $x_D$ ),  $V$  (boil-up rate) is used to control the composition of the bottom product ( $x_B$ ), and  $Q_{cw}$  (cooler duty) is used to control the composition of vapour stream leaving the absorber. The configuration behaves as a 3 x 3 square system in which the number of manipulated and control variables are equal and three in number. In reality this system is higher order, but can be considered 3 x 3 if the assumption of near perfect inventory control holds.

Table 8-9. The RGA, REEFA and REDA results for the whole MCB plant

<i>Configuration</i>	<i>RGA</i>	<i>REEFA</i>	<i>REDA</i>
$LVQ_{cw}$	$\begin{bmatrix} 3.80 & -2.80 & 0.02 \\ -1.40 & 2.60 & -0.23 \\ -1.40 & 1.20 & 1.20 \end{bmatrix}$	$\begin{bmatrix} 0.0 & 0.01 & 0.99 \\ 0.99 & 0.0 & 0.01 \\ 0.01 & 0.99 & 0.0 \end{bmatrix}$	$\begin{bmatrix} -2.80 & 0.02 & 3.80 \\ 2.60 & -0.23 & -1.40 \\ 1.20 & 1.20 & -1.40 \end{bmatrix}$
$LBQ_{cw}$	$\begin{bmatrix} 0.84 & -1.60 & 1.76 \\ 0.18 & 0.38 & 0.43 \\ -0.03 & 2.20 & -1.19 \end{bmatrix}$	$\begin{bmatrix} 0.0 & 0.0 & 1.0 \\ 1.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 \end{bmatrix}$	$\begin{bmatrix} -1.60 & 1.76 & 0.84 \\ 0.38 & 0.43 & 0.18 \\ 2.20 & -1.19 & -0.03 \end{bmatrix}$
$DVQ_{cw}$	$\begin{bmatrix} 0.91 & 0.03 & 0.06 \\ 0.03 & 1.02 & -0.05 \\ 0.06 & -0.05 & 0.99 \end{bmatrix}$	$\begin{bmatrix} 0.0 & 0.0 & 1.0 \\ 1.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 \end{bmatrix}$	$\begin{bmatrix} 0.03 & 0.06 & 0.91 \\ 1.02 & -0.05 & 0.03 \\ -0.05 & 0.99 & 0.06 \end{bmatrix}$

The RGA results in Table 8-9 show that the leading diagonal elements of the  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are positive, although large for  $LVQ_{cw}$ . The RGA results of the  $LBQ_{cw}$  control configuration are far away from 1, except for one element.  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are further selected to check for their eco-efficiency, but  $LBQ_{cw}$  control configuration is not because its RGA leading diagonal elements are away from 1.

Table 8-10. The EEFs for the whole MCB plant

Diagonal pairs	$(L, x_D)$	$(D, x_D)$	$(V, x_B)$	$(B, x_B)$	$(Q_{cw}, x_{HCl})$
EEF	94.3	3.41	78.72	1.08 E3	1.28 E4
Off-Diagonal pairs	$(L, x_B)$	$(D, x_B)$	$(V, x_D)$	$(B, x_D)$	$(L, x_{HCl})$
EEF	1.14 E10	8.78 E7	3.38 E8	2.03 E7	1.22 E5
Other pairs	$(Q_{cw}, x_D)$	$(Q_{cw}, x_B)$	$(V, x_{HCl})$	$(B, x_{HCl})$	$(D, x_{HCl})$
EEF	7.75 E12	1.55 E12	9.21 E5	5.55 E4	940.70

The EEFs for different diagonal, off-diagonal and other pairs (other than diagonal and off-diagonal pairs) control loop pairs are shown in Table 8-10. From Table 8-10, the control pairing  $(Q_{cw}, x_{HCl})$  will use the most exergy and be the least eco-efficient control pair, and the control pairing  $(D, x_D)$  is the most eco-efficient pairing. The sums of the EEFs for the  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are 1.30 and 1.28 ( $\times 10^4$  kW) respectively. From Table 8-9 and Table 8-10, both  $LVQ_{cw}$  and  $DVQ_{cw}$  control configurations are controllable, but the process with a  $DVQ_{cw}$  control configuration is more eco-efficient than the same process with an  $LVQ_{cw}$  control configuration. Specifically, the  $DVQ_{cw}$  control configuration (EEF =  $1.28 \times 10^4$  kW) can save up to 1.3% more exergy compared with the  $LVQ_{cw}$  control configuration (EEF =  $1.30 \times 10^4$  kW), as calculated from Table 8-10.

The REEFA results of  $LVQ_{cw}$ ,  $LBQ_{cw}$  and  $DVQ_{cw}$  show that their leading diagonal elements are away from 1 and close to 0, This means that, pairing diagonal elements of  $LVQ_{cw}$ ,  $LBQ_{cw}$  and  $DVQ_{cw}$  control configurations is more eco-efficient than pairing off-diagonal elements, as shown in Table 8-9.

REDA results show that MCB plant has leading diagonal elements closer to 0 (0.03, -0.05 and 0.06) under the  $DVQ_{cw}$  control configuration than when the plant is under the  $LVQ_{cw}$  control configuration (-2.80, -0.23 and -1.40). This means that the MCB plant is more eco-efficient under the  $DVQ_{cw}$  control configuration than it is under the  $LVQ_{cw}$  control configuration, as shown in Table 8-9. This result agrees with the result based on summation of the EEFs in Table 8-10.

## 8.5. Summary

Control loop configuration has traditionally focused only on control loop analysis and controllability. However, in this present era of increasing energy crisis and climate change, engineers should also consider energy costs and environmental impacts in their design. Eco-efficient processes and plant can be achieved by integrating control loop configuration and eco-efficiency, and a new tool proposed in this paper can assist in this goal. The REDA integrates control loop configuration and eco-efficiency to measure the relative eco-efficiency of a MIMO process. The REDA results are explained with the help of a simple illustrative example and three more complex case studies: a MCB distillation column (2 x 2), a heat exchanger network (3 x 3), and a MCB whole plant (higher order/pseudo 3 x 3). The results of the REDA are verified with the results of EEFs. The REDA can help process designers to find a quick, optimal and eco-efficient control design during early process design stages in a cost effective manner.

## 8.6. Conclusions

A new tool, the REDA, which integrates the controllability and measurements of eco-efficiency of a process, was developed. This new tool measures the relative eco-efficiency of a process and provides a measure that can be used to compare eco-efficiency of MIMO processes for different combinations of control structures, based on steady state information. In other words, it compares the eco-efficiency of a process with several process control structures. The tool is simple and easy to use during early process design stages.

## References

- Alonso, A. A., B. E. Ydstie and J. R. Banga (2002). "From irreversible thermodynamics to a robust control theory for distributed process systems." Journal of Process Control **12**(4): 507-517.
- Bristol, E. (1966). "On a new measure of interaction for multivariable process control." Automatic Control, IEEE Transactions on **11**(1): 133-134.
- DeSimone, L. D. and F. Popoff (1998). Eco-efficiency. The business link to sustainable development. Cambridge, MA., MIT press.
- Dincer, I., M. M. Hussain and I. Al-Zaharnah (2004). "Energy and exergy use in public and private sector of Saudi Arabia." Energy Policy **32**(14): 1615-1624.
- Dincer, I. and M. A. Rosen (2007). Exergy: Energy, Environment and Sustainable Development. Amsterdam, Elsevier.
- Hinderink, A. P., F. P. J. M. Kerkhof, A. B. K. Lie, J. De Swaan Arons and H. J. Van Der Kooi (1996). "Exergy analysis with a flowsheeting simulator - I. Theory; calculating exergies of material streams." Chemical Engineering Science **51**(20): 4693-4700.
- Luyben, W. L., B. D. Tyreus. and M. L. Luyben. (1998). Plantwide Process Control. New York, McGraw-Hill.
- Marlin, T. E. (2000). Process control: design process and control system for dynamic performance. New York, McGraw Hill.
- McAvoy, T. J. (1983). Interaction Analysis: Principles and Applications. Research Triangle Park, NC, Instrument Society of America.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2007). "An exergy calculator tool for process simulation." Asia-Pacific Journal of Chemical Engineering **2**(5): 431-437.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2009). The Relative Exergy Array - A tool for integrated process design and control. Chemeca 2009. Perth, Australia.
- Montelongo-Luna, J. M., W. Y. Svrcek and B. R. Young (2010). "The relative exergy array—a new measure for interactions in process design and control." The Canadian Journal of Chemical Engineering **89**(3): 545-549.
- Moran, M. J. and E. Sciubba (1994). "Exergy Analysis: Principles and Practice." Journal of Engineering for Gas Turbines and Power **116**(2): 285-290.
- Morari, M. and Z. Evangelhos (1989). Robust Process Control. Englewood Cliffs, NJ, Prentice Hall.
- Muangnoi, T., W. Asvapoositkul and S. Wongwises (2007). "An exergy analysis on the performance of a counterflow wet cooling tower." Applied Thermal Engineering **27**(5-6): 910-917.
- Munir, M. T., J. J. Chen and B. R. Young (2010). A computer program to calculate the stream exergy using the visual basic graphical interface. Chemeca 2010. Adelaide, Australia.
- Munir, M. T., W. Yu and B. R. Young (2012). Control loop configuration and eco-efficiency. FOCAPO/CPC-VIII. Savannah, Georgia, USA.

- Munir, M. T., W. Yu and B. R. Young (2012). Determination of Plant-wide Control Loop Configuration and Eco-Efficiency, G.P. Rangaiah and V. Kariwala (Eds.). Plantwide Control: Recent Developments and Applications, John Wiley & Sons, ISBN:9780470980149.
- Rosen, M. A. and I. Dincer (1997). "On exergy and environmental impact." International Journal of Energy Research **21**: 643-654.
- Rosen, M. A. and I. Dincer (1999). "Exergy analysis of waste emissions." International Journal of Energy Research **23**: 1153-1163.
- Seborg, D. E., T. F. Edgar and D. A. Mellichamp (1989). Process Dynamics and Control. New York, John Wiley & Sons.
- Seider, W. D., J. D. Seader. and D. R. Lewin. (2004). Product and Process Design Principles: Synthesis, Analysis, and Evaluation. New York, John Wiley.
- Svrcek, W. Y., D. P. Mahoney and B. R. Young (2006). A Real-Time Approach to Process Control. Chichester, John Wiley & Sons.
- Szargut, J., D. R. Morris. and F. R. Steward (1988). Exergy analysis of thermal, chemical, and metallurgical processes. New York, Hemisphere.
- Ydstie, B. E. (2002). "Passivity based control via the second law." Computers & Chemical Engineering **26**(7-8): 1037-1048.

## **Chapter 9. Discussion, conclusions and recommendations for future work**

In this chapter a general discussion of the project, and the applications of the VMGSim based exergy calculator, plantwide RGA/REA, EEF and REDA are presented. The advantages and disadvantages of these tools (the VMGSim based exergy calculator, plantwide RGA/REA, EEF and REDA) are also discussed in this chapter. Finally, conclusions, recommendations and possible future work are also presented in this chapter.

### **9.1. Discussion**

#### **9.1.1. Process simulator based Exergy Calculator**

VMGSim is one of the latest commercial process simulators; it was used in this research for the exergy calculation of material streams, as explained in chapters 3 and 4. The VMGSim based exergy calculator was developed to design the REA, EEF, REDA and the eco-efficiency tools also developed in this work. These tools help with integrating process design, control, and thermodynamics into a single domain.

There are many advantages of the process simulator based exergy calculator developed in this work. The calculator helps to determine thermodynamic efficiency quickly in order to identify key areas where most exergy is being destroyed. This approach helps in process improvement and can provide significant savings. The development of the process simulator based exergy calculator has also helped in the development of tools/methods (REA, EEF, REDA and eco-efficiency), which facilitate controllable and eco-efficient process design.

The VMGSim based exergy calculator is simple and easy to use but also needs manual input of data (thermodynamic properties) for the exergy calculation of a material stream. The VMGSim based exergy calculator can be further improved in order to avoid any manual input by using VMGSim's process simulator COM (Component object modular) automation. More details of VMGSim's COM automation are given in the VMGSim COM automation manual (Virtual Materials Group Inc. 2009). Details of the VMGSim based exergy calculator are discussed in chapters 3 and 4.

### **9.1.2. Plantwide RGA and REA**

Plantwide RGA and REA evaluate plantwide controllability and exergy interaction/eco-efficiency within the scope of a plant's control loops. It is necessary to study plantwide controllability and exergy interactions because, in practice, individual units are connected with other units of the plant in a plantwide layout through recycles. The development of plantwide REA is an attempt to unify the application of thermodynamics (exergy) and process control. With plantwide RGA and REA, process engineers can obtain information about plantwide controllability and exergy interaction/eco-efficiency at the early design stage. This information (plantwide controllability and exergy interaction/eco-efficiency) at the early design stage allows process engineers to compare a variety of possible control configurations simultaneously and determine what impact a control configuration will have on the controllability/economics of the process when operating.

Plantwide RGA and REA results provide a screening tool to quickly evaluate and compare several control structure candidates and rank them according to their controllability /exergy interactions/eco-efficiency. This screening tool (Plantwide RGA/REA) can be used in deciding a final control scheme for the unit or even for a whole plant. Plantwide RGA/REA and recycle effect on REA are discussed in chapters 3 and 4.

Plantwide RGA and REA also have certain limitations: they are only applicable to linear systems, applicable only to steady state control scheme evaluation, and require dynamic simulation validation.

### **9.1.3. Exergy Eco-efficiency Factor (EEF)**

The REA is simple and easy to use but it has a limitation of measuring eco-efficiency within the scope of a plant or unit's control loops only, which is not a true eco-efficiency of a process. To minimize the limitations of REA, the EEF was developed in this research, as discussed in chapters 5 and 6. The EEF provides means to determine the true eco-efficiency of the whole process. The EEF is based on the steady state information of total exergy in and out of the process, using manipulated and control variables. A higher EEF value for a control configuration implies that the selection of that control configuration will result in more exergy destruction, and vice versa. The EEF provides a qualitative and quantitative measure for selecting the most eco-efficient control scheme. The EEF results also need dynamic simulation validation. More details in regard to the EEF are given in chapter 5.

The EEF results are also affected by the recycling of material and energy streams. As recycle loops can have a significant effect on controllability and eco-efficiency of a unit, therefore in this research, the effect of recycle loops on the EEF is also studied. The effect of recycle loops on the EEF results is presented in chapter 6. VMGSim and Excel are used to develop an EEF calculator. The EEF calculator can calculate the EEF for different cases with all possible control structure combinations in a single MIMO process. The EEF calculator details are presented in chapter 7.

#### **9.1.4. Relative Exergy Destroyed Array (REDA)**

In a MIMO process, normally there are various possible control schemes. The REDA is a simple screening tool used to simultaneously compare the eco-efficiencies of a MIMO process under different control schemes. The REDA combines the controllability and eco-efficiency of a process in a single domain. It helps to quickly evaluate and compare several control structure candidates and rank them according to their controllability and eco-efficiency. The results and details of the REDA are explained and interpreted with the help of simple case studies in chapter 8.

The REDA also has the limitation that it is based on steady state information (RGA and REEFA). The REDA results are in the form of a number which can also require dynamic simulation validation. The REDA is a simple screening tool to quickly find an optimal and eco-efficient control structure design during the early process design stage, based on steady state information.

## **9.2. Conclusions**

In this research, the objectives presented and described in chapter 1 have mostly been achieved, as explained below.

A VMGSim based exergy calculator was developed and implemented for the exergy calculation of multi-component material streams. An integrated approach of using VMGSim and the MS Excel unit operation was used to extend the use of VMGSim for exergy analysis, exergy interaction and eco-efficiency measurements. The Exergy calculator also facilitated the determining of the REA, EEF and REDA controllability methods based on exergy results. This calculator was also applied to three complex process/plant case studies: an ethylene glycol plant, an ethyl benzene plant, and an MCB plant.

The plantwide RGA and REA concepts were applied for the determination of plantwide controllability and eco-efficiency. The plantwide RGA can only integrate process design and control. For eco-efficient process design, a plantwide REA which integrates process design, control and eco-efficiency was proposed. The combined use of the plantwide RGA and REA provides a measure of the controllability and eco-efficiency of the process under a certain design, although the final decision for control scheme requires dynamic simulation validation.

The plantwide REA was used to simultaneously compare the thermodynamic efficiency of various possible control schemes. It provides useful information about eco-efficiency but its application to a process with one or more recycle loops can provide biased information, which in turn can mislead the process designer to select the wrong control scheme. So plantwide REA must be determined with the consideration of recycle loops.

The EEF was developed to minimize the limitations of the plantwide REA (the REA evaluates the eco-efficiency only within the scope of the control loops studied). The EEF was used to determine the eco-efficiency of an entire unit or plant. The EEF integrates control loop configuration and eco-efficiency into a single domain. The EEF provides a qualitative and quantitative measure to select the most eco-efficient control scheme out of the possible control schemes. The EEF also needs dynamic simulation validation as it is only based on steady state information.

The EEF results are also affected by the consideration of recycle loops in a plantwide layout. The EEF value of a unit/plant decreases because recycles of material/energy decrease the exergy destruction. The effect of recycle on the EEF was studied, as the final selection of control configuration for a unit must be based on the plantwide layout of that unit, and the EEF results given without consideration of recycle loops can be misleading and biased. The EEF results based on isolated units can only be utilized for start-up periods.

The disadvantages of EEF are that it only determines the eco-efficiency of a single control scheme one at a time, and also that EEF results need dynamic simulation validation which increases the computation load for practising engineers. In this research, the REDA is proposed to minimize the limitations of the EEF. The REDA also integrates the controllability and eco-efficiency of a process. The REDA measures the relative eco-efficiency of a MIMO process to compare the eco-efficiencies of that process with several

possible control schemes simultaneously. It is simple and easy to use during the early process design stage, even though it is based only on steady state information.

### **9.3. Limitations**

There are some limitations of the tools developed in this work which are considered below.

The plant-wide REA definition proposed in Chapter 3 is analogous to the plant-wide RGA definition, thus it implies that the control structure under consideration applies to a linear system. In other words, the application of the REA to a highly non-linear system is limited to the range in which the model is evaluated. For instance, the distillation column shown in Chapters 3 and 4 is a highly non-linear system. However, the results are valid for the range in which the distillation column RGA and REA were evaluated.

The REA is, as is the RGA, strictly applicable to steady control scheme evaluation. This drawback is due to the definition of the REA which indicates that only values from steady state (open and closed loop) are used in the calculation of the interaction matrix. In other words, the interactions reflect the final new steady state but not necessarily the path to it. Similarly, EEF and REDA are applicable to steady state control schemes, because their results are based on steady state information. Another limitation of the proposed tools (REA, EEF, and REDA) is that these are not applicable to unstable systems.

The software package for automatic EEF calculation proposed in Chapter 7 has a limitation of manual inputs of physical properties for exergy calculation. This limitation can be avoided by using VMGSim COM automation technique.

The manual testing to perform the controllability/eco-efficiency assessments for each possible design/topology is very time consuming task especially for large scale or complex processes.

The proposed tools (REA, EEF and REDA) are not integrated into the profitability of designs/operations which acts as one of the major objective in the selection of design. This is an optimization problem not considered in this research.

The REDA for a MIMO process with different possible control schemes compares destroyed exergies qualitatively during a step input disturbance simultaneously and helps to select a control scheme which destroys the least exergy among all possible control schemes. It does

not help to compare relative destroyed exergies quantitatively for different possible control schemes of a MIMO process.

The proposed REA, EEF and REDA measures are based on steady state information of exergies and do not consider the exergy path (dynamics) between two steady states. For preliminary selection of the eco-efficient control schemes during early process design stages, these steady state tools (REA, EEF and REDA) are good enough to compare different possible control schemes. This does not necessarily hold for a detailed analysis. The eco-efficient control schemes selected after REA, EEF and REDA analysis then need to be further evaluated for their controllability by doing dynamic controllability analysis. This is a hybrid approach.

The proposed REA, EEF and REDA measures still need to give more information on the level of difficulty of the application of the proposed methodology to industrial systems or processes. Still there is a knowledge gap about application of these tools to industrial processes.

#### **9.4. Recommendations for future work**

The development of the plantwide RGA/REA, EEF and REDA tools are new contributions to research aimed at integrating process design, control and thermodynamics/eco-efficiency. They help to minimize the knowledge gaps in the integration of process design, control and thermodynamics/eco-efficiency. They open up some new perspectives for determining plantwide control loop interactions, plantwide exergy interactions, the process eco-efficiency and relative eco-efficiency of a MIMO process. This research can assist process engineers in the designing of controllable and eco-efficient processes.

The new tools/methods (the plantwide RGA/REA, EEF and REDA) developed in this research also have limitations; these, are discussed in section 9.1 of this chapter and in their assigned chapters (3, 4, 5, 6, 7 and 8). Future research in this area should also focus on these identified limitations. Based on reducing the limitations of these new tools, there are many possible topics for proposed future research. A list of proposed research topics in this area is given below.

1. Further improvement of the VMGSim based exergy calculator by using VMGSim COM automation to avoid manual inputs.

2. Extension of the plantwide RGA/REA for non-square systems, in which the MV and CV are not equal in number.
3. Improvement of the plantwide REA by developing a plantwide dynamic REA (DREA). As the plantwide REA is based on steady state information, without dynamic validation, its results can therefore be biased and misleading; DREA could address this.
4. Study of the controller performance effect on eco-efficiency and the EEF results of a process. As controller performance can have an impact on EEF results/eco-efficiency, it is therefore necessary to quantify the role of controller performance in the EEF results.
5. Extension of steady state EEF analysis to dynamic EEF analysis to avoid the necessity of the dynamic simulation validation of EEF results, which increases the computational load on practising engineers. EEF analysis can be extended to the dynamic state after considering the exergy path (dynamics) between two steady states.
6. Further investigation of the REDA to quantify the relative differences of exergy destroyed between different possible control schemes. This could help to quantify the exergy saving of a given control scheme.
7. An extension of the proposed tools (REA, EEF, and REDA) to unstable systems.
8. Extension of the plantwide RGA/REA, EEF and REDA to other non-linear and complex systems to provide a means of evaluating a control scheme over the full range of operating conditions/plants.
9. Further investigation of the strategies available for automatic selection of the best plant design/topology using different measures to perform the controllability/eco-efficiency assessment of different designs/topology.
10. The profitability of design/operations could be integrated into the proposed assessments (REA, EEF and REDA).
11. Use of exergy factor to convert dynamic energy plots to dynamic exergy plots to avoid the onerous computations involved in dynamic exergy validation. Exergy dynamic plots can also be obtained after normalizing energy dynamic plots with the exergy factor.

12. Extension of the proposed REA, EEF and REDA to industrial systems and provision of information on its level of difficulty. This will build more a solid ground in terms of the validity and applicability of these proposed tools.

## Appendix A: List of Publications

### A.1. Journal articles and Book Chapters

1. Determination of plantwide control loop configuration and Eco-efficiency (Munir, M. T., W. Yu and B. R. Young (2011), Determination of Plant-wide Control Loop Configuration and Eco-Efficiency, In G.P. Rangaiah and V. Kariwala (Eds.), Plant-Wide Control: Recent Developments and Applications, John Wiley & Son, ISBN:9780470980149).
2. Munir, M. T., W. Yu and B. R. Young (2012). Recycle effect on the relative exergy array. Chemical Engineering Research and Design 90(1): 110-118.
3. Munir, M. T., W. Yu and B. R. Young (2012). Eco-efficiency and control loop configuration for recycle systems. AIChE Journal (Submitted).
4. Munir, M. T., W. Yu and B. R. Young (2012). Plantwide control: Eco-efficiency and control loop configuration. Industrial engineering & chemistry research (Submitted).
5. Munir, M. T., W. Yu and B. R. Young (2011). A software algorithm/package for control loop configuration and eco-efficiency. IEEE transactions on industrial informatics. (Submitted).
6. Munir, M. T., W. Yu and B. R. Young (2012). Dynamic exergy plots using exergy factor. Transaction on control and Mechanical Systems. (Submitted).
7. Munir, M. T., W. Yu and B. R. Young (2012). The Relative Exergy-destroyed a new tool for process design and control. The Canadian Journal of chemical engineering. (Submitted).

### A.2. Conference articles

1. Munir, M. T., J. J. Chen and B. R. Young (2010). A computer program to calculate the stream exergy using the visual basic graphical interface. Chemeca 2010. Adelaide, Australia.
2. Munir, M. T., W. Yu and B. R. Young (2011). Analysis of control configuration changes with relative gain array and relative exergy array for units in plants with recycle. Chemeca 2011. Sydney, Australia.
3. Munir, M. T., W. Yu and B. R. Young (2011). Dynamic exergy plots using exergy factor. SCENZ – IChemE annual conference. Hamilton, New Zealand.

## Appendix A –List of Publications

4. Munir, M. T., W. Yu and B. R. Young (2012). Control loop configuration and eco-efficiency. CPC-VIII. Savannah, Georgia, USA.
5. Munir, M. T., W. Yu and B. R. Young (2012). Eco-efficiency and control loop configuration for recycle systems. ACC 2012. Montreal, Canada (Accepted).
6. Munir, M. T., W. Yu and B. R. Young (2012). The Relative Exergy destroyed array. ADCHEM 2012. Singapore (Accepted).