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Computer Aided Assessment and Design of Occupationally Healthier Process during Research and Development Stage

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Systematic computer-aided tool was developed for early inherent health hazards assessment during process research and development stage. Themethodis based on the earlier manual-basedapproach called the Inherent Occupational Health Index method. The tool was developed using MATLAB®(R2010b) and is presented in the Graphical User Interface (GUI). Electronic chemical properties database of almost 800 chemicals was constructed and this database was integrated with the computer-aided tool. The database further enhances the attractiveness of the proposed tool as users need only to key in process conditions data and the remaining materialrelated data will be directly imported from the database. The tool was applied on six process routes to produce methyl methacrylate. It was found that with the proposed computer-aided tool the inherent occupational health evaluation has now become much easier and faster. Besides, the method also can be integrated with existing CAPE tools.

1. Introduction

During the 1980s and particularly after Rio conference in 1992, the term'sustainability' has become increasingly popular. Sustainabilitycan be defined as 'meeting the needs of the present without comprising the ability of future generations to meet their own needs' (Anon, 1987). Safety and health areamong the vital sustainable indicators, which indirectly implied by the increased awareness on process hazards particularly associated with chemical substances.

In recent decades, the production of chemical substances and the use of hazardous chemicals have tremendously increased, which consequently brought significant risk to both workers and general public.Therefore it is important to evaluate process hazards early especially before the plant is built.The idea of inherent safety is to design better chemical processes by focusing on hazard elimination or minimization. This can be achieved by using less hazardous materials and process conditions (Hassim and Hurme, 2010a). Early hazard assessment allows process modifications to be made easier and at lower cost. This idea was later extended to environmental, before adopted recently by occupational health aspect.

Occupational health concerns with the two-way relationship between work and health (Hassim and Hurme, 2010a). Health risks to workers could be reduced by proper selection of chemical synthesis route during the research and development (R&D) stage. In order to choose the 'healthiest' one from a number of alternative routes, the potential health hazards must be quantified. Ranking of alternative chemical synthesis routes based on the severity of potential health effects to the workers exposed could provide an assessment method for avoiding potential harm to humans.Compared to safety and

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environmental criteria, research on inherent occupational health is considered relatively new especially for chemical process design. Nevertheless several works have been published notably by Hassim and Edwards (2006) and Hassim and Hurme (2010a-e). All the existing methods involve manual-based assessment. Hassim and Hurme (2008) presented a framework for integrating the methods with computer aided design tools. However till the date, no effort has been made towards developing computer-based tools for assessing inherent health hazards like for the other two aspects.
Since nowadays most of project design works are done by using CAPE tools, such computer aided methods are clearly in need. The aim of this paper is to develop a physical computer-based tool for evaluating inherent health hazards during process R&D stage based on the Inherent Occupational Health Index (IOHI) (Hassim and Hurme, 2010a). The development involves two major tasks of 1) constructing electronic chemical properties database and 2) developing computer-aided IOHI method.

2. Methodology

2.1 Construction of electronic chemical properties database

At the R&D stage, much of the detailed information is still missing because the process is not yet designed. Therefore the IOHI was developed based on reaction conditions and material properties data. Material properties data are mostly obtained from the literature e.g. Material Safety Data Sheet (MSDS) or International Chemical Safety Cards (ICSC). In order to computerize the IOHI method, a comprehensive and user-friendly electronic chemical database is constructed. The database comprises of chemical, physical and toxicity properties needed for health hazard evaluation. It includes almost 800 chemical substances with the following information reported: chemical name, chemical formula, molecular weight, atmospheric boiling point (^{0}C), corrosiveness, vapor pressure (bar), long and short-term exposure limits (ppm and mg/m^3) and R-phrases.The chemical and physical properties are collected from different sources includinghandbooks, ICSC and reliable MSDS. The exposure limitvalues are extracted from the extensive list of Permissible Exposure Limits (PEL). For missing chemicals, values from Threshold Limit Values (TLV) and Workplace Exposure Limits (WEL) are also used. Since the collected data are in various measurement units, major unit conversion works were performed to ensure unit consistency across all chemicals for each material property.The selected units are those utilized in the IOHI method. The database was constructed in Excel® spreadsheet(see Figure 1).Microsoft Excel® spreadsheet is chosen as it is common among users, very user-friendly and most importantly, it is compatible with wide range of existing computer-aided tools includingthe most common process simulators e.g. HYSYS®, Aspen plus®, PRO/II®, iCON® and programming software e.g. MATLAB® and Visual Basic®.

2.2 Development of computer-aided IOHI method

After the database construction, computer-aided tool is developed for systematic inherent occupational health assessment of chemical processes at the R&D stage.The aim is to simplify and speed-up the assessment.This is because during early process screening quite a number of alternative processes need to be evaluated from different criteria and the number can go up to more than a hundred. A study conducted by Gupta and Edwards (2002) revealed that among the reasons for poor adoption of Inherently Safer Design (ISD) in industries that is the existing indexes are too complicated. Therefore, a computer-aided tool is developed in this study based on the earlier manual method called the Inherent Occupational Health Index (IOHI) (Hassim and Hurme, 2010a).The IOHI is a reaction step-oriented methodthatcomprises of two indexes; Index for Physical and Process Hazards (I_{PPH}) and Index for Health Hazards (I_{HH}).The I_{PPH} represents the possibility for workers to be exposed to chemicals and physical hazards, whereas the I_{HH} evaluates the health impacts due to the exposure (Hassim and Hurme, 2010a). The IOHIfor each process route is calculated as a sum of the two indexes as shown in equations1, 2 and 3.

$$I_{IOHI} = I_{PPH} + I_{HH} \tag{1}$$

$$I_{PPH} = I_{PM} + I_P + I_T + [\![max(I]\!]_{MS}) + [\![\max(I]\!]_V) + [\![\max(I]\!]_C) \tag{2}$$

$$I_{HH} = [\![\max(I]\!]_{EL}) + [\![\max(I]\!]_R) \tag{3}$$

No.	Name	Formula	Molecular Weight	Material Phase[a]	Boiling Point(^{0}C) @1bar	Corrosivity[c]	Vapour Pressure mmHg at 20^{0}C	Exposure Limit TWA$_8$ ppm	Exposure Limit TWA$_8$ mg/m^3	Exposure Limit STEL ppm	Exposure Limit STEL mg/m^3	Risk phrase
1	Acetaldehyde	C_2H_4O	44.04	L	21	1	750	100	180	25	45	R12, R36/37,R40
2	Acetic acid	$C_2H_4O_2$	60.05	L	118	2	11	10	21	15	-	R10, R35
3	Acetic anhydride	$C_4H_8O_3$	102.09	L	139.9	1	4	5	21	-	-	R10,R20/22, R34
4	Aceton	C_3H_6O	58.08	L	56.2	0	181	500	1187	750	3620	R11,R36, R66/67
5	Aceton cyanohydrin	C_4H_7NO	85.11	L	69	1	0.8	1.56	-	4.7	5	R 26/27/28,R50
6	Acetonitrile	CH_3CN	41.05	L	81.6	2	67.5	40	67	60	102	R11, R 20/21/22,R36
7	Acetophenone	C_8H_8O	120.15	L	201.7	1	0.75	10	49	-	-	R22, R 36/37,38, R41

Figure 1: Snapshot of chemical properties database

where I_{PM} is process mode, I_P is pressure, I_T is temperature, I_{MS} is material state, I_V is boiling point, I_C is corrosiveness, I_{EL} is exposure limits and I_R is R-phrase subindexes.

The program code for developing the IOHI tool is written using MATLAB (R2010b) and presented to the userin theGraphical User Interface (GUI) (see Figure 2).

The subindexes selection, penalty assignment and index formulation are directly based on the IOHI method.

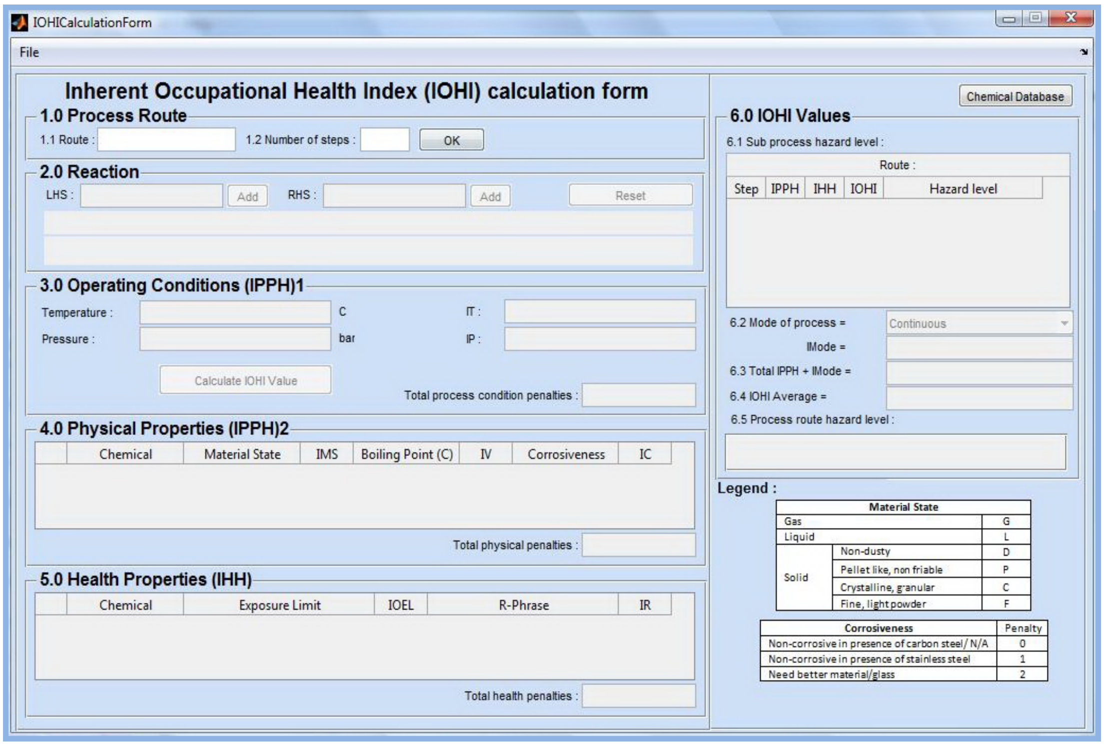

Figure 2: Snapshot of computer-aided IOHI tool

The tool is developed in such a way that it minimizes manual work where users just need to key in process conditions related data (the I_{PM}, I_T and I_P) since these vary from one process to another. Before that, users need to specify the reaction chemistry (subprocess) to be evaluated. This is also computerized. Users only need to select the chemicals involved as reactants and products from the database. Once the chemicals are selected, all material properties data required for the assessment will be imported from the database. Subsequently, the associate penalty for each subindex will be automatically assigned and the IOHI index value for the subprocess will be calculated. In addition, the

subprocess will be characterized with different hazard level (safe, moderately safe, moderately hazardous or hazardous) based on the IOHI value calculated. The tool is also capable of computerizing the IOHI index for the whole process route, which may comprises of more than one subprocesses.
For route evaluation consisting of more than one subprocess, the tool is able to ‘save’ the IOHI value calculated for each subprocess before providing a summary of the index values calculated for all the alternative processes so the users can assess the hazard level of different processes easily and make decision based on the results presented. Besides, the tool also highlights the major source of hazards in the process e.g. too extreme operating temperature, toxic/highly volatile chemical. Early hazards assessment allows appropriate countermeasures to be taken earlier at almost no cost. Besides, the tool will automatically recalculate the new index value upon any modification is made on the process. This process can be iterated easily until the desired hazard reduction is achieved or modification has reached the limit.The flowchart of user guideline for computer-aided inherent occupational health assessment during the R&D stage is shown in Figure 3.

3. Case study

In this study the production of methyl methacrylate (MMA) is used as case study. The routes are acetone cyanohydrin based route (ACH), ethylene via propionaldehyde based route (C2/PA), ethylene via methyl propionate based route (C2/MP), propylene based route (C3), isobutylene based route (i-C4) and tertiary butyl alcohol based route (TBA). For more details, see Hassim and Hurme (2010a).

3.1 Results and discussion

The inherent occupational health hazard of each subprocess of the MMA routes is assessed using the computer-aided IOHI tool. This is the same case study used by Hassim and Hurme (2010a) in their manual IOHI method. However, the evaluation now becomes so much easier and faster with the aid of the new tool. After key in the process related data, the IOHI for the subprocess is automatically calculated. Since all routes have several subprocesses (three to four each), the process is repeated until all the subprocesses’ evaluation is done. Overall the IOHI index values calculated for all the MMA routes are similar to those obtained from the manual IOHI calculations. However small variations are observed in terms of the sub index penalties received by certain subprocesses. This is due to the different sources of exposure limits data used in the case study calculations in both methods. E.g. in Hassim and Hurme (2010a), the exposure limits values are taken from the UK Occupational Exposure Limits (OELs) whereas the values in the electronic database presented in this paper are based on the Malaysia Permissible Exposure Limits (PELs). However both values are not so varied except for a few particular chemicals.
The tool is capable to keep the calculation history for all the subprocesses of a single route in order to generate a route’s index summary at the end of the evaluation. *Figure 4* presents a result summary for the C2/PA subprocesses as an illustration taken from the tool. Also all routes are characterized as moderately hazardous based on the standard developed by Hassim and Hurme (2010a) (see *Table 1*). More detailed results on the case study i.e. process ranking and sources of hazards are reported by Hassim and Hurme (2010a) and cannot be discussed here due to the limited space. Moreover, the purpose of this paper is to introduce the new computer-aided tool, which is developed based on the original manual IOHI method.

Table 1: Hazard level characterization for MMA routes (computer-generated)

Route	No. of Steps	Status
ACH	3	Moderately Hazardous
C2/PA	4	Moderately Hazardous
C2/MP	3	Moderately Hazardous
C3	4	Moderately Hazardous
i-C4	3	Moderately Hazardous
TBA	3	Moderately Hazardous

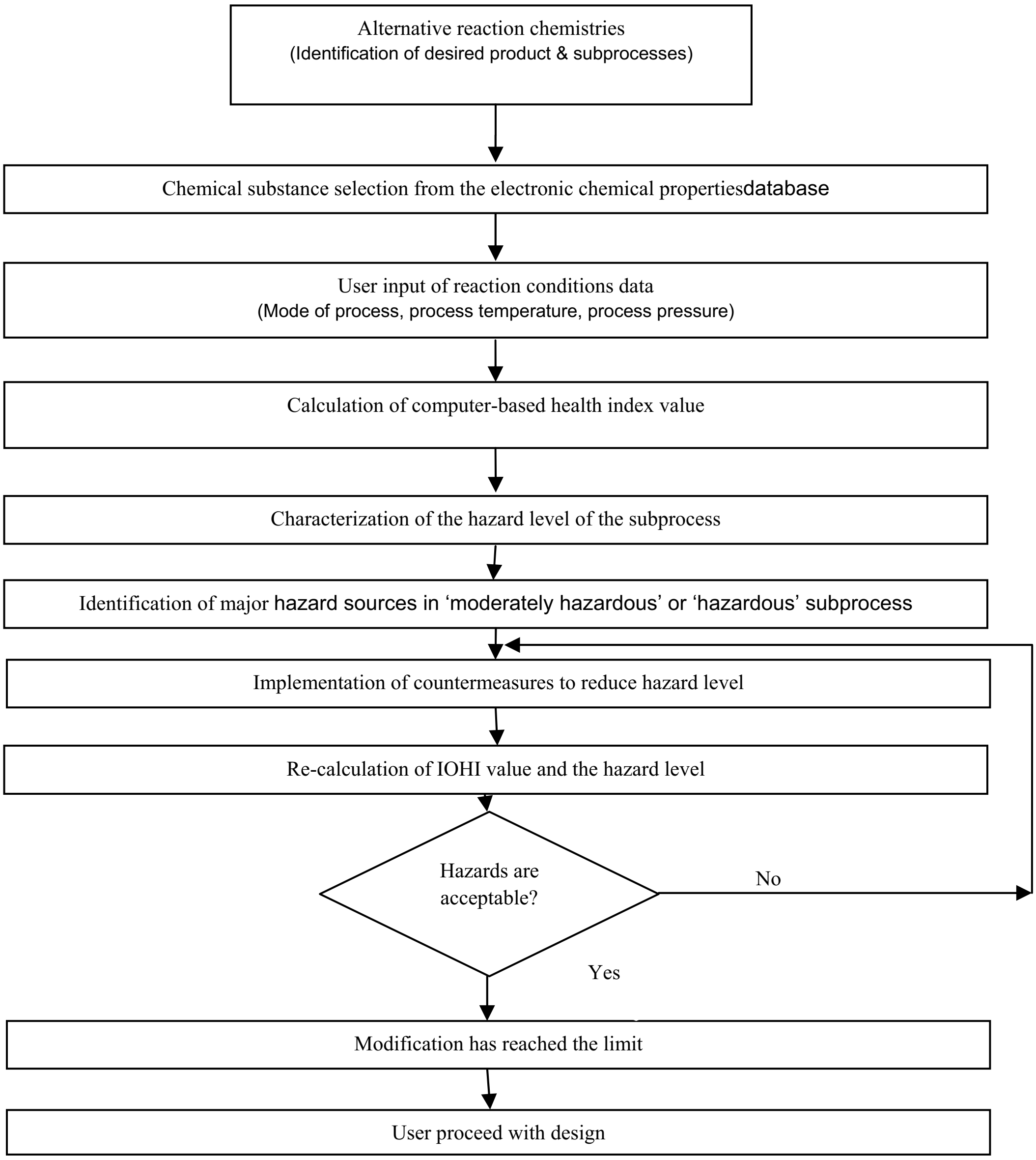

Figure 3: User guideline for computer-aided IOHI tool

4. Conclusion

A computer-aided tool is proposed for assessing inherent occupational health hazard of chemical synthesis routes during the R&D stage. The tool is developed based on Inherent Occupational Health Index (IOHI). The method can be used either for ranking processes based on their health properties or characterizing the hazard level of single process. Besides it is able to analyze the sources of hazards of process design for improvement and modification.

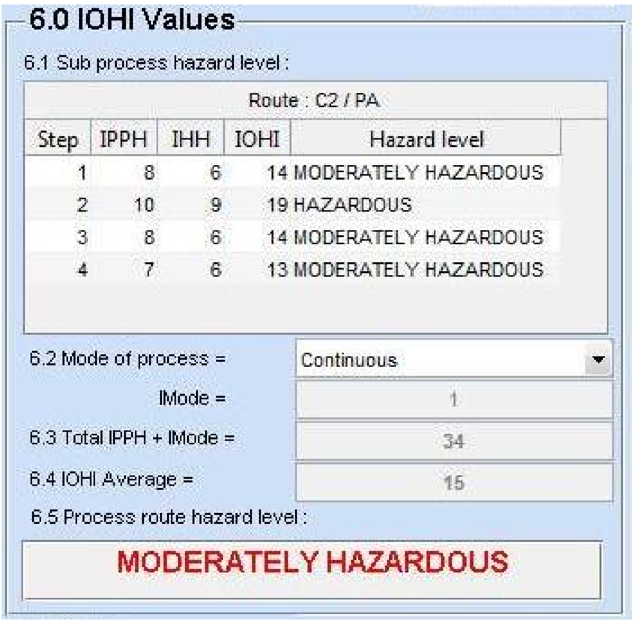

Figure 4: Snapshot of results summary for C2/PA route assessment

A material properties database, which is required for the tool, is constructed using Excel spreadsheet, involving almost 800 chemicals. The program code for the tool is written using MATLAB® R2010b and is presentedto the user in the Graphical User Interface (GUI). With the proposed tool, inherent occupational health hazards can now be evaluated earlier, easier and faster. The tool is also readily integratedwith the existing CAPE tools.

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