

**RISK-BASED CHEMICAL PROCESS ROUTE  
SELECTION CONSIDERING INHERENT  
ENVIRONMENTAL FRIENDLINESS**

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Doctor of Philosophy

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Thesis submitted in partial fulfillment of the requirements for the degree

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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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The above candidate has carried out research for the PhD thesis under my supervision.

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Signature of the Supervisor:

Date: 01.04.2024.

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## Abstract

Chemical process route selection is one of the key decisions taken during the preliminary design stage of process plant development. A chemical process route is defined as the raw material(s) and the sequence of reaction step(s) that convert them to the desired product. In the past, the 'best' process route was selected solely considering economic factors. However, with the disastrous chemical plant accidents experienced in the past, attention has been drawn to select process routes considering other factors such as inherent environmental friendliness. Therefore, methodologies that assess chemical process routes considering environmental aspects are needed for the development of inherently environmentally friendly chemical process plants. The work presented in this thesis proposes a risk-based methodology to assess and rank chemical process routes considering inherent environmental friendliness using the data available during preliminary design stage of chemical process plant design and development. The environmental impacts that could occur due to chemical plant accidents such as accidental chemical releases, fires and explosions are considered when developing the methodology. In the proposed methodology, the chemical process routes are assessed in three approaches. They are fires and explosions, accidental chemical releases and all these three accidents in combination. Therefore, three risk indices are proposed namely, the Inherent Environmental Risk Index for Fires and Explosions (F&E-IERI), the Inherent Environmental Risk Index for accidental Chemical Releases (Chem-IERI), and the Inherent Environment Risk Index (Chem F&E-IERI). A lower risk index of a process route indicates a lower environmental risk and, thus the most inherently environmentally friendly route among the alternate process routes. The proposed methodology is applied in four potential process routes in acetone production. The results obtained show that the process route that has the lowest environmental risk due to fires and explosions in the chemical plant is the p-diisopropyl benzene oxidation process. The dehydrogenation of 2-propanol process route shows the lowest environmental risk due to accidental chemical release. The chemical route that has the lowest environmental risk due to all three major chemical plant accidents, fires, explosions, and chemical releases is the dehydrogenation of 2-propanol process.

**Keywords:** Environmental risk assessment, chemical process route selection, accidental chemical releases, fires and explosions, inherent safety

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## LIST OF ABBREVIATIONS

Abbreviation	Description
$AcTL_j$	Minimum risk level of chemical $j$ that is likely to be without appreciable risk of adverse non-cancer human health effects
$aqlife$	Aquatic life
BI	Burn injury impact
Chem-IERI	Inherent environmental risk index for accidental chemical release
$CL_j$	Concentrations ( $\text{mol}/\text{m}^3$ ) in the atmosphere above which direct adverse effects on plants may occur according to present knowledge
F&E-IERI	Inherent Environmental Risk Index for Fires and Explosions
$f_{k,i,j}$	Frequency Index of chemical plant accident that results in environmental impact $k$ due to chemical $j$ in process equipment $i$
$f_{ref}$	Reference frequency of occurrence of fire and explosion event
GW	Global warming impact
$i$	Process equipment
$inhLC50_j$	Inhalation lethal concentration of chemical $j$ that kills 50% of the test population of an animal species in 4 hours by inhalation, $\text{mol}/\text{m}^3$
$IR_{abs_j}$	IR absorption strength of the chemical $j$ in the interval of 500–1400 $\text{cm}^{-1}$ , $\text{cm}^{-2}\text{atm}^{-1}$
$j$	Chemical in process equipment $i$
$k$	Environmental impact
$k_{OH(C_3H_6)}$	Rate constant for the reaction between the OH radical and propene
$k_{OH(j)}$	Rate constant for the reaction between the OH radical and substance $j$
$LC50_j$	Concentration of chemical $j$ in water, which kills 50% of a test population of the most sensitive species over a 96 h period, $\text{mol}/\text{m}^3$
$LD50_j$	Lethal dose of chemical $j$ that kills 50% of the test population ( $\text{mg}/\text{kg}$ )
LOC	Loss of containment
$MM_j$	Molecular mass of chemical $j$ , $\text{g mol}^{-1}$
$M_{k,i,j}$	Magnitude of environmental impact $k$



$n_{Cl}, n_{Br}$	Number of Cl atoms per molecule, number of Br atoms per molecule
$PEC_{Ca,j}$	Predicted environmental concentration of the chemical $j$ in the atmospheric compartment ( $\text{mol}/\text{m}^3$ )
$PEC_{Ca}(j)$	Predicted environmental concentration of substance $j$ in ppbC in the atmospheric compartment when a quantity $Q_j$ is released
$PEC_{s,j}$	Predicted environmental concentration of chemical $j$ in soil compartment ( $\text{mol}/\text{m}^3$ )
$PEC_{w,j}$	Predicted environmental concentration of chemical $j$ in water compartment ( $\text{mol}/\text{m}^3$ )
$Q_j$	Quantity of the chemical $j$ released into the atmosphere
$g$	acceleration due to gravity
$RI_k$	Risk index of environmental impact $k$
$SD$	Structural damage impact
$SM_{k,i,j}$	Scaled magnitude of environmental impact $k$ of chemical $j$ in process equipment $i$
$s^n$	Vulnerability score of $n^{\text{th}}$ influencing factor
$TDI_{f,x}$	Daily food intake of species $x$ ( $\text{m}^3/\text{day}$ )
$TDI_{w,x}$	Daily fluid intake of species $x$ ( $\text{m}^3/\text{day}$ )
<i>terran</i>	Terrestrial animal population
<i>terrhab</i>	Terrestrial inhabitants
<i>veg</i>	Vegetation
$V_{gas,k}$	Vulnerability score of the environmental element affected by environmental impact $k$ due to accidental gas release
$V_{liquid,k}$	Vulnerability score of the environmental element affected by environmental impact $k$ due to accidental liquid release
$w_k$	Weighting factor for environmental impact $k$
$W_{t,x}$	Weight of species $x$ (kg)
$\tau_j$	Atmospheric life (years) of chemical $j$

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