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

Hewa Batagodage Buddika Anuradha

(158059X)

Degree of Master of Philosophy

Department of Chemical & Process Engineering

University of Moratuwa

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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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Buddika Anuradha

TABLE OF CONTENTS

LIST OF FIGURES

LIST IF TABLES

LIST OF ABBREVIATION

A_{Floor} - cumulative value of average floor area of each unit operation

ADacc - the acid deposition impact due to accidental chemical release (Kmol equivalence of SO_2)

AQacc1, AQacc2, 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)

$CF_{AD\textit{i}}$ - characterization factor for acidification of chemical i

EPA - environment protection agency

EHS - Environment Health and Safety

FEcont - 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_{GWPi} - global warming potential of chemical i (equivalence of CO_2)

GHG - greenhouse gases

GWIacc-fire - the global warming impact due to GHG emission of accidental fire (Kmol equivalence of CO_2)

GWIacc-che - the Global Warming Impact due to greenhouse gas emission of accidental chemical releases (Kmol equivalence of CO_2)

GWIcon - the global warming impact due to GHG emission of continuous operation (kmol equivalents of CO_2/hour)

HAQacc - health impact of work place accidental release airborne quantity of a chemical route

INVche - chemical safety impact of a chemical route (te)

LC - Lethal concentration

LD - Lethal dose

MMA - manufacture methyl methacrylate

M_i - molar mass (g/mol)

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m_{AQ} - airborne quantity (kg/s)

$m_{i,FE}$ - 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
TWAi	- time weighted average value of substance i (kg/m^3)
Tpro	- 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 faction of chemical i in the stream
Yi	- mass fraction of chemical i
τ_i	- atmospheric life (years) of chemical i
ΔH_{CO2}	- heat of combustion of carbon (kJ/mol)