

**CHEMICAL PROCESS ROUTE SELECTION BASED  
ON ASSESSMENT OF INHERENT ENVIRONMENTAL  
HAZARD, OCCUPATIONAL HEALTH AND SAFETY  
(IEHS)**

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Degree of Master of Science

Department of Chemical & Process Engineering

University of Moratuwa  
Sri Lanka

September 2013

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Thesis submitted in partial fulfillment of the requirements for the degree

Master of Science

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## DECLARATION OF THE CANDIDATE & SUPERVISOR

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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The above candidate has carried out research for the Masters Thesis under my supervision.

Signature of the supervisor: ..... Date: .....

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## Abstract

Chemical process route selection is one of the main design decisions that needs to be taken during the preliminary stages of chemical plant design and development. A chemical process route is considered as the raw materials and the sequence of reaction steps that converts them in to desired products. Previously, the most important factor considered in selecting the chemical process route was plant economics. However, now other issues such as safety, environment and occupational health have also become important considerations. Therefore, at early stages of chemical process plant design and development it is necessary to apply methodologies to identify and assess environmental, occupational health and safety hazards involved in the process routes.

This work proposes a methodology for assessing chemical process routes to manufacture a chemical based on inherent environmental, occupational health and safety hazards. The method developed in this work can be used during early design stages of a chemical process plant. The process route selection is done based on impacts due to emissions from the ongoing operational conditions of the plant. It considers the potential toxicological impacts on the environment, potential impacts on the occupational health due to fugitive emissions and the potential chemical and process safety impacts within the plant.

As the outcome of the methodology, an integrated index called “Inherent Chemical Process Route Index” (ICPRI) is proposed which can be used for the selection of the ‘best’ chemical process route for a chemical process plant, based on inherent environmental hazard, occupational health and safety (IEHS). The lower the ICPRI the more inherently environmentally friendly, inherently occupational healthier and inherently safer the route is. The methodology developed in this work can also rank alternative chemical process routes based on inherent environmental hazard or occupational health hazard and or safety hazard separately. The method was applied on four possible process routes to produce acetone. The propene oxidation route showed the lowest ICPRI value indicating potentially the ‘best’ chemical process route for acetone manufacturing process based on the IEHS assessment.

Keywords:

Inherent Environmental hazard, occupational health, Inherent Safety, Chemical process route

## DEDICATION

*I dedicate this thesis to my wonderful family.*

*Without their patience, understanding, support and most of all love, the*

*completion of this work would not have been possible....*



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## ACKNOWLEDGEMENT

Completion of this thesis has been one of the most significant academic challenges I have ever had to face. This research becomes a reality because of the untiring efforts of many knowledgeable people and I would like to thank all of those people who helped make this dissertation possible.

In the first place I would like to give my sincere gratitude to my main supervisor, Dr. M. Y. Gunasekera for her inspiring and motivating guidance throughout this research with supervision.

I am indebted to Dr. Shantha Walpolage who is the former postgraduate coordinator in the department and provided a helping hand to move my M.Sc. forward.

I am immensely grateful to Dr. A.D.U.S. Amarasinghe, former Head of the Department of Chemical and Process Engineering, University of Moratuwa, for giving me the opportunity to do the M.Sc. in the department.



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Also I gratefully acknowledge, Dr. H.M.R. Premasiri, Department of Earth Resources Engineering, for his great advices and comments as the chairperson of the progress review committee.

My grateful thank to Dr. P.G, Rathnasiri, Head of the Department of Chemical and Process Engineering, University of Moratuwa and the coordinator of the MSc in Sustainable Process Development course for assisting me with my course work component. .

I would like to thank all members of the academic staff of Department of Chemical & Process Engineering for advising and helping me in many ways.

My special thanks go to the University of Moratuwa Senate Research Grant for their financial support. This research project was supported by University of Moratuwa Senate Research Grant Number SRC/LT/2011/13.

It is my pleasure to remind Sri Lanka Custom Department for providing organic chemicals import data in order to select my case study.

I am thankful to non academic staff of Department of Chemical & Process Engineering for helping me in many ways.



Last but not the least I would like to thank all the colleagues, Staff members of PG division, Examination branch, Accounts division and Library for the help and cooperation given.

Most importantly, none of these would have been possible without the love and patience of my family. I am deeply indebted to my loving parents and parents in-law who have given me their fullest support, my understanding and patient husband Nalin, who is behind me in my every step, our loved son Navitha, who is the joy of our lives and my brothers and sisters who always supported and encouraged me, in my entire endeavour.

I thank all who helped me in numerous ways and regret my inability to mention them individually.

S. Warnasooriya

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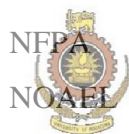
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## LIST OF ABBREVIATIONS & NOTATIONS

Abbreviation	Description
ACP	Acetophenone
AHI	Atmospheric Hazard Index
AHP	Analytical Hierarchy Process
AP	<i>Acidification Potential</i>
CAHI	Chemical Atmospheric Hazard Index
CEL	Chemical Exposure Limit
CFC	Chlorofluorocarbon
CHP	Cumenehydroperoxide
ChV	Chronic concentration Value
CRSI	Chemical Route Safety Index
CSI	Chemical Safety Index
CTHI	Chemical Terrestrial Hazard Index
CWHI	Chemical Water Hazard Index
DMPC	Dimethylphenylcarbinol
ECOSAR	ECOLOGical Structure Activity Relationship
EHI	Environmental Hazard Index
EHS	Environment, Health and Safety
EI	Explosiveness Index
EPA	Environment Protection Agency
ETHI	Environmental Toxicity Hazard Index
FI	Flammability Index
GWP	Global Warming Potential
HI	Hazard Index
HQI	Health Quotient Index
IBI	Inherent Benign-ness Index
ICPRI	Inherent Chemical Process Route Index

IEHS	Inherent Environmental hazard, occupational Health and Safety
IETH	Inherent Environmental Toxicity Hazard
inhChL	inhalation Chronic toxicity Level
inhLC <sub>50</sub>	Inhalation LC <sub>50</sub> of chemical
InI	Inventory Index
IOHI	Inherent Occupational Health Index
IPB	Isopropylbenzene
IRIS	Integrated Risk Information System
ISI	Inherent Safety Index
ISPI	Inherent Safety Potential Index
LC <sub>50</sub>	Lethal Concentration of chemical that that kills 50% of the test population, mol/m <sup>3</sup>
LD <sub>50</sub>	Lethal Dose of chemical that kills 50% of the test population, mg/kg body weight
LEL	Lower Explosive Limit
NFPA	National Fire Protection Association
NOAEL	No Observable Adverse Effect Level
OHHI	Occupational Health Hazard Index
OhHI	Occupational health Hazard Index
OHI	Occupational Health Index
oralChL	oral Chronic toxicity Level
OSHA	Occupational Safety and Health Administration
OSI	Overall Safety Index
<i>p</i> -DIPB	<i>p</i> -diisopropylbenzene
<i>p</i> -DIPBDHP	<i>p</i> - diisopropylbenzenedihydroperoxide
PEC	Predicted Environmental Concentration
PFD	Process Flow Diagram
PI	Pressure Index
PID	Piping and Instrumentation Diagram
PIIS	Prototype Index for Inherent Safety
<i>ppb</i>	<i>parts</i> per billion



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PRHI	Process Route Healthiness Index
PSI	Process Safety Index
RAHI	Route Atmospheric Hazard Index
RfD	Reference Dose
RI	Reactivity Index
RTHI	Route Terrestrial Hazard Index
RWHI	Route Water Hazard Index
SHE	Safety, Health and Environmental
TI	Temperature Index
TLV	Threshold Limit Value
TLV-C	Threshold Limit Value-Ceiling
TLV-STEL	Threshold Limit Value-Short Term Exposure Limit
TLV-TWA	Threshold Limit Value-Time Weighted Average
UEL	Upper Explosive Limit
UV	Ultraviolet
VOCs	Volatile Organic Compounds
WCC	Workplace Chemical Concentration



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## NOTATIONS

$CEL_i$	Chemical exposure limit for chemical $i$ , $mg/m^3$
$ChV_i$	Chronic concentration value of chemical $i$ for aquatic organisms, $mol/m^3$
$C^S$	solubility in water, $mol/m^3$
$E_i$	Emission rate of chemical $i$ to the unit world, $mol/h$
$f$	fugacity, Pa
$FE_i$	Fugitive emissions rate of chemical $i$ , $kg/hr$
$FE_k$	pre-calculated fugitive emission rate for process unit $k$
$F_{NFPA}$	NFPA scores for flammability
$i$	chemical $i$ involved with the route.
$inhChL_i$	Inhalation chronic toxicity level of chemical $i$ , $mol/m^3$
$k_A$	first order rate constant in air, $h^{-1}$



$K_{ow}$	octanol water partition coefficient
$k_s$	first order rate constant in soil, $h^{-1}$
$k_w$	first order rate constant in water, $h^{-1}$
$L$	mass fraction organic matter
$M$	Molecular weight of chemical, g/mol
$MF_{ik}$	Mass fraction of chemical $i$ in process unit $k$
$n$	number of chemicals in the route
$oralChL_x$	Oral Chronic toxicity Level of species $x$ , mg/kg body weight/day
$p$	number of process units involved in the route
$PEC_{ai}$	PEC of chemical $i$ in air compartment from daily operational releases, $mol/m^3$
$PEC_{si}$	PEC of chemical $i$ in soil compartment from daily operational releases, $mol/m^3$
$PEC_{wi}$	PEC of chemical $i$ in water compartment from daily operational releases, $mol/m^3$
$P^S$	vapor pressure, Pa
$R$	gas constant ( $8.314 Pa m^3/mol K$ )
$R1$	Cumene oxidation route
$R2$	2-Propanol dehydrogenation route
$R3$	Propene oxidation route
$R4$	<i>p</i> -Diisopropyl benzene oxidation route
$R_{NFPA}$	NFPA scores for reactivity
$T$	emission temperature, K
$TDI_{fx}$	daily food intake of animal species $x$ , g/kg body weight/day
$TDI_{wx}$	daily fluid intake of animal species $x$ , g/ kg body weight /day
$V$	Volumetric air flow rate, $m^3/hr$
$V_A$	Volume of air compartment, $m^3$
$V_S$	Volume of soil compartment, $m^3$
$V_W$	Volume of water compartment, $m^3$
$W_A$	Weight factor for the atmospheric environment
$WCC_i$	Workplace Chemical Concentration of chemical $i$ , $mg/m^3$



$WF_E$	Weight Factor for explosiveness
$WF_F$	Weight Factor for flammability
$WF_{In}$	Weight Factor for inventory
$WF_P$	Weight Factor for pressure
$WF_R$	Weight Factor for reactivity
$WF_T$	Weight Factor for temperature
$W_T$	Weight factor for the terrestrial environment
$W_W$	Weight factor for the aquatic environment
$Z_A$	fugacity capacity of air, mol/m <sup>3</sup> Pa
$Z_S$	fugacity capacity of soil, mol/m <sup>3</sup> Pa
$Z_W$	fugacity capacity of water, mol/m <sup>3</sup> Pa
$\rho_s$	density of soil, kg/m <sup>3</sup>
$\rho_w$	density of water, kg/m <sup>3</sup>



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