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Computer Aided Design of Occupationally Healthier Processes

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Abstract

Computer aided approaches for assessing inherent occupational health hazards and ranking process concepts based on their health properties were developed for the first stages of a process lifecycle; the process development, preliminary design, and basic engineering steps. The methods are tailored to the process design lifecycle steps in terms of their principle and information requirement. The methods can be integrated with existing computer aided design tools as described. A case study is given to illustrate the approach.

Keywords: occupational health evaluation, CAPE, process development and design.

1. Introduction

Occupational health concerns with the two-way relationship between work and health. Each year, more people die from diseases caused by work than are killed in industrial accidents. Still unlike in process safety, there are only a very limited number of methods available for evaluating occupational health hazards during the chemical process design (Hassim and Edwards, 2006). Such computer aided methods are clearly needed as most of design work is done by using CAPE tools now.

2. Assessment stages

Although inherent occupational health concept can be applied throughout the process lifecycle, the opportunity of implementation decreases as the design proceeds. Basic engineering is the last step to make the changes at a moderate cost.

The aim of this research has been to develop a set of occupational health assessment methods for the three early stages of a process lifecycle; 1) process research and development (R&D), 2) preliminary process design and 3) basic engineering. These stages differ in terms of the type and extent of information available (see Table 1). This will eventually affect the assessment procedure as well as the accuracy of the results. At later stages, a more comprehensive assessment is possible due to the better availability of process information.

3. Approaches to Occupational Health Assessment

The methods developed for evaluating occupational health properties of process alternatives are described in the following.

3.1. Process R&D Stage

For process R&D a qualitative index-based method, called the Inherent Occupational Health Index (IOHI) was developed (Hassim, *et al.*, 2006). The method is reaction step-oriented. Therefore a whole reaction step is considered as one entity (see Fig.1). Only chemical and health properties and reaction operating conditions are used in the index, because of their availability and their ability to represent the inherent occupational

health hazards in the R&D stage. The main objective of the method is to rank alternative chemical process routes for the production of the desired product. The required information are the chemicals present, their chemical properties (boiling point (I_v), toxicity, corrosiveness (I_C) and phase (I_{MS})), the pressure (I_P), temperature (I_T) and the mode (I_{PM}), e.g. batch mode of the main process item (typically reactor).
The IOHI consists of two parts; the Index for Physical and Process Hazards (I_{PPH}) and the Index for Health Hazards (I_{HH}). The I_{PPH} represents process related physical hazards. The I_{HH} is evaluating acute and chronic toxicity hazards by considering the exposure limits (I_{EL}) and R-phrases (I_R) of the compounds present. The eight evaluation factors were selected based upon their availability in this phase of design. In the method each factor is assigned with a set of penalty; a higher penalty indicates a higher hazard posed by the factor. The sum of the two scores is the IOHI index value (Hassim, *et al.*, 2006).

Table 1. Information Availability at Different Process Design Stages

Stage:	R&D	Process predesign	Basic engineering
Information available:	Reaction steps Type of chemicals Physical/chemical/ toxicity properties Process conditions Product yield	All in Stage 1 Flowsheet Mass/energy balances Unit operations	All in Stage 1 and 2 P&I diagram Equipment, instrumentation, piping details Process layout Manual working procedures

3.2. Flowsheet Stage

A more detailed method, called the Health Index (HI), is proposed for assessment in the predesign phase. This semi-quantitative method is capable of both ranking process options and indicating the presence of chronic health risks due to chemical exposures from fugitive airborne emissions. The fugitive emissions are mainly due to leaks in process components such as valves, flanges and pump seals. Since the mechanical details of the process in this design stage are still unknown, the index utilizes precalculated standard process modules for fugitive emissions. The standard process modules represent typical operations in chemical plants such as distillation, flash, reactors, absorption etc. systems (see Fig. 1). The fugitive emission rates for the modules were created by evaluating the number of leak sources in these operations by studying typical piping and instrumentation diagrams (PID) of the sub processes.
To implement the HI method, the information needed are process flow diagrams (PFDs), chemical exposure limits, vapor pressures, phases and concentrations of the compounds present in the process. The main task in HI method is to estimate the chemical exposure concentrations. It involves two steps: The fugitive emission rates (FE) are calculated from the standard process modules present. This is then combined with data on typical process layout dimensions and typical wind speed to evaluate the air volume flow rate (Q) and concentrations (C) of the most hazardous chemicals in air (see Section 4.2). The concentrations are then compared to acceptable exposure limits (EL) such as threshold limit values both as individual chemicals and a chemicals mixture. The higher the estimated exposure value is compared to the limit value, the greater the risk from chemical exposure. HI evaluates only the risks from chronic exposures of airborne emissions. It is a non additive-type index unlike the IOHI.

3.3. PID Stage

The Occupational Health Index (OHI) method developed for the PID stage is an extension of the HI method presented earlier for the flowsheet stage. OHI covers both chronic and acute exposures, whereas HI assessed only chronic inhalation based exposures. In OHI chronic exposures, the non-carcinogenic and carcinogenic risks are assessed separately. The assessment of acute and dermal exposures from manual operations is also done. Consequently there are four different sub indices in the method. One of the subindices is the HI for chronic airborne exposures but it is evaluated in more exact way than in flowsheeting stage. It is now based on the calculation of fugitive emissions by considering pipe and equipment details from PID's and 3D plans (Fig. 1).
OHI can be used as a more quantitative health risk assessment tool during detailed process design phase. It aims to assess the occupational health hazards of process concepts rather than only to rank process options by their risk level as the Stage 1 and 2 methods. The aim is also to highlight the main health hazards of each process concept. Therefore by using OHI the process design can be improved based on the index values evaluated.

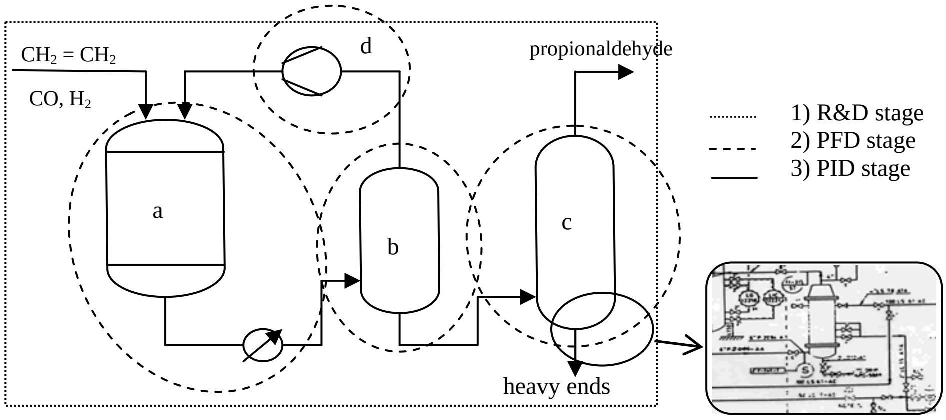

Figure 1. Utilization of Evaluation Levels on the Different Stage Methods in the Case Study Process; 1) process step at R&D stage, 2) standard modules of the predesign stage, 3) piping details at basic engineering stage (a=reactor, b=flash, c=distillation system, d=compressor)

4. Case Study

To depict the method, a case study is presented. The case study selected is the first sub process in the ethylene via propionaldehyde based route for methyl methacrylate (MMA) production (Fig. 1). Ethylene, carbon monoxide and hydrogen are reacted to produce propionaldehyde (Eq. 1). The reaction takes place at 100 °C and 15 bar.

$$CH_2 = CH_2 + CO + H_2 \rightarrow CH_3CH_2CHO \quad (1)$$

4.1. Process R&D Stage

The IOHI is calculated based on the properties of chemicals, process conditions and a process block diagram. The process is divided into main, typically reaction steps (see Fig. 1). The reaction operating conditions determine the process mode, temperature and pressure sub indices. Sub indices values for the other factors (such as volatility etc.) are

taken as the worst values in the reaction step. The sub index evaluation tables are presented by Hassim *et al.* (2006).
The results below show that the sub process falls under 'moderate risk' category:

$$I_{PPH} = I_{PM} + I_P + I_T + Max(I_{MS}) + Max(I_V) + Max(I_C) = 1 + 1 + 1 + 2 + 3 + 0 = 8 \quad (2)$$

$$I_{HH} = Max(I_{EL}) + Max(I_R) = 2 + 4 = 6 \quad (3)$$

$$IOHI = I_{PPH} + I_{HH} = 8 + 6 = 14 \quad (4)$$

4.2. Flowsheet Stage

In the Health Index method the fugitive emissions are evaluated based on sub process module data. Therefore the process is represented as standard process modules (see Section 3.2 and Fig. 1). Based on the chemical composition and vapor pressure data, service type of each module stream is classified as light liquid, heavy liquid or gas service. If the stream is in liquid phase and it contains mostly highly volatile chemicals, it is light liquid service. Other liquids fall under the category of heavy liquid service. The fugitive emissions of the streams are then estimated based on EPA average emission factors. The most hazardous chemical in each stream is determined; that is the major component that has the lowest emission limit value. The emission stream rates which have the same dominant chemical are totaled up. Then, the volumetric wind rate within the sub process is estimated based on average wind speed, a typical floor area and height of the each module. The emission concentrations in air are calculated from emission rates and volumetric air rate. Finally; the HI for individual chemical (HI_i) is estimated by comparing the concentration in air to the respective exposure limit value, EL (Table 2). The HI for chemical mixture (HI_{mix}) is also calculated, assuming that the chemicals have additive effects (worst-case scenario). Since the HI index value in Table 2 < 1, the risk from chronic airborne emissions is absent.

4.3. PID Stage

The main principle of estimating the risk of *chronic inhalative* exposures is similar as in the flowsheet stage. However, real emission source data, e.g. number of flanges from PID (see Fig.1) and 3D plans are used instead of typical module values. Also knowledge on the type of leak source (e.g. pump shaft with single mechanical seal) is used instead of the average values (e.g. 'typical' pump seal) due to the more detailed information available at this stage. In the case study, there is no *carcinogen* present so only non-carcinogenic risk is assessed.
To analyze acute inhalation and dermal exposures the manual operations are identified. In the sub process, a manual sampling point exists in the top product stream of the distillation column. It may pose a source of acute inhalative or dermal exposure during sampling. The risk of *acute inhalation* exposure is estimated based on the comparison between the chemical’s vapor equilibrium concentration at 20 ^oC (C_{eq}) with its short-term (15 min) exposure limit value (EL). The index can be calculated both for individual chemicals and mixture of chemicals (Table 4). Index value greater than 5000 indicates a dangerous condition (Lipton and Lynch, 1994).
Eye and dermal exposures are also evaluated. In the acute exposure source (sampling point), only propionaldehyde may cause irritation to eye and skin, as indicated by its R-phrases (R36 and R38). R36 and R38 fall under the group of low toxicity. Based on a qualitative assessment using a matrix concept, risk of dermal and eye exposure to propionaldehyde in this sub process is minor but present.

As a summary the calculations reveal that the results in PID stage (Table 3) are somewhat lower than those obtained by using the average emission factors in the flowsheeting stage (Table 2). It can be seen that chronic non-carcinogenic risks are absent (Table 3). There is neither carcinogenic risk. The risk of acute inhalation is present (Table 4) due to propionaldehyde, as well as the minor but existing risk to eye and dermal exposures.

Table 2. Calculating the HI for Flowsheet Stage

Chemical	FE mg/s	Q m^3/s	C mg/m^3	EL mg/m^3	HI_i	HI_{mix}	Risks present?
Carbon monoxide	148		0.24	35	0.007		Absent (<1)
Propionaldehyde	399	621	0.64	46	0.014	0.021	Absent (<1)

Table 3. Calculating the HI in the PID Stage

Chemical	FE mg/s	Q m^3/s	C mg/m^3	EL mg/m^3	HI_i	HI_{mix}	Risks present?
Carbon monoxide	89		0.14	35	0.004		Absent (<1)
Propionaldehyde	224	621	0.36	46	0.008	0.012	Absent (<1)

Table 4. Calculating the Acute Toxicity Index (C_{eq}/EL) for PID Stage

Chemical	C_{eq} mg/m^3	EL (15-min) mg/m^3	C_{eq}/EL	Risks present?
Propionaldehyde	8.10E+05	138	5870	Present (>5000)

5. Adaption to Computer System

The three methods presented are intended for different process development and design stages. Therefore their data requirements and integration needs are somewhat different. The data requirements are divided to three main sources: 1) health and safety data, 2) fugitive emission related data and 3) process data. Figure 2 presents the configuration of the computer system for all the three methods.

1. Health and safety data includes typical commonly needed safety data; short term and long term threshold limit values, R-phrases, vapor pressures at 20 ^oC and atmospheric boiling points. These are available e.g. from International Chemical Safety Cards (ICSC) by ILO. A *database of safety properties* therefore needed.
2. Fugitive emission related data includes the *database of standard process modules* (e.g. distillation, absorption and various reaction systems). These are ready made modules for fugitive emissions evaluations as described earlier. For more detailed evaluations a *database of fugitive emissions* from different components (such as various types of valves etc.) is needed.
3. Process related data comes in the R&D evaluation stage from the process block diagram and the user, in the second stage from flowsheets or flowsheeting programs and in the third evaluation stage from flowsheets, PID's and 3D design models.

As a conclusion it can be said that the proposed computer system is quite straight-forward in the stages I and II. Stage III requires more complicated data and design software integration.

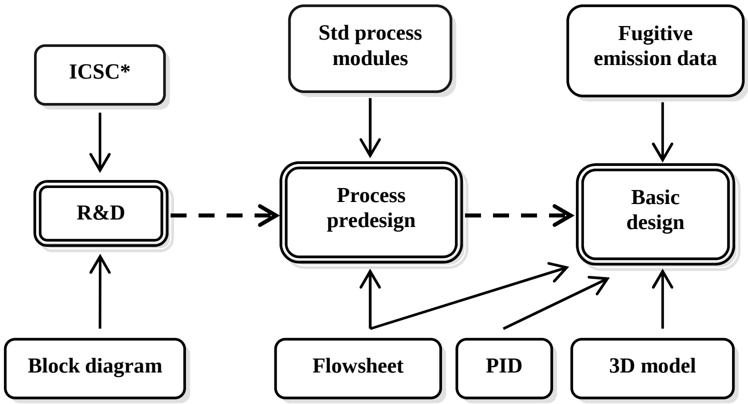

Figure 2. Configuration of the Computer System for the Three Evaluation Methods
*) ICSC=International Chemical Safety Cards database

6. Conclusion

Three methods are proposed for assessing process concepts and designs based on occupational health hazards during R&D, preliminary design, and basic engineering stages of chemical processes. The methods can evaluate chronic and acute hazards except the method for flowsheet stage. The chronic hazard evaluation is based on estimation of process fugitive emissions either by a simplified standard module method or by a more detailed component based approach. The methods can be used either for ranking processes based on their health properties or for analyzing the weak points of process design for improvement or modification.

The methods can be implemented into the existing CAPE tools as described. New databases are needed for safety properties of chemicals and for fugitive emission evaluation. The integration of tools is quite straightforward except for the evaluation in basic engineering step which requires more elaborate CAPE tool integration.

Nomenclature

C	concentration
C_{eq}	vapour equilibrium concentration
EL	exposure limits
FE	fugitive emission rate
HI	Health Index
HI_i	Health Index for individual chemical
HI_{mix}	Health Index for chemical mixture
I_C	corrosiveness sub index
I_{EL}	exposure limits sub index
I_{HH}	Index for Health Hazards
I_{MS}	material state sub index
IOHI	Inherent Occupational Health 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	boiling point sub index
OHI	Occupational Health Index
Q	air volume flow rate

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