COMPUTER AIDED APPROACH FOR OCCUPATIONALLY HEALTHIER CHEMICAL PROCESSES ASSESSMENT AND SELECTION

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I would like to dedicate this thesis to my parents…

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ABSTRACT

The purpose of this study is to develop computer aided approach of inherently healthier chemical process selection during early design stage. The study is divided into two major parts, which are to develop 1) a computer-aided index tool for inherent occupational health assessment and 2) a systematic approach to design an inherently healthier chemical process. Early hazard assessment during early design stage is critical as process modifications can still be made with high degree of freedom and at minimal cost. In this study, an electronic database was created for 1625 chemicals to provide all the chemical, physical and toxicity properties required for the index calculations for a comprehensive list of chemicals. The tool can be used to screen the alternative chemical synthesis routes to the desired product by their health properties as well as to characterise the hazard level of single process. The results of the hazards calculation are presented as a summary in tabulated as well as graphical forms which further ease the hazard assessment process. In the second part of the thesis, a flowchart is proposed for designing an inherently healthier process using Inherently Safer Design (ISD) principles (minimisation, substitution, moderation and simplification). Based on the guideline, the users may design a process which poses the lowest health hazards to workers by selecting less hazardous chemical substances and operating conditions but still within a constraint of ensuring the improved reaction chemistry is technically feasible for synthesising the desired product. With both the hazard assessment tool and design approach, the users are able to efficiently obtain reliable results.

ABSTRAK

Tujuan kajian ini ialah bagi menghasilkan reka bentuk berbantu komputer untuk pemilihan proses kimia sedia ada lebih sihat semasa peringkat reka bentuk awal. Kajian ini dibahagikan kepada dua bahagian utama, iaitu penghasilan 1) alatan indeks berbantu komputer untuk penilaian kesihatan pekerjaan yang sedia ada dan 2) pendekatan sistematik untuk menghasilkan proses kimia yang sedia ada lebih sihat. Pengenalpastian peringkat bahaya awal semasa reka bentuk awal adalah kritikal kerana pengubahsuaian proses masih boleh bebas dilakukan dalam kadar yang tinggi pada kos yang minimum. Dalam kajian ini, satu pangkalan data elektronik telah dihasilkan untuk 1625 bahan kimia bagi menyediakan ciri-ciri kimia, fizik dan ketoksikan yang diperlukan untuk pengiraan menyeluruh senarai indeks semua bahan kimia. Kemudahan ini boleh digunakan untuk menyaring laluan alternatif bagi sintesis kimia kepada produk yang diingini melalui ciri-ciri kesihatan dan juga untuk pengkategorian peringkat bahaya bagi proses tunggal. Keputusan bagi pengiraan bahaya telah dibentangkan dalam bentuk ringkasan jadual dan juga grafik yang seterusnya memudahkan proses penilaian. Pada bahagian kedua tesis ini, sebuah carta aliran untuk proses rekaan lebih sihat yang sedia ada telah dicadangkan menggunakan prinsip reka bentuk lebih selamat (ISD), (meminimum, mengganti, kesederhanaan dan memudahkan). Berdasarkan garis panduan ini, pengguna boleh merekabentuk proses yang menunjukkan bahaya kesihatan paling rendah pada para pekerja dengan memilih bahan kimia dan keadaan operasi yang kurang berbahaya tetapi masih dalam kawalan bagi memastikan tindak balas kimia yang lebih baik dapat dilaksanakan secara teknikal bagi mensintesis produk yang dikehendaki. Dengan kedua-dua alat penilaian dan pendekatan reka bentuk, pengguna boleh mendapatkan keputusan dengan cepat dan tepat.

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Pandian, S., Hassim, M. H., and Hurme, M. Computer Aided of Occupationally Healthier Processes During Research and Development Stage. *Journal of Loss Prevention in the Process Industries*, 2013; 26(1) 705-713.

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LIST OF ABBREVIATIONS

ACH	-	Acetone cyanohydrin based route
ACGIH	-	American Conference of Govermental Industrial Hygienist
BAT	-	Biologische Arbeitsplatztoleranzwerte
CAPE	-	Computer Aided Process Engineering
COSHH	-	Control of Substances Hazardous to Health Regulations
C2/MP	-	Ethylene via methyl propionate based route
C2/PA	-	Ethylene via propionaldehyde based route
C3	-	Propylene based route
EL	-	Exposure limit
EU	-	European Union
GPA	-	Global Plan of Action on workers health
HAZOP	-	Hazard and Operability
H&MB	-	Heat and Material Balance
HQI	-	Hazard Quotient Index
HTP	-	Haitallisiksi Tunnetut Pitoisuudet
i-C4	-	Isobutylene based route
I2SI	-	Integral Inherent Safety Index
iRET	-	Integrated Risk Estimation Tool
ISD	-	Inherently Safer Design
ISHE	-	Inherent Safety Health and Environment
ISL	-	Inherent Safety Level
ISI	-	Inherent Safety Index
ISIM	-	Inherent Safety Index Module
IOHI	-	Inherent Occupational Health Index
LPCVD	-	Low Pressure Chemical Vapour Deposition

MAK	-	Maximale Arbeitsplatz-Konzentration
MMA	-	Methyl Methacrylate
MSDS	-	Material Safety Data Sheet
NIEHS	-	National Institute of Environmental Health Sciences
OEL	-	Occupational Exposure Limits
OELV	-	Occupational Exposure Limit Value
OHHI	-	Occupational Health Hazards Index
OHI	-	Occupational Health Index
PEL	-	Permissible Exposure Limit
PFD	-	Process Flow Diagram
P&ID	-	Piping and Instrumentation Diagram
PIIS	-	Prototype Index for Inherent Safety
PRHI	-	Process Route Healthiness Index
PSI	-	Process Stream Index
QAISD	-	Quality Assessment for Inherently Safer Design
R&D	-	Research and Development
SHE	-	Safety, Health and Environment
STEL	-	Short Term Exposure Limit
TBA	-	Tertiary butyl alcohol based route
TLV	-	Threshold Limit Value
TORCAT	-	Toxic Release Consequences Analysis Tool
QI2SD	-	Quantitative Index of Inherently Safer Design
WHO	-	World Health Organisation

NOMENCLATURE

I_C	-	Corrosiveness sub index
I_{EL}	-	Exposure limit sub index
I_{HH}	-	Index for Health Hazards
I_{MS}	-	Material state sub index
I_P	-	Pressure sub index
I_{PM}	-	Process mode sub index
I_{PPH}	-	Index for Physical and Process Hazards
I_R	-	R-phrases sub index
I_T	-	Temperature sub index
I_V	-	Volatility sub index

CHAPTER 1

INTRODUCTION

1.1 Research background

Occupational health is the protection of the bodies and minds of people from illness resulting from materials, processes, or procedures used in the workplace (Hughes and Farrett, 2008). The assessment of occupational health is related to the identification and control of the risks arising from physical, chemical, and other workplace hazards in order to establish and maintain a safe and healthy working environment. These hazards can be divided into five major categories of chemical, physical, biological, and ergonomics/mechanics as well as psychosocial factors (Hartley, 1999; Negash, 2002). The National Institute of Environmental Health Sciences (NIEHS) has supported training and education programs since 1986 in order to protect workers in Malaysia. This is mainly to protect them from being exposed to toxic materials during hazardous waste operations and chemical emergency response. They have also arranged safety and health training for the workers who are involved in hazardous waste removal. Apart from that, residents who are living near heavily polluted industrial waste sites were also given comprehensive training and environmental restoration. This kind of effort shows that chemical-related safety and health issues are highly critical matter that should be considered seriously at different level including the workers, the communities, and even the environments.

Globally, World Health Organization (WHO) also takes an effort to educate the society by organizing and promoting occupational health. They endorsed the WHO Global Plan of Action on Workers Health (GPA) for a period of 2008 to 2017. There are five main objectives of GPA (WHO, 2012). The primary objective relies in strengthening the governance and leadership function of national health systems. This is in order to respond to the specific health needs of the working group of people. Besides, it is also to establish basic levels of health protection at all workplaces to decrease inequalities in workers' health between and within countries. Moreover, this effort also includes strengthening the promotion of health at work. The third objective is to ensure preventive health services and link occupational health to primary health care are accessible to all workers. In addition, improving the knowledge base for action on protecting and promoting the health of workers and establish linkages between health and work is also put in place. Last but not least, stimulating incorporation of actions on workers' health into other policies is also part of the objectives. The policies include sustainable development, poverty reduction, trade liberalisation, environmental protection and employment.

In principle workers do not create hazards if the working guidelines are proper and they are followed (Kletz, 1991). Therefore, it is important to make work environment to be safer by designing a workplace inherently safer than trying to get workers to adapt to hazardous conditions. This idea aligns with 'inherent safety' concept, which professes that hazards should be eliminated or reduced rather than controlled or managed. Inherent occupational health is often given less attention if compared to inherent safety and inherent environmental friendliness because of its complicated principles. However there are still several existing works published related to the health hazard evaluation. These include research works such as the COSHH Essential (Russell *et al.*, 1998), Occupational Health Hazards Index (OHHI) (Johnson, 2001), Process Route Healthiness Index (PRHI), (Hassim and Edwards, 2006), and the latest is Inherent Occupational Health Index (IOHI) by Hassim and Hurme, (2010a).

All the works mentioned above are done only with manual intervention. As a result, the assessments consume a lot of time in obtaining the end results. Thus a faster, simpler means of assessment is preferred seeing to the advancement of technology nowadays. Especially during early design stage, in which a high number of alternative synthesis routes need to be screened within a limited time. This recognises a need for the development of a computerised tool to be in par with the technology growth. The tool is not only simple and fast, but most importantly can minimise human errors.

As important as an assessment could be, the assessment means nothing if the results or findings obtained are not further used for improving the evaluated process. Therefore it is critical to extent any assessment done by progressing to the next step in a chemical process lifecycle, which is to design a process with fundamentally lower level of hazards. The design can already be done during the early design stage, when selecting or formulating the reaction chemistry towards synthesising the desired product. This is what the concept of ISD is all about. There are quite a number of publications available discussing the ISD applications in process design, but mostly they were focusing on the safety aspect only. On the other hand, such efforts for health aspect are still lacking, but very much in need since each year hundreds of million people are exposed to hazardous material in their working place (Eijkemans, 2005).

Therefore a systematic approach is needed for designing an inherently healthier process for the workers in chemical process industries. With this approach in place, a route to the desired product can be formulated to make it operate at more moderate conditions and using less hazardous chemicals so that to reduce the level of potential health hazards to the workers.

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1.2 Problem statement

The occupational health assessment has received much less attention from researchers and industries compared to safety and health criteria, especially from chemical process design perspective. The few existing methods for occupational health assessment however, show that the calculations are performed manually. There are yet any computational tools developed. During early design stage, there are large numbers of chemical synthesis routes that need to be screened. Apart from that, there are also no methods available to design an inherently healthier process by reducing the health hazards during early design stage. These remain the research gap that needs to be filled in. The aim of this study is to develop a computer-aided tool during early design stage which is highly demanded as nowadays most of design works are done using computer aided process engineering (CAPE) tools and also to propose a systematic approach to design an inherently healthier process with reduce if not eliminate the health hazards in a chemical process plant.

1.3 Objectives of the study

The primary objectives of this research work are as the following:

a) To develop a computer-aided method for assessing inherent occupational health in early chemical process design stage.

b) To develop a systematic design approach for selecting alternative chemical routes with reduced the health hazards.

1.4 Scopes of the study

To achieve the intended research objectives, the scopes of work had been drawn as following:

1. To perform a comprehensive data collection by referring to literature review and chemical properties handbooks.

2. To create an electronic chemical properties database based on the collected data.

3. To develop a computer-aided tool based on the Inherent Occupational Health Index method for early design stage.

4. To develop a systematic design approach to reduce the health hazards.

5. To demonstrate the developed tools by applying to case studies.

1.5 Contribution of the study

The study on occupational health aspect from chemical process design has been poorly researched compared to the other sustainability criteria such as safety, environment, and economic. However extensive works on this area are highly demanded since each year more people die from occupational related diseases then are killed in industrial accidents (Wenham, 2002). To date, there are only a very limited number of methods available for evaluating occupational health hazards during the chemical process design (Hassim and Edward, 2006). Computer-aided methods are clearly in need as most of design works are now done by using CAPE tools. Besides, such tools are lacking in early design stage of process lifecycle.

Therefore this research study is definitely very critical and does offer significant benefits, among others are as follows:

- It is able identify the potential occupational health hazards earlier during early design stage of chemical processes.

- It is able eliminate or reduce the identified hazards so that the problems in the process can be tackled earlier before the plant is even constructed.

- It is able to make appropriate changes on the process with high degree of freedom and at minimal cost.

- It can incorporate inherently healthier design features into the process to make it fundamentally healthier.

- It will be ease and fasten the hazard assessment of the whole chemical process (typically very large and complex), which needs to be done repeatedly.

- It is able to support a sound decision on the process design made by the management.

- Able to educate plant designers, chemical engineers, and managers about inherently healthier processes.

- It is also helps to have a better management of health and safety risks, now and in the future.

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