

**METHODOLOGY FOR COMPARISON OF CHEMICAL
PROCESS ROUTES BASED ON ENVIRONMENT,
HEALTH AND SAFETY ASPECTS AT EARLY STAGES
OF CHEMICAL PROCESS PLANT DESIGN**

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Degree of Master of Philosophy

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University of Moratuwa

Sri Lanka

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Thesis submitted in partial fulfillment of the requirements for the degree Master of
Philosophy

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DECLARATION

I declare that this is my own work and this thesis does not incorporate without acknowledgement any material previously submitted for a Degree or Diploma in any other University or institute of higher learning and to the best of my knowledge and belief it does not contain any material previously published or written by another person except where the acknowledgement is made in the text.

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Abstract

The chemical process route selection is one of the important decisions that needs to be taken during initial stages of plant design and development. Although conventionally the economic factor has been considered in this selection process, presently the environmental, health and safety (EHS) issues have also become main concerns as hazards related to EHS can be largely reduced by avoiding them during initial stages of plant development. Therefore, in order to select a route, the assessment of alternate chemical process routes based on EHS aspects and their comparison need to be carried out. For this assessment, comparison and selection methodologies are needed. Most of the methodologies available for chemical process routes assessment and selection, consider mainly environmental or health or safety hazards individually or in combination of two of them. Although few methodologies are available that consider all three EHS aspects, those that consider EHS hazards posed by both types of releases namely daily plant operational and accidental are lacking.

In this work fuzzy based inherent environmental, health and safety hazard index called EHS-Fuzzy Index is developed to compare chemical process routes based on integrated EHS hazards due to daily operational activities of the plant as well as accidental releases. The EHS-Fuzzy Index includes information of thirteen EHS related parameters which is available during routes selection stage. The lower the EHS-Fuzzy Index the more environmental friendly, occupational healthy and safer the chemical route. Further, this methodology can be used to compare and rank alternative chemical routes based on environmental hazard or health hazard and safety impact separately as well. The EHS-Fuzzy Index was applied in a case of six routes to manufacture methyl methacrylate (MMA). The Tertiary Butyl Alcohol (TBA) chemical route to manufacture MMA showed the least EHS-Fuzzy Index value. By applying the MMA case study in the radial polygon diagram method, the results obtained using the EHS-Fuzzy Index methodology were verified.

Keywords:

Chemical process route, Plant releases, Inherent safety, Environmental and health hazards, Fuzzy based index

DEDICATION

I dedicate this thesis to my wonderful family who have always been a great source of inspiration and support.

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TABLE OF CONTENTS

DECLARATION	i
Abstract	ii
DEDICATION	iii
ACKNOWLEDGEMENT	iv
LIST OF FIGURES	xi
LIST IF TABLES.....	xiii
LIST OF ABBREVIATION	xv
Chapter 1	1
INTRODUCTION	1
1.1 Research objective and Scope	3
1.2 Thesis structure.....	3
Chapter 2	5
LITERATURE REVIEW.....	5
2.1 Inherent environmental hazards assessment.....	6
2.1.1 Environmental impact assessment based on plant releases	6
2.1.1.1 Toxicity	6
2.1.1.2 Global warming.....	7
2.1.1.3 Acid deposition	7
2.1.1.4 Ozone depletion	8
2.1.2 Environmental impact assessment based on chemical characteristics.....	8
2.2 Inherent occupational health hazards assessment.....	9
2.2.1 Health impact assessment based on accidental plant releases	9
2.2.2 Health impact assessment based on continuous plant releases.....	10
2.2.3 Health impact assessment based on process parameters	11
2.2.4 Health impact assessment methodology guidelines.....	11
2.3 Inherent safety hazards assessment methodologies.....	12

2.3.1 Inherent safety assessment parameters	13
2.4 EHS hazards combined assessment methods	16
2.5 Multi criteria decision making	17
Chapter 3	19
DEVELOPMENT OF THE ASSESSMENT METHODOLOGY.....	19
3.1 Framework for proposed assessment approach.....	19
3.1.1 Selection of impacts due to EHS hazards	20
3.2 Quantification of impacts	22
3.2.1 Environmental impacts	22
3.2.1.1 Global warming impact due to greenhouse gas emission of accidental chemical release	22
3.2.1.2 Toxicity impact on living things	23
3.2.1.3 Ozone depletion	25
3.2.1.4 Acid deposition	26
3.2.1.5 Global warming impact due to greenhouse gas emission of accidental fire	27
3.2.1.6 Global warming impact due to greenhouse gas emission of continuous operation.....	27
3.2.2 Health impacts	29
3.2.2.1 Occupational health impact from work place accidental release airborne quantity	29
3.2.2.2 Occupational health impact due to fugitive emissions.....	31
3.2.3 Safety	32
3.2.3.1 Inventory	32
3.2.3.2 Flammability	33
3.2.3.3 Explosiveness.....	34
3.2.3.4 Operating pressure	34
3.2.3.5 Operating temperature.....	35

3.3 Multi criteria decision- making methodology	35
3.3.1 Proposed Fuzzy logic- based assessment method.....	36
3.3.2 Fuzzy inference system for primary parameters.....	38
3.3.2.1 Initialization for primary parameters	38
3.3.2.2 Fuzzification and Defuzzification of primary parameters	39
3.3.3 Definition of membership function and IF-THEN rules for primary parameters.....	41
3.3.3.1 Membership functions and IF-THEN rules for global warming impact due to greenhouse gas emission of accidental chemical releases	41
3.3.3.2 Membership functions and IF-THEN rules for toxicity due to accidental chemical releases	44
3.3.3.3 Membership functions and IF-THEN rules for ozone depletion due to accidental chemical release	47
3.3.3.4 Membership functions and IF-THEN rules for acid deposition due to accidental chemical release	50
3.3.3.5 Membership functions and IF-THEN rules for global warming impact due to greenhouse gas emission of accidental fire	53
3.3.3.6 Membership functions and IF-THEN rules for global warming impact due to greenhouse gas emission of continuous operation	55
3.3.3.7 Membership functions and IF-THEN rules for health impact due to continuous emission in the plant	58
3.3.3.8 Membership functions and IF-THEN rules for occupational health impact from work place accidental release airborne quantity at the plant premises.....	61
3.3.3.9 Membership function and IF-THEN rules for explosiveness of chemical substances	64
3.3.3.10 Membership functions and IF-THEN rules for flammability of chemical substance.....	67
3.3.3.11 Membership functions and IF-THEN rules for to inventory of chemical substance.....	69

3.3.3.12 Membership function and IF-THEN rules for operating temperature of chemical reaction	72
3.3.3.13 Membership functions and IF-THEN rules for operating pressure of chemical reaction	75
3.3.4 Fuzzy inference system for intermediate parameters	77
3.3.4.1 Definition of linguistic variables for intermediate parameters	77
3.3.4.2 Fuzzy hierarchical model for EHS-Fuzzy Index.....	78
3.3.4.2.1 Aggregation of de-fuzzified primary parameters (Level IV) by addition	80
3.3.4.2.2 Aggregation of intermediate parameters (Level III, II and I) by pair wise comparison.....	81
3.3.4.3 Definition of Universe of Discourse for intermediate parameters in level IV.....	82
3.3.5 Fuzzy aggregation of intermediate parameters according to the hieratical model	82
3.3.5.1 The pair wise aggregation for intermediate parameters of ENVACC	83
3.3.5.2 The pair wise aggregation for intermediate parameters of ENV2REL87	
3.3.5.3 The pair wise aggregation for intermediate parameters of HEL2REL90	
3.3.5.4 The pair wise aggregation for intermediate parameters of SAF2CHPR	94
3.3.5.5 The pair wise aggregation for intermediate parameters of HANDS...	97
3.3.5.6 The pair wise aggregation for determination of EHS-Fuzzy Index ..	101
3.6 Comparison of EHS–Fuzzy Index methodology with EHS assessment using radial polygon diagram method.....	104
3.7 Case Study Application	105
3.7.1 MMA Chemical process routes description.....	106
3.7.1.1 Acetone Cyanohydrin based route (ACH)	106
3.7.1.2 Ethylene via Propionaldehyde based route (C2/PA).....	106
3.7.1.3 Ethylene via Methyl Propionate based route (C2/MP)	107

3.7.1.4 Propylene based route (C3).....	107
3.7.1.5 Tertiary Butyl Alcohol based route (TBA)	107
3.7.1.6 Isobutylene based Route (i-C4).....	107
Chapter 4	108
RESULTS AND DISCUSSION	108
4.1 Ranking routes to manufacture Methyl Methacrylate	109
4.2 Comparison of chemical process routes based on environmental impacts	110
4.3 Comparison of chemical process routes based on occupational health impacts	111
4.4 Comparison of chemical process routes based on safety	112
4.5 Ranking chemical process routes based on individual environmental, health and safety aspects	113
4.6 Verification of the results by radial polygon diagram method.....	114
Chapter 5	120
CONCLUSIONS.....	120
Chapter 6	121
RECOMMENDATIONS	121
REFERENCES.....	122
Appendix A.1	127
Example calculation for Tertiary Butyl Alcohol based Route (TBA)	127
Appendix A.2	137
The STEL, TWA, LC50 and molecular weight values	137
Appendix B.1	139
Hazard potential calculation for primary parameters.....	139
Appendix B.2	142
Hazard potential calculation for intermediate parameters (pair wise comparison)..	142

LIST OF FIGURES

Figure 1.1: Chemical plant process development stages.....	1
Figure 3.1: Framework for ranking routes based on EHS-Fuzzy Index	19
Figure 3.2: EHS based impacts for a chemical process route.....	21
Figure 3.3: The model environment showing compartment volumes.....	24
Figure 3.4: Fuzzy based multicriteria decision making approach for EHS- fuzzy Index.....	37
Figure 3.5: Input membership functions of GWIacc-che.....	43
Figure 3.6: Output membership functions of GWIacc-che.....	43
Figure 3.7: Input membership functions of TOXacc.....	46
Figure 3.8: Output membership functions of TOXacc.....	46
Figure 3.9: Input membership functions of ODacc.....	49
Figure 3.10: Output membership functions for ODacc.....	49
Figure 3.11: Input membership functions of ADacc.....	51
Figure 3.12: Output membership functions for ADacc.....	52
Figure 3.13: Input membership functions of GWIacc-fire.....	54
Figure 3.14: Output membership functions for GWIacc-fire.....	54
Figure 3.15: Input membership functions of GWIcon.....	57
Figure 3.16: Output membership functions of GWIcon.....	57
Figure 3.17: Input membership functions of FEcon.....	60
Figure 3.18: Output membership functions for FEcon.....	60
Figure 3.19: Input membership functions of HAQacc.....	63
Figure 3.20: Output membership functions for HAQacc.....	63
Figure 3.21: Input membership functions of EXPche.....	65
Figure 3.22: Output membership functions for EXPche.....	66
Figure 3.23: Input membership functions for FLAche.....	68
Figure 3.24: Output membership function for FLAche.....	68
Figure 3.25: Input membership functions for INVche.....	71
Figure 3.26: Output membership functions for INVche.....	71
Figure 3.27: Input membership functions for Tpro.....	73
Figure 3.28: Output membership functions for Tpro.....	74
Figure 3.29: Input membership functions for Ppro.....	76
Figure 3.30: Output membership functions for Ppro.....	76

Figure 3.31: The fuzzy hierarchical model for EHS hazard assessment of a chemical process route.....	79
Figure 3.32: Input membership functions for ENVCHE.....	85
Figure 3.33: Input membership functions for ENVFIRE.....	85
Figure 3.34: Output membership functions for ENVACC.....	86
Figure 3.35: Input membership functions for ENVACC.....	88
Figure 3.36: Input membership functions for ENVCON.....	89
Figure 3.37: Output membership functions for ENV2REL.....	89
Figure 3.38: Input membership functions for FECON.....	92
Figure 3.39: Input membership functions for HAQACC.....	92
Figure 3.40: Output membership functions for HEL2REL.....	93
Figure 3.41: Input membership functions for SAFCHE.....	95
Figure 3.42: Input membership functions for SAFPRO.....	96
Figure 3.43: Output membership functions for SAF2CHPR.....	96
Figure 3.44: Input membership functions for HEL2REL.....	99
Figure 3.45: Input membership functions for SAF2CHPR.....	99
Figure 3.46: Output membership functions for HANDS.....	100
Figure 3.47: Input membership functions for HANDS.....	102
Figure 3.48: Input membership functions for EHV2REL.....	103
Figure 3.49: Output membership functions for EHS-fuzzy Index.....	103
Figure 3.50: Radial polygon diagram for a chemical process route.....	105
Figure 4.1: Radial polygon diagram for TBA route.....	116
Figure 4.2: Radial polygon diagram for I/C4 route.....	116
Figure 4.3: Radial polygon diagram for C3 route.....	117
Figure 4.4: Radial polygon diagram for C2/MP route.....	117
Figure 4.5: Radial polygon diagram for C2/PA route.....	118
Figure 4.6: Radial polygon diagram for ACH route.....	118

LIST OF TABLES

Table 3.1: NFPA fire ratings.....	33
Table 3.2: List of input and output notations to the FISs used for the primary parameters.....	38
Table 3.3: Fuzzy sets of GWIacc-che and the shape of the input and output membership functions.....	42
Table 3.4: Fuzzy IF-THEN rules for GWIacc-che.....	44
Table 3.5: Fuzzy sets of TOXacc and the shape of the for input and output membership functions.....	45
Table 3.6: Fuzzy IF-THEN rules for TOXacc.....	47
Table 3.7: Fuzzy sets of ODacc and shape of input and output membership functions.....	47
Table 3.8: Fuzzy IF-THEN rules for ODacc.....	50
Table 3.9: Fuzzy sets of ADacc and the shape of input and output memberships....	50
Table 3.10: Fuzzy IF-THEN rules for ADacc.....	52
Table 3.11: Fuzzy sets of GWIacc-fire and shape of input and output membership functions.....	53
Table 3.12: Fuzzy IF-THEN rules for GWIacc-fire.....	55
Table 3.13: Fuzzy sets of GWIcon and shape of input and output membership functions.....	56
Table 3.14: Fuzzy IF-THEN rules for GWIcon.....	58
Table 3.15: Fuzzy sets of FEcon and shape of for input and output memberships....	58
Table 3.16: Fuzzy IF-THEN rules for FEcon.....	61
Table 3.17: Fuzzy sets of AQacc and the shape of input and output memberships..	61
Table 3.18: Fuzzy IF-THEN rules for HAQacc.....	64
Table 3.19: Fuzzy sets of EXPche and shape of input and output memberships.....	64
Table 3.20: Fuzzy IF-THEN rules for EXPche.....	66
Table 3.21: Fuzzy sets of FLAche and shapes of for input and output membership functions.....	67
Table 3.22: Fuzzy IF-THEN rules for FLAche.....	69
Table 3.23: Fuzzy sets of INVche and shapes of the input and output membership functions.....	70
Table 3.24: Fuzzy IF-THEN rules for INVche.....	72

Table 3.25: Fuzzy sets of Tpro and shape of the for input and output membership functions.....	72
Table 3.26: Fuzzy IF-THEN rules for Tpro.....	74
Table 3.27: Fuzzy sets of Ppro and shapes of input and output memberships.....	75
Table 3.28: Fuzzy IF-THEN rules for Ppro.....	77
Table 3.29: Notation of intermediate parameters.....	77
Table 3.30: Summary of aggregation method used in EHS-Fuzzy Index hierarchy...	79
Table 3.31: Fuzzy sets and shapes of input and output memberships for ENVACC..	83
Table 3.32: Fuzzy IF-THEN rules for ENVACC.....	86
Table 3.33: Fuzzy sets and shapes of input and output memberships for ENV2REL..	87
Table 3.34: Fuzzy IF-THEN rules for ENV2REL.....	90
Table 3.35: Fuzzy sets and shapes of input and output memberships for HEL2REL..	90
Table 3.36: Fuzzy IF-THEN rules for HEL2REL.....	93
Table 3.37: Fuzzy sets and shapes of input and output memberships for SAF2CHPR.....	94
Table 3.38: Fuzzy IF-THEN rules for SAF2CHPR.....	97
Table 3.39: Fuzzy sets and shapes of input and output memberships for HANDS....	97
Table 3.40: Fuzzy IF-THEN rules for HANDS.....	100
Table 3.41: Fuzzy sets and shapes of input and output membership functions for EHS-Fuzzy Index.....	101
Table 3.42: Fuzzy IF-THEN rules for EHS-Fuzzy Index.....	104
Table 3.43: Notation for MMA manufacturing process routes.....	106
Table 4.1: Quantified impacts representing EHS aspects in the MMA routes assessment.....	108
Table 4.2: Routes to produce MMA ranked based on EHS fuzzy Index.....	109
Table 4.3: Hazard potential values for environment impact assessment parameters..	111
Table 4.4: Hazard potential values for health impact assessment parameters.....	112
Table 4.5: Hazard potential values for safety impact assessment parameters.....	113
Table 4.6: The ranking according to the result.....	114
Table 4.7: The Universe of Discourse for 13 parameters.....	115
Table 4.8: Comparison of radial polygon diagram and EHS-Fuzzy Index values for chemical routes to manufacture MMA	119
Table 4.9: Comparison of chemical routes to manufacture MMA ranked based on radial polygon diagram and EHS-Fuzzy Index	119

LIST OF ABBREVIATION

A_{Floor}	- cumulative value of average floor area of each unit operation
AD_{acc}	- the acid deposition impact due to accidental chemical release (Kmol equivalence of SO_2)
$AQ_{\text{acc}1}, AQ_{\text{acc}2}, \text{etc.}$	- the health impact value of each work place accidental release scenario
CEI	- Chemical Exposer Index
CED_i	- cumulative energy demand of chemical i (kJ/mol)
CF_{ADi}	- characterization factor for acidification of chemical i
EPA	- environment protection agency
EHS	- Environment Health and Safety
FE_{cont}	- health impact due to fugitive emission of a chemical route
FLAche	- flammability hazard of a chemical route
Fi	- flammability of chemical i (NFPA fire rating)
$f_{\text{GWP}i}$	- global warming potential of chemical i (equivalence of CO_2)
GHG	- greenhouse gases
$GW_{\text{Iacc-fire}}$	- the global warming impact due to GHG emission of accidental fire (Kmol equivalence of CO_2)
$GW_{\text{Iacc-che}}$	- the Global Warming Impact due to greenhouse gas emission of accidental chemical releases (Kmol equivalence of CO_2)
GW_{Icon}	- the global warming impact due to GHG emission of continuous operation (kmol equivalents of CO_2/hour)
HAQ_{acc}	- health impact of work place accidental release airborne quantity of a chemical route
INV_{che}	- chemical safety impact of a chemical route (te)
LC	- Lethal concentration
LD	- Lethal dose
MMA	- manufacture methyl methacrylate
M_i	- molar mass (g/mol)
M_i	- molar mass (g/mol)
m_{AQ}	- airborne quantity (kg/s)
$m_{i,\text{FE}}$	- fugitive emission rate of chemical substance i (kg/s)
n	- number of chemicals associated with the chemical process route

NFPA	- National fire and protection agency
$N_{i(Cl)}$ and $N_{i(Br)}$	- the number of Cl and Br atoms respectively, per molecule
$N_{i(C)}$	- the number of C atoms of substance i, per molecule
ODacc	- ozone depletion impact of a chemical route (years)
PEC	- Predicted Environmental Concentration
q_i	- molar feed rate of chemical i (kmol/hour)
Q_i	- total quantity of chemical i released to the environment (te)
$STEL_i$	- short-term exposer limit of chemical i (kg/m^3)
TLV	- threshold limit value
TWA_i	- time weighted average value of substance i (kg/m^3)
T_{pro}	- process safety impact due to operating temperature of chemical route (K)
T_j	- difference between operating temperature and ambient temperature of reaction step j (K)
VF	- volumetric flow rate (m^3/s) of air in the work place
x_i	- mass fraction of chemical i in the stream
Y_i	- mass fraction of chemical i
τ_i	- atmospheric life (years) of chemical i
ΔH_{CO_2}	- heat of combustion of carbon (kJ/mol)