



**Islamic Azad University  
Tehran South Branch  
Graduate School**

**Dissertation for the Partial Fulfillment for the Degree of  
Master of Science**

**Chemical Engineering - Process Design**

**Subject:**

**Computer Aided Risk Reduction Tool (CARRT)**

**An Inherently Safer Approach**

**Advisor:**

**Consulting Advisor:**

**By:**



دانشگاه آزاد اسلامی  
واحد تهران جنوب  
دانشکده تحصیلات تکمیلی

پایان نامه برای دریافت درجه کارشناسی ارشد “M. Sc.”  
مهندسی شیمی – طراحی فرآیند

**عنوان:**

ابزار کاهش ریسک بکمک کامپیوتر  
(CARRT)  
با نگرش طراحی ذاتا ایمن تر

**استاد راهنما:**

**استاد مشاور:**

**نگارش:**

## **ABSTRACT**

The term 'inherently safer' implies that the process is safe by its very nature and not externally constrained to be safe by the use of add-on systems and devices, hence making it a proactive approach to process safety. It is very effective in risk reduction if applied at the beginning stages of design, leading to cost effective and timely solutions and modifications. In this thesis, after elements of risk and its management strategies are briefly discussed, Inherently Safer Design (ISD) - as well as its quantification by indices both developed non-specifically and specifically for ISD - is elaborated, in order to rank alternative processes based on their inherent safety adaptability. Considering the advantages and the shortcomings of ISD quantification indices in the literature, a new modified ISD index is proposed, covering ISD aspects of a process at conceptual design stage, which leads to better ranking in comparison with its predecessor.

Finally, in order to heuristically validate the new ISD index, the details of inherently safer analysis at conceptual design stage are illustrated by comparing three competing processes for acrylonitrile manufacture. These processes are simulated using a well-known commercial process simulator, with a program added capable of extracting the necessary data from the simulation cases to calculate new ISD index value, incorporating great flexibility and speed in risk reduction through inherently safer analysis of processes.

# TABLE OF CONTENTS

<u>Chapter</u>	<u>Page</u>
DEDICATION.....	iv
ACKNOWLEDGEMENTS.....	v
ABSTRACT.....	vi
TABLE OF CONTENTS.....	vii
LIST OF TABLES.....	xi
LIST OF FIGURES.....	xiii
INTRODUCTION .....	1
I SCOPE OF THE PROJECT.....	2
II ELEMENTS OF RISK & ITS MANAGEMENT.....	5
2.1 Elements of risk.....	6
2.2 Layers of protection.....	7
2.3 Risk reduction and management strategies.....	8
III INHERENTLY SAFER CHEMICAL PROCESS DESIGN.....	12
3.1 Definition of an inherently safer process.....	13
3.2 History of inherently safer process design.....	14
3.3 Inherently safer process design strategies.....	17
3.3.1 Minimize.....	18
3.3.2 Substitute.....	22
3.3.3 Moderate.....	25

	3.3.4 Simplify.....	29
	3.4 Inherent safety and the process life cycle.....	30
	3.5 Inherent safety conflicts.....	32
	3.6 Resolving inherent safety conflicts.....	33
IV	A REVIEW OF INHERENTLY SAFER CHEMICAL PROCESS DESIGN	
	HAZARD INDICIES.....	35
	4.1 Introduction to hazard indices.....	36
	4.2 Hazard indices <i>not specifically</i> developed for inherent safety.....	37
	4.2.1 Dow indices.....	37
	4.2.1.1 Dow's fire and explosion index.....	37
	4.2.1.2 Dow's chemical exposure index.....	41
	4.2.2 Mond index.....	43
	4.2.3 The instantaneous fractional annual loss (IFAL) index.....	46
	4.2.4 Hazard identification and ranking (HIRA).....	49
	4.2.5 Safety weighted hazard index (SWeHI).....	53
	4.3 hazard indices <i>specifically</i> developed for inherent safety.....	57
	4.3.1 INSIDE project and INSET toolkit.....	57
	4.3.2 Fuzzy based inherent safety index.....	63
	4.3.3 Integrated inherent safety index (I2SI).....	69
	4.3.4 Graphical method.....	76
V	CRITICAL REVIEW OF MAINSTREAM INHERENTLY SAFER CHEMICAL	
	PROCESS DESIGN HAZARD INDICIES.....	81
	5.1 Introduction to mainstream indices.....	82

5.2	Prototype index of inherent safety (PIIS).....	82
5.3	Inherent safety index (ISI).....	92
5.4	Modified inherent safety index (m-ISI).....	101
VI	A NEW INHERENTLY SAFER DESIGN INDEX.....	108
6.1	Introduction.....	109
6.2	Corrosion.....	109
6.3	Inventory.....	110
6.4	Toxicity.....	110
6.5	Flammability.....	112
6.6	Explosiveness.....	113
6.7	Temperature.....	114
6.8	Pressure.....	114
6.9	Yield.....	114
6.10	Chemical reactivity.....	115
6.11	The new inherently safer design index (ISDI).....	116
VII	THE COMPUTER TOOL: CARRT.....	119
7.1	Computerized inherent safety evaluation.....	120
7.2	Computer aided risk reduction tool (CARRT).....	120
VIII	CASE STUDY.....	123
8.1	Acrylonitrile and its production.....	124
8.2	Process description.....	125
8.3	Computer simulation and CARRT results.....	128

IX	CONCLUSIONS & FUTURE WORK.....	132
	9.1 Conclusions.....	133
	9.2 Future work.....	134
	APPENDIX.....	135
	A. Three significant disasters.....	136
	A.1. Flixborough, England.....	136
	A.2. Bhopal, India.....	138
	A.3. Seveso, Italy.....	140
	FARSI ABSTRACT.....	142
	REFERENCES.....	143

## LIST OF TABLES

<b><u>Table</u></b>		<b><u>Page</u></b>
2.1	Risk management strategies.....	9
3.1	Effect of refrigeration on distance to ERPG-3 concentration for a 5.1 cm monomethylamine pipe rupture.....	27
4.1 (a, b)	Relative values of p factor for some plants and relative contribution of hazards on an EB plant in IFAL.....	49
4.2	INSET stages, key issues & information used.....	60
4.3	List of tools in INSET.....	61
4.4	List of required input parameters (linguistic variables).....	64
4.5	List of required input parameters for adaptive membership design.....	65
4.6	Fuzzy IF-THEN rules for ISI.....	67
4.7	Guidelines for the extent of requirement of add-on system.....	72
4.8	Guidelines for the extent of applicability of IS guidewords.....	74
5.1	Parameters considered and selected in PIIS.....	83
5.2 (a ~ g)	Scores in PIIS.....	84
5.3	Routes to MMA production.....	85
5.4	Scores for each step of each route to MMA production.....	86
5.5	Scores each route to MMA production.....	87
5.6	Process safety experts who commented on PIIS.....	88
5.7	Criteria used in PIIS and ISI and their source.....	93
5.8	ISI symbols of sub-indices.....	93
5.9 (a ~ k)	ISI scores of sub-indices.....	94 ~ 96
5.10	Routes to acetic acid production.....	104

5.11	Individual chemical index calculation in M-ISI for carbonylation process for acetic acid production.....	104
5.12	M-ISI for carbonylation process for acetic acid production.....	105
5.13	M-ISI for routes to acetic acid production.....	105
6.1 (a ~ c)	Process sub-indices for the new ISD Index.....	117
6.2 (a ~ e)	Chemical sub-indices for the new ISD Index.....	117
8.1	Route to acrylonitrile synthesis.....	125
8.2	Basic data for routes to acrylonitrile synthesis simulation.....	128 ~ 129
8.3 (a ~ c)	ISD indices for routes to acrylonitrile synthesis: (a) chemical sub-indices, (b) process sub-indices and (c) total.....	130

## LIST OF FIGURES

<u>Figure</u>		<u>Page</u>
2.1	The elements of risk.....	6
2.2	Layers of protection, when they are degraded and when inherently safer design approach is applied.....	7
2.3	Inherently safer design approach aims the heart of process.....	11
3.1	The conventional design for the manufacture of methyl acetate.....	21
3.2	The reactive distillation design for the manufacture of methyl acetate.....	22
3.3	Comparison of centerline vapor cloud concentration as a function of distance from the release for anhydrous and 28% aqueous ammonia storage for two release scenarios (Weather - D Stability, 3.4 mph wind speed).....	26
3.4	Address safety at the very beginning of project life cycle.....	31
4.1	Procedure for calculating Dow's F&EI.....	38
4.2	Procedure for calculating Mond's F, E&TI.....	45
4.3	Procedure for calculating The IFAL index.....	48
4.4	Methodology of HIRA computation.....	50
4.5	Methodology of SWeHI computation.....	54
4.6 (a)	Hierarchical tree for Layer 1 and Layers 2.1 and 2.2.....	66
4.6 (b, c)	Hierarchical tree for (b) the evaluation of fire and explosion hazards (c) the evaluation of hazards due to chemical properties.....	66
4.6 (d)	Hierarchical tree for the evaluation of mechanical failure.....	67
4.7	Methodology of I2SI computation.....	70
4.8	Monograph for PHCI.....	72

4.9	ISI for different guidewords a) minimization b) substitution c) attenuation d) limiting of.....	74
4.10	Graphical IS measurement for MMA routes.....	78
5.1	Number of usage of keywords by the eight process safety experts.....	98
6.1	Relative toxicity at different dose.....	112
7.1	Inherent safety evaluation embedded in automated process synthesis.....	121
8.1	Simplified process flow diagram – SOHIO process for acrylonitrile.....	126
8.2	An operating acrylonitrile production plant in India.....	127