

# Safety and health index development for formulated product design: Paint formulation

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**Abstract.** Over the years, safety and health effects among consumers due to the exposure of formulated products have been reported. Thus, there is a need for systematic methodologies to assess the safety and health effects of the candidate's ingredients in the early stages of formulated product design. Therefore, an index-based methodology was proposed to assess the safety and health effects in formulated product design. Product Safety and Health Index (PSHI) highlights the health sub-indexes based on the exposure routes including eye, inhalation, ingestion, and dermal. Each exposure route has its corresponding health sub-indexes that have to be applied. There are also new sub-indexes introduced for ingestion and dermal exposure. A case study on paint formulation was used to illustrate the developed methodology. The results show that the newly proposed index is able to identify hazardous chemical ingredient(s) with its corresponding adverse safety and health effects.

## 1 Introduction

Formulated product design is the process of selecting the right product to fulfil consumer needs of a specific application. In order to develop products that meet the required product function, formulation of the products may contain different classes of chemicals such as active ingredients, solvent mixtures, and additives. Some of the ingredients used in formulated products have been found to increase safety and health hazards to consumers. For instance, exposure to an active ingredient in paint (lead) not only causes abdominal pain, but also skin irritation and even has been identified as carcinogenic to human [1]. At the moment, there is still lack of systematic methodology available to quantify the safety and health effects of the choices of potential ingredients in the early stages of formulated product design. It is pivotal to perform the assessment in the early stages to ensure that the identified hazardous ingredient can be avoided in the future product formulation. Therefore, in this research, Product Safety and Health Index (PSHI) was proposed to assess the safety and health aspects of the chemical ingredients used in the early stages of product formulation. The established index-based approaches employed in chemical process design such as the Inherent Safety Index (ISI) [2] and Inherent Occupational Health Index (IOHI) [3] were adopted to assess safety and health aspects in formulated product design. Based on the assessment, not only can the potential safety risk and adverse health impacts arising from using the products be mitigated, in fact, it can also be eliminated.

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## 2 Literature review

The challenge for formulated product design is to develop a product that fulfils consumer needs without compromising the safety and health impact from exposure to the product. Such formulated products contain chemical ingredients that have been reported to be harmful to humans. However, not much research has been done to estimate the potential safety hazard and health effects from the chemical ingredients during the preliminary design stage. In formulated product design, the main focus is to identify the chemical ingredients that meet consumer needs, which is the principal product function. For instance, the chemical ingredients must satisfy the sensorial properties of the product such as smoothness and softness [4, 5, 6]. Most of the previous research placed an emphasis on safety issues, whereby flammability and toxicity were selected as the target properties during computer-aided design stage [4], as well as during the experimental testing [5]. The research by [6] was conducted to provide knowledge-based ingredient formulation system for personal care industry. Nevertheless, the aspect of safety was not considered. On the other hand, [7] subsequently incorporated safety and health aspects into a computer-aided molecular design (CAMD) method to synthesise solvents that do not possess harmful conditions and health hazards to consumers. However, most of the above-mentioned research only included the flammability and toxicity properties during the design of formulated products. To date, limited research has been conducted on other important safety and health properties, such as the potential of eye illness due to eye exposure to the ingredients used in product formulation.

Although the methodologies for safety and health assessment in formulated product design have not been well developed, there are numerous established safety and health assessment methodologies in chemical process design. The pioneer in index-based methods such as Prototype Index of Inherent Safety (PIIS) [8], ISI [2], and i-Safe Index [9] were developed to estimate the hazards in order to select safer process alternatives. These methods focus on the assessment at the early stage of process design, in which only basic information is available such as the chemicals used in the process and process conditions. The safety properties such as flammability, explosiveness, reactivity, and toxicity are taken into account in evaluating inherent safety of a chemical process route. Moreover, for inherent occupational health, the methods available for the assessment at the research and development (R&D) stage include Process Route Healthiness Index (PRHI) [10] and IOHI [3]. Some of the health properties considered are exposure limit, acute and chronic effects, inhalation, and dermal contact. The prominent inherent safety and occupational health assessment methodologies employed during the early stage of process design are suitable to be adapted during the preliminary stage of formulated product design. This is because the safety and health properties employed at this stage are applicable to assess the safety and health hazards of the chemical ingredients used in product formulation. Consumers are prone to safety and health risks (e.g., explosivity, toxicity, and acute effects) when they are in contact with some of the ingredients, either during application or storage of the product.

## 3 Development of Product Safety and Health Index

The goal of developing safety and health index for formulated product design is to provide estimation of the potential safety and health effects from each chemical ingredient used in product formulation. Furthermore, the index is designed to identify the most hazardous exposure route for each chemical ingredient based on the score. A score is therefore allocated for each safety and health sub-index respectively. For instance, a high score signifies a higher severity of the effects and vice versa.

### **3.1 Inherent safety index**

A consumer may be exposed to safety hazards during application and storage of a chemical product. The safety hazards include accidental emission of chemical ingredients, leakage, and spillage of chemicals from the container, which would result in fire and explosion. The development of safety sub-indexes includes dust explosiveness, explosiveness, flammability, toxicity, and chemical reactivity.

### **3.2 Inherent health index**

A chemical ingredient in a product may enter a human body during the application, storage, as well as in the event of any unintentional incident. There are four major routes where chemical ingredients may enter a human body, namely eye contact, inhalation, ingestion, and dermal contact. In this present work, the health sub-indexes were modified based on the exposure route to highlight the source of the effects from the chemical ingredients. The modified sub-indexes are based on the established IOHI that was developed by [3]. The new sub-index of gastrointestinal hazards via ingestion is presented in Section 3.3.1 whereas dermal exposure is described in Section 3.3.2. Table 1 shows the health sub-indexes according to the exposure route. In addition, Table 2 presents the allocation of the score based on hazard statements to indicate the degree of severity of adverse health effects.

#### **3.2.1 Eye contact**

When a chemical ingredient (solid or liquid) comes into contact with eyes, it could lead to the exacerbation of eye condition. A consumer can also come into contact with a chemical ingredient during the application of a product, for example, a pigment in paint such as iron. If the consumer is exposed to excessive amount, it may lead to eye defects or remain in the tissue of the eye [11]. Furthermore, the consumer may also be exposed to a chemical ingredient through eye contact if they have the habit of not washing their hands after the application of a formulated product. The risk of eye contact to the consumer can be evaluated based on the hazard statements of the Global Harmonised System (GHS) developed by the United Nation [12].

#### **3.2.2 Inhalation exposure**

Inhaled chemical substances may harm respiratory tract, ranging from simple symptoms to severe diseases. For instance, the emission of a volatile compound present in a scented product may contribute to headaches or even respiratory difficulties [13]. Moreover, the inhaled substances are mostly found in the form of gases and vapours. Nevertheless, liquids and solids can also be inhaled in the form of finely divided mists, aerosols, or dusts [14]. The degree of potential inhalation of volatile liquid ingredients is presented by the volatility sub-index. The data of boiling point of a chemical ingredient are required to indicate the level of volatility.

Inhalation of various types of mists, aerosols, and dusts may cause disturbance and respiratory system failure. The varying particle sizes of chemical dusts may settle at different areas of respiratory tract. A sub-index of respiratory hazards is used to estimate the potential health effects based on the dust particle sizes (aerodynamic diameter).

Exposure to chemical ingredients through inhalation can also be estimated by referring to the hazard statements stated in the material safety data sheet (MSDS) of a chemical ingredient. On the other hand, occupational exposure limit (OEL) outlined by the United Kingdom Health and Safety Commission (HSE) is used to describe the concentration of an

airborne substance in a workroom. OEL concerns on workers that may be exposed repeatedly to chemicals on a daily basis (8 h of exposure duration). The sub-indexes of volatility, respiratory tract hazard, hazard statements, and OEL are listed in Table 1.

## 4 New development of inherent health sub-index

### 4.1 Ingestion exposure

Chemical ingredients in formulated products such as pigments in paints contain heavy metals including lead, cadmium, and chromium. International POPs Elimination Network (IPEN) [15] found that young children may swallow chipped paint. They come in close contact with paint flakes on cribs, playpens, tables, chairs, and playground equipment that are covered with leaded paint. Therefore, ingestion of even a small amount of chipped paint may give rise to the accumulation of lead in the children's blood above the safe limits. Lead can cause mental retardation and has carcinogenic properties that cause cancer. The ingestion of chemical particles results in the transportation of the chemical through the gastrointestinal tract. Particle size is one of the most important factors in determining the extent and pathway of the uptake. Thus, the sub-index of gastrointestinal hazards is developed based on the size of the ingredient's particle. Another option to assess the potential hazard due to ingestion is by referring to the hazard statements. Table 2 lists the hazard statements used specifically for ingestion with the assigned scores.

### 4.2 Dermal exposure

Dermal contact occurs when the skin is exposed to chemical substances, regardless by means of absorption or merely superficial for a period of time. Splashes, spills, or drift during mixing or loading may occur during the application of a product or from contaminated surfaces. The health impacts from dermal exposure can be estimated using the hazard statements published in the chemical ingredients' MSDS. The allocation of the scores for the sub-index of hazard statements are shown in Table 2. Furthermore, health and safety authorities worldwide utilise skin notation to indicate the chemicals that may contribute to skin effects. The HSE utilises the skin notation to over 120 chemicals, whereas the American Conference of Governmental Industrial Hygienists (ACGIH) applies the skin notation to over 160 substances [16]. Moreover, the United States National Institute for Occupational Safety and Health (NIOSH) has published NIOSH pocket guide to chemical hazards where descriptions of chemicals with skin effects are stated. Thus, another sub-index for dermal hazards is introduced *via* the chemical lists published by HSE, ACGIH, and NIOSH.

**Table 1.** Health sub-indexes.

Exposure Route	Material Phase	Sub-index
Eyes	Solid/liquid/gas	Hazard statement
Inhalation	Liquid	Volatility (boiling point, $T_b$ )
	Solid	Respiratory tract (dust particle size)
	Solid/liquid/gas	Hazard statement OEL ( $\text{mg m}^{-3}$ )
Ingestion	Solid	Gastrointestinal tract (dust particle size)
	Solid/liquid/gas	Hazard statement
Dermal	Solid/liquid/gas	Hazard statement
		HSE, ACGIH, and NIOSH

**Table 2.** Score of health sub-index based on hazard statement.

Exposure Route	Score Information	Score
Eyes	H319	1
	H318	2
Inhalation	H332	1
	H331, H335	2
	H330, H334	3
Ingestion	H302	1
	H301	2
	H300, H304	3
Dermal	H315	1
	H312	2
	H311, H317	3
	H310, H314	4

## 5 Case study

A case study of two paint formulations are presented to demonstrate the proposed index methodology. The solvent-borne paint formulation (Formulation 1) consists of titanium dioxide (pigment), diethylene glycol monoethyl ether (DEGEE), and toluene as a solvent, as well as sodium dioctyl sulfosuccinate (SDS) as an additive [17]. Meanwhile, the ingredients in water-borne paint formulation (Formulation 2) also used titanium dioxide as a pigment, styrene acrylic copolymer as a binder, water as a solvent, silicone, and butyl glycol as an additive [18]. Next, the data required in regard to the physical and chemical properties were obtained from MSDS. Since water is not hazardous, it was excluded in this assessment.

The health sub-indexes based on the data of hazard statements were taken as examples to illustrate the score received by the ingredients in the formulation. The results from the score obtained will reveal the level of potential hazard from each chemical ingredient in product formulation. Tables 3 and 4 show the score received from the exposure route of eye, inhalation, ingestion, and dermal contact for Formulation 1 and Formulation 2, respectively. The pigment in Formulation 1 and 2, titanium dioxide, only received a score from exposure of eyes, which indicates the potential of irritation to eyes (H319). Likewise, exposure to DEGEE elicits similar eye effects. Furthermore, toluene obtained a score of 3 for ingestion and score of 1 for inhalation exposure. The score of 3 refers to fatality if toluene is consumed and thus, enters the airways. Evidently, high concentration of toluene has been reported by [19], which causes disturbances in respiration and can even result in fatality. Meanwhile, the highest score of 3 for SDS is from dermal contact, which has the potential to cause sensitisation to skin. In addition, SDS is also prone to the risks from eyes and inhalation, respectively, with the score obtained of 2. Eye and inhalation exposures to SDS will cause serious eye damage and respiratory irritation, respectively. Among the ingredients in the formulation, SDS was identified as the hazardous ingredient as it received higher scores for multiple exposure routes in comparison to other ingredients.

In Formulation 2, the binder, styrene acrylic copolymer, received the highest score of 2 for inhalation exposure, which may cause irritation to respiratory system. It is noted that silicone obtained a low score of 1 for all exposure routes, thereby indicating that the risk of handling silicone is low. On the other hand, butyl glycol received a high score of 2 for eyes and dermal exposures and a score of 1 for inhalation and ingestion, respectively. Overall, the hazardous ingredient in this formulation was butyl glycol because there were two exposure routes with a high score of 2. Table 5 summarises the significant health hazard exposure routes of each ingredient in both formulations based on the score obtained.

The scores of all the hazards from the exposure routes in Formulation 2 are notably less than 3 in comparison to Formulation 1, which possesses two hazard potential with the high score of 3. Thus, the result of the assessment revealed that Formulation 2 (water-borne paint) can be considered as a healthier formulation due to its lower score compared to Formulation 1 (solvent-borne paint). Nevertheless, the results discussed here are based solely on the health effects from the hazard statements, whereas other safety and health sub-indexes are not included. Further assessment has to be carried out in order to determine other potential hazards for a more detailed result.

**Table 3.** The score of health sub-index based on hazard statements for Formulation 1.

Ingredient / Exposure Route	Titanium Dioxide		DEGEE		Toluene		SDS	
	Hazard	Score	Hazard	Score	Hazard	Score	Hazard	Score
Eyes	H319	1	H319	1	No effect	0	H318	2
Inhalation	No effect	0	No effect	0	H332	1	H335	2
Ingestion	No effect	0	No effect	0	H304	3	H302	1
Dermal	No effect	0	No effect	0	No effect	0	H317	3

**Table 4.** The score of health sub-index based on hazard statements for Formulation 2.

Ingredient/ Exposure Route	Titanium Dioxide		Styrene Acrylic Copolymer		Silicone		Butyl Glycol	
	Hazard	Score	Hazard	Score	Hazard	Score	Hazard	Score
Eyes	H319	1	H319	1	H319	1	H319	2
Inhalation	No effect	0	H335	2	H332	1	H332	1
Ingestion	No effect	0	H302	1	H302	1	H302	1
Dermal	No effect	0	H315	1	H315	1	H312	2

**Table 4.** Highly hazardous exposure route identification.

Ingredient	Highly Hazardous Exposure Route
<b>Formulation 1</b>	
Titanium Dioxide	Eyes
DEGEE	Eyes
Toluene	Ingestion
SDS	Dermal
<b>Formulation 2</b>	
Titanium Dioxide	Eyes
Styrene Acrylic Copolymer	Inhalation
Silicone	Eyes, inhalation, ingestion, and dermal
Butyl Glycol	Eyes and dermal

## 6 Conclusion

In this work, Product Safety and Health Index (PSHI) was developed to assess the safety and health risks of the chemical ingredients used in product formulation. The developed index can be used to identify the potential source of safety and health hazard from the exposure of each ingredient in product formulation. In addition, the score obtained by the ingredients will serve as a guide in determining the level of hazard for all sub-indexes. Future works can be performed by extending the case study of the assessment for other formulated products such as cosmetics and detergents.

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