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A molecular design methodology by the simultaneous optimisation of performance, safety and health aspects

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HIGHLIGHTS

- CAMD techniques are applied to design molecules with optimum functionality.
- Inherent safety and occupational health are integrated into CAMD framework.
- Disjunctive programming is employed to translate molecular properties into indexes.
- Fuzzy optimisation is utilised to synthesis molecules with multiple design criteria.
- Case study on the design of amine-based solvent for gas sweetening process.

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ABSTRACT

Computer aided molecular design (CAMD) techniques have been implemented to design molecules or mixtures that satisfy a set of desirable target properties as specified by the customers. Molecular physical and thermodynamic properties are often selected as the target properties during the design stage. However, the incorporation of safety and health aspects into CAMD is not strongly emphasised in many design problems. Because of this, many chemical substances available in the market may lead to adverse health impacts following prolonged and repeated exposure. Therefore, the integration of safety and health aspects as design criteria in the existing CAMD methods is of paramount importance. This is to ensure that the synthesised product does not bring harm and health-related hazards to the consumers. In this work, a novel chemical product design methodology has been developed to integrate both safety and health aspects, as well as the target physicochemical properties into a single-stage CAMD framework. The assessment of safety and health parameters are based on the molecular properties that have significant impact on both aspects. Each property is introduced with an index value depending on the degree of potential hazards. Disjunctive programming algorithm is employed to assist in allocating index scores to the molecules depending on their property values. Fuzzy optimisation is applied to optimise two principal design criteria in this work: product target properties and its safety and health performance. A case study on solvent design for gas sweetening process has been carried out to determine the optimal molecule with reasonably low safety and health hazards level, and at the same time, achieves the target properties.

Abbreviations: AHP, Analytic hierarchy process; CAMD, Computer-aided molecular design; F_p, Flash point; GCM, Group contribution method; H_v, Heat of vaporisation; I_{AH}, Penalty for acute health hazard; I_{EL}, Penalty for exposure limit; I_{EX}, Penalty for explosiveness; I_{FL}, Penalty for flammability; I_{MS}, Penalty for material phase; IOHI, Inherent Occupational Health Index; I_{SHI}, Total penalty score of molecule; $I_{SHI,w}$, Total weighted penalty score of molecule; ISI, Inherent Safety Index; I_V, Penalty for volatility; I_η, Penalty for viscosity; LC_{50}, Acute inhalation toxicity; LD_{50}, Acute oral toxicity (rat); $LD_{50,dermal}$, Acute dermal toxicity; *LEL*, Lower explosion limit; *LFL*, Lower flammability limit; log K_{oc}, Soil sorption coefficient; log K_{ow}, Octanol-water partition coefficient; MEA, Monoethanolamine; M_w, Molecular weight; OHHI, Occupational Health Hazard Index; *PEL*, Permissible exposure limit; PIIS, Prototype Index for Inherent Safety; PRHI, Process Route Healthiness Index; *S*, Explosiveness (UEL-LEL); T_b, Normal boiling point; T_m, Normal melting point; *UEL*, Upper explosion limit; *UFL*, Upper flammability limit; V_m, Liquid molar volume; *VP*, Vapour pressure; V_p, Target property value; V_p^L, Lower bound of target property; V_p^U, Upper bound of target property; η, Viscosity; λ, Degree of satisfaction for least satisfied objective; λ_I, Degree of satisfaction for total penalty score of molecule; λ_p, Degree of satisfaction for target property *p*; Ω_p, Property operator for target property *p*

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1. Introduction

In a conventional process and product design problem, the engineering technical aspects and economic factor are the two key components commonly considered as the decision-making criteria. However, one of the major concerns in chemical process industries is the growing number of industrial accidents. Most of these accidents were reported to be due to mishandling of hazardous materials, combustible dusts and reactive chemicals (Chen et al., 2015). Following these tragedies, process safety has received much attention to serve as a key decision-making component in the chemical and petrochemical industries (Ee et al., 2015). One way to eliminate and minimise such hazards is to operate the process with milder conditions and replace those hazardous substances with less hazardous materials. Any unintentional release of safer chemicals will not bring much adverse effects to the workers and surrounding community. This concept of 'embedding' safety by eliminating or minimising process hazards is known as inherent safety, which was initiated by Trevor Kletz (Kletz, 1978).

In addition to process safety, other aspects of sustainability such as environment and health are also deemed as paramount decision-making components in process plant development and design (Rathnayaka et al., 2014). Generally, health differs from safety in terms of several aspects. The most obvious difference is, safety hazards may cause acute effects, whereas health impacts often deal with chronic diseases, due to prolonged exposure, and it is also known as noncommunicable diseases (NCDs). This has caused health related events to receive much less attention compared to safety since the effects of health hazards can only be seen after some time. Despite such issue, occupational health should not be neglected, as it is equally as significant as process safety in industrial plants. This gives rise to the establishment of inherent occupational health (Hassim and Edwards, 2006), which strives to minimise the inherent occupational health hazards posed by chemical processes to the workers.

As mentioned previously, mishandling of hazardous materials is one of the main factors that result in industrial catastrophe. Both inherent safety and occupational health aim to reduce the usage of hazardous chemicals in manufacturing process. A highly toxic chemical can be substituted with a less or non-toxic chemical that exhibits a similar or higher performance compared to the replaced chemical. This is to ensure that the performance of the process plant is not compromised by the substitution of chemical with improved safety and health characteristics. The conventional approach used to search for new chemicals often involves trial and error methods in which large amount of compounds are synthesised and tested in the laboratory. An alternate approach known as chemical product design technique can be applied for the search of a promising chemical candidate with reduced time and effort (Duvedi and Achenie, 1996). This approach begins with the identification of product needs to archive, followed by the development of molecule that offers the desired properties to achieve the product needs (Gani et al., 1991). Existing databases containing a few chemical groups or molecular building blocks can be employed to explore a vast number of conventional or novel molecular structures that can fulfil the product needs of interest. This systematic search can be achieved with the utilisation of computer-aided molecular design (CAMD) technique, which has already been recognised as a powerful tool to determine molecules having a desirable set of physicochemical properties (Harper and Gani, 2000). Since the properties in the design problem are known while the chemical identities or their mixture remained unknown, property models are coupled with CAMD method in a 'generate and test' solution approach (Gani, 2004a). A comprehensive review on a variety of molecular design algorithms and applications are presented by Ng et al. (2015). The problem can also be formulated using a mathematical programming model to generate the optimal solution (Churi and Achenie, 1996). In this work, CAMD approach is applied to design molecule that not only possesses the specified target properties, but also provides a favourable safety and health characteristics. The concept of inherent safety and health is integrated into the CAMD framework to generate molecule with high performance in terms of product functionality and the aspects of safety and health.

2. Inherent safety and occupational health

The Basic Principles of Inherent Safety include intensification, substitution, attenuation and limitation of effects (Kletz, 1991). These inherent safety principles can be employed at any phase of process design and operation, such as process concept assessment, design of process route, plant layout development, process safety management, process life cycle and more (Okoh and Haugen, 2014). However, as the process design progresses to a later stage, it will not be feasible to modify the process decisions during this stage as most technical and financial decisions would have already been finalised (Heikkilä, 1999). The best way to integrate inherent safety principles to their full extent is to implement them during the earlier design phase. One of the commonly used methods to quantify and compare the level of inherent safety and occupational health of different process routes is using the index-based approach, in which each process route will be evaluated depending on its safety and health factors or indicators. It is able to provide quick and reliable results that can assist users in deciding the process route with better safety and health attributes (Gnoni and Bragatto, 2013).

The first inherent safety index approach was the Prototype Index for Inherent Safety (PIIS), introduced by Edwards and Lawrence (1993). It aims to rank the inherent safety of different chemical synthesis routes by assigning index values to each of the process candidates. The method was a breakthrough in 'quantifying' inherent safety level of chemical processes – process route with lower total index value is considered to be inherently safer and vice versa. Edwards and Lawrence (1993) have identified seven inherent safety parameters based on their data availability from the literature during the conceptual design stage. These seven parameters can be divided into two categories, namely chemical score and process scores. Chemical score is made up of inventory, flammability, explosiveness and toxicity; while process score contains temperature, pressure and yield. The total index value of a process route is the summation of index score for all seven parameters of each reaction step in the route.

Besides PIIS, another prominent safety index is named Inherent Safety Index (ISI) developed by Heikkilä (1999). It takes into account of a wider scope of safety parameters, in which their data must be readily available during the preliminary process design phase. ISI can be classified into two categories, namely the Chemical Inherent Safety Index and the Process Inherent Safety Index. The former category consists of sub-indexes for chemical reactivity, flammability, explosiveness, toxicity and corrosiveness of chemical species present in the process. The Process Inherent Safety Index includes sub-indexes for inventory, process temperature, process pressure, equipment safety and safe process structure. Meanwhile, i-Safe index established by Palaniappan et al. (2002) is derived from both PIIS and ISI, but it also considers additional factors to rank different process routes. Khan and Amyotte (2004) have presented the Integrated Inherent Safety Index (I2SI) to take into account the entire life cycle of the process by focussing on economic assessment and hazard potential identification for each process option. Ahmad et al. (2014) have developed a novel method to evaluate inherent safety known as the