Sustainability **2014**, *6*, 3993-4009; doi:10.3390/su6073993

OPEN ACCESS

sustainability

ISSN 2071-1050

www.mdpi.com/journal/sustainability

Article

The Chemistry Scoring Index (CSI): A Hazard-Based Scoring and Ranking Tool for Chemicals and Products Used in the Oil and Gas Industry

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Received: 2 April 2014; in revised form: 4 June 2014 / Accepted: 9 June 2014 / Published: 26 June 2014

Abstract: A large portfolio of chemicals and products is needed to meet the wide range of performance requirements of the oil and gas industry. The oil and gas industry is under increased scrutiny from regulators, environmental groups, the public, and other stakeholders for use of their chemicals. In response, industry is increasingly incorporating "greener" products and practices but is struggling to define and quantify what exactly constitutes "green" in the absence of a universally accepted definition. We recently developed the Chemistry Scoring Index (CSI) which is ultimately intended to be a globally implementable tool that comprehensively scores and ranks hazards to human health, safety, and the environment for products used in oil and gas operations. CSI scores are assigned to products designed for the same use (e.g., surfactants, catalysts) on the basis of product composition as well as intrinsic hazard properties and data availability for each product component. As such, products with a lower CSI score within a product use group are considered to have a lower intrinsic hazard compared to other products within the same use group. The CSI provides a powerful tool to evaluate relative product hazards; to review and assess product portfolios; and to aid in the formulation of products.

Keywords: hazard assessment; product evaluation; product stewardship; green chemistry; hydraulic fracturing

1. Introduction

The oil and gas industry uses a wide variety of chemical products during the drilling, stimulation, and production of oil and gas wells. These products are formulated with various chemicals (hereafter referred to as "components") at variable concentrations to meet the performance requirements for a particular use or operation. Components are selected from a wide spectrum of chemical classes (e.g., organics, inorganics, naturally-occurring materials, *etc.*) and exhibit a wide range of potential hazards to human health, physical safety, and the environment (HSE). Historically, product performance, and to a lesser extent cost, have been the primary criteria for product formulation. However, we have developed a comprehensive evaluation of component hazards that can also be used to guide product formulation. This approach is not without precedent. For example, new regulatory requirements regarding the use of hazardous substances as part of oil and gas exploration in the marine environment have added criteria for environmental hazards for product development and selection. For instance, the objective of the OSPAR Commission Hazardous Substances Strategy, one of six strategies under the 1992 OSPAR convention [1], is to prevent pollution of the maritime area by reducing discharges, emissions and losses of hazardous substances. Guiding principles of the OSPAR Convention, implemented through its Harmonized Mandatory Control System for the Use and Reduction of Discharge of Offshore Chemicals [2], include the principle of substitution with less hazardous or non-hazardous substances where such substances are available. While these OSPAR regulatory requirements incorporated environmental hazards as a consideration, hazards to human health and physical safety were not included. However, regulatory safety assessments that take into account a more comprehensive view of hazard are increasingly required for market and/or specific use authorizations of chemicals and products, such as under the REACH regulation in the European Union [3] and the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) in Australia [4].

Increasingly, the oil and gas industry has been taking into consideration the potential hazards of its products; however, no comprehensive method for evaluating HSE performance of products is currently available. This issue is not unique to the oil and gas industry. While a range of scoring and ranking systems has been developed over the last decade using both hazard-based and risk-based approaches (e.g., [5–11]), broadly accepted approaches for selecting safer products and product components are lacking.

To address the lack of a suitable system for evaluating and comparing the potential HSE hazards of products used in the oil and gas industry, we developed the Chemistry Scoring Index (CSI). The CSI is a hazard ranking system that is intended to provide a comprehensive evaluation of the potential hazards associated with products used in oil and gas exploration and production. The CSI tool assigns hazards to product components and generates numerical product scores based on component hazard assignments and product composition.

In the CSI, HSE hazards are assigned to product components based on their presence on a Minimum Set of Lists (described in more detail below) that are contained within the LOLI (List Of Lists) Database. LOLI is a subscription service database, developed and maintained by ChemADVISOR, Inc. (Pittsburgh, PA, USA). As of January, 2014, the LOLI database contains nearly 5000 regulatory lists from around the world, including HSE hazard assessments, international inventories, and other reference material necessary for Safety Data Sheet (SDS) preparation. Following hazard assignment using LOLI, the CSI product score is calculated using the percentage composition of each component in the product and the CSI scoring matrix. The scoring matrix specifies scores for each hazard category considered in the CSI based on the percentage of that component in the product. To account for uncertainties associated with lack of hazard data, the scoring matrix also assigns scores to components for which data are not available. In the CSI, a lower product score implies that a product is less hazardous than others in the same use group, *i.e.*, a lower CSI score implies a safer product alternative within a use group. The CSI also includes an option to further refine product scores by filling data gaps using reliable and well-documented information obtained from non-LOLI sources. While initially developed for use by the oil and gas industry, the CSI provides an approach to product hazard scoring and ranking that could be applied more broadly by other industries.

2. The Chemistry Scoring Index (CSI)

2.1. CSI Minimum Input Requirements

The CSI tool is currently implemented as a semi-automated worksheet application in Microsoft Excel. A customized software solution is under development with the objective of documenting hazard assignments, organizing associated metadata, automating product scoring, and minimizing user error.

The minimum data inputs needed to derive a CSI product score include: (1) the identity and percent composition by weight of components making up at least 70% of the total composition of the product to be scored; and (2) hazard assignments for each product component or a determination that data are not available to assign hazards for a component.

Component composition of the product to be scored is typically available from internal sources (e.g., internal formulation data or SDS) or external sources (e.g., information provided by a chemical supplier). If a component cannot be identified based on its Chemical Abstract Service (CAS) registry number or other chemical identifier (e.g., International Union of Pure and Applied Chemistry [IUPAC] name, International Organization for Standardization [ISO] name, common chemical name, Simplified Molecular-Input Line-Entry Specification [SMILES] notation), then it is categorized in the CSI as having "No Data Available". If more than 30% of a product's composition is due to the contribution of components with "No Data Available", then that product is designated "Do Not Evaluate" in the CSI, and re-evaluated at a later time when more information may be available.

2.2. Hazard Categories Evaluated in the CSI

Selection of the appropriate hazard categories is a key component of chemical and product safety assessment, requiring a balance between comprehensiveness, complexity, and redundancy. The three broad groupings of "hazard categories" evaluated by the CSI—hazards to the environment, physical safety, and human health—are referred to as "hazard criteria". Each criterion within the CSI includes a number of hazard categories as defined by the United Nations' (UN) Globally Harmonized System (GHS) of Classification and Labeling of Chemicals [12], supplemented with additional non-GHS hazard categories in the environmental criterion (Table 1).

The GHS is an international system for standardizing and harmonizing the classification and labeling of chemicals [12]. While current chemical management systems may be similar in content and approach, their differences are significant enough to require multiple classifications, labels and safety data sheets for the same product when marketed in different countries, or even in the same country when parts of the life cycle are covered by different regulatory authorities. The GHS was developed to provide greater consistency across jurisdictions. It is a voluntary international system, not a regulation or a standard, and no international implementation schedule has been defined. However, implementation has been initiated, or is actively being discussed, by several international bodies and various countries, including the U.S., have incorporated the GHS into their chemical regulatory programs. It is therefore anticipated that the GHS will continue to be implemented over the coming years and serve as a harmonizing standard for chemical hazard communication in the future. Since a key objective of the CSI is to be applicable and relevant as a global tool for product hazard evaluation, the GHS was selected as an appropriate starting point.

The CSI includes or addresses all hazards defined by the GHS [12], with some modifications under the environmental, physical safety, and health criteria (see Table 1 and Supplementary Material). Additional environmental hazards included in the CSI, but not considered under the GHS, are "volatile organic compounds" (VOCs), "hazardous air pollutants" (HAPs), "hazardous water pollutants" (HWPs), and "endocrine disruptors", and the use of two separate biodegradability hazard categories as opposed to one in the GHS. These two separate, but mutually exclusive, biodegradation hazard categories, "biodegradation-persistent" and "biodegradation-inherent", are used in the CSI to be consistent with regulatory environmental testing requirements for oil and gas operations under OSPAR regulations [2]. Also, the GHS "chronic aquatic toxicity" hazard is not scored as a separate hazard but chronic aquatic toxicants are covered by the CSI through individual scoring of "acute aquatic toxicity", "biodegradation", and "bioaccumulation". Similarly, acute toxicity, biodegradation and bioaccumulation are used as separate environmental hazards to classify chronic aquatic toxicants in the GHS classification scheme when no adequate chronic aquatic toxicity data are available. Consequently, the CSI approach for chronic aquatic toxicity hazard assignment is consistent with the GHS.

The primary reason for the inclusion of additional environmental hazards is that the CSI uses a broader definition of environmental hazards than the GHS. Under the CSI, the health criterion focuses on worker health (note that although there is a focus on worker health, many of the hazard categories included under the health criterion are relevant to general population exposures as well). In contrast, hazards that may result from a chemical being released into the environment, migrating off-site and subsequently affecting the general population that is exposed to the resulting environmental conditions are included in the environmental criterion. Accordingly, the environmental criterion in the CSI includes both ecological hazards and certain types of hazards that may ultimately affect human health. For example, HAPs, HWPs, and VOCs are not included as environmental hazards in the GHS, but are considered in the CSI because they relate to the health hazards to which populations may be exposed in the event of a release and off-site migration of components through environmental media. “Endocrine disruptors” were included in the CSI, but not in the GHS, based on a concern for potential endocrine-disruptive properties of product components to humans and wildlife. The inclusion of these additional environmental hazards in the CSI allows for a more thorough identification of potential hazards and is intended to result in a comprehensive hazard identification that is appropriate for a typical operational setting in the oil and gas industry.

The physical hazards evaluated by the CSI mirror those defined by the GHS, with two minor exceptions. The GHS considers “explosives” more broadly by including “pyrotechnic components”, while the CSI evaluates these as separate physical hazard categories (Table 1). Also, the GHS “flammable aerosols” hazard is not included in the CSI because these kinds of components are not typically used in the oil and gas industry.

Table 1. Chemistry Scoring Index (CSI)—Hazard Categories.

Environmental Criterion	Physical Criterion	Health Criterion
Acute Aquatic Toxicity (Category 1, 2, and 3)	Explosive	Carcinogenicity (Category 1 and 2)
Chronic Aquatic Toxicity (Category 1, 2, 3, and 4) [1]	Pyrotechnic	Mutagenicity
Biodegradation—Persistent [2]	Flammable Gas	Reproductive Toxicity
Biodegradation—Inherent [2]	Oxidizing Gas	Sensitizers
Bioaccumulation	Gases Under Pressure	Acute Toxicity (Category 1, 2, 3, and 4)
Ozone Depleting Substance	Flammable Liquid (Category 1, 2, 3, and 4)	Corrosivity (Category 1 and 2)
Volatile Organic Compound (VOC) [3]	Flammable Solid	Acute Target Organ Toxicity
Hazardous Air Pollutant (HAP) [3]	Self-Reactive Substance	Chronic Target Organ Toxicity
Hazardous Water Pollutant (HWP) [3]	Pyrophoric (Liquids and Solids)	Aspiration hazard
Endocrine Disruptor [3]	Self-Heating Substance Emit Flammable Gases in Contact with Water Oxidizing Liquid Oxidizing Solid Organic Peroxide Corrosive to Metals	

Notes: [1] A component that is classified as a “chronic aquatic toxicant” based on the Minimum Set of Lists (see Supplementary Material) is scored under the respective “acute aquatic toxicant” hazard category (note, a “chronic aquatic toxicant category 4” is not scored as an acute aquatic toxicant but is assigned “No Hazard” for aquatic toxicity) AND under the “biodegradation/persistent” and “bioaccumulation” hazard categories, unless data are available for that component to demonstrate that it is not bioaccumulative or persistent. For example, a component that is classified as a “chronic aquatic toxicant category 3” is scored as an “acute aquatic toxicant category 3” AND under the “biodegradation/persistent” and “bioaccumulation” hazard categories, unless data are available for that component to demonstrate that it is not bioaccumulative or persistent; [2] These categories deviate from those in the GHS, and are based on definitions presented in the OSPAR HOCNF [2]; [3] These hazard categories are not addressed by the GHS [12].

While the CSI health hazards are largely based on the GHS, the CSI includes a number of modifications. The "reproductive toxins" hazard contains multiple categories in the GHS (*i.e.*, reproductive toxicity categories 1A, 1B, and 2; there is also a separate category for effects on or *via* lactation), but is represented by only one category in the CSI, thus treating all reproductive toxins as equally hazardous. Similarly, the "mutagens" hazard contains multiple categories in the GHS (*i.e.*, germ cell mutagenicity categories 1A, 1B, and 2), but is represented by only one category in the CSI, thus treating all mutagens as equally hazardous. The CSI has two categories for carcinogenicity: Category 1 encompasses the GHS carcinogenicity classification 1A and 1B, while Category 2 corresponds to GHS carcinogenicity classification 2. GHS "category 3 skin irritants (mild irritants)" are not scored in the CSI because some countries/regions have not adopted the class 3 category and they are of minimal public health concern. Also, "serious eye damage/eye irritation" (a distinct health hazard in the GHS) is evaluated jointly with skin corrosion/irritation under "corrosivity" in the CSI. And finally, the CSI does not include GHS "category 5 acute toxicants" because category 5 acute toxicants are considered to have very low acute toxicity and the GHS, based on animal welfare concerns, discourages animal testing in this range unless there is a reason to believe a chemical (at this dose magnitude) may pose a hazard to a vulnerable population. Overall, the modifications to the GHS scheme implemented in the CSI increase the likelihood of identifying a health hazard and therefore represent a conservative approach to hazard assessment.

The CSI approach allows sufficient flexibility that addition or removal of hazard categories could be relatively easily implemented by other users, if deemed necessary.

2.3. CSI Hazard Assignments Using LOLI

The CSI assigns hazards to product components based on their presence on a "Minimum Set of Lists" contained within the LOLI database (see Supplementary Material). The LOLI database is considered a highly reliable hazard data source because it is based on determinations made by regulatory authorities or other widely recognized authorities from around the world. Also, the LOLI database is updated on a weekly basis, and licensed users of the database are notified of changes/updates on a quarterly basis.

The Minimum Set of Lists was defined for the purposes of hazard assignments within the CSI. It contains lists that have been populated with chemicals in accordance with the GHS definitions for each of the GHS hazard categories. For example, the GHS defines an oxidizing gas as "*any gas which may, generally by providing oxygen, cause or contribute to the combustion of other material more than air does as determined through specified ISO test methods*." The CSI implements this definition by identifying a number of regulatory lists in the LOLI database that categorize gases using this same definition, including lists published by authorities from the European Union, Japan and New Zealand (see Supplementary Material). Similarly, for non-GHS hazard categories (*i.e.*, biodegradation/persistent, biodegradation/inherent, VOCs, HAPs, HWPs, and endocrine disruptors), relevant lists were identified within LOLI and included in the Minimum Set of Lists. The Minimum Set of Lists is updated annually to reflect changes to the LOLI database.

There are sometimes instances where various lists on the Minimum Set of Lists provide conflicting hazard classifications for a particular component. For example, a component may be listed as a hazard on a list issued by one country but not another list issued by a different country, or different lists may categorize components in different (higher or lower) categories for the same hazard (e.g., carcinogenicity category 1B *versus* carcinogenicity category 2). In such cases, the CSI conservatively scores the component in the more stringent hazard category unless there is compelling evidence to suggest that the hazard assignment is inappropriate. These determinations require professional judgment using the weight-of-evidence approach outlined in the GHS [12]. When decisions on hazard assignment are made in this manner, the ultimate basis is always documented in the CSI product scoring materials to aid in transparency and allow for future reference. Note that weight-of-evidence decisions are typically not needed when the hazard assignment is based directly on analytical measurements (e.g., "bioaccumulation" assignment based on an experimentally-derived bioconcentration factor or octanol-water partitioning coefficient).

While the CSI relies on the Minimum Set of Lists and LOLI as its primary data sources for making hazard assignments, it also provides users with the flexibility to rely on additional non-LOLI data sources to make hazard assignments, such as internal toxicity or other test data, additional database sources not included in LOLI, SDS information, *etc.* In such cases, the user is encouraged to select sources with the highest reliability. The same weight-of-evidence approach used for LOLI data sources, including documentation of expert judgment decisions, is used when non-LOLI data are used to assign hazards. While currently not implemented in the CSI, a future version may incorporate data reliability flags associated with component hazard assignments, and ultimately, confidence levels associated with CSI product scores.

When hazard data are lacking for a product component, the component is assigned to the "No Data Available" category. However, for several hazard categories (*i.e.*, ozone depleting substances, endocrine disruptors, VOCs, HAPs, and HWPs), absence of a component from the Minimum Set of Lists shown in the Supplementary Material is used to classify that component as "No Hazard Identified" (referred to as "No Hazard" hereafter). For example, if a component is not on the VOC Minimum Set of Lists, then that is not considered a data gap, but evidence that it is not a VOC.

2.4. CSI Hazard Scoring Using the CSI Scoring Matrix

Following hazard assignment, the CSI assigns hazard scores based on the percent composition by weight of each component in the finished product using the CSI scoring matrix (Table 2). The matrix assigns numeric values for hazard categories that vary based on (1) nature and severity of the hazard; and (2) the concentration of a particular component within a product.

Within each hazard criterion, professional judgments were made regarding the relative importance of certain hazard categories by assigning different maximum scores to different hazard categories. In general, the hazards judged as most significant under each of the criteria are assigned a maximum value of 100 points (Table 2). For example, for the health criterion, the maximum score is assigned to known human carcinogens and category 1 acute toxicants. Similarly, the maximum score is assigned to components with acute aquatic toxicity in category 1 in the environmental criterion and components that are considered explosive and organic peroxides in the physical criterion. While these categories represent very different hazards to potentially different receptors, these endpoints were judged to be of similar impact in terms of evaluating intrinsic hazard in the CSI. Under the environmental hazard criterion, the highest maximum scores are given to the categories that describe toxicity rather than component properties that may or may not result in subsequent toxicity, such as biodegradation or bioaccumulation. For the physical hazard criterion, the highest maximum scores are assigned to the explosives and organic peroxides, as components in these categories have the greatest potential to endanger physical safety. For human health, higher scores were given to categories that have the potential for more significant adverse outcomes (e.g., fatality, cancer, birth defects). Components for which data are lacking ("No Data Available") for all hazard categories within a particular criterion are conservatively assigned a maximum value of 100 points for that criterion, thereby assuming that they may be as hazardous as the most severe hazard categories. This approach ensures that potentially hazardous components that are unreported, or for which hazard data are not available, do not result in a favorable score due to this lack of information.

The same types of relative scoring judgments also extend to the maximum scores assigned to hazard categories within a given hazard criterion. While the maximum score of 100 is assigned to the hazard(s) within each criterion judged to have the greatest impact, and to the "No Data Available" category, other hazards within a criterion are assigned lesser maximum scores. For example, the maximum score assigned to a known or presumed human carcinogen is 100, which is 10 times the maximum score assigned to an irritant. By assigning higher values to hazard categories of greatest impact or components for which data is lacking, components which have a mode of action that results in serious adverse effects under multiple categories or for which hazard data are unavailable will be highlighted by receiving a higher hazard score.

As noted, the scores assigned by the CSI scoring matrix also vary based on the concentration of a component in a product. The CSI weighting matrix assumes a defined quantitative relationship between the concentration at which a component is found in a product and degree of hazard. For example, in the environmental hazard category "acute aquatic toxicity category 1", the CSI tool assumes that a component which makes up 5%–9.9% of a product is five times more hazardous than a component present at greater than 0.1%–0.9% (Table 2). This represents a simplified approach given that a defined quantitative relationship between a component's percent composition and degree of hazard is a function of component-specific toxicity information and properties. Nevertheless, the generic approach taken in the CSI is preferable to assuming that a component's hazard is equal at all concentrations. Furthermore, this approach allows for distinctions to be made between products that contain a high percentage of a hazardous component and those containing a low percentage of the same component.

The GHS also considers the concentration of a component in a product but relies on generic percent composition cut-offs/concentration limits below which components are not considered hazardous. The cut-off values used in the GHS are 0.1%, 1%, or higher (for irritants), depending on the health and environmental hazards (cut-offs are not used for physical hazards). In contrast, the CSI evaluates and assigns a score to every product component regardless of its concentration in the product. However, that score may be zero if the percent composition is below the percent-based threshold for the hazard category or if the component was assigned "No Hazard" for all categories in a hazard criterion (Table 2). For example, carcinogenicity is not considered in the GHS at concentrations below 0.1%, whereas a component present at a concentration of less than 0.1% and classified as a carcinogen category 1 would receive a score of 25 in the CSI. Therefore, the CSI approach is more inclusive in assigning hazards in the low concentration range than is the GHS approach.

Table 2. Chemistry Scoring Index (CSI)—Hazard Scoring Matrix.

Hazard Criteria	Hazard Categories [1]	Max. Score	Product Component Percent Range (by weight)						
			>0%–0.09%	0.1%–0.9%	1%–4.9%	5%–9.9%	10%–29.9%	30%–59.9%	60%–100%
ENVIRONMENTAL [2]	No Data Available [3]	100	10	25	50	75	100	Do not evaluate	Do not evaluate
	Acute Aquatic Toxicity Cat. 1	100	1	5	10	25	50	75	100
	Acute Aquatic Toxicity Cat. 2	75	0	1	5	10	25	50	75
	Acute Aquatic Toxicity Cat. 3	50	0	0	1	5	10	25	50
	Ozone Depletion	50	5	10	50	50	50	50	50
	Volatile Organic Compounds	50	5	10	50	50	50	50	50
	Hazardous Air Pollutants	50	1	5	10	25	40	50	50
	Hazardous Water Pollutants	50	1	5	10	25	40	50	50
	Biodegradation-Persistent	50	5	10	50	50	50	50	50
	Biodegradation-Inherent	10	1	10	10	10	10	10	10
	Bioaccumulation	50	5	10	50	50	50	50	50
	Endocrine Disruptors	50	10	25	50	50	50	50	50
	No Hazard [4]	0	0	0	0	0	0	0	0
PHYSICAL [5]	No Data Available [3]	50	0	5	10	25	50	Do not evaluate	Do not evaluate
	Explosive	100	25	75	100	100	100	100	100
	Organic Peroxide	100	5	10	75	75	100	100	100
	Flammable Gas	75	5	10	25	50	75	75	75
	Flammable Liquid Cat. 1	75	0	5	10	25	50	75	75
	Flammable Liquid Cat. 2	50	0	1	5	10	25	50	50
	Flammable Liquid Cat. 3	25	0	0	1	5	10	25	25
	Flammable Liquid Cat. 4	10	0	0	0	1	5	10	10
	Flammable Solid	75	1	5	50	75	75	75	75
	Oxidizing Gas	75	5	10	25	50	75	75	75
	Oxidizing Solid	75	1	5	50	50	50	75	75
	Pyrotechnic	75	5	10	25	50	75	75	75
	Pyrophoric (Liquids and Solids)	75	1	5	10	25	50	75	75
	Oxidizing Liquid	50	0	1	5	10	25	50	50
	Self-Reactive Substance	50	0	1	5	10	25	50	50

Table 2. *Cont.*

Hazard Criteria	Hazard Categories [1]	Max. Score	Product Component Percent Range (by weight)						
			>0%–0.09%	0.1%–0.9%	1%–4.9%	5%–9.9%	10%–29.9%	30%–59.9%	60%–100%
PHYSICAL [5]	Gases Under Pressure	25	1	5	25	25	25	25	25
	Self-Heating Substance	10	0	0	1	1	5	10	10
	Emit Flammable Gases in Contact with Water	10	0	0	1	1	5	10	10
	Corrosive to Metals	5	0	0	1	1	5	5	5
	No Hazard [4]	0	0	0	0	0	0	0	0
HEALTH	No Data Available [3]	100	10	25	50	75	100	Do not evaluate	Do not evaluate
	Carcinogenicity Cat. 1	100	25	100	100	100	100	100	100
	Carcinogenicity Cat. 2	75	10	75	75	75	75	75	75
	Acute Toxicity Cat. 1	100	10	25	50	75	75	100	100
	Acute Toxicity Cat. 2	75	5	10	25	50	50	75	75
	Acute Toxicity Cat. 3	50	0	1	5	10	25	50	50
	Acute Toxicity Cat. 4	10	0	0	1	5	5	10	10
	Mutagenicity	50	10	25	25	50	50	50	50
	Reproductive Toxicity	50	10	25	40	50	50	50	50
	Acute Target Organ Toxicity	50	1	5	10	25	25	50	50
	Chronic Target Organ Toxicity	50	1	5	10	25	25	50	50
	Sensitizers	25	5	10	25	25	25	25	25
	Corrosivity Cat. 1	25	0	1	5	5	10	25	25
	Corrosivity Cat. 2 (Irritant)	10	0	0	1	5	5	10	10
	Aspiration Hazard	10	0	0	0	1	5	10	10
	No Hazard [4]	0	0	0	0	0	0	0	0

Notes: [1] Hazards are assigned based on the Minimum Set of Lists contained within LOLI (see Supplementary Material). The Minimum Set of Lists is updated annually to reflect changes to the LOLI database; [2] Chronic Aquatic Toxicants are not scored separately, but are scored in the respective Acute Aquatic Toxicant (*i.e.*, a Chronic Cat 1 is scored as an Acute Cat 1) AND Biodegradation/Persistent AND Bioaccumulation hazard categories, unless data are available to indicate that the component is not persistent or bioaccumulative; [3] If data are not available for ≥30% of a product's composition by weight, then the product is not scored in the CSI; [4] "No Hazard" indicates that a component is not assigned to any of the listed hazard categories for the criterion, *i.e.*, no hazard was identified; [5] A component is scored in either the liquid, the solid OR the gas phase—*i.e.*, a component cannot be assigned to both the flammable gas and the flammable liquid categories.

In the CSI, an environmental hazard score, a physical hazard score, and a health hazard score are calculated based on each of the product's individual components. As discussed earlier, these three hazard criterion scores for the product incorporate scores given to each component, including components for which information was not available to assign hazards (*i.e.*, assigned "No Data Available" in Table 2). This ensures that products are not identified as non-hazardous solely based on a lack of data. The environmental, physical, and health hazard criterion scores are added together to compile a total hazard or CSI score for the product. The three hazard criteria are weighted equally when added together to generate the final CSI score; *i.e.*, no hazard criteria score is added in multiples when deriving the total hazard score for a product. However, caution must be exercised in comparing the health hazards of a particular product to its physical hazards or environmental hazards given that the weighting matrix and the CSI were not designed to facilitate such comparisons.

Overall, the CSI is designed to allow all of the hazards associated with one product to be compared with all of the hazards associated with other products in the same product use group. Products that score lower within a product use group are considered to have a lower intrinsic hazard compared to other products within the same use group that have higher scores, as illustrated below by a CSI example analysis for five products.

A range of sensitivity analyses were conducted on the CSI scoring matrix to evaluate the robustness of the overall relative CSI scores within a product use group (full analyses available upon request). The sensitivity analyses were conducted using eight product use groups, consisting of a total of 127 products. As part of the sensitivity analysis, several alternative approaches to scoring were evaluated. For example, we evaluated a binary scoring system (*i.e.*, if a chemical is assigned to a hazard category, it is given a score of 1; otherwise, it is given a score of 0), different approaches for addressing components for which no data are available, use of combined hazard scores for components assigned to the same hazard category, and assigning differential weights to the individual CSI criteria scores to derive a combined total score. The impact of each approach on scoring and ranking within each product use group was then evaluated. These analyses showed that the different evaluated approaches did not significantly affect CSI scores and relative ranking of products within the use groups evaluated. That is, products that were either significantly more or less hazardous than the average product within a use group were relatively unaffected by slight modifications to the weighting matrix.

3. CSI Example and Results Interpretation

When CSI scores are calculated for products within the same use group, the CSI tool allows CSI scores—and therefore the relative hazards—of those products to be compared. This comparison can be taken into account when selecting products for use in particular applications, typically alongside other factors such as product performance and cost. It is important to recognize that, while the CSI allows for relative ranking of products, small differences in scores among products in a use group may not be significant. For instance, a product with a CSI score of 180 is not necessarily significantly less hazardous than a product in the same use group that received a CSI score of 220. However, differences in scores that are of greater magnitude when compared to other products in the same use group may be more likely to be significant, and might form the basis of a decision about product substitution. This concept is incorporated into the CSI by calculating an average CSI score and a standard deviation on that average for each use group. A difference in CSI scores among products in a use group that is within one standard deviation of the average score for the use group is not considered significant, whereas a difference that is greater than one standard deviation of the average score for the use group is considered more meaningful.

To illustrate the use of the CSI and the aforementioned concept of significance in product hazards within a use group, five generic products belonging to the same use group were evaluated. Compositions of these five products and the associated CSI evaluation are summarized in Table 3. Product 1 was not evaluated because greater than 30% of its composition was assigned to the "No Data Available" category in the physical safety criterion based on information in the Minimum Set of Lists. Products 4 and 5 each contain tributyl tetradecyl phosphonium chloride, which lacks information in the Minimum Set of Lists for both the environmental and physical hazard criteria. Since this component is present at less than 30% of the total product composition, both products could be scored despite data gaps. Figure 1 shows the final scores for the four example products that could be evaluated using the CSI. The three qualifiers shown in Figure 1 (*i.e.*, "Typical Product Scores in Use Group", "Less Hazardous than Typical Products in Use Group", and "More Hazardous than Typical Products in Use Group") are derived using the average CSI score of the four example products and the standard deviation on that average. As shown in Figure 1, Product 2 received a higher hazard score than Products 3, 4, and 5, which all have "Typical" scores for the use group. The CSI score for Product 4 is actually equal to the use group average minus one standard deviation (*i.e.*, 293 − 188 = 105). Much of this score is driven by data gaps and therefore addressing data gaps for Product 4 under the environmental and physical hazard criteria may result in a future categorization of "Less Hazardous than Typical Products in Use Group". The latter illustrates the usefulness of the CSI for informing data gathering within a product portfolio.

Figure 1. CSI evaluation of five example products with similar use. AVE = Average Score (293) for Use Group; SD = Standard Deviation (188) for Use Group; * Products 4 and 5 contained some data gaps, but could be scored (*i.e.*, containing component(s) with data gaps at total mass percent <30%); ** Product 1 did not receive a CSI score because of substantial data gaps (*i.e.*, containing components with data gaps at total mass percent ≥30%).

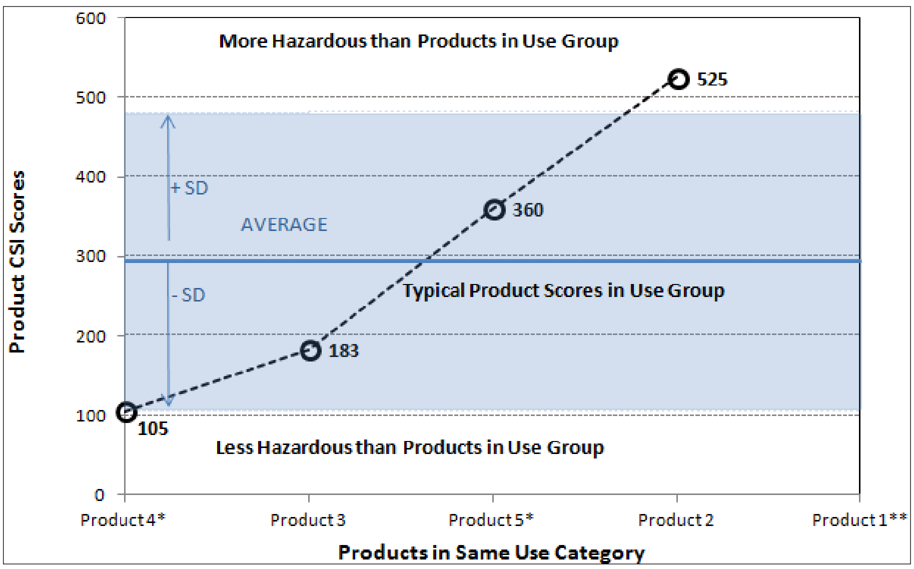

Table 3. CSI evaluations for five example products with similar use.

Product [1]	Component CAS#	Component Name	Component Percent Range (by weight)	Environmental Hazards [2]	Physical Hazards [2]	Health Hazards [2]	CSI Scores [3]
Product 1	1113-55-9	2-Monobromo-3-nitrilpropionamide	1%–4.9%	No Data Available (50)	No Data Available (Do Not Evaluate)	No Data Available (50)	ENV = 250
							PHY = NA [4]
							HEA = 200
	10222-01-2	2,2-Dibromo-3-nitrilopropionamide	60%–100%	Acute Aquatic Toxicity Cat. 1 (100)	No Data Available (Do Not Evaluate)	Acute Toxicity Cat. 2 (75)	**TOTAL = NA** [4]
				Biodegradation-Persistent (50)		Corrosivity Cat. 1 (25)	
				Bioaccumulation (50)		Chronic Target Organ Toxicity (50)	
Product 2	52-51-7	2-Bromo-2-nitro-1,3-propanediol	60%–100%	Acute Aquatic Toxicity Cat. 1 (100)	Flammable Solid (75)	Acute Toxicity Cat. 2 (75)	ENV = 200
				Biodegradation-Persistent (50)	Self-Reactive Substance (50)	Corrosivity Cat. 1 (25)	PHY = 125
				Bioaccumulation (50)		Acute Target Organ Toxicity (50)	HEA = 200
						Chronic Target Organ Toxicity (50)	**TOTAL = 525**
Product 3	1310-73-2	Sodium hydroxide	1%–4.9%	Acute Aquatic Toxicity Cat. 3 (1)	Corrosive to Metals (1)	Acute Toxicity Cat. 4 (1)	ENV = 101
						Corrosivity Cat. 1 (5)	PHY = 26
						Acute Target Organ Toxicity (10)	HEA = 56
	7681-52-9	Sodium hypochlorite	10%–29.9%	Acute Aquatic Toxicity Cat. 1 (50)	Oxidizing Liquid (25)	Acute Toxicity Cat. 4 (5)	**TOTAL = 183**
				Bioaccumulation (50)		Corrosivity Cat. 1 (10)	
						Acute Target Organ Toxicity (25)	
	7732-18-5	Water	Remainder	No Hazard (0)	No Hazard (0)	No Hazard (0)	
Product 4	81741-28-8	Tributyl tetradecyl phosphonium chloride	5%–9.9%	No Data Available (75)	No Data Available (25)	Corrosivity Cat. 1 (5)	ENV = 75
							PHY = 25
							HEA = 5
	7732-18-5	Water	Remainder	No Hazard (0)	No Hazard (0)	No Hazard (0)	**TOTAL = 105**

Table 3. *Cont.*

Product [1]	**Component CAS#**	**Component Name**	**Component Percent Range (by weight)**	**Environmental Hazards** [2]	**Physical Hazards** [2]	**Health Hazards** [2]	**CSI Scores** [3]
Product 5	67-56-1	Methanol	10%–29.9%	Acute Aquatic Toxicity Cat. 3 (10)	Flammable Liquid Cat. 2 (25)	Reproductive Toxicity (50)	ENV = 175
				Volatile Organic Compounds (50)		Acute Toxicity Cat. 3 (25)	PHY = 50
				Hazardous Air Pollutants (40)		Corrosivity Cat. 2 (Irritant) (5)	HEA = 135
						Acute Target Organ Toxicity (25)	**TOTAL = 360**
						Chronic Target Organ Toxicity (25)	
	81741-28-8	Tributyl tetradecyl phosphonium chloride	5%–9.9%	No Data Available (75)	No Data Available (25)	Corrosivity Cat. 1 (5)	
	7732-18-5	Water	Remainder	No Hazard (0)	No Hazard (0)	No Hazard (0)	

Notes: [1] Five generic products belonging to the same Use Group and their corresponding composition by weight are presented; [2] Hazard categories were assigned using the Minimum Set of Lists (see Supplementary Material). The corresponding hazard score is shown in parentheses and is based on the component percent range and the CSI Scoring Matrix (Table 2). Note that the Minimum Set of Lists is updated annually to reflect changes to the LOLI database. Therefore, future changes to the Minimum Set of Lists may result in changes to the hazards and scores presented here; [3] CSI Scores for the Environmental (ENV), Physical (PHY), and Health (HEA) Hazards Criteria and the TOTAL (ENV, PHY, and HEA combined); [4] ≥30% of product composition lacks data ("No Data Available"). Consequently, TOTAL hazards for this product were not evaluated using the CSI.

4. Discussion

A detailed comparison of the CSI to other chemical or product ranking and scoring systems is beyond the scope of this manuscript and will be published elsewhere. Briefly, many existing systems are relatively consistent with regard to approach and the hazard categories evaluated. For instance, other hazard ranking and scoring systems, such as USEPA's Design for the Environment Master Criteria for Safer Ingredients [11] and the Clean Production Action's Green Screen [5], similarly base their hazard evaluation on the GHS [12]. Given the addition of several non-GHS hazard categories, the CSI is generally more comprehensive with respect to the hazards that are evaluated compared to other systems. Hazards with the greatest impact under each of the three CSI criteria (*i.e.*, carcinogenicity category 1 and acute toxicity category 1 under health, explosivity and organic peroxide under physical, and acute aquatic toxicity under environmental) are assigned the same maximum value, *i.e.*, 100 points. A number of other existing ranking systems likewise assign equal values to hazards such as carcinogenicity (or other measures of chronic health hazards) and acute aquatic toxicity as part of their scoring processes, or use similar hazard levels (e.g., low, medium, high, very high) to characterize these types of hazards (e.g., [13]).

It is recognized that the regulatory lists compiled in LOLI may have been established over an extended period of time, potentially following public debate, such that they may not always reflect the most current scientific information on potentially new emerging hazards or chemicals of emerging concern. However, there are significant advantages in relying principally on LOLI as a single broad data compilation source in that: (1) the LOLI database is widely recognized and easily accessible; (2) the LOLI database is considered a highly reliable data source because it is based on determinations made by regulatory authorities or other widely recognized authorities; (3) reliance on the LOLI database allows for quick hazard scoring and ranking; (4) the LOLI database is automatically and regularly updated; (5) hazard scores can be more easily automated and implemented; (6) the effort is less labor-intensive; and (7) ideally, different users should obtain the same CSI scores (or, in case of differences in obtained score using the LOLI database, this should be a result of well-documented best professional judgment decisions). In addition, the CSI provides a framework that can be used to include additional hazard information from sources outside of LOLI if the user desires.

It is important to point out that the CSI calculates hazard scores for products based on a product's intrinsic ability to cause adverse effects. The CSI is therefore not directly indicative of risk, which is the probability that such effects will occur in the various applications and exposure scenarios in which the product will be used and/or discharged. While the CSI is not a tool to evaluate risks associated with products, it can be used to alert formulators/users to the presence of an intrinsic hazard. This hazard information can be used to minimize the use of hazardous product components, thus potentially reducing risk.

5. Conclusions

One of the challenges facing the oil and gas industry today is addressing concerns about potential health, safety, and environmental (HSE) hazards that may be associated with its operations. Although great strides have been made in this area, a comprehensive and universally-accepted method for comparing and communicating overall HSE performance of comparable products is lacking. The CSI addresses this challenge by quantifying HSE properties of products based on the intrinsic hazards of their components. The CSI approach for product hazard scoring and ranking could be implemented more broadly to provide an industry-wide standard for product safety evaluations. Furthermore, the approach could be easily tailored to serve specific needs of other types of industries or future users.

Acknowledgments

This work was funded by Halliburton Energy Services, Inc. (HESI) (Houston, TX, USA). The authors have no conflicts of interest related to this manuscript.

Author Contributions

All authors were involved in the development of the CSI and the writing of the manuscript. All authors read and approved the final manuscript.

Conflicts of Interest

The authors declare no conflict of interest.

Disclaimer

The CSI was developed to provide a means for comparing the relative environmental, physical safety and health hazards of its products used in the process of oil and natural gas exploration and production. We make no warranties or representations regarding the risks associated with the use of any particular product based on the score assigned to a product through the use of the CSI. We also make no representations regarding, and are not in any way responsible for, any scoring or ranking of products through the application of the CSI in a manner that is inconsistent with its intended use.

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