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A Schematic Method for Sustainable Material Selection of Toxic Chemicals in Design and Manufacturing

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A Schematic Method for Sustainable Material Selection of Toxic Chemicals in Design and Manufacturing

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Toxic chemicals used in product design and manufacturing are grave concerns due to their toxic impact on human health. Implementing sustainable material selection strategies on toxic chemicals can substantially improve the sustainability of products in both design and manufacturing processes. In this paper, a schematic method is presented for characterizing and benchmarking the human health impact of toxic chemicals, as a visual aid to facilitate decision-making in the material selection process for sustainable design and manufacturing. In this schematic method, the human health impact of a toxic chemical is characterized by two critical parameters: daily exposure risk R and environmental persistence T. The human health impact of a toxic chemical is represented by its position in the $R-T$ two-dimensional plot, which enables the screening and benchmarking of toxic chemicals to be easily made through comparing their relative positions in the characterization plot. A case study is performed on six toxic chemicals commonly used as solvents for cleaning and degreasing in product development and manufacturing.
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1 Introduction

Toxic chemicals are heavily used in product design and manufacturing processes for a wide range of purposes and operations. Applications of toxic chemicals in product design and manufacturing generate huge amount of toxic wastes and emissions into the environment [1]. Once released, these toxic chemicals will be subject to a series of environmental transport and transformation processes and may produce serious adverse effects on human health via such impact pathways as air, water, soil, food, etc., and such impact routes as inhalation, ingestion, and dermal uptake. In order to monitor and control the emissions of toxic chemicals, many industrialized countries including Unites States, European Union nations, Australia, Canada, Japan, Korea, etc., have established national regulatory programs to collect the toxic chemical release data and information from the industry [1–3]. In the United States, the toxic chemical release information is collected and is available through the U.S. Environmental Protection Agency's toxic release inventory (TRI) database [1]. These toxic chemicals, based on their release patterns, can be categorized into four groups: air emissions, surface water discharges, land releases, and underground injections. Figure 1 below shows the toxic release inventory of the United States in 2001 [1]. The total amount released was 5.616×10^9 lbs. Based on weight, the air emissions roughly account for 30% of the total toxic release, the total land releases take roughly 62% share, and surface water discharges and underground injections are both around 4%. It should be noted here that the total amount disclosed in the TRI database is an underestimate of the toxic chemical released in the United States since many small scale production facilities are not required to report their toxic chemical emissions.

Due to the severe adverse effects and damages toxic chemicals can cause on human health, a number of environmental laws and regulations have been enacted worldwide to control the application and proliferation of toxic chemicals in the exposure routes and pathways to humans. Typical examples include the U.S.' Clean Air Act, Clean Water Act, and Toxic Substance Control Act, which regulate the restriction and control of toxic chemicals and their concentration in the environmental media, and the European Restriction of Hazardous Substances directive, which bans the application of six toxic chemicals including mercury, lead, cadmium, hexavalent chromium, polybrominated biphenyls, and polybrominated diphenyl ethers in any new electrical and electronic appliances.

Controlling the toxic impact of chemicals can be implemented in the material selection process during the product design and manufacturing process planning stage. Material selection has been recognized as one of the most effective processes in reducing the environmental impact of products [4–6]. A number of methodologies have been developed to integrate sustainable material selection strategies to improve the environmental performance of products during the mechanical design stage [7–9]. While these methodologies consider the environmental impact mainly in such aspects of reducing energy consumption and material use, few studies have been done on material selection of toxic chemicals from human health impact perspective to support sustainable design and manufacturing practices [10].

In this paper, we report a study on the sustainable material selection of toxic chemicals by integrating human health impact assessment into the standard material selection processes for improving the sustainability of design and manufacturing. A schematic method is developed and used as a visual decision tool for characterizing and benchmarking the human health impact of toxic chemicals. Finally, a case study is conducted on sustainable material selection of six toxic chemicals, which are commonly used as solvents for cleaning and degreasing in product development and manufacturing.

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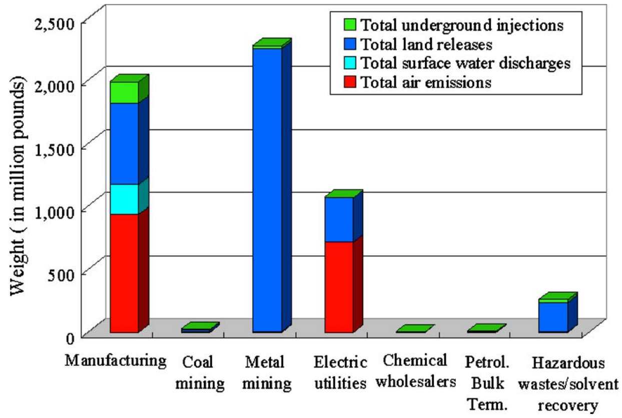

Fig. 1 U.S. toxic release inventory in 2001

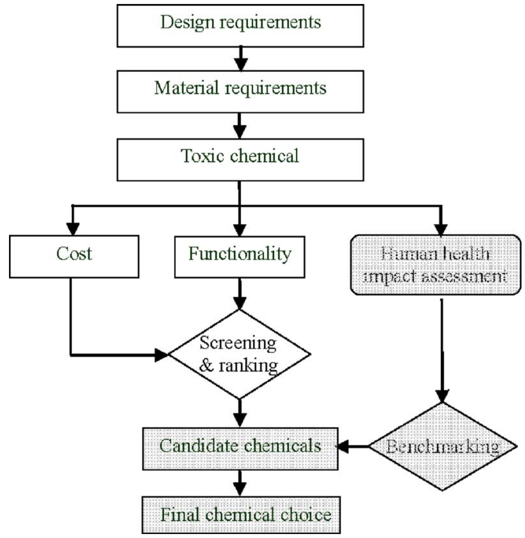

Fig. 2 Sustainable material selection process of toxic chemicals

2 Sustainable Material Selection of Toxic Chemicals in Design and Manufacturing

Sustainable material selection is critical for improving the sustainability of design and manufacturing since the environmental impacts of wastes and emissions resulting from material use are mainly determined in the material selection process. Conventional material selections in product design and manufacturing are made primarily based on functionality by considering such material properties as strength, hardness, density, etc., and by including both material acquisition and processing costs. For toxic chemicals, their potential impact on human health needs to be considered in the material selection process, so as to use the chemical material, which has the minimum human health impact, while it meets the requirements of the functional and cost criteria.

Ashby structured the material selection in mechanical design into a standard four-step process: translating design requirements into material requirements, screening materials based on functional requirements, ranking screened materials to improve performance, and seeking supporting information to select the final material [11]. The Ashby method, providing schematic benchmarking of material properties of different classes in the constructed material property chart, is widely adopted to aid decision-making in material selection in the stage of mechanical design for functional optimization [12,13] and of environmental impact reduction [4,6,7,14]. In the Ashby's material property chart, the fundamental relationships between material properties become self-evident and it becomes easy for designers and engineers to select the optimal material based on the selection criteria by comparing the relative positions of the candidate materials in the two-dimensional chart [15].

Here, we integrate the human health impact assessment into the Ashby's standard material selection structure to perform a sustainable material selection of toxic chemicals by benchmarking those candidate chemicals on their human health impact, so as to reduce their overall impact on human health throughout their life cycle applications in design and manufacturing processes. The integrated sustainable material selection process of toxic chemicals is shown in Fig. 2 below [16].

Human health impact assessment of toxic chemicals is a complicated process, which needs to consider not only those intrinsic physical-chemical properties of the chemical material but also the release patterns and exposure pathways of the chemical in the environment. Integration of human health impact assessment into the material selection processes for decision support requires the human health impact assessment method to be transparent, reliable, and convenient to use in the real practice.

In this study, the human health impact assessment is considered parallel to the conventional material selection process, which includes functionality and cost considerations. It should be noted that in this study, the human health impact assessment of toxic chemicals is used as a decision support tool only for the final benchmarking of those top ranked candidate chemicals, which are selected from the conventional material selection process, as shown by the shaded process flows in Fig. 2 above, while the human health impact assessment can also used in the initial material screening and ranking simultaneously with the conventional material selection process to support decision-making. For conventional material selections based on functionality and cost, a large number of research results and useful methodologies have been published [17–20].

3 Human Health Impact of Toxic Chemicals

Current human health impact assessment of toxic chemicals is generally conducted by following the risk assessment principles by using a five-tiered hierarchy process: mass, toxicity, persistence, concentration, and intake [21–25], as demonstrated in Fig. 3 below. Risk in human health impact assessment is characterized as the probability of an individual subject to the adverse health effects through various exposure routes and pathways. For toxic chemicals, there are two types of adverse effects on human health: carcinogenic and noncarcinogenic. In current practice, the human health impact of a toxic chemical release is assessed by computing an impact score within the life cycle impact assessment (LCIA)

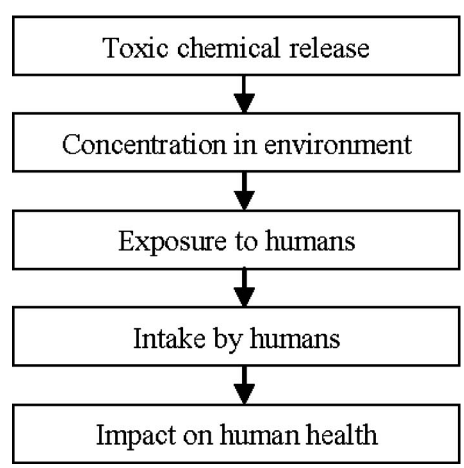

Fig. 3 Human health impact of toxic chemical release

framework, either separately for the carcinogenic and noncarcinogenic effects [26] or a combined overall score [27].

The human risk assessment starts from quantifying the source of a toxic chemical release, which is determined from the disposal of product or manufacturing operations. The mass of a chemical release dictates the concentrations of the chemical in the environmental media and the concentrations consequently determines the final intake of the toxic chemical among the exposed population through various exposure pathways and routes, as demonstrated in Fig. 3 above. In this way, the intake of a toxic chemical release can be taken as a multimedia function of mass and environmental concentrations, as demonstrated in the risk flowchart. The human health impact assessment of toxic chemicals can be reduced to a three-tiered hierarchy, which includes toxicity, persistence, and intake of a toxic chemical release in the environment. In the following part, the three factors are described in more details for assessing the impact of a toxic chemical release on human health.

Toxicity is regarded as an inherent material property of a chemical substance and is counted as a critical factor in assessing the toxic impact of a chemical on human health. For carcinogenic and noncarcinogenic effects, different toxicity indicators are derived for use from the dose-response modeling. Noncarcinogenic effect is generally assessed by using indicators derived from the threshold value of the chemical inducing adverse effect on the dose-response curve while carcinogenic effect is measured by using a potency factor, which is the slope of the dose-response curve at a very low level of dose. There are numerous toxicity indicators developed and used in toxic chemical risk assessment and benchmarking. Threshold limit value has been used for benchmarking toxic chemicals in the TRI database [28]; acceptable daily intake (ADI), an indicator widely adopted by the Council of Europe, WHO, U.S. FDA, etc., has been applied for risk assessment of toxic chemicals on both carcinogenic and noncarcinogenic effects [29,30], and ED_{10}, defined as an effective dose inducing a response over a background of 10% for humans, has been recently developed for assessing human health response from toxic chemical exposure for both carcinogenic and noncarcinogenic effects [31,32]. ED_{10} is also recommended as a preferred benchmark measure for toxic chemical risk assessment in a recent SETAC panel review [33]. In this schematic characterization method, both ED_{10} and ADI are used for toxicity assessment and result verifications.

Besides toxicity, the persistence of a chemical in the environment is another important factor for the human health impact assessment. Those chemicals with longer persistence in the environment would bring larger exposure to the human beings in the model environment and accordingly, pose higher risks to the exposed population than those chemicals with shorter persistence. Persistence of chemicals has been systematically investigated by researchers in the past decade and various methods have been developed for its calculations [34–40]. It has been well understood that the persistence of a chemical substance in the environment is jointly determined by its material properties and environmental conditions. The half-life of a chemical was widely used as an indicator of its persistence in the regulatory context while recent research results found that overall persistence should be used since it integrates both single media half-lives and phase partitioning of a chemical in various environmental media [40]. The overall persistence of a chemical substance in the environment can be generally calculated by means of [35]

$$T = \frac{\sum M_j}{\sum M_j k_j} \tag{1}$$

where T is the persistence of the chemical in the environment, M_j is the mass in the environmental compartment j, and k_j is the decay rate of the chemical in the compartment j.

In human health impact assessment, it is the intake of a toxic chemical, which generates the adverse impact on human health.

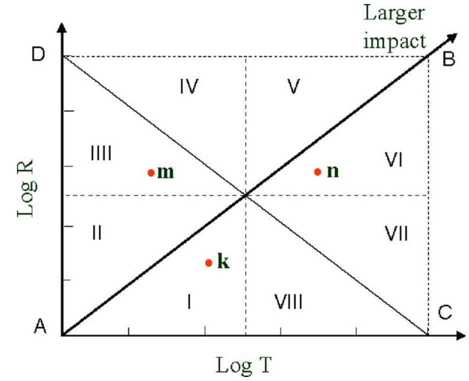

Fig. 4 Human health impact characterization concept

Intake of a toxic chemical can result from various exposure pathways such as air, water, soil, food, etc., and a number of exposure routes such as inhalation, ingestion, and dermal uptake, etc. Intake of a chemical release is usually calculated as the product of the chemical's concentrations in the environmental media and an intake factor (for inhalation and ingestion) or an uptake factor (for dermal contact) of the environmental media, which the population is exposed to [38]. In current practices, the intake of a toxic chemical for human health impact assessment is computed by using multimedia exposure analysis models such as CalTOX for the U.S. region [26] or USES-LCA for the Europe [27]. In the risk assessment, the total intake of a chemical release is usually integrated over the persistence time of the chemical in the environment. Since the adverse effect of a toxic chemical exposure is not determined by the total intake amount but by the intake over a unit time period (per day in common practice), here, we employ a daily intake in this method for a human health impact assessment of a toxic chemical exposure from various environmental media. A daily intake is the total amount an average person takes during a typical 24 h period in the model environment. As a result, the human health impact of a toxic chemical release can be characterized by a multimedia function of such three factors: daily intake, toxicity, and persistence, as shown in the following:

$$\text{Impact} = f(\text{daily intake,} \quad \text{toxicity,} \quad \text{and} \quad \text{persistence}) \tag{2}$$

The human health impact characterization function (2) can be further simplified because the two factors: daily intake D and toxicity Y can be combined into a dimensionless daily risk R, as defined by the following expression:

$$R = \frac{D}{Y} \tag{3}$$

As a result, the human health impact of a toxic chemical release can be characterized through daily risk R and persistence T, these two independent factors. For a chemical i, its human health impact I_i can be characterized through the following expression:

$$I_i = f(R_i, T_i) \tag{4}$$

By using Eq. (4), the human health impact of a toxic chemical can be schematically characterized in a two-dimensional $R-T$ plot. In this schematic characterization method, the potential impact of a toxic chemical on human health is represented by the position of the chemical material in the plot. Here we use three chemicals, m, n, and k, as examples to demonstrate the schematic characterization of their human health impact, as shown in Fig. 4 above.

In the characterization plot, the two axes are both set on logarithmic scales due to the large differences of R and T magnitudes. In this schematic method, the sustainable material selection of toxic chemicals can be made by benchmarking the relative positions of the candidate chemicals in this $R-T$ two-dimensional plot. The fundamental benchmarking principle is that the chemical

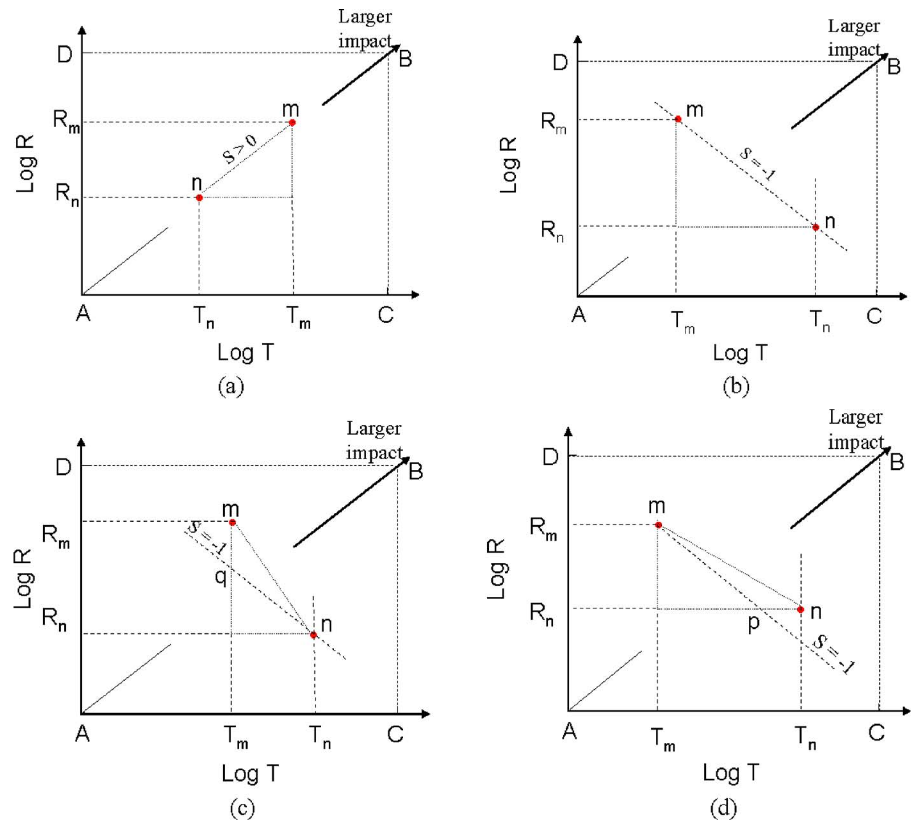

Fig. 5 Schematic benchmarking of human health impact of two toxic chemicals *m* and *n* for the human health impact: (*a*) $I_m > I_n$, (*b*) $I_m = I_n$, (*c*) $I_m > I_n$, and (*d*) $I_m < I_n$

with a higher risk and a longer persistence has a higher impact on human health. So in Fig. 4, those chemicals with relatively high impact on human health are characterized in the upper right corner of the characterization plot while those with relatively low impact on human health are in the lower left corner of the plot. To facilitate rapid decision-making in material selections, the characterization plot is divided into eight regions, as shown in Fig. 4. Those chemicals characterized in regions V and VI have higher human health impact than those in regions I and II because both R and T values of chemicals in regions V and VI are larger than those of chemicals in regions I and II. While for those chemicals in such regions as III, IV and VII, and VIII, the tradeoffs are analyzed by evaluating the slope value of the line between the two chemicals. For two chemicals m and n, the slope value of line mn S_{mn} is calculated through

$$S_{m,n} = \frac{\log R_n - \log R_m}{\log T_n - \log T_m} \tag{5}$$

Different tradeoff scenarios are shown in Fig. 5 above. If $S_{m,n} > 0$, the human health impact of the two chemicals: $I_m > I_n$, as shown in Fig. 5(*a*). If $S_{m,n} = -1$, then $I_m = I_n$, as shown in Fig. 5(*b*);when $S_{m,n} < -1$, then $I_m > I_n$, as shown in Fig. 5(*c*); when $0 > S_{m,n} > -1$, then $I_m < I_n$, as shown in Fig. 5(*d*). A summary of the benchmarking principles of the two chemicals' human health impact under various scenarios is presented in Table 1 below [41].

Because those chemicals positioned on a line with a slope value of −1 have the same impact on human health, in the characterization plot, the magnitude of the human health impact of a chemical can be represented by the vector distance from the chemical's position to a line with a slope value of −1. A larger vector distance means a larger human health impact. For multiple chemical benchmarking, reference lines with a slope value of −1 can be drawn on the plot to compare the vector distance of chemicals to determine their scale of human health impact.

In the characterization plot, as the relative positions of chemicals are determined by the absolute R and T values, the final benchmarking results are not influenced by the scales of the R and T coordinates. But for a convenient visual representation, the R and T scales are suggested to have the same orders of magnitude difference, for example R and T, each with five orders of magnitude difference as scaled from 10^{-13} to 10^{-8} and 10^{1} to 10^{6}, respectively. In this way, the reference line with a slope value of −1 will be positioned parallel to the diagonal line of the characteriza-

Table 1 Human health impact benchmarking of two chemicals

Condition		Result
If $R_m > R_n$ and $T_m > T_n$		$I_m > I_n$
If $R_m > R_n$ and $T_m < T_n$	$\frac{R_m}{R_n} > \frac{T_n}{T_m}$	$I_m > I_n$
	$\frac{R_m}{R_n} = \frac{T_n}{T_m}$	$I_m = I_n$
	$\frac{R_m}{R_n} < \frac{T_n}{T_m}$	$I_m < I_n$
If $R_m = R_n$ and $T_m > T_n$		$I_m > I_n$
If $R_m > R_n$ and $T_m = T_n$		$I_m > I_n$

Table 2 Schematic characterization parameters of six chemical solvents used in semiconductor manufacturing

Chemical	Case No.	ED_{10} (mg kg day)	Individual daily risk (R)	Persistence (T days)
1,1,2-trichloroethane	79-00-5	5.1	1.63E-13	1024
Carbon tetrachloride	56-23-5	1.19	1.37E-11	73.40
Methylene chloride	75-09-2	42	1.95E-13	124.86
Tetrachloroethylene	127-18-4	5.8	1.75E-13	875.60
Carbon disulfide	75-15-0	3.1	2.14E-13	935.33
1,1,1,2-tetrachloroethane	630-20-6	10.3	6.51E-13	161.60

tion plot (parallel to line CD in Fig. 4 above). Such a schematic characterization improves the transparency of conventional human health impact assessment of toxic chemicals by reflecting the intrinsic factors behind the complicated impact assessment process and can be used as a visualization tool for rapid benchmarking of the human health impact of toxic chemicals to facilitate decision-making in the sustainable material selection of toxic chemicals.

4 Case Study

In order to illustrate the applications of the schematic method on characterizing and benchmarking the human health impact of toxic chemicals for a sustainable material selection, here, we conduct a case study on six toxic chemicals commonly used as solvents for cleaning and degreasing in product development and manufacturing, which includes: 1,1,2-trichloroethane, carbon tetrachloride, methylene chloride, tetrachloroethylene, carbon disulfide, and 1,1,1,2-tetrachloroethane. In the schematic characterization and benchmarking of these six toxic chemicals, the daily intake of each chemical is modeled by using the CalTOX multimedia exposure analysis model [42]. Persistence time of each chemical is obtained from the CalTOX database by aggregating the residence time of the chemical substance in the nine environmental compartments under continuous emission pattern and LCIA exposure factors set in U.S. landscape conditions [42]. Like the conventional human health assessment model [26], in the schematic characterization process, we also consider that the whole U.S. population is subject to the multimedia exposure of these toxic releases. The primary toxicity indicator used is the ED_{10}, a benchmark measure recommended by the SETAC panel [33]. Based on 1 kg emission into air, the process parameters for characterizing the human health impact of these six chemicals are shown in Table 2 above. The ED_{10} values of 1,1,2-trichloroethane, carbon tetrachloride, methylene chloride, and 1,1,1,2-tetrachloroethane are from Ref. [31], the ED_{10} of carbon disulfide is from Ref. [32], and the ED_{10} of tetrachloroethylene is calculated from Refs. [31,43].

Based on the daily risk and persistence parameters, the schematically characterized impacts of these six toxic chemicals are shown in Fig. 6 below. To improve the visualization of benchmarking, the R and T scales of the characterization plot are both set on three orders of magnitude. In the plot, three parallel lines with a slope of −1 are drawn to facilitate the benchmarking of the human health impact of these six toxic chemicals. As indicated by the vector distance between each chemical's position and the three reference lines, the chemical carbon tetrachloride has the most significant impact on human health among these six chemicals, followed by the carbon disulfide, 1,1,2-trichloroethane, tetrachloroethylene, 1,1,1,2-tetrachloroethane, and methylene chloride. From the plot, the three chemicals, carbon disulfide, 1,1,2-trichloroethane, and tetrachloroethylene, have very comparable impact on human health, as clustered on the lower right corner of the plot. Taking into account the high uncertainty of multimedia analysis and data inputs, the human health impact of these three chemicals could be considered at the same level based on the schematic characterization results. From the schematic benchmarking of the human health impact, methylene chloride is the chemical with the least human health impact and accordingly, should be selected as the final solvent chemical for cleaning and degreasing among these six toxic chemicals from the perspectives of sustainable process design and manufacturing.

5 Sensitivity of Toxicity Indicator

In the schematic characterization, the selection of different toxicity indicators may affect the risk value R and consequently, change the final benchmark result. As there is a large number of toxicity indicator being developed and under development for both regulatory and benchmark purposes, a detailed assessment of all these toxicity indicators is beyond the scope of this study. In order to check the sensitivity of the toxicity indicator on the benchmarking results of the schematic method, here, we use another toxicity indicator, ADI, for the schematic characterization and benchmarking of these six toxic chemicals and for comparing the benchmark results from the two ED_{10} and ADI based characterizations. The schematically characterized result by using ADI toxicity indicator is shown in Fig. 7 below.

It demonstrated that the ADI characterized result is exactly the same with that of the ED_{10} based result, indicating again that the chemical carbon tetrachloride has the most significant impact on human health while the chemical methylene chloride has the least. The two chemicals, carbon disulfide and 1,1,2-trichloroethane, have been confirmed on their same level of human health impact by the overlapped positions of the two chemicals in Fig. 7. The ADI based characterization lowers the chemical tetrachloroethylene a little bit further from the cluster of carbon disulfide and 1,1,2-trichloroethane. The small discrepancy could result from the uncertainty of toxicity indicators [44,45].

The two characterized results from the ED_{10} and ADI benchmark measures indicate that the schematic method is insensitive to certain toxicity indicators. Based on the structure of the schematic method, the same benchmark results would be obtained if using

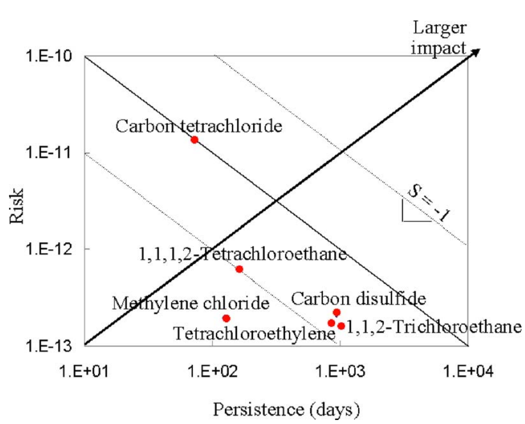

Fig. 6 Human health impact characterization of six toxic chemicals with ED_{10}

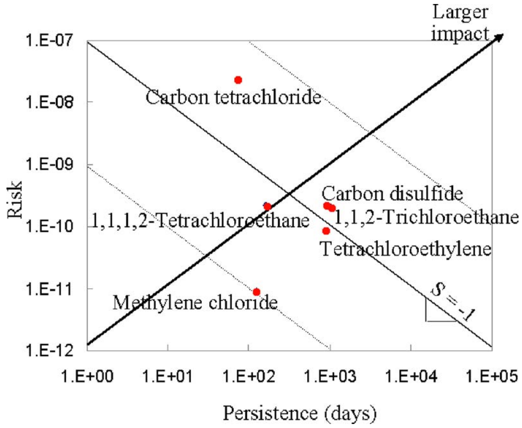

Fig. 7 Human health impact characterization of six toxic chemicals with ADI

those toxicity indicators, which are highly correlated with each other, through uncertainty and safety factors. But further analysis is still needed in the future on those toxicity indicators, which are independent with each other or have a low correlation coefficient.

The reliability of the schematic method has been checked and validated by comparing the benchmark results of the schematic method with those of the conventional scoring method, human toxicity potential on 104 toxic chemicals by using the ADI as the toxicity indicator [46]. A very high correlation coefficient $R = 0.985$ has been obtained on impact rank of the 104 toxic chemicals between these two methods [46].

6 Concluding Remarks

Toxic chemicals are heavily used in product design and manufacturing processes, which generates significant impact on human health after being released into the environment. Human health impact assessment is necessary for providing decision support in the material selection process to improve the sustainability of design and manufacturing practices. In this paper, we integrate the human health impact assessment into the standard material selection process to provide an integrated sustainable material selection metric for toxic chemicals in design and manufacturing.

A schematic method is presented in this paper to characterize the human health impact of toxic chemicals. In this schematic method, the human health impact of a toxic chemical is characterized by two critical parameters: daily risk R and environmental persistence T. The human health impact of a toxic chemical is represented by its position in the $R-T$ two-dimensional plot, which enables the screening and benchmarking of toxic chemicals to be easily made through comparing their relative positions in the characterization plot. With a streamlined characterization process and a visualized representation, this schematic method can improve the understanding of the intrinsic factors behind the human health impact of a toxic chemical release and can be used for rapid benchmarking of various chemical materials to facilitate decision-making in the industrial implementation of sustainable design and manufacturing strategies. In the assessment of the human health impact, the schematic characterization method does not specifically address the release differences between various environmental media, as that is reflected separately in the intake and persistence of the chemical materials. As a result, chemicals released to different environmental media can be benchmarked on the same plot through this schematic method.

A case study is conducted on sustainable material selections of six toxic chemicals including 1,1,2-trichloroethane, carbon tetrachloride, methylene chloride, tetrachloroethylene, carbon disulfide, and 1,1,1,2-tetrachloroethane. These chemicals are commonly used as solvents for cleaning and degreasing in product development and manufacturing. The human health impact of these six chemicals are characterized and benchmarked in the schematic plot for decision support in selecting the chemical with the least impact on human health. The benchmarked results show that methylene chloride has the least impact on human health among these six chemicals while carbon tetrachloride has the most. Sensitivity of the toxicity indicator in the schematic method is checked and validated by comparing the schematic results from ED_{10} and ADI based characterizations. The benchmark results from these two characterizations are exactly the same on these six chemicals, which indicates that this schematic method is insensitive to some toxicity indicators but further analysis is still needed in the future on those toxicity indicators, which are independent with each other or have a low correlation coefficient.

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