Postprint of: Tobiszewski M., Bystrzanowska M.: Monetary values estimates of solvents emissions, GREEN CHEMISTRY (2020), pp.1-16, DOI: 10.1039/D0GC03210G

Monetary values estimates of solvents emissions

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Abstract:

The impact values for environmental emissions of 52 solvents are estimated and expressed in monetary units. The impact values of solvents present in the air are calculated on the basis of 13 impact indicators and for solvents present in water on additional 2 impact indicators. These impact values are weighted with the results obtained with multi-compartment distribution model, allowing to calculate the fraction of solvent emitted to the environment present in each of the compartments. The results show that the impact values of solvents emissions are in range 0.7 – 1179.51 \$ L^{-1}, with mean value 20.69 \$ L^{-1}, expressed in USD_{2019}. These impacts are considerably lower for short chain aliphatic hydrocarbons, alcohols, ethers, aldehydes, ketones and esters. High impact values are obtained for long chain aliphatic hydrocarbons, aromatic hydrocarbons, terpenes and extremely high value for carbon tetrachloride. Monetary values calculated to assess the solvents emissions impact have the advantage that they are quantitative, and easily applicable.

Keywords: solvents; monetary accounting; monetary valuation; green chemistry; greenness assessment

1. Introduction

Solvents are applied in many industries as cleaning or degreasing agents, media for chemical reactions, are applied in separation technology, for dilution or as carriers of other substances.[1] Organic solvents have many undesired environmental properties, high oral, inhalation or aquatic toxicity, potential to form tropospheric ozone or secondary atmospheric particles and some of them due to volatility are easily emitted to the environment.[2,3] Therefore, one of the trends in green chemistry is application of greener solvents, minimization of amounts of organic solvents used or application of solventless processes.[4] Also more detailed solvents environmental impact assessment methods are needed.

The assessment of the solvent greenness should take into consideration multiple criteria of different dimensions, units and importance. To make the assessment easily interpretable, it is good to bring all hazards impacts to single dimension and single unit. It has been done before, by the application of carbon footprint, which brings many impact categories into equivalent of CO_2 kilogram emission.[5] However, impact categories such as human or ecosystem toxicity, resources depletion or land use are poorly expressed as CO_2 equivalents. Another good candidate may be monetary value as the value of one dollar is single estimation of multiple hazards and human, biological or physical impacts can be translated to money and as a result can be directly compared.[6] The drawback of monetary valuation approach is that some aspects, such as the value of human life or biodiversity, are not easily directly measurable with monetary units. Another drawback is that the results are usually accompanied with rather large uncertainties.[7] Monetary

units were used to assess ammonium and imidazolium ionic liquids, acetone and glycerol in terms of direct production costs and ecosystem quality, resources damage and human health impact during their production.[8] These indirect costs can contribute to more than 50% of total solvent production cost. Economic sustainability was assessed for olive leaf waste valorization by different processes with and without solvent recovery.[9]

The aim of the study is to calculate the total impacts of solvents emitted to the environment, expressed as monetary values. It should be clearly stated that other aspects of solvents impacts, such as manufacturing or operational safety are not included. Distribution of solvents in the evaluative environment is considered as a good estimation of their environmental fate. The aim of the study is to assess the monetary values of emissions as a tool applied to solvents greenness assessment in the environmental emissions impacts. Monetary values estimates are based on solvent global warming potential, ozone depletion potential, potential to form secondary particles, oxygen demands to biodegrade and acute oral toxicity towards rats.

2. Materials and Methods

2.1. Data collection

The input data to monetary accounting model are global warming potentials (GWP), photochemical ozone creation potentials (POCP), secondary organic aerosol (SOA) formation potentials. The most accurate estimates are taken from publications – GWP[10] (following "Monetary valuation of environmental impacts: models and data" handbook), POCP[11,12,13,14] and SOA formation potentials.[15,16,17] The values for these parameters may differ for respective sources, depending on geographical region, assumptions on meteorological factors, insolation and others. In such cases values representative for larger areas or calculated for more general environmental assumptions are taken. In case of some missing points for POCP and SOA

formation potentials are substituted with mean values for given class of chemicals. Such approach is applied in assessment of chemicals.[18] If all two or three of these parameters are missing, to avoid excessive substitution of missing points, such solvents are excluded from the analysis (but the examples breaking this rule are shown later).

The data for level I mass balance model is rather easily available and is taken mainly from material safety data sheets. The data extracted here is molar mass, water solubility, vapour pressure, $\log K_{OW}$ and melting point.

2.2. Monetary accounting

The calculations of monetary values related to VOCs emissions and assumed uncertainty factors are made exactly after Steen [[19]]. However, in many cases different values of GWP, POCP and SOA are introduced to the model. Generally, the model incorporates the potential of solvent to cause cancer, form secondary particles, tropospheric ozone and contribute to global warming and water oxygen loss due to biodegradation. The details are presented in Supplementary Information.

2.3. Level I mass balance model

Level I mass balance model is the simplest from the family of multi-compartment models for prediction of environmental fates of chemicals.[20] It is applied to calculate the distribution of organic chemical between atmospheric air, water, soil and sediment. It is done on the basis of chemical physicochemical properties and within defined volumes of environmental compartments. In this case the assumed volumes of compartments are 10^{14} m^3 for the atmospheric air, 2×10^{11} m^3 for water, 9×10^9 m^3 for soil and 10^8 m^3 for sediments as presented in the figure 1. It is simplified regional 100,000 km^2 environment applied before,[21] simplification

is by neglecting fish and aerosols phases. Such evaluative environment is not real but realistic in terms of physicochemical properties of compartments and is representative for the habitat of the majority of human population. It is also representative as solvents are compounds with rather short environmental lifetimes have rather local impact, so this environment seems to be better estimation than global model.

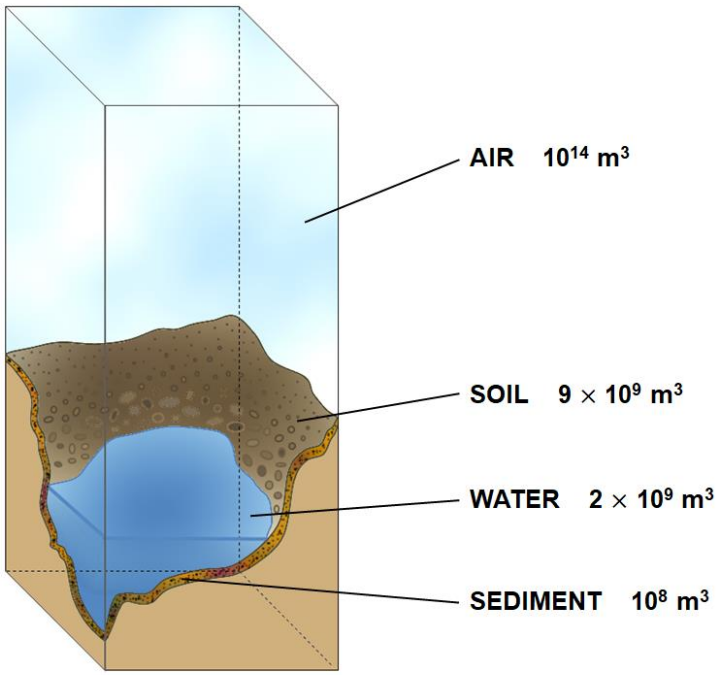

Figure 1. The evaluative environment used in this study.

In Level I model it is not important to which environmental compartment the compound is emitted, it will be distributed in the compartments according to its partitioning coefficients. This allows to neglect the type of emission of solvent. The amount of compound emitted is also not important, only percentage distribution is further needed as the output from this model. The software is downloadable from https://tuspace.ca/~dmackay/models.html

The Excel sheet with all calculations is attached as Supplementary Information. It can be applied to assess other solvents if new endpoints will be available in literature. It can be also used in case of appearance of better, updated, more specific or more general (depending on the needs) data.

112 It can be applied with data originating from other evaluative environment, applied in multimedia
113 modelling.
114
115 **3. Results and Discussion**
116 3.1. The results of monetary accounting
117 The results of impact values for different solvents, according to methods presented in
118 Supplementary Information are presented in the table 1. IV_{AIR} are in
119 the range of 0.6-1181.78 \$ L^{-1} with mean equal to 42.19 \$ L^{-1}. The solvents with higher IV_{AIR} are
120 aromatic hydrocarbons, long chain aliphatic hydrocarbons, terpenes and some of chlorinated
121 solvents. This is mainly due to SOA formation potentials of some solvents (terpenes and aromatic
122 hydrocarbons). The sums of impact values of YLL and YLD via secondary particles are in ranges
123 20.18 – 52.75 \$ L^{-1} for aromatic hydrocarbons and 72.59 – 77.70 \$ L^{-1} for terpenes and contribute
124 to >89% of total impact values of solvents emitted to air. The solvent with extreme IV_{air} is carbon
125 tetrachloride, because of its high GWP, equal to 2019. As a result impact values of YLL,
126 undernutrition, working capacity and crop loss via climate change are 650, 35.7, 439 and
127 13.3 \$ L^{-1}, respectively. The solvents with low IV_{air} are C_5-C_7 aliphatic hydrocarbons
128 (1.32 – 1.95 \$ L^{-1}), ethers (1.2 – 1.32 \$ L^{-1}), aldehydes (1.46 – 1.88 \$ L^{-1}), ketones
129 (0.9 – 2.03 \$ L^{-1}) and organic acids (0.60 – 1.17 \$ L^{-1}). They have low or moderate GWP and
130 POCP values and they have SOA formation potentials equal to 0.
131 IV_{WAT} for solvents are in range 0.03 – 333.80 \$ L^{-1}, with mean value 23.18 \$ L^{-1}, so they are
132 considerably lower in comparison to IV_{AIR} values. IV_{BOD} seems to be negligible in comparison to
133 IV_{WAT}, as the contribute to <1 % of IV_{WAT}. As IV_{DRINK} are dependent on LD_{50} towards rats and
134 biodegradability half-lifes, solvents such as benzene, methanol, butanol, o-cresol, formic acid or
135 chlorinated solvents are characterized by high IV_{DRINK} values.

136
137 Table 1. The impact values for solvents emitted to atmospheric air and to water.

Group	Compound	Impact value for solvents emission to air [$ L^{-1}]*	Impact value for solvents emission to water [$ L^{-1}]*
hydrocarbons	pentane	1.32	2.20
	hexane	1.38	0.03
	cyclohexane	3.02	16.29
	heptane	1.95	5.12
	octane	9.60	12.02
	nonane	21.73	12.02
	decane	31.82	12.02
	undecane	43.83	12.02
	dodecane	57.54	3.01
	benzene	56.34	7.79
	toluene	50.98	2.20
	o-xylene	51.85	3.62
	m-xylene	50.38	17.59
	p-xylene	23.25	6.04
alcohols	methanol	13.16	0.91
	ethanol	10.17	0.04
	propanol	9.56	3.21
	isopropanol	8.91	0.73
	butanol	9.20	8.68
	isobutanol	8.64	7.27
	sec-butyl alcohol	9.03	7.50
	tert-butyl alcohol	8.17	7.03
	o-cresol	25.04	2.35
ethers	diethyl ether	1.32	1.19
	tert-butyl methyl ether	1.20	1.79
aldehydes	ethanal	1.46	3.31
	propanal	1.83	12.82
	butanal	1.88	5.18
ketones	acetone	0.95	1.91
	2-butanone	1.44	11.06
	2-pentanone	1.69	6.65
	3-pentanone	0.90	8.08
	methyl isobutyl ketone	1.72	11.93
	2-hexanone	1.79	5.12
	cyclohexanone	2.03	7.83
terpenes	(R)-(+)-limonene	78.36	5.63
	p-cymene	80.21	10.67

	α-pinene	82.05	18.67
	β-pinene	76.22	16.13
organic acids	formic acid	0.60	1.11
	acetic acid	0.86	1.87
	propionic acid	1.17	1.02
esters	ethyl acetate	14.37	3.28
	methyl formate	15.29	2.56
	methyl acetate	12.41	1.72
	methyl lactate	7.55	3.01
chlorinated	dichloromethane	5.80	12.17
	chloroform	11.32	36.40
	carbon tetrachloride	1181.78	333.80
	trichloroethene	3.94	133.44
	tetrachloroethene	3.15	234.21
	1,1,1-trichloroethane	94.54	162.96

* in USD_{2019}

3.2.Combination of monetary accounting with multimedia model

The second step is combination of IV_{AIR} and IV_{WAT} to calculate total impact value. The information from Level I mass balance model is very useful to evaluate the risk related to the presence in each environmental compartment. The fractions of solvent present in air and water are used to calculate total impact values (IV_{TOTAL}) and it is done according to:

$$IV_{TOTAL} = IV_{AIR} * A_{AIR} + IV_{WAT} * A_{WAT}$$

Where A_{AIR} and A_{WAT} are amounts of solvent, expressed in % of total amount, present in air and water in evaluative environment under equilibrium. A_{SOIL} and A_{SED}, being amounts of solvent in soil and sediment, are neglected. Except of some high molecular weight solvents, they do not tend to be present in soil nor sediment and the potential impacts are also not well studied and probably negligible. The results of partitioning of solvents in the environment are presented in table 2.

156 Table 2. The distribution of solvents emitted to evaluative environment and total impact value

Group	Compound	A_{AIR} [%]	A_{WAT} [%]	A_{SOIL} [%]	A_{SED} [%]	IV_{TOTAL} [\$ L^{-1}]*	Purchase cost [\$ L^{-1}]*+
hydrocarbons	pentane	99.993	0.002	0.005	0	1.32	79.70
	hexane	99.97	0	0.03	0	1.38	105.00
	cyclohexane	99.89	0.03	0.08	0	3.02	105.00
	heptane	99.95	0	0.05	0	1.95	102.00
	octane	99.73	0	0.26	0.01	9.58	301.00
	nonane	99.61	0	0.38	0.01	21.65	641.00
	decane	74.11	0.03	25.3	0.56	23.58	117.00
	undecane	73.64	0	25.78	0.58	32.28	342.00
	dodecane	40.44	0	58.26	1.3	23.27	309.00
	benzene	98.67	0.846	0.473	0.011	55.66	96.30
	toluene	98.99	0.74	0.26	0.01	50.48	65.50
	o-xylene	96.99	1.37	1.6	0.04	50.34	110.00
	m-xylene	97.72	0.94	1.31	0.03	49.39	142.00
	p-xylene	97.97	0.91	1.1	0.02	22.83	108.00
alcohols	methanol	9.83	90.15	0.02	0	2.12	67.10
	ethanol	6.59	93.37	0.04	0	0.70	128.00
	propanol	10.73	89.13	0.14	0	3.89	99.00
	isopropanol	14.62	85.29	0.09	0	1.92	73.00
	butanol	15.25	84.17	0.57	0.01	8.71	87.10
	isobutanol	46.97	52.97	0.06	0	7.91	95.20
	sec-butyl alcohol	14.06	85.61	0.32	0.01	7.69	62.30
	tert-butyl alcohol	27.36	72.49	0.14	0.01	7.33	113.00
	o-cresol	4.37	88.02	7.44	0.17	3.16	79.30
ethers	diethyl ether	93.66	6.3	0.04	0	1.32	100.00
	tert-butyl methyl ether	91.99	7.95	0.06	0	1.24	81.80
aldehydes	ethanal	80.53	19.42	0.05	0	1.82	208.00
	propanal	62.18	37.69	0.13	0	5.97	167.00
	butanal	85.14	14.76	0.1	0	2.36	128.00
ketones	acetone	61.54	38.44	0.02	0	1.32	68.20
	2-butanone	42.02	57.88	0.1	0	7.01	77.10
	2-pentanone	43.92	55.7	0.37	0.01	4.45	103.00
	3-pentanone	48.84	50.79	0.36	0.01	4.55	114.00
	methyl isobutyl ketone	73.06	26.37	0.56	0.01	4.40	88.30
	2-hexanone	37.57	61.1	1.3	0.03	3.80	-
	cyclohexanone	11.89	87.6	0.5	0.01	7.10	48.70
terpenes	(R)-(+)-limonene	97.82	0.08	2.05	0.05	76.66	153.60
	p-cymene	95.41	0.44	4.06	0.09	76.58	56.60
	α-pinene	99.31	0.03	0.65	0.01	81.48	290.00

	β-pinene	98.25	0.08	1.63	0.04	74.90	96.70
organic acids	formic acid	0.48	99.49	0.03	0	1.11	131.00
	acetic acid	5.07	94.89	0.04	0	1.82	65.10
	propionic acid	3.72	96.1	0.18	0	1.03	36.10
esters	ethyl acetate	73.51	26.36	0.13	0	11.43	81.30
	methyl formate	90.11	9.89	0	0	14.03	132.00
	methyl acetate	88.6	11.38	0.02	0	11.19	79.70
	methyl lactate	0.53	99.46	0.01	0	3.03	-
chlorinated	dichloromethane	97.51	2.45	0.04	0	5.95	67.10
	chloroform	98.66	1.25	0.09	0	11.62	84.90
	carbon tetrachloride	99.76	0.17	0.07	0	1179.51	451.00
	trichloroethene	99.32	0.56	0.12	0	4.66	113.00
	tetrachloroethene	99.58	0.31	0.11	0	3.87	124.00
	1,1,1-trichloroethane	99.61	0.31	0.08	0	94.68	-

157 * in USD_{2019}
158 + price for one liter container of reagent grade or anhydrous solvent. Taken from Sigma-Aldrich
159 webpage. Accessed 19.05.2020.
160
161 Organic solvents tend to be present in atmospheric air (mean 66.7 %), then in water
162 (mean 30.7 %), in minor amounts in soil (mean 2.6 %) and sediments (mean 0.06 %). There is
163 clear distinction between nonpolar solvents, such as aliphatic and aromatic hydrocarbons, ethers,
164 terpenes and chlorinated solvents that are generally partitioned towards air and polar ones, such
165 as alcohols and organic acids, that are present in water. Aldehydes, ketones and esters partition to
166 both phases in considerable amounts. The application of multimedia distribution model makes the
167 results valid for any emission regarding type of emission source, environmental compartment or
168 the amount of solvent emitted.
169 IV_{TOTAL} are in range 0.7 – 1179.51 \$ L^{-1} (mean 20.69 \$ L^{-1}), following the pattern of IV_{AIR}
170 values, with higher impact of aromatic hydrocarbons, terpenes and some of chlorinated solvents.
171 Solvents with low IV_{TOTAL} are C_5-C_7 aliphatic hydrocarbons, ethanol, isopropanol, ethers,
172 aldehydes, ketones, organic acids and methyl lactate. The purchase costs of these solvents are in
173 range 36.1 – 641 \$ L^{-1} (mean 132.41 \$ L^{-1}), what means that calculated IV_{TOTAL} contribute to
174 0.54 – 261.43 % of purchase cost (mean 20.69 %). The solvents with the highest IV_{TOTAL} to

purchase cost ratio are carbon tetrachloride (261.43 %), p-cymene (135.30 %), β-pinene (77.46 %), toluene (77.07 %), benzene (57.80 %). This is strong implication that estimated monetary values of solvents emissions should be considered during extended economic, feasibility assessments of various processes and products, wherever solvents are applied. It is advised to select as first preferences solvents with IV_{TOTAL} less than 8 \$ L^{-1} and avoid those with higher IV_{TOTAL}. As environmental aspects are taken into consideration not overall greenness, it is recommended to support the assessment with other metrics.

The results are useful in economic – environmental analyses of chemical processes. For example, hexane and ethanol are applied for soybean oil extraction in closed system but the losses of ethanol are 0.0063 and 0.0051 kg kg^{-1} of soybean oil and for ethanol and hexane, respectively.[22] The costs of these emissions (calculated in our study as IV_{TOTAL}) if considered in this economic assessment would be 0.006 and 0.019 \$ kg^{-1} of oil for ethanol and hexane. Another example of solvent emission costs incorporation is the process of methacrylic acid extraction from water.[23] The costs of cyclohexane (1012.37 \$ t^{-1}), toluene (914.16 \$ t^{-1}) and hexane (1000 \$ t^{-1}) would be corrected with IV_{TOTAL} of 2123, 58022 and 3922 \$ t^{-1}, for cyclohexane, toluene and hexane, respectively, multiplied by solvent loss fraction in this process. The third example can be the application of heptane and decane for lipid extraction from microalgae.[24] In this continuous process heptane is lost at rate of 0.921 kmol h^{-1} and decane loss rate is 0.099 kmol h^{-1}. The calculated IV_{TOTAL} of these losses would be 264.3 and 454.1 \$ h^{-1} for heptane and decane, respectively. These simple considerations show that emission costs can be significant.

3.3. Assessment of green solvents

The assessment procedure is applied to assess solvents that are generally considered to be green. They are solvents from solvent selection guide[18] and PolarClean[25], Cyrene,[26] butylpyrrolidone[27],

recently applied green solvents. As for these compounds the values of GWP, ODP and SOA formation potentials are not available the mean values for chemical class these solvent belongs to are substituted. Therefore, the results presented in Table 3 should be treated as the best estimate for present time.

Green solvents are characterized by rather low estimated IV_{TOTAL} monetary values. Two solvents with slightly deviated values are 1-octanol, because it is readily biodegradable in water and Cyrene because mean SOA value for terpenes is substituted.

Table 3. The estimates for IV_{TOTAL} for green solvents

Solvent	IV_{TOTAL} [\$ L^{-1}]	Purchase cost [\$ L^{-1}]
1-pentanol	6.57	70.80
1-hexanol	7.42	50.80
1-heptanol	6.87	62.70
1-octanol	0.11	83.00
t-amyl alcohol	7.08	115.00
isobutyl acetate	6.06	67.80
amyl acetate	5.77	79.00
isoamyl acetate	5.98	103.00
2-ethylhexyl acetate	5.97	62.00
diethyl carbonate	6.90	48.90
methyl oleate	5.16	-
dimethyl succinate	3.94	104.00
glycerol diacetate	6.28	70.00
glycerol triacetate	2.77	191.00
polarclean (5-(dimethylamino)-2-methyl-5-oxopentanoate)	2.56	-
lactic acid	2.69	104.00
furfural	2.51	103.00
Cyrene (dihydrolevoglucosenone)	15.70	191.00
butylpyrrolidinone	1.69	-

3.4. Sensitivity and uncertainty analyses

Sensitivity analysis is performed to investigate how variations in the input data influence the final result. We assume that the values of GWP, ODP, SOA formation potential, oral LD_{50} towards

rats and biodegadation half-lifes can change randomly in the range of ± 50 % of initial value with uniform distribution. The values of IV_{TOTAL} are calculated 25 times with randomly changed input data and the results are resented in form of mean value ± standard deviation in Table S1. The average relative standard deviation is 0.27 what is acceptable in this type on analysis.

The uncertainty analysis is performed with Monte Carlo simulation to investigate how the initial assumptions on calculation respective impact indicators influence the final result. The uncertainty factors are taken from Steen (2019) handbook[17] and normal distribution is assumed. The analysis is repeated 500 times and the calculated mean values with standard deviations are presented in Table S1. The average relative standard deviation is 1.96, which is not unusual uncertainty for monetization studies,[28,29] as many components with high uncertainty factors are considered.

3.5. Metrics limitations

The presented metric despite having merits is characterized by certain limitations:

- The availability of input data is limited. The values of GWP, ODP, SOA generation potentials are not available for many solvents. They may be substituted with values for similar compounds or mean value for the chemical group solvent belongs to. However, this generates additional uncertainty of result.
- Link of acute or chronic solvents toxicity towards fish with monetary impacts is the problem to overcome.
- The model does not consider information on solvents operational safety issues nor environmental problems during production, information if solvents origin from fossil fuels or bio-based, renewable sources. So the applicability as greenness metric tool is limited.

- Uncertainties for the estimated values are large.
- Presence of solvents in soils and sediments is neglected.

4. Conclusions

In this study we present the methodology to estimate the monetary estimates of solvents emissions to the evaluative environment and calculate impact values for 52 solvents. Solvents with lower impact values are alcohols, esters, aldehydes, ketones and organic acids. These with higher impact values are aromatic hydrocarbons, terpenes and carbon tetrachloride. The results can be used during environmental-economic assessment studies of various products, materials or chemical processes. Few examples show that emissions monetary impact values can be large in chemical processes.

As this is one of the first attempts to calculate monetary impact values of solvents emissions the procedure and the results probably could be improved when new data will be available. For example toxicity towards aquatic organisms, DALY related to inhalation exposure through non-cancer diseases and soil and sediment related impacts could make the results more complete.

Conflict of interests

There are no conflict of interests to declare.

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