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

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(118010E)

Degree of Master of Science

Department of Chemical & Process Engineering

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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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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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S. Warnasooriya

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LIST OF ABBREVIATIONS & NOTATIONS

Abbreviation	Description
ACP	Acetophenone
AHI	Atmospheric Hazard Index
AHP	Analytical Hierarchy Process
AP	*Acidification Potential*
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$_{50}$	Inhalation LC$_{50}$ 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$_{50}$	Lethal Concentration of chemical that that kills 50% of the test population, mol/m^3
LD$_{50}$	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
p-DIPB	*p*-diisopropylbenzene
p-DIPBDHP	*p*- diisopropylbenzenedihydroperoxide
PEC	Predicted Environmental Concentration
PFD	Process Flow Diagram
PI	Pressure Index
PID	Piping and Instrumentation Diagram
PIIS	Prototype Index for Inherent Safety
ppb	*parts* per billion

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

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	*p*-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^3Pa
Z_S	fugacity capacity of soil, mol/m^3Pa
Z_W	fugacity capacity of water, mol/m^3Pa
ρ_s	density of soil, kg/m^3
ρ_w	density of water, kg/m^3