Supplementary information

Monetary values estimates of solvents emissions

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Environmental impact indicators related to air emissions.

Environmental impact indicators (where YLL is years of lost life expectancy, estimated to be 107067 $, and YLD is years lived with disability) are calculated in following way:[1]

- YLL via climate change – it is 1.88E-06 YLL kg^{-1} CO_2, so for solvent *S* the impact is calculated from 1.88E-06*GWP_S, assumed uncertainty factor = 2.7;
- YLL via oxidants – it is estimated to be 6.97E-06 YLL kg^{-1} NO_X. POCP for NO_X is 0.46 so for solvent *S* the impact is calculated with 6.97E-06*$(0.46*POCP_S)^{-1}$, assumed uncertainty factor = 2.7;
- YLL via secondary particles – it is estimated to be 1.34E-03 YLL kg-1 PM2.5. The impact is calculated from 1.34E−03*SOA_S YLL kg^{-1} of solvent, assumed uncertainty factor = 2;
- YLL via cancer – from the solvents dataset only benzene is categorized by IARC as human carcinogen. The impact is calculated as 5.13E-06 YLL kg^{-1} of benzene, for details please see [17], assumed uncertainty factor = 3; for other compounds being IARC class 1 carcinogens the value is also 5.13E-06 YLL kg^{-1}, while for IARC class 2 compounds the value is 2.57E-06 YLL kg^{-1}

- Undernutrition via climate change – it is 1.72E-06 personyears kg^{-1} CO_2, so the impact is calculated from 1.72E-06*GWP_S, assumed uncertainty factor = 2.7.
- Working capacity via climate change – it is estimated to be 4.53E-03 personhours kg^{-1} CO_2, so the impact is calculated with 4.53E-03*GWP_S, assumed uncertainty factor = 2.7.
- Diarrhea via climate change – it is 2.69E-10 personyears kg^{-1} of CO_2. The impact of indicator is calculated with formula 2.69E-10*GWP_S, assumed uncertainty factor = 3.7.
- YLD via secondary particles – it is 6.16E-05 YLD kg^{-1} PM2.5. The formula 6.16E-05*SOA_S YLL kg^{-1} VOC is applied to calculate this impact, assumed uncertainty factor = 3.2.
- Crop loss via climate change – it is 1.42E-02 kg crop kg^{-1} CO_2, so for solvent *S* it is calculated with 1.42E-02*GWP_S, assumed uncertainty factor = 3.7.
- Crop loss via oxidants – it is 0.120 kg crop kg^{-1} NO_X, so for solvent *S* it is 0.120*(0.46*$POCP_S)^{-1}$ for solvent S, assumed uncertainty factor = 2.7.
- Meat production capacity via climate change – it is 3.72E-04 kg meat kg^{-1} CO_2, for solvent *S* it becomes 3.72E-04*GWP_S, assumed uncertainty factor = 3.7.
- Drinking water production capacity via climate change – it is 9.06E-04 m^3 drinking water kg^{-1} CO_2, for solvent S it is calculated with 9.06E-04*GWP_S, assumed uncertainty factor = 3.
- Decreased biodiversity via climate change – it is estimated to be 1.69E−16 per kg of CO2, so the formula applied is 1.69E−16*GWP_S, assumed uncertainty factor = 4.

YLL and YLD are summed to DALY, which are disability-adjusted life years that refer to years lost in good health. Weights are applied to YLD to be comparable with YLL.

The methodology of calculation of one kg of solvent impact on atmospheric air is presented in details in Supplementary Information. The equation to combine all impacts is following:

*IV_{AIR} = (YLL via climate change + YLL via oxidants + YLL via secondary particles + YLL via cancer) * YLL + Undernutrition via climate change * U_{IV} + Working capacity via climate change * WC_{IV} + Diarrhea via climate change * D_{IV} + YLD via secondary particles * YLL + (Crop loss via climate change + Crop loss via oxidants) * CL_{IV} + Meat production capacity via climate change * MP_{IV} + Drinking water production capacity * DW_{IV} + Decreased biodiversity via climate change * DB_{IV}*

Where IV_{AIR} - impact value for solvent *S* emitted to the air [$ kg^{-1}]; YLL is year of lost life expectancy (107067 $); U_{IV} is undernutrition impact value - 6424 $ $personyear^{-1}$; WC_{IV} is working capacity impact value 30 $ $personhour^{-1}$; D_{IV} is diarrhea impact value 11242 $ $personyears^{-1}$; CL_{IV} is crop loss impact value 0.289 $ kg^{-1}; MP_{IV} is meat production impact value 2.59 $ kg-1 of meat; DW_{IV} is drinking water impact value 1.87 $ m^{-3}; DB_{IV} is decreased biodiversity impact value equal to 7.61E+10 $ kg^{-1}. All values are taken from Steen (2019).[1]

Finally, the results are solvent density corrected to be expressed in $ L^{-1}. As the results presented by Steen is for USD_{2018} the correction to USD_{2019} is done.

Impact values for solvents in water

The solvent that is well studied in terms of monetary valuation of exposure is ethanol. It is estimated that the exposure through gastrointestinal track results in the cost of 107.44 $ L^{-1}, expressed as USD_{2006}.[2] Taking into consideration inflation the value in USD_{2019} is 136.25 $ L^{-1}. It was estimated that the same biological effect is caused by 40 times lower concentration of toluene than given concentration of ethanol.[3] This estimation is based on the equation:[18]

$$\text{Ethanol}_{\text{EQUIV}} = \exp(0.599(\ln(TOL)) - 2.95)$$

which is valid for small solvent concentrations, what is reasonable as such are expected for environmental conditions. For low concentrations of solvents the relation between concentration and biological effect can be assumed to be linear. Therefore, the cost of toluene oral exposure is calculated to be 5450 $ L^{-1}. Because of availability of data, the best parameter to relate biological effect of many solvents is LD_{50} towards rats through oral exposure. LD_{50}

for ethanol is 10900 mg kg^{-1}, while for toluene it is 5000 mg kg^{-1}. Based on this proportion, to relate the impact values of oral exposure towards other solvents the equation was used:

$$IV_{ORAL} = -0.9006 \times LD_{50} + 9933$$

The equivalence relationships based on single effect are fulfilled for solvents because assumptions are met[4] - a common dose metric was concentration of ethanol and toluene in blood, common effect is the best estimate – oral LD_{50} towards rats and the common mode of action is assumed for all solvents.

The global population is 7.7 billion of people, with mean daily consumption of 1 L of tap water [[5]]. The volume of water consumed yearly is calculated as 2.8 km^3. As solvents are not persistent pollutants and their residence times are short, the global volume of water in which emitted solvents are present is not convenient to be taken. The volume of water in which the solvent can be present is taken from multimedia Level I model = 200 km^3. As the volume of consumed water is for one year perspective, we introduce relation of solvent water hazard to one year by multiplying of biodegradation half-life (expressed in days) by 3.5 (which equals to concentration drop to 10% of initial one) and dividing by 365 to obtain normalization to one year. Therefore, the impact value due to drinking water consumption (IV_{DRINK}) is calculated by multiplying IV_{ORAL} by factor 0.014 (obtained by dividing volume of water consumed yearly – 2.8 km^3 by volume of water where solvent is present – 200 km^3) multiplied by (BOD $t_{1/2}$*3.5*365^{-1}).

To incorporate biological oxygen demand (BOD), theoretical oxygen demand (ThOD) is calculated (as good estimation),[6] so first the molecular formula of solvent is considered. The amount of oxygen needed to oxidize the mole of solvent is calculated from:

$$\text{Moles of } O_2 = 0.5*(\text{moles of C} *2 + \text{moles of H} * 0.5 - \text{moles of O})$$

Then the mass of O_2 that oxidize the kilogram of solvent is calculated. The value of BOD is established to be 0.000352 \$ kg^{-1} O_2 and it is the sum of impacts resulting from fish productivity loss and biodiversity loss.[17] Finally, the impact value for BOD IV_{BOD} is calculated by multiplication of the mass of O_2 needed to oxidize kg of solvent times 0.000352 \$ kg^{-1} O_2.

The impact values for IV_{DRINK} and IV_{BOD} are summed up to calculate the impact value of solvents emitted to water (IV_{WAT}). Finally, the results are solvent density corrected to be expressed in \$ L^{-1}.

The results of sensitivity and uncertainty estimations

Table S1. The results of sensitivity and uncertainty analyses, methodology described in section 3.4.

Group	Compound	IV_{TOTAL} [\$ L^{-1}]*	Sensitivity results analysis [\$ L^{-1}]	Uncertainty estimation [\$ L^{-1}]
hydrocarbons	pentane	1.32	1.32 ± 0.36	1.34 ± 2.02
	hexane	1.38	1.39 ± 0.31	1.51 ± 1.97
	cyclohexane	3.02	2.83 ± 0.63	3.16 ± 3.74
	heptane	1.95	1.84 ± 0.31	2.00 ± 2.46
	octane	9.58	10.27 ± 2.55	9.33 ± 14.98
	nonane	21.65	20.37 ± 6.36	21.16 ± 39.37
	decane	23.58	23.87 ± 6.00	23.43 ± 42.07
	undecane	32.28	32.27 ± 7.17	34.38 ± 62.16
	dodecane	23.27	23.68 ± 5.80	24.28 ± 43.75
	benzene	55.66	54.19 ± 16.48	54.80 ± 100.62
	toluene	50.48	50.54 ± 13.76	55.29 ± 91.31
	o-xylene	50.34	55.47 ± 14.03	49.96 ± 88.41
	m-xylene	49.39	46.47 ± 13.09	44.08 ± 94.47
	p-xylene	22.83	23.51 ± 6.28	22.76 ± 39.18
alcohols	methanol	2.12	1.97 ± 0.36	2.27 ± 3.49
	ethanol	0.70	0.60 ± 0.63	0.71 ± 1.18
	propanol	3.89	4.10 ± 0.88	3.66 ± 9.35
	isopropanol	1.92	1.86 ± 0.42	2.19 ± 2.87
	butanol	8.71	8.88 ± 2.37	8.80 ± 22.02
	isobutanol	7.91	7.86 ± 1.85	8.32 ± 13.13
	sec-butyl alcohol	7.69	7.37 ± 2.22	8.91 ± 18.99
	tert-butyl alcohol	7.33	8.03 ± 1.53	7.43 ± 15.42
	o-cresol	3.16	3.05 ± 0.62	3.32 ± 6.33
ethers	diethyl ether	1.32	1.41 ± 0.27	1.27 ± 1.97
	tert-butyl methyl ether	1.24	1.27 ± 0.23	1.27 ± 1.75
aldehydes	ethanal	1.82	1.75 ± 0.40	1.8 ± 2.74
	propanal	5.97	5.74 ± 1.32	6.46 ± 14.13
	butanal	2.36	2.49 ± 0.40	2.44 ± 3.46

ketones	acetone	1.32	1.28 ± 0.36	1.38 ± 2.44
	2-butanone	7.01	7.01 ± 1.76	5.54 ± 18.05
	2-pentanone	4.45	4.81 ± 1.36	4.86 ± 10.71
	3-pentanone	4.55	4.09 ± 1.24	4.84 ± 13.04
	methyl isobutyl ketone	4.40	4.45 ± 1.11	4.78 ± 9.78
	2-hexanone	3.80	3.80 ± 0.83	3.37 ± 9.21
	cyclohexanone	7.10	7.08 ± 1.81	7.57 ± 20.29
terpenes	(R)-(+)-limonene	76.66	78.32 ± 23.88	66.32 ± 145.52
	p-cymene	76.58	72.50 ± 24.29	73.33 ± 140.17
	α-pinene	81.48	80.20 ± 23.93	84.93 ± 144.88
	β-pinene	74.90	76.66 ± 20.48	79.96 ± 140.14
organic acids	formic acid	1.11	1.26 ± 0.28	0.92 ± 3.50
	acetic acid	1.82	1.86 ± 0.57	1.95 ± 5.46
	propionic acid	1.03	1.02 ± 0.33	0.30 ± 3.02
esters	ethyl acetate	11.43	11.03 ± 3.07	10.74 ± 19.97
	methyl formate	14.03	13.39 ± 3.92	11.31 ± 26.21
	methyl acetate	11.19	11.42 ± 2.94	11.66 ± 20.09
	methyl lactate	3.03	3.11 ± 1.87	2.95 ± 8.68
chlorinated	dichloromethane	5.58	5.43 ± 1.36	5.25 ± 10.06
	chloroform	11.21	11.08 ± 2.77	10.97 ± 20.42
	carbon tetrachloride	1179.06	1236.57 ± 305.29	1318.84 ± 2158.24
	trichloroethene	4.66	4.67 ± 0.78	4.91 ± 5.61
	tetrachloroethene	4.32	4.14 ± 0.84	4.50 ± 6.26
	1,1,1-trichloroethane	94.68	94.46 ± 27.23	103.86 ± 178.94

[1] B. Steen, Monetary Valuation of Environmental Impacts. CRC Press, Boca Raton, FL, USA, 2019.

[2] E.E. Bouchery, H.J. Harwood, J.J. Sacks, C.J. Simon and R.D. Brewer, *Am. J. Prev. Med.*, 2011, **41(5)**, 516-524.

[3] V.A. Benignus, P.J. Bushnell and W.K. Boyes, *Risk Anal.*, 2005, **25(2)**, 447-456.

[4] P.J. Bushnell, W.K. Boyes, T.J. Shafer, A.S. Bale and V.A. Benignus, *Neurotoxicology*, 2007, **28(2)**, 221-226.

[5] EPA, Update for Chapter 3 of the Exposure Factors Handbook, *Ingestion of Water and Other Select Liquids, 2019*

[6] J.R. Baker, M.W. Milke and J.R. Mihelcic, *Water Res.*, 1999, **33(2)**, 327-334.