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SUSTAINABLE MATERIAL SELECTION OF TOXIC CHEMICALS IN DESIGN AND MANUFACTURING FROM HUMAN HEALTH IMPACT PERSPECTIVE

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ABSTRACT

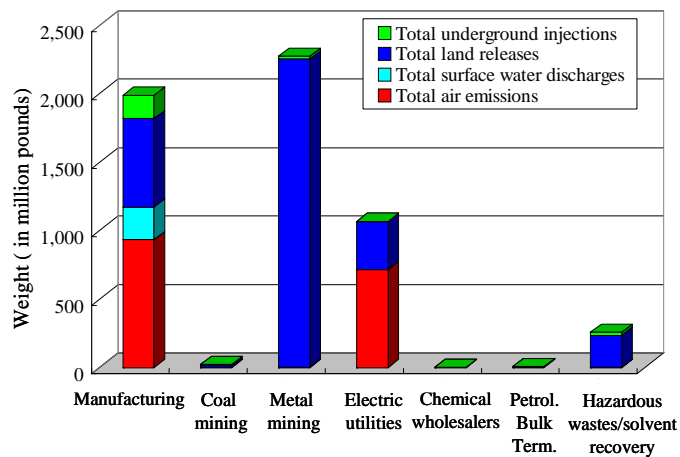
Toxic chemicals used in product design and manufacturing are grave concerns due to their significant impact on human health. Sustainable material selections are needed by industry to reduce the overall impact of toxic chemicals in both design and manufacturing. In this paper, we integrate the human health impact assessment into standard material selection process for developing a sustainable material selection metric for decision support in design and manufacturing. A schematic method is presented for characterizing and benchmarking the human health impact of toxic chemicals. A case study is performed on six toxic chemicals used as solvents in semiconductor manufacturing. Reliability of the schematic benchmarking results is checked and validated by comparing the results with that of conventional Human Toxicity Potential (HTP) method.

Keywords: Sustainable material selection, toxic chemical, human health impact, schematic method.

INTRODUCTION

Toxic chemicals used in product design and manufacturing are grave concerns due to their significant impact on human health. In the United States, facility level of toxic chemical release information from the manufacturing industry and seven related industrial sectors are available through the U.S. Environmental Protection Agency's Toxic Release Inventory (TRI) database [1]. Such inventory programs for collecting toxic chemical information from industrial emissions have also been established by many other countries including European Union nations, Australia, Canada, Japan and Korea, etc. [2-3]. 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 billion pounds. Based on weight, the air emissions roughly account for 30% of the total toxic release; the total land releases take roughly 62% share; surface water discharges and underground injections are both around 4%.



Total release: 5.616 billion pounds

Fig.1 US Toxic Release Inventory in 2001

It should be noted here that the total amount disclosed in the TRI database is an underestimate of toxic chemical released in the United States since many small scale manufacturing entities are not required to report their toxic chemical emissions. Such an enormous amount of toxic chemical release,

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as exposed to human beings in the environment, would generate significant impact on public health through various exposure routes and pathways. Sustainable material selection of toxic chemicals aims to reduce the overall impact of toxic chemicals used in design and manufacturing by picking less impact chemical materials through material screening and benchmarking. In the industrial operations, sustainable material selection is identified as one of the most effective strategies for reducing the environmental impact of industrial operations and supporting the efforts of sustainable design and manufacturing.

In real practice, there are a wide variety of toxic chemicals used in product development and manufacturing processes for various operations including etching, forming, catalyzing, cleaning, etc. Different toxic chemicals have different physical-chemical properties and lead to different impact on public health and the environment. For sustainable material selection of toxic chemicals, both the material properties and environmental factors need to be considered in the human health impact assessment for providing decision support in material screening and benchmarking.

In this paper, we report a study on 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 visualization 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 semiconductor manufacturing.

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 phase. Conventional material selections in product design and manufacturing are made primarily based on functionality by considering such material properties like strength, hardness, density, etc., and cost including both the material acquisition cost and processing cost. 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 meets the requirements of the functional and cost criteria.

Ashty has 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 the screened materials to improve performance, and seeking supporting information to select the final material [4]. Here we integrate the human health impact assessment into this standard material selection structure to perform a sustainable material selection of toxic chemicals by benchmarking the top-ranked candidate

chemicals on their human health impact, so as to reduce their overall impact on human health throughout their life cycle applications in the design and manufacturing processes. The integrated sustainable material selection process of toxic chemicals is shown in figure 2 below [5].

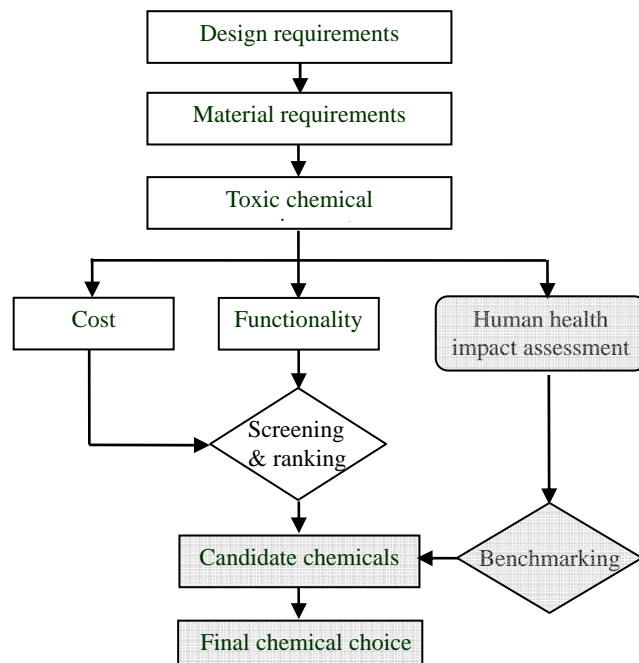


Fig.2 Sustainable material selection process of toxic chemicals

Human health impact assessment of toxic chemicals is a complicated process which needs to consider not only the physical-chemical properties of the chemical material but also the release pattern and exposure pathways of the chemical release 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 top ranked candidate chemicals which are selected from the conventional material selection process, as shown by the shaded process flows in figure 2 above, while the human health impact assessment can also be 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 [6-10].

HUMAN HEALTH IMPACT OF TOXIC CHEMICALS

Current human health impact assessment of toxic chemicals is based on risk assessment by considering the fate and transport of the released chemical in the environment, and the final dose (intake) of the chemical on an exposed human being through multiple exposure routes and pathways.

In current practice, Human Toxicity Potential (HTP) is used for the human health impact assessment of toxic chemicals. HTP is a computed weighting index, proposed by Guinée and Heijungs [11], calculated by using multimedia environmental fate, exposure and risk analysis models based on the inherent toxicity and final dose delivered from the toxic release to an individual in the model environment [12][13]. HTP is a powerful metric for toxic chemical assessment and benchmarking, but it has a limited coverage and lacks transparency, and accordingly has limited practical applications in the industry for sustainable material selection of toxic chemicals. Here we present the development of a schematic method for characterizing and benchmarking the human health impact of toxic chemicals, to improve the transparency and promote the benchmarking efficiency of toxic chemicals to support the efforts of sustainable design and manufacturing. Current human health impact assessment of toxic chemicals is generically conducted by following the risk assessment principles as described in [14]. The standard human health impact assessment uses a five-tiered hierarchy process: mass, toxicity, persistence, concentration and intake [15-19], as demonstrated in figure 3 below.

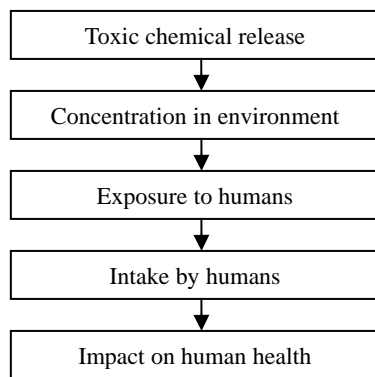


Fig. 3 Human health impact of toxic chemical release

The mass of a toxic chemical release, as determined from the production process operations, dictates the concentrations of the chemical release in the environment, which consequently determines the final intake of the toxic chemical among the exposed population through various exposure pathways and routes, as demonstrated in figure 3 above. Accordingly, the intake of a toxic chemical release can be taken as a multi-media function of the mass and environmental concentrations. In this way, 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 impact of chemicals on human health. Toxicity of a chemical substance is typically evaluated through a material equivalency approach by using threshold values obtained from dose-response modeling studies. There are some commonly used toxicity indicators in human health impact studies such as the Threshold Limit Value (TLV) [20], Permissible Exposure Limit (PEL) [21], Human Limit Value (HLV) [22], Acceptable Daily Intake (ADI) [23], etc. In this method, we use ADI as the toxicity indicator for human health impact assessment. The ADI indicator is usually expressed with a value in the unit of mg/kg bw/day. The ADI indicator is widely adopted by the Council of Europe, WHO, U.S.FDA, etc., in the human risk and exposure analysis.

Besides toxicity, 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 a shorter persistence time. Persistence of chemicals has been systematically investigated by researchers in the past decade, and various methods have been developed for its calculations [24-29]. Persistence of a chemical substance in the environment is jointly determined by its material properties and environmental conditions including both geographic and meteorological conditions. The half-life of a chemical material 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 [30]. The overall persistence of a chemical substance in the environment can be generally calculated by means of [25]:

$$T = \frac{\sum M_j}{\sum M_j k_j} \quad (1)$$

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

In human health impact assessment, it is the intake amount of a toxic chemical which generates the adverse impact on human health. Intake of a toxic chemical can result from various exposure pathways like 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 [27].

In conventional risk assessment, the total intake of a chemical release is 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 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 human health impact assessment of a toxic chemical exposure from various environmental media, by making the intake and persistence factors independent with each other. A daily intake is the total amount an average person takes during a typical 24 hour period in the model environment. As a result, the human health impact of a toxic chemical release can be characterized by a multi-media function of such three factors: daily intake, toxicity and persistence, as shown in the following:

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

In this method, we employ the following simplified formula to calculate the daily intake of a toxic chemical release by an average individual in the model environment [31]:

$$D = \frac{E \times IF \times 10^6}{N \times BW \times T} \quad (3)$$

Where D is the average individual daily intake with units of mg/kg bw/day; E is the released amount of the chemical material, with unit of kg; IF is the intake fraction of the chemical; N is the total number of people exposed to the release; BW is the average body weight of an individual (set at 70 kg in common practice); and T is the overall persistence of the chemical in the environment, in days.

To simplify the human health impact characterization, here we have the daily intake, D , and toxicity, ADI , combined into a dimensionless daily risk, R , as defined by the following expression:

$$R = \frac{D}{ADI} \quad (4)$$

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:

$$I_i = f(R_i, T_i) \quad (5)$$

By using equation (5), 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 , k , to demonstrate the schematic characterization of their human health impact, as shown in figure 4 below. In the characterization plot, the two axes are both set on logarithmic scales due to the large differences of R and T magnitude. Such a schematic characterization improves the transparency of the 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 sustainable material selection of chemical substances. 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 with a higher risk and a longer persistence has a higher impact on human health.

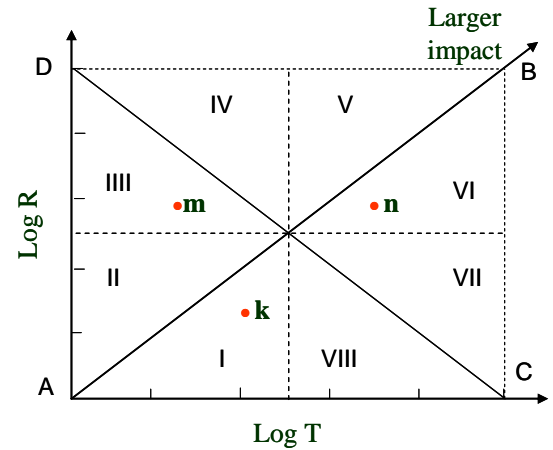


Fig.4 Human health impact characterization concept

In the cases where tradeoffs need to be assessed between R and T factors, the benchmarking is made by evaluating the slope value of the line between the two chemicals. For two chemicals m , n , the slope value of line mn , $S_{m,n}$, can be calculated through:

$$S_{m,n} = \frac{\text{Log}R_n - \text{Log}R_m}{\text{Log}T_n - \text{Log}T_m} \quad (6)$$

Different tradeoff scenarios are shown in figure 5 below. If $S_{m,n} > 0$, the human health impact of the two chemicals: $I_m > I_n$, as shown in figure 5(a). If $S_{m,n} = -1$, then $I_m = I_n$, as shown in figure 5(b); when $S_{m,n} < -1$, then $I_m > I_n$, as shown in figure 5(c); when $0 > S_{m,n} > -1$, then $I_m < I_n$, as shown in Figure 5(d).

In the schematic 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.

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 characterization plot (parallel to line CD in figure 4 above).

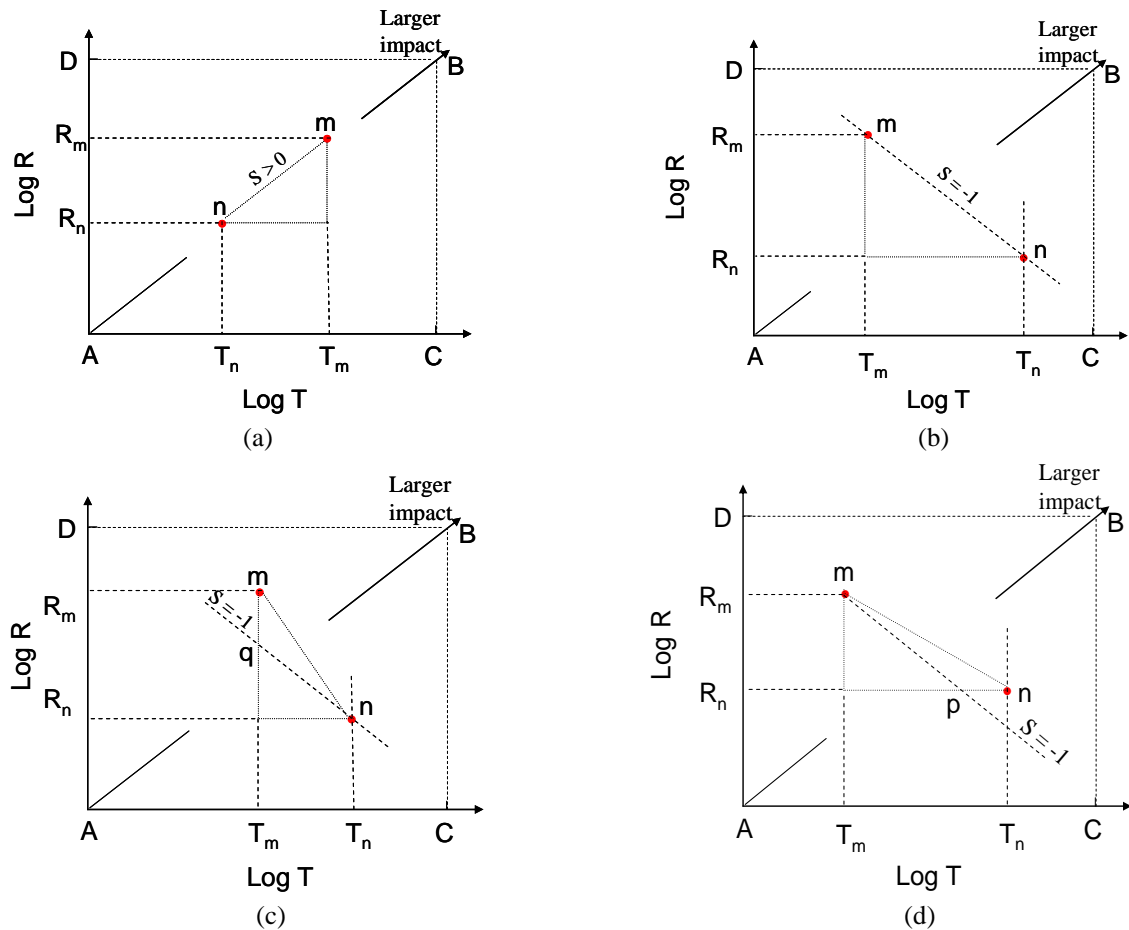


Fig. 5 Schematic benchmarking of human health impact of two toxic chemicals m , n
For the human health impact: (a) $I_m > I_n$; (b) $I_m = I_n$; (c) $I_m > I_n$; (d) $I_m < I_n$.

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 in semiconductor manufacturing, which includes: trichloroethylene, 1,1,1-trichloroethane, carbon tetrachloride, methylene chloride, tetrachloroethylene, and chlorinated fluorocarbons. These chemicals are found mainly for use of cleaning and degreasing in semiconductor manufacturing and have been listed in F001 group of wastes in the RCRA act [32].

As for these six toxic chemicals, there are four chemicals including carbon tetrachloride, tetrachloroethylene, trichloroethylene, and 1,1,1-trichloroethane are included in the EPA's TRI database, as reported by various manufacturers for both their onsite and offsite releases. As a demonstration, here we have the 2006 release data of these four chemicals in the United States, as shown in figure 6 below [1].

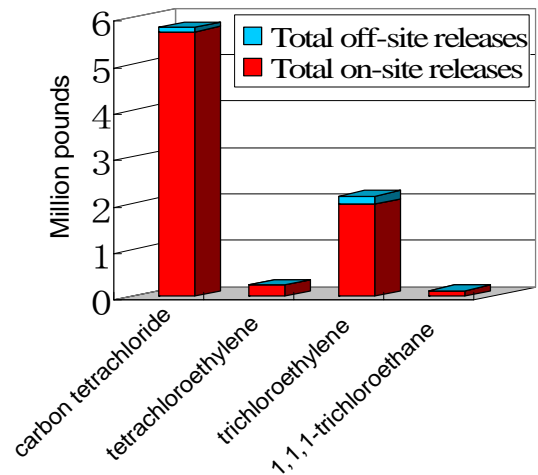


Fig. 6 2006 TRI release of four toxic chemicals in the U.S.

In the schematic characterization and benchmarking of these six toxic chemicals, the intake is modeled by using the CalTOX multi-media exposure analysis model [33]. Persistence

Chemical	Daily intake (mg/kg/day)	ADI (mg/kg/day)	Individual daily risk (R)	Persistence (T, days)
Trichloroethylene	1.50E-13	0.17143	8.72E-13	1270.00
1,1,1-trichloroethane	2.01E-12	3	6.72E-13	588.93
Carbon tetrachloride	1.63E-11	0.0007	2.33E-8	73.40
Methylene chloride	8.19E-12	0.9	9.10E-12	124.86
Tetrachloroethylene	1.01E-12	0.0114	8.88E-11	875.60
Chlorinated fluorocarbons	2.01E-12	25.71	7.81E-14	600.14

Table 1 Schematic characterization parameters of six chemical solvents used in semiconductor manufacturing

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 [33]. Like conventional human health assessment model [12], in the schematic characterization process we also consider the whole U.S. population is subject to the multi-media exposure of these toxic releases. The U.S. population data is 304.6 million and the average body weight is taken at 70 kg. The process parameters for characterizing the human health impact of these six chemicals are shown in table 1.

Based on the intake, toxicity, and persistence, the schematically characterized impacts of these six toxic chemicals are shown in figure 7 below. In the plot, three parallel lines with slope of -1 are drawn for facilitating the benchmarking of the human health impact of these six toxic chemicals.

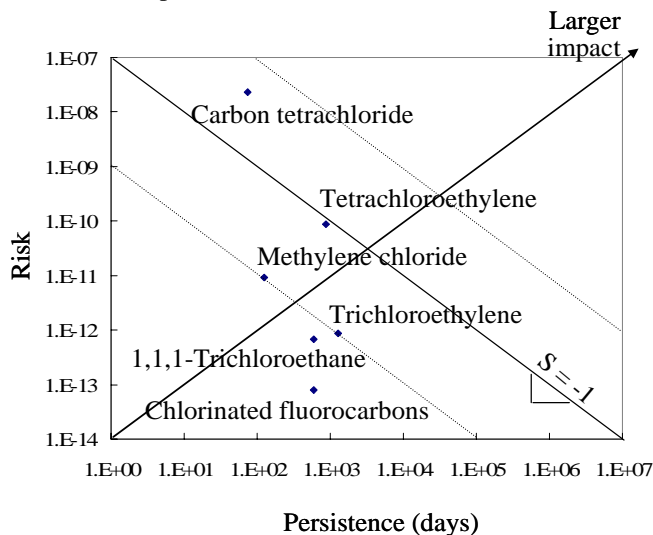


Fig 7. Human health impact characterization of six chemicals used as solvents in semiconductor manufacturing

As indicated by the vector distance between the chemical's position and the line with a slope of -1, the chemical carbon tetrachloride has the most significant impact on human health among these six chemicals, with tetrachloroethylene next, followed by methylene chloride, trichloroethylene, 1,1,1-trichloroethane, and chlorinated fluorocarbons. From the plot, methylene chloride and trichloroethylene have very comparable

impact on human health although their risks and persistence times are completely different. From the analysis, the risk of methylene chloride is 10.43 times of that of trichloroethylene, while the persistence of trichloroethylene is 10.17 times of that of methylene chloride. As a result, methylene chloride has a little bit higher impact on human health than trichloroethylene.

Based on the schematic benchmarking of the human health impact, chlorinated fluorocarbons should be selected as the final solvent chemical for cleaning and degreasing among these six toxic chemicals for improving the sustainability of the semiconductor industry.

RELIABILITY CHECK

In this part, the reliability of the schematic characterization results is checked by comparing the schematic ranking with that from the conventional HTP method. In the conventional HTP assessment, the human health impacts of toxic chemicals are assessed for cancer and non-cancer effect, respectively, with an impact value calculated for each of the cancer and non-cancer effect [12].

Among these six toxic chemicals used as solvents for cleaning and degreasing in semiconductor manufacturing, 1,1,1-trichloroethane and chlorinated fluorocarbons have non-cancer effects only while the other four chemicals including carbon tetrachloride, trichloroethylene, methylene chloride and tetrachloroethylene have both cancer and non-cancer effects [18]. In order to benchmark the toxic chemicals on the overall human health impact, here we combine the cancer and non-cancer effects into a single value by weighting cancer risk 10^6 times non-cancer effect, following the suggested ratio in [12]. Based on the two assessments, the benchmarking results of the conventional HTP method and the schematic characterization method are exactly the same on these six toxic chemical solvent materials as used in semiconductor manufacturing. The correlation of the two assessed results is demonstrated in figure 8 below.

The results indicate that this schematic method is reliable to use for characterizing and benchmarking the human health impact of toxic chemicals. Moreover, this schematic method characterizes the human health impact of a toxic chemical release through a reduced three-tiered hierarchy process which increases the transparency of the human health impact assessment method and also provides a convenient way for

facilitating decision-making in material selection processes for sustainable design and manufacturing.

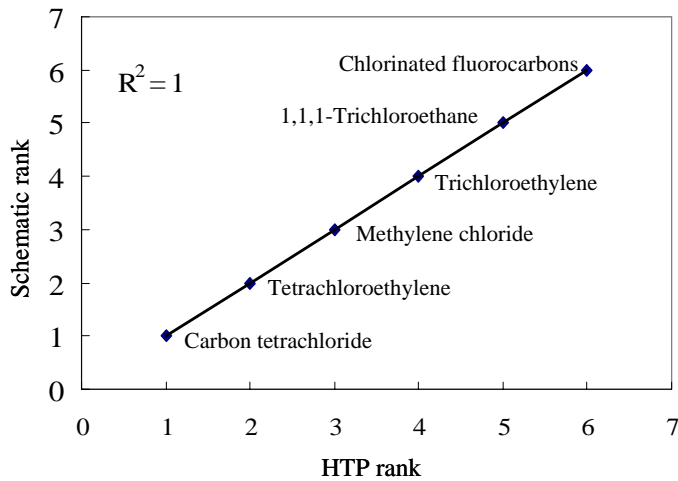


Fig 8. Correlation of the impact rank between HTP and schematic method

CONCLUDING REMARKS

Toxic chemicals are extensively used in product development and manufacturing processes which could generate significant impact on human health and the environment after being released into the environment. Human health impact assessment is necessary for providing decision support in 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. This method uses a reduced three-tiered hierarchy process which needs daily intake, toxicity and persistence of a chemical release for its impact characterization. This schematic method is transparent, and convenient to use. With a streamlined characterization process and a visualized evaluation, 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 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. Like

conventional HTP method, severity of human health damages is not addressed in this schematic method either.

A case study is conducted on sustainable material selections among six toxic chemicals including trichloroethylene, 1,1,1-trichloroethane, carbon tetrachloride, methylene chloride, tetrachloroethylene, and chlorinated fluorocarbons, which are commonly used as solvents for cleaning and degreasing in semiconductor manufacturing. The human health impact of these six chemicals are characterized and benchmarked in the schematic plot, and ranked for supporting decision-making in material selections of design and manufacturing. The benchmarked results show that chlorinated fluorocarbons have the least impact on human health among these six chemicals, while carbon tetrachloride has the most. Reliability of the benchmarked results is checked and validated by comparing the schematic results with that of conventional HTP method. The benchmarked results from these two methods are exactly the same on these six chemicals, which indicates that this schematic characterization method is reliable to use for human health impact characterization and to provide decision support in sustainable material selection of toxic chemicals.

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