Cost effective method for determining the Relative Hazardousness of substances and compounds

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Abstract: Evaluation of substance hazardousness is of large interest. Here a method describing how the total hazards statement indicator (HSI) - associated with any substance - is used to estimate the HSI of CdS, Pb(CN)₂, thallium(I) carbonate, several other compounds and a full life cycle inventory of aluminum smelting. The proposed method is based on the following parameters: hazards statement (HS), numerical values for each HS based on class, and calculated values for HS combinations. The proposed HSI method is simple, fast, efficient, low in cost, easy to use and enables risk assessment as regulations change. The HSI method seems also very easy to popularize, and the market has broad application prospects. Two other hazardousness life cycle impact assessment indicators – the ReCiPe (H) Human Toxicity and BEES+ Ecotoxicity in LCIA - give different and similar results compared to HSI for a life cycle inventory of aluminum smelting unit process, respectively. HSI applied to tungsten production shows that the hazardousness of smaller mass flows can indeed be captured. Carbon monoxide is not included in ReCiPe (H) human toxicity or in any other toxicity indicator except BEES+ ecotoxicity. The HSI method does not need guesswork whenever the HSs are known.

Keywords: Hazards, Hazard Statements, Hazardous Substance Process Management, Materials, Risks. Substances.

1. INTRODUCTION

There is a huge number of possible chemical substances and compounds. The global GDP growth will globally also require additional amounts of chemicals e.g. herbicides, insecticides and fungicides in industrial agriculture [1]. Thousands of new chemicals are introduced each year and hundreds of millions of tonnes are emitted [2, 3]. The world is demanding more and more compounds (compounds consist of more than two elements), substances and chemicals many of which have unknown risks, hazards and toxicity [4]. For instance, nanomaterials [5,6] and microplastics [7,8] released from single-use plastics means extra output of substances in the oceans [9]. Miele identified 14 steps towards global environmental compliance of which identification of material risk is one of them [10]. There is a general need for:

- 1) Identification and risk management of substances of concern;
- 2) Safe and sustainable use of chemicals by industry;
- 3) Sustainable management of chemicals.

In this context, the European Commission published a report [11] of gaps, challenges and weaknesses of the most relevant chemicals legislation (excluding REACh).

The report addresses the need for simplifying and streamlining hazard and risk assessment processes and providing better consumer information.

The present method globalizes the German Toxic Potential Indicator (TPI) [12,13] in a simplified manner. Apart from TPI there are at least three other methods to mention: GreenScreen [14], Chemical Prioritization Protocol (GPP) [15] and Environmental Score (ES) [16]. All three have shortcomings as far as transparency which is however natural as they are commercial methods. On the other hand, the present *Hazard Statements Indicator (HSI)* is fully transparent and repeatable.

GreenScreen is a commercial/proprietary method for chemical hazard assessment. The rapid version of GreenScreen – the GreenScreen List Translator - aims to identify chemicals of great concern. As such it is similar to the present *HSI* method. Each chemical is given a benchmark score of 1, 2, 3 or 4. GreenScreen has been used to conduct Chemical Hazard Assessment [17] of printed wiring board manufacturing [18]. GPP is

based on GreenScreen and is a multi-criteria evaluation framework that synthesizes information about chemical hazard, use, exposure potential, and public concern into a set of quantitative indicators. GPP is not transparent enough to be tested. ES is comprehensive but also not fully transparent.

Neither TPI, GreenScreen, GPP nor ES are transparent enough to be tested. However, all of them probably work well practically for their respective application.

In the present research a new methodological framework is developed: the *HSI*. Existing life cycle impact assessment mid-point indicators for human and ecotoxicity are exposed for a lack of comprehensiveness compared to the *HSI* method and others.

A falsifiable hypothesis tested in the present research is:

The present *HSI* method gives different conclusions for aluminum smelting unit process regarding contributing compounds to the overall score than ReCiPe (H) Human toxicity and BEES+ Ecotoxicity.

2. MATERIALS AND METHODS

In this section the *HSI* method is explained.

2.1 Categorization of hazard statement classes

Table I lists the categorization and description of the hazard statement classes inspired by [19].

Table I. Categorization and description of hazard statement classes

Hazard Statement Categorization, A_i	Description
0	Zero hazard
1	Very low hazard
2	Low hazard
3	Moderately low hazard
4	Moderate hazard
5	Considerably low hazard
6	Considerable hazard
7	High hazard
8	Very high hazard
9	Extreme hazard
10	Extremely high hazard

Where

 A_i = Categorization of Hazard Statement i, minimum 0 (zero hazard), 10 (extremely high hazard)

2.2 Classification of Hazard Statements

In Table II a non-exhaustive list of existing Hazard Statements (*HSs*) are each given a score from 0 to 10 according to Table I. Extreme toxicity to aquatic life and fatality to human health are given very high classification compared to explosion hazardousness.

Table II. Scaling of Hazard Statements

Hazard Statements	Description	Score (0 to 10) assumed in this research
	PHYSICAL	
H200	Unstable explosive	4
H201	Explosive; mass explosion hazard	5
H202	Explosive; severe projection hazard	7
H203	Explosive; fire, blast or projection hazard	5
H204	Fire or projection hazard	4
H205	May mass explode in fire	3

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H206	Fire, blast or projection hazard: increased risk of explosion if desensitizing agent is reduced	5
H207	Fire or projection hazard: increased risk of explosion if desensitizing agent is reduced	4
H208	Fire hazard: increased risk of explosion if desensitizing agent is reduced	4
H220	Extremely flammable gas	7
H221	Flammable gas	3
H222	Extremely flammable aerosol	7
H223	Flammable aerosol	5
H224	Extremely flammable liquid and vapor	7
H225	Highly flammable liquid and vapor	3
H226	Flammable liquid and vapor	3
H227	Combustible liquid	3
H228	Flammable solid	3
H229	Pressurized container: may burst if heated	4
H230	May react explosively even in the absence of air	5
	May react explosively even in the absence of air at	3
H231	elevated pressure and/or temperature	4
H232	May ignite spontaneously if exposed to air	5
H240	Heating may cause an explosion	6
H241	Heating may cause a fire or explosion	6
H242	Heating may cause a fire	6
H250	Catches fire spontaneously if exposed to air	7
H251	Self-heating; may catch fire	4
H252	Self-heating in large quantities; may catch fire	4
H232	In contact with water releases flammable gases which	4
H260	may ignite spontaneously	4
H261	In contact with water releases flammable gas	4
H270	May cause or intensify fire; oxidizer	3
H271	May cause fire or explosion; strong oxidizer	3
H272	May intensify fire; oxidizer	
H272 H280	Contains gas under pressure; may explode if heated	3 3
H280	Contains gas under pressure; may explode it heated Contains refrigerated gas; may cause cryogenic burns or	3
H281		2
H290	injury May be corrosive to metals	3
H290		3
H300	HEALTH Fatal if swallowed.	10
H301	Toxic if swallowed	8
	Harmful if swallowed	
H302		<u>6</u> 3
H303	May be harmful if swallowed	
H304	May be fatal if swallowed and enters airways	6
H305	May be harmful if swallowed and enters airways	4
H310	Fatal in contact with skin	10
H311	Toxic in contact with skin	8
H312	Harmful in contact with skin	5
H313	May be harmful in contact with skin	3
H314	Causes severe skin burns and eye damage	8
H315	Causes skin irritation	4
H316	Causes mild skin irritation	3
H317	May cause an allergic skin reaction	4

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H318	Causes serious eye damage	8		
H319	Causes serious eye irritation	5		
H320	Causes eye irritation	4		
H330	Fatal if inhaled	10		
H331	Toxic if inhaled	8		
H332	Harmful if inhaled	5		
H333	May be harmful if inhaled	4		
H334	May cause allergy or asthma symptoms or breathing	2		
11225	difficulties if inhaled	3		
H335	May cause respiratory irritation	4		
H336	May cause drowsiness or dizziness	3		
H340	May cause genetic defects	9		
H341	Suspected of causing genetic defects	9		
H350	May cause cancer	10		
H351	Suspected of causing cancer	10		
H360	May damage fertility or the unborn child	10		
H361	Suspected of damaging fertility or the unborn child	10		
H361d	Suspected of damaging the unborn child	10		
H361e	May damage the unborn child	9		
H361f	Suspected of damaging fertility	9		
H361g	may damage fertility	9		
H362	May cause harm to breast-fed children	7		
H370	Causes damage to organs	10		
H371	May cause damage to organs	8		
H372	Causes damage to organs through prolonged or repeated exposure	9		
	May cause damage to organs through prolonged or			
H373	repeated exposure	7		
H300+H310	Fatal if swallowed or in contact with skin	10		
H300+H330	Fatal if swallowed or if inhaled	10		
H310+H330	Fatal in contact with skin or if inhaled	10		
H300+H310+H330	Fatal if swallowed, in contact with skin or if inhaled	10		
H301+H311	Toxic if swallowed or in contact with skin	9		
H301+H331	Toxic if swallowed or if inhaled	9		
H311+H331	Toxic in contact with skin or if inhaled	9		
H301+H311+H331	Toxic if swallowed, in contact with skin or if inhaled	8		
H302+H312	Harmful if swallowed or in contact with skin	6		
H302+H332	Harmful if swallowed or if inhaled	6		
H312+H332	Harmful in contact with skin or if inhaled	6		
H302+H312+H332	Harmful if swallowed, in contact with skin or if inhaled	7		
11302 11312 11332	Training it swanowed, in contact with skin of it inhaled	8		
H303+H313		O		
*******	May be harmful if swallowed or in contact with skin			
H303+H333	May be harmful if swallowed or if inhaled	4		
H313+H333	May be harmful in contact with skin or if inhaled	4		
H303+H313+H333	May be harmful if swallowed, in contact with skin or if inhaled	4		
H315+H320	Causes skin and eye irritation	5		
ENVIRONMENTAL				
H400	Very toxic to aquatic life	9		
H401	Toxic to aquatic life	7		
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H402	Harmful to aquatic life	6
H410	Very toxic to aquatic life with long-lasting effects	10
H411	Toxic to aquatic life with long-lasting effects	9
H412	Harmful to aquatic life with long-lasting effects	7
H413	May cause long-lasting harmful effects to aquatic life	4
H420	Harms public health and the environment by destroying	
H420	ozone in the upper atmosphere	4
H433	Harmful to terrestrial vertebrates	4

Combination of HSs are calculated using (1):

$$A_{HS_i} = ln(\sum_{i}^{n} e^{A_i} - n + 1)$$
 (1)
IF($A_{HS_i} > 10$, THEN $A_{HS_i} = 10$)

where

 A_{HS_i} = Classification of Hazard Statement *i* consisting of one or more *HSs*.

If a combination of HS_i leads to a score of more than 10 it still gets 10 according to (2).

2.3 Constituents of the Hazard Statement Indicator method

A specific HSI score, HSI_C , per mg material (compound) is calculated by using (3)-(6).

$$HS_{n,C} = \ln(e^{A_{HS_1}} + e^{A_{HS_2}} + e^{A_{HS_3}} + \cdots + e^{A_{HS_n}})$$
 (3)

$$HS_{n,C,max} = ln\left(\sum_{i=1}^{1} e^{10}\right) = 10$$
 (4)

$$SF = \frac{\left(e^{HS}n.C.max - 1\right)}{100} = \frac{\left(e^{10} - 1\right)}{100} = 220.25$$
 (5)

$$HSI_{C} = \frac{\left(e^{HS_{n,C-1}}\right)}{SF} \tag{6}$$

where

 $HS_{n,C}$ = Non normalized HS for compound C

 $HS_{n,C,max=}$ Non normalized maximum HS for compound C

SF = Scaling Factor for normalization and projection on the exponential scale HSI_C = HSI for compound C, HSI/mg

3. RESULTS

In this section the HSI method is applied to several compounds and two life cycle inventories (LCI).

 HSI_{c} are calculated for CdS, Pb(CN)₂, LiOH and SO₂ and some other compounds and unit processes. The HSs used are obtained from [20].

3.1 Example HSI for metallic Cadmium Sulfide (CdS)

Table III shows the classified HSs for cadmium sulfide.

Table III. Classification of Hazard Statements for Cadmium Sulfide, CAS No. 1306-23-6

HSs for CdS	Ai
H302	6
H341	8
H350	10
H361fd	10
H372	9
H413	4

$$HS_{n,cds} = ln (e^6 + e^8 + e^{10} + e^{10} + e^9 + e^4) = 10.87$$

$$HSI_{CdS} = \frac{\left(e^{HS_{n,CdS}}-1\right)}{SF} = 239.67 \text{ HSI/mg}$$

3.2 Example HSI for Pb(CN)₂

Table IV shows the classified Hazard Statements for lead dicyanide.

Table IV. Classification of Hazard Statements for Pb(CN)₂, CAS No. 592-05-2

HSs for Pb(CN) ₂	Ai
H341	9
H350	10
H360	10
H372	9

$$HS_{n,Pb(CN)2} = ln (e^9 + e^{10} + e^{10} + e^9) = 10.9$$

$$HSI_{Pb(CN)2} = \frac{\left(e^{HS_{n,Pb(CN)2}}-1\right)}{SF} = 247.94 \text{ HSI/mg}$$

3.3 Thallium (I) carbonate

Table V shows the classified Hazard Statements for thallium (I) carbonate.

Table V. Classification of Hazard Statements for thallium (I) carbonate, CAS No. 6533-73-9

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HSs for	
Thallium(I)carbonate	Ai
H300	10
H330	10
H373	7
H411	9

$$HS_{n,Tl2CO3} = ln (e^{10} + e^{10} + e^7 + e^9) = 10.8$$

$$HSI_{Tl2CO3} = \frac{\left(e^{HS_{n,Tl2CO3}} - 1\right)}{sF} = 229.7 \text{ HSI/mg}$$

Occasionally H300 and H330 are not separated for thallium (I) carbonate hazard and safety information and then

HSI_{Tl2C03} will be lower.

3.4 Other examples

In Table VI are shown several other examples of application results of the HSI method.

Table VI. Classification of Hazard Statements for various compounds

	Chemical		HSI/mg
	Abstract		
	Service		
	(CAS)	Globally Harmonized System of Classification and	
Compound	number	Labelling of Chemicals (GHS) Hazard Statements	
Carbon nanotubes	308068-56-6	H30, H373	105.74
N-	1071-83-6		37.5
(phosphonomethyl)gl ycine) "Glyphosate"		H318, H411	
Beryllium oxide	1304-56-9	H301, H315, H317, H319, H330, H335, H350i, H372	239
Amoxicillin	61336-70-7		24.29
trihydrate		H317, H334, H400	
Indium phosphide	22398-80-7	H350,H361f, H372	147.9
	7786-81-4	H302, H315,H317,H332,H334,H341,H350I,	298.94
Nickel sulphate		H360D,H372, H400, H410	
Nickel sulfamate	13770-89-3	H317,H334,H341,H350i,H360D,H372,H400, H410	373.59
	7791-13-1		351.79
Cobalt dichloride		H302, H317,H334,H341,H350,H360,H400,H410	
	10124-43-3	11202 11217 11224 11241 11250: 112505 11400 11410	351.79
Cobalt sulphate		H302,H317,H334,H341,H350i,H360F,H400,H410	0.450
Carbon dioxide	124-38-9	H280 ; H281	0.178
Trioctylamine	1116-76-3	H315, H319, H335, H360, H372, H400, H410, H411	311.55
Ammonia gas	7664-41-7	H221, H314, H331, H400	63.946
1-Decanol	112-30-1	H335	0.243
Hydrogen sulfide	7704-34-9	H220, H330, H400	141.772
Molybdenum disulfide	1317-33-5	H350	100.002
Sodium Sulfate	7757-82-6	H315, H318	13.778
Hydrogen	1333-74-0	H220	4.974
Nitrogen	7727-37-9	H280, H281	0.178

3.5 Aluminium smelting life cycle inventory – several compounds released and combined to one HSI score In this section The *HSI* method is applied to a life cycle inventory of aluminium smelting from Table 3 "Detailed inventories of the processes considered in aluminum production (inputs and outputs)." in [21]. The functional unit (f.u.) is 1 kg of aluminum smelt. The choice of released compounds (Table VII) from the inventory for aluminum smelting is done based on presumed physical, health and environmental hazards. The inventory is more diverse than shown in Tables VII-IX.

Table VII. HSI calculation for life cycle inventory of aluminium smelting

Table VII. HSI calculation for the	T Tributa	l	I	
Released compounds to air	HSI/mg	Amount (kg)/functional unit (f.u.) [21]	HSI/f.u.	% of Total HSI score
Carbon monoxide	143.25	0.06	8.59×10^6	94.92%
Carbonyl sulfide	20.61	1.12×10 ⁻³	2.31×10 ⁴	0.25%
Ethane, hexafluoro-, HFC-116	0.08	2.28×10 ⁻⁵	1.80	0%
Hydrocarbons, chlorinated (HCCl ₃ used)	240.26	1.2×10 ⁻⁴	2.88×10 ⁴	0.32%
Hydrogen cyanide	228.95	3.7×10 ⁻⁵	8.47×10^3	0.09%
Hydrogen fluoride	313.55	6.2×10 ⁻⁴	1.94×10 ⁵	2.15%
Nitrogen oxides (nitric oxide (NO) used)	146.52	1.1×10 ⁻⁴	1.61×10^4	0.18%
NMVOC, non-methane volatile organic compounds, unspecified origin (Toluene used)	108	9.1×10 ⁻⁴	9.83×10 ⁴	1.09%
PAH, polycyclic aromatic hydrocarbons (Benzo[a]pyrene used]	348.19	1.15×10 ⁻⁴	4.00×10 ⁴	0.44%
Particulates, unspecified (Carbon Nanotubes used)	105.74	4.75×10 ⁻⁴	5.02×10 ⁴	0.55%
Released compounds to water				
Ammonium, ion (Ammonium hydroxide used)	37.5	5.7×10 ⁻⁷	2.14×10^{1}	0%
Iron	0.41	2.2×10 ⁻⁶	9.00×10 ⁻¹	0%
Lead (Pb(CN) ₂ used)	247.94	4.6×10 ⁻⁹	1.14	0%
Mercury	347.95	4×10 ⁻¹⁰	1.39×10 ⁻¹	0%
Nitrogen	0.16	4.9×10 ⁻⁷	7.75×10 ⁻²	0%
Oils, unspecified (1-Octene is used)	150.1	9.9×10 ⁻⁹	1.49	0%
Phenol	83.84	1.8×10 ⁻⁷	1.51×10 ¹	0%
Sodium	13.86	6.2×10 ⁻⁶	8.6×10 ¹	0%
TOTAL score			9.05×10^6	

In Table VIII the aluminum smelting inventory is assessed with the ReCiPe Midpoint (H) Human toxicity [22] with the purpose of comparing the relative score to the *HSI* score.

Table VIII. ReCiPe Midpoint (H) Human toxicity calculation for life cycle inventory of aluminium smelting

Released compounds to air [21]	kg 1,4- Dibromobenzene (DB) equivalents/kg (ReCiPe Midpoint (H) Human toxicity)	Amount (kg)/f.u.	kg 1,4- DB/f.u.	% of Total 1,4-DB score
Carbon monoxide	Not included (N.i.)	0.06	0	0.00%
Carbonyl sulfide	N.i.	1.12×10 ⁻³	0	0%
Ethane, hexafluoro-, HFC-116	N.i.	2.28×10 ⁻⁵	0	0%
Hydrocarbons, chlorinated	52.5	1.2×10 ⁻⁴	6.30×10 ⁻³	3.55%
Hydrogen cyanide	105	3.7×10 ⁻⁵	3.89×10 ⁻³	2.19%
Hydrogen fluoride	266	6.2×10 ⁻⁴	0.165	93.00%
Nitrogen oxides	N.i.	1.1×10 ⁻⁴	0	0%
NMVOC, non-methane volatile	N.i.	9.1×10 ⁻⁴	0	0%

organic compounds, unspecified origin				
PAH, polycyclic aromatic hydrocarbons (Benzo[a]pyrene				
used]	19.3	1.15×10 ⁻⁴	2.22×10 ⁻³	1.25%
Particulates, unspecified	N.i.	4.75×10 ⁻⁴	0	0%
Released compounds to water			0	0%
Ammonium, ion	N.i.	5.7×10 ⁻⁷	0	0%
Iron	N.i.	2.2×10 ⁻⁶	0	0%
Lead	220	4.6×10 ⁻⁹	1.01×10 ⁻⁶	0%
Mercury	25100	4×10 ⁻¹⁰	1.00×10 ⁻⁵	0.01%
Nitrogen	N.i.	4.9×10 ⁻⁷	0	0%
Oils, unspecified (1-Octene is used)	N.i.	9.9×10 ⁻⁹	0	0%
Phenol	0.0113	1.8×10 ⁻⁷	2.03×10 ⁻⁹	0%
Sodium	N.i.	6.2×10 ⁻⁶	0	0%
TOTAL score			0.177	

In Table IX the aluminum smelting inventory is assessed with the BEES+ Ecotoxicity [23] with the purpose of comparing the relative score to the *HSI* score.

Table IX. BEES+ ecotoxicity calculation for life cycle inventory of aluminium smelting

				% of Total
Released compounds to air	kg 2,4-Dichlorophenoxyacetic acid (2,4-D) equivalents/kg (BEES+ Ecotoxicity)	Amount (kg)/f.u.	Kg 2,4- D/f.u.	2,4-D score
compounds to an	equivalents/kg (BEES+ Ecotoxicity)	(Kg)/1.u.	1.23×10 ⁻	SCOLE
Carbon monoxide	0.0205	0.06	3	94.45%
		2	3.45×10	
Carbonyl sulfide	0.0308	1.12×10 ⁻³	3	2.65%
Ethane, hexafluoro-		_		
, HFC-116	Not included (N.i.)	2.28×10 ⁻⁵	0	0%
Hydrocarbons,			7.39×10	
chlorinated	0.0616	1.2×10 ⁻⁴	6	0.57%
			3.42×10 ⁻	
Hydrogen cyanide	0.0924	3.7×10 ⁻⁵	6	0.26%
			1.91×10	
Hydrogen fluoride	0.0308	6.2×10 ⁻⁴	5	1.47%
			2.26×10	
Nitrogen oxides	0.0205	1.1×10 ⁻⁴	6	0.17%
NMVOC, non-				
methane volatile				
organic				
compounds,		,		
unspecified origin	N.i.	9.1×10 ⁻⁴	0	0%
PAH, polycyclic				
aromatic			5.50×10	
hydrocarbons	0.0478	1.15×10 ⁻⁴	6	0.42%
Particulates,				
unspecified	N.i.	4.75×10 ⁻⁴	0	0%

Released compounds to water				
Ammonium, ion	N.i.	5.7×10 ⁻⁷	0	0%
Iron	N.i.	2.2×10 ⁻⁶	0	0%
Lead	0.0635	4.6×10 ⁻⁹	2.92×10 ⁻	0%
Mercury	58.8	4×10 ⁻¹⁰	2.35×10 ⁻	0%
Nitrogen	N.i.	4.9×10 ⁻⁷	0	0%
Oils, unspecified	N.i.	9.9×10 ⁻⁹	0	0%
Phenol	0.467	1.8×10 ⁻⁷	8.41×10 ⁻	0.01%
Sodium	N.i.	6.2×10 ⁻⁶	0	0%
TOTAL score			1.3×10 ⁻³	

Table VIII shows that one of the most well-known life cycle impact assessment methods to emerge in the last decades, ReCiPe [22], has failed to include carbon monoxide which dominates the *HSI* score. BEES+ [23] on the other hand does indeed correctly characterize carbon monoxide as an ecotoxin and it dominates the total 2,4-D score for aluminium smelting.

To further explore the applicability of the proposed *HSI* it is applied to an LCI of tungsten carbide production [24]. Here the third to sixth most contributing flow to the total released mass flow, trioctylamine, contributes the most to the *HSI* score in all three cases (Table X). This is different from e.g. hydrogen fluoride in Table VII.

Table X. HSI calculation for life cycle inventory data for the typical non-Chinese production of tungsten carbide with cobalt (WC-Co) – from Table 4 in [24]

Released compounds	Baseline case - kg	Low environmental impact case - kg	High environmental impact case - kg
Carbon dioxide	0.411	0.2284	0.599
Trioctylamine	0.11	0.1	0.55
Ammonia gas	0.196	0.0138	0.39
1-Decanol	0.11	0.1	0.12
Hydrogen sulfide	0.0035	0	0.0081
Molybdenum disulfide	0.02	0	0.046
Sodium Sulfate	0.84	0.23	1.9
Hydrogen	0.0027	0.00031	0.0054
Nitrogen	0.13	0.073	0.21

Fig. 1 shows that trioctylamine contributes to 56, 88 and 75% of the total *HSI* score for the baseline, low environmental impact and high environmental impact, respectively.

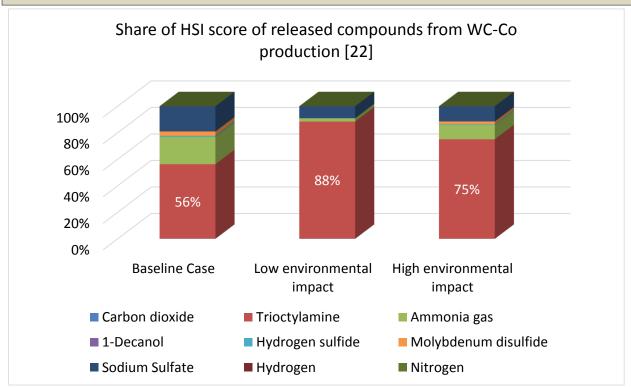


Figure 1: Share of HSI score of released compounds from WC-Co production.

4. DISCUSSION

Apparently *HSI* can be used as either a product tool identifying material risks, or as a company hazardous material risk indicator tool.

HSI can be used in a factory within the ISO14001 system to monitor the most critical compounds from a hazardousness perspective. The advantage is that all compounds that have been classified with HSs can be given a HSI score and updated regularly. This is more straightforward than the mid-point LCIA methodologies used in LCA. Those have still a little bit more focus on hazardousness differences between emissions to air and water.

A potential problem with the usability of the HSI method is that the mass of the different materials to be evaluated for a product or a process might range from a few billions parts of a gram (nanogram) to several dozens of grams. This dilemma was found in a method development project aiming to classify raw materials regarding their criticality [25]. The HSI score "ratio" in Table VII between the highest and lowest is 348.19 (hydrogen fluoride)/0.08(HFC-116) = 4350 and the maximum mass "ratio" is 0.06 (carbon monoxide)/ 4.60×10^{-10} (mercury) = 1.3×10^{8} . With such ratios it might be argued that the HSI method will always point out the material in greater quantity as the most hazardous. However, the opposite is shown in Table X in which trioctyleamine is mostly contributing to the overall HSI score for the LCI at hand despite not being the biggest mass flow.

In general, environmental science in companies should strive for operationability and data availability. Several approaches such as the present *HSI*, Circularity Scoring [26] and Eco Rating [27] are similar "KPI"-methods as LCA [27] as the LCA result is actually a parametrized short cut of relative results. The present *HSI* score may be used along Circularity Scoring Indicators in the Eco Rating for smartphones and other products.

5. CONCLUSION

The cost-effective, transparent, and systematic *HSI* method can act as an enhancer of traditional midpoint life cycle impact assessment indicators for human toxicity and ecotoxicity.

The present *HSI* method gives different conclusions for aluminum smelting unit process - regarding contributing compounds to the overall score - than ReCiPe (H) Human toxicity, but not for BEES+ Ecotoxicity.

6. NEXT STEPS

It would be worthwhile to analyze which questions about hazardousness cannot be answered by the present *HSI* method. Naturally the Analytical Hierarchy Process and fuzzy theories might be applied to quantification of value judgements.

"Cocktail" effects - which may occur when chemicals act in combination in mixtures - are also not addressed. Usually mid-point LCIA methods present different toxicity potentials for emissions to air and water. For example, mercury emissions to air have a much larger relative score when emitted to air than water. The *HSI* methodology does not yet have a way of separating emissions to air, water and soil.

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