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4 Monetary values estimates of solvents emissions

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12 Abstract:

13 The impact values for environmental emissions of 52 solvents are estimated and expressed in

14 monetary units. The impact values of solvents present in the air are calculated on the basis of 13

15 impact indicators and for solvents present in water on additional 2 impact indicators. These

16 impact values are weighted with the results obtained with multi-compartment distribution model,

17 allowing to calculate the fraction of solvent emitted to the environment present in each of the

18 compartments. The results show that the impact values of solvents emissions are in range

19 $0.7 - 1179.51$ \$ L^{-1}, with mean value 20.69 \$ L^{-1}, expressed in USD_{2019}. These impacts are

20 considerably lower for short chain aliphatic hydrocarbons, alcohols, ethers, aldehydes, ketones

21 and esters. High impact values are obtained for long chain aliphatic hydrocarbons, aromatic

22 hydrocarbons, terpenes and extremely high value for carbon tetrachloride. Monetary values

23 calculated to assess the solvents emissions impact have the advantage that they are quantitative,

24 and easily applicable.

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29 **1.   Introduction**

30 Solvents are applied in many industries as cleaning or degreasing agents, media for chemical

31 reactions, are applied in separation technology, for dilution or as carriers of other substances.[1]

32 Organic solvents have many undesired environmental properties, high oral, inhalation or aquatic

33 toxicity, potential to form tropospheric ozone or secondary atmospheric particles and some of

34 them due to volatility are easily emitted to the environment.[2,3] Therefore, one of the trends in

35 green chemistry is application of greener solvents, minimization of amounts of organic solvents

36 used or application of solventless processes.[4] Also more detailed solvents environmental impact

37 assessment methods are needed.

38 The assessment of the solvent greenness should take into consideration multiple criteria of

39 different dimensions, units and importance. To make the assessment easily interpretable, it is

40 good to bring all hazards impacts to single dimension and single unit. It has been done before, by

41 the application of carbon footprint, which brings many impact categories into equivalent of CO_2

42 kilogram emission.[5] However, impact categories such as human or ecosystem toxicity, resources

43 depletion or land use are poorly expressed as CO_2 equivalents. Another good candidate may be

44 monetary value as the value of one dollar is single estimation of multiple hazards and human,

45 biological or physical impacts can be translated to money and as a result can be directly

46 compared.[6] The drawback of monetary valuation approach is that some aspects, such as the value

47 of human life or biodiversity, are not easily directly measurable with monetary units. Another

48 drawback is that the results are usually accompanied with rather large uncertainties.[7] Monetary

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49   units were used to assess ammonium and imidazolium ionic liquids, acetone and glycerol in

50   terms of direct production costs and ecosystem quality, resources damage and human health

51   impact during their production.[8] These indirect costs can contribute to more than 50% of total

52   solvent production cost. Economic sustainability was assessed for olive leaf waste valorization by

53   different processes with and without solvent recovery.[9]

54   The aim of the study is to calculate the total impacts of solvents emitted to the environment,

55   expressed as monetary values. It should be clearly stated that other aspects of solvents impacts,

56   such as manufacturing or operational safety are not included. Distribution of solvents in the

57   evaluative environment is considered as a good estimation of their environmental fate. The aim of

58   the study is to assess the monetary values of emissions as a tool applied to solvents greenness

59   assessment in the environmental emissions impacts. Monetary values estimates are based on

60   solvent global warming potential, ozone depletion potential, potential to form secondary

61   particles, oxygen demands to biodegrade and acute oral toxicity towards rats.

62

63   **2.   Materials and Methods**

64   2.1.   Data collection

65   The input data to monetary accounting model are global warming potentials (GWP),

66   photochemical ozone creation potentials (POCP), secondary organic aerosol (SOA) formation

67   potentials. The most accurate estimates are taken from publications – GWP[10] (following

68   "Monetary valuation of environmental impacts: models and data" handbook), POCP[11,12,13,14] and

69   SOA formation potentials.[15,16,17] The values for these parameters may differ for respective

70   sources, depending on geographical region, assumptions on meteorological factors, insolation and

71   others. In such cases values representative for larger areas or calculated for more general

72   environmental assumptions are taken. In case of some missing points for POCP and SOA

73 formation potentials are substituted with mean values for given class of chemicals. Such

74 approach is applied in assessment of chemicals.[18] If all two or three of these parameters are

75 missing, to avoid excessive substitution of missing points, such solvents are excluded from the

76 analysis (but the examples breaking this rule are shown later).

77 The data for level I mass balance model is rather easily available and is taken mainly from

78 material safety data sheets. The data extracted here is molar mass, water solubility, vapour

79 pressure, $\log K_{OW}$ and melting point.

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81   2.2.   Monetary accounting

82 The calculations of monetary values related to VOCs emissions and assumed uncertainty factors

83 are made exactly after Steen [[19]]. However, in many cases different values of GWP, POCP and

84 SOA are introduced to the model. Generally, the model incorporates the potential of solvent to

85 cause cancer, form secondary particles, tropospheric ozone and contribute to global warming and

86 water oxygen loss due to biodegradation. The details are presented in Supplementary

87 Information.

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89   2.3.   Level I mass balance model

90 Level I mass balance model is the simplest from the family of multi-compartment models for

91 prediction of environmental fates of chemicals.[20] It is applied to calculate the distribution of

92 organic chemical between atmospheric air, water, soil and sediment. It is done on the basis of

93 chemical physicochemical properties and within defined volumes of environmental

94 compartments. In this case the assumed volumes of compartments are 10^{14} m^3 for the

95 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

96 in the figure 1. It is simplified regional 100,000 km^2 environment applied before,[21] simplification

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97   is by neglecting fish and aerosols phases. Such evaluative environment is not real but realistic in

98   terms of physicochemical properties of compartments and is representative for the habitat of the

99   majority of human population. It is also representative as solvents are compounds with rather

100   short environmental lifetimes have rather local impact, so this environment seems to be better

101   estimation than global model.
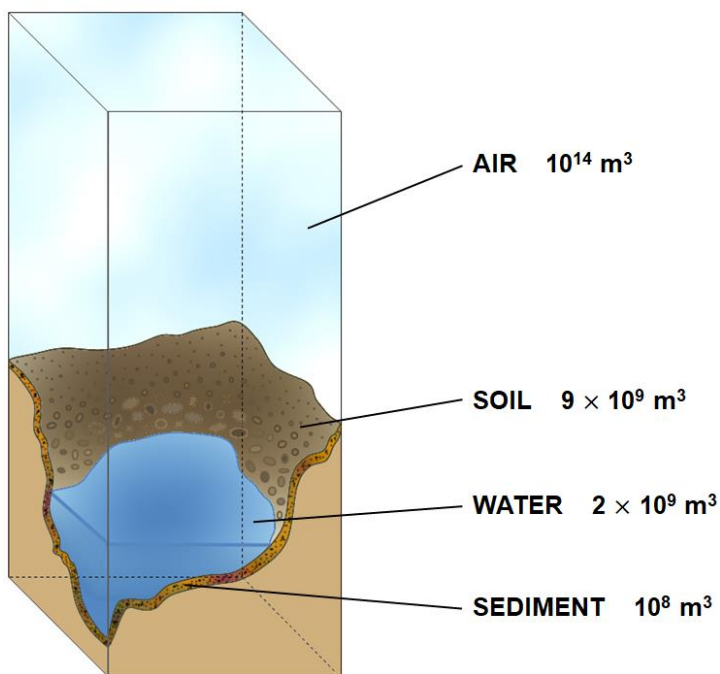
102
103   Figure 1. The evaluative environment used in this study.

104   In Level I model it is not important to which environmental compartment the compound is

105   emitted, it will be distributed in the compartments according to its partitioning coefficients. This

106   allows to neglect the type of emission of solvent. The amount of compound emitted is also not

107   important, only percentage distribution is further needed as the output from this model.

108   The software is downloadable from https://tuspace.ca/~dmackay/models.html

109   The Excel sheet with all calculations is attached as Supplementary Information. It can be applied

110   to assess other solvents if new endpoints will be available in literature. It can be also used in case

111   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-lives, 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

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	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

138 * in USD_{2019}

140 3.2.Combination of monetary accounting with multimedia model

141 The second step is combination of IV_{AIR} and IV_{WAT} to calculate total impact value.

142 The information from Level I mass balance model is very useful to evaluate the risk related to the

143 presence in each environmental compartment. The fractions of solvent present in air and water

144 are used to calculate total impact values (IV_{TOTAL}) and it is done according to:

145 $$IV_{TOTAL} = IV_{AIR} * A_{AIR} + IV_{WAT} * A_{WAT}$$

146 Where A_{AIR} and A_{WAT} are amounts of solvent, expressed in % of total amount, present in air and

147 water in evaluative environment under equilibrium. A_{SOIL} and A_{SED}, being amounts of solvent in

148 soil and sediment, are neglected. Except of some high molecular weight solvents, they do not

149 tend to be present in soil nor sediment and the potential impacts are also not well studied and

150 probably negligible. The results of partitioning of solvents in the environment are presented in

151 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

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	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	-

* in USD$_{2019}$

+ price for one liter container of reagent grade or anhydrous solvent. Taken from Sigma-Aldrich webpage. Accessed 19.05.2020.

Organic solvents tend to be present in atmospheric air (mean 66.7 %), then in water (mean 30.7 %), in minor amounts in soil (mean 2.6 %) and sediments (mean 0.06 %). There is clear distinction between nonpolar solvents, such as aliphatic and aromatic hydrocarbons, ethers, terpenes and chlorinated solvents that are generally partitioned towards air and polar ones, such as alcohols and organic acids, that are present in water. Aldehydes, ketones and esters partition to both phases in considerable amounts. The application of multimedia distribution model makes the results valid for any emission regarding type of emission source, environmental compartment or the amount of solvent emitted.

IV_{TOTAL} are in range 0.7 – 1179.51 $ L^{-1} (mean 20.69 $ L^{-1}), following the pattern of IV_{AIR} values, with higher impact of aromatic hydrocarbons, terpenes and some of chlorinated solvents. Solvents with low IV_{TOTAL} are C_5-C_7 aliphatic hydrocarbons, ethanol, isopropanol, ethers, aldehydes, ketones, organic acids and methyl lactate. The purchase costs of these solvents are in range 36.1 – 641 $ L^{-1} (mean 132.41 $ L^{-1}), what means that calculated IV_{TOTAL} contribute to 0.54 – 261.43 % of purchase cost (mean 20.69 %). The solvents with the highest IV_{TOTAL} to

175 purchase cost ratio are carbon tetrachloride (261.43 %), p-cymene (135.30 %), β-pinene

176 (77.46 %), toluene (77.07 %), benzene (57.80 %). This is strong implication that estimated

177 monetary values of solvents emissions should be considered during extended economic,

178 feasibility assessments of various processes and products, wherever solvents are applied. It is

179 advised to select as first preferences solvents with IV_{TOTAL} less than 8 \$ L^{-1} and avoid those with

180 higher IV_{TOTAL}. As environmental aspects are taken into consideration not overall greenness, it is

181 recommended to support the assessment with other metrics.

182 The results are useful in economic – environmental analyses of chemical processes. For example,

183 hexane and ethanol are applied for soybean oil extraction in closed system but the losses of

184 ethanol are 0.0063 and 0.0051 kg kg^{-1} of soybean oil and for ethanol and hexane, respectively.[22]

185 The costs of these emissions (calculated in our study as IV_{TOTAL}) if considered in this economic

186 assessment would be 0.006 and 0.019 \$ kg^{-1} of oil for ethanol and hexane. Another example of

187 solvent emission costs incorporation is the process of methacrylic acid extraction from water.[23]

188 The costs of cyclohexane (1012.37 \$ t^{-1}), toluene (914.16 \$ t^{-1}) and hexane (1000 \$ t^{-1}) would be

189 corrected with IV_{TOTAL} of 2123, 58022 and 3922 \$ t^{-1}, for cyclohexane, toluene and hexane,

190 respectively, multiplied by solvent loss fraction in this process. The third example can be the

191 application of heptane and decane for lipid extraction from microalgae.[24] In this continuous

192 process heptane is lost at rate of 0.921 kmol h^{-1} and decane loss rate is 0.099 kmol h^{-1}.

193 The calculated IV_{TOTAL} of these losses would be 264.3 and 454.1 \$ h^{-1} for heptane and decane,

194 respectively. These simple considerations show that emission costs can be significant.

195

196   3.3. Assessment of green solvents

197 The assessment procedure is applied to assess solvents that are generally considered to be green.

198 They are solvents from solvent selection guide[18] and PolarClean[25], Cyrene,[26] butylpyrrolidone[27],

199 recently applied green solvents. As for these compounds the values of GWP, ODP and SOA

200 formation potentials are not available the mean values for chemical class these solvent belongs to

201 are substituted. Therefore, the results presented in Table 3 should be treated as the best estimate

202 for present time.

203 Green solvents are characterized by rather low estimated IV_{TOTAL} monetary values. Two solvents

204 with slightly deviated values are 1-octanol, because it is readily biodegradable in water and

205 Cyrene because mean SOA value for terpenes is substituted.

206

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	-

207

208 3.4. Sensitivity and uncertainty analyses

209 Sensitivity analysis is performed to investigate how variations in the input data influence the final

210 result. We assume that the values of GWP, ODP, SOA formation potential, oral LD_{50} towards

211   rats and biodegadation half-lifes can change randomly in the range of ± 50 % of initial value with

212   uniform distribution. The values of IV_{TOTAL} are calculated 25 times with randomly changed input

213   data and the results are resented in form of mean value ± standard deviation in Table S1. The

214   average relative standard deviation is 0.27 what is acceptable in this type on analysis.

215   The uncertainty analysis is performed with Monte Carlo simulation to investigate how the initial

216   assumptions on calculation respective impact indicators influence the final result. The uncertainty

217   factors are taken from Steen (2019) handbook[17] and normal distribution is assumed. The analysis

218   is repeated 500 times and the calculated mean values with standard deviations are presented in

219   Table S1. The average relative standard deviation is 1.96, which is not unusual uncertainty for

220   monetization studies,[28,29] as many components with high uncertainty factors are considered.

221

222   3.5. Metrics limitations

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

224   • The availability of input data is limited. The values of GWP, ODP, SOA generation

225   potentials are not available for many solvents. They may be substituted with values for

226   similar compounds or mean value for the chemical group solvent belongs to. However,

227   this generates additional uncertainty of result.

228   • Link of acute or chronic solvents toxicity towards fish with monetary impacts is the

229   problem to overcome.

230   • The model does not consider information on solvents operational safety issues nor

231   environmental problems during production, information if solvents origin from fossil

232   fuels or bio-based, renewable sources. So the applicability as greenness metric tool is

233   limited.

234 • Uncertainties for the estimated values are large.

235 • Presence of solvents in soils and sediments is neglected.

236

237 **4. Conclusions**

238 In this study we present the methodology to estimate the monetary estimates of solvents

239 emissions to the evaluative environment and calculate impact values for 52 solvents. Solvents

240 with lower impact values are alcohols, esters, aldehydes, ketones and organic acids. These with

241 higher impact values are aromatic hydrocarbons, terpenes and carbon tetrachloride. The results

242 can be used during environmental-economic assessment studies of various products, materials or

243 chemical processes. Few examples show that emissions monetary impact values can be large in

244 chemical processes.

245 As this is one of the first attempts to calculate monetary impact values of solvents emissions the

246 procedure and the results probably could be improved when new data will be available. For

247 example toxicity towards aquatic organisms, DALY related to inhalation exposure through non-

248 cancer diseases and soil and sediment related impacts could make the results more complete.

249

250 **Conflict of interests**

251 There are no conflict of interests to declare.

252
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