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Scoring of solvents used in analytical laboratories by their toxicological and exposure hazards

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ABSTRACT

Green analytical chemistry, although a well recognised concept, still lacks reliable environmental impact assessment procedures. This article describes scoring of solvents, frequently used in analytical laboratories, with CHEMS-1 model. The model uses toxicological and exposure data to calculate hazard values related to the utilisation of solvents.

The original model was modified to incorporate hazards related to the volatility of chemicals. The scoring of hazard values showed that polar solvents are less hazardous. The scoring results were applied to assess the total hazard values in terms of solvent consumption. The hazard scores calculated for each chemical were multiplied by the volumes of solvent used during the analytical procedure. The results show that calculation of total procedural hazard values is valuable in the green analytical chemistry assessment procedure. Moreover, the assessment procedure can be combined with other procedural greenness assessment methods.

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1. Introduction

Analytical chemistry laboratories consume high-purity solvents, which are widely applied in procedures as extraction agents, cleaning agents and mobile phases in liquid chromatography (Mohamed, 2015). Solvents mentioned above come from a variety of chemical groups, from polar alcohols to nonpolar aliphatic or aromatic hydrocarbons and halogenated solvents. Their physicochemical properties are relatively diverse, similarly to their inhalation and oral toxicities, influence on the environment (especially aquatic ecosystem) and the exposure parameters. Preparation of analytical sample solvents consumption, related to this analytical step, are concerned as the most polluting and hazardous of the whole analytical procedure (Spietelun et al., 2013; Li et al., 2013).

Green analytical chemistry is the concept that recently finds more acceptance among the analysts. It assumes that the results of chemical measurements can be obtained with minimising the consumption of chemicals, reduction of emission and exposure without sacrificing the quality of analytical parameters (Armenta et al., 2008; Moros et al., 2010). Environmental impact is the factor that makes statistical difference between the analytical procedures, while parameters like limits of detection, recoveries and precisions are in most of the cases at comparable levels (Tobiszewski et al., 2013). Green analytical chemistry favours the procedures that minimise their impact by miniaturisation, application of solventless extraction techniques, greener reagents and alternative solvents.

Only few propositions of techniques are known for assessment of the environmental impact or "greenness" of analytical procedures and these include NEMI labelling (Keith et al., 2007), analytical Eco-scale (Gałuszka et al., 2012), application of HPLC-EAT tool (Gaber et al., 2011) or multivariate statistics (Tobiszewski et al., 2013). The details of techniques mentioned are accessible in the references and have been discussed recently (Tobiszewski and Namiesnik, 2014). All of them are characterised by severe drawbacks, like tedious assessment procedures, lack of data availability as well as lack of information about the structure or nature of the hazards carried by application of the procedure. Still, this field requires new solutions to give easy-to-use, based on easily available information and clear-to-read "greenness" assessment procedures.

The aim of the study is to perform scoring of the solvents commonly used in analytical laboratories with CHEMS-1 model (Swanson et al., 1997). Such scores can be useful at initial stages of procedure development, when solvents are selected. The scores can be also successfully used as one of the factors when assessing greenness of analytical procedures.

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2. Materials and methods

The CHEMS-1 procedure was developed for relative scoring and ranking of chemicals with respect to their hazard. For the detailed discussion about CHEMS-1 the reader should kindly refer to the source article (Swanson et al., 1997) but brief introduction to the scoring procedure is presented below. Although the CHEMS-1 model was developed to score the risk of using chemicals in industry, we find such approach very attractive for scoring of solvents used in analytical laboratories. The procedure considers toxicity of chemicals to human and the environment as well as chemical exposure potential. The input data are toxicological and ecotoxicological endpoints collected from material safety data sheets (MSDS). Such data sources are easily available, which is very important to perform the chemical scoring by potential user. The assessment procedure involves transformation and scaling of the numerical values to give similar weights to each parameter. For non-toxic compounds the value for respective hazard values is set to 0, while for very toxic compounds the hazard value is set to maximum value of 5. Parameters included in the algorithm are hazards related to oral toxicity (HV_{ORAL}), inhalation toxicity (HV_{INH}), carcinogenicity (HV_{CAR}), other hazardous effects (HV_{HE}), aquatic acute toxicity (HV_{FA}), aquatic chronic toxicity (HV_{FC}) and exposure-related parameters like biodegrability (HV_{BOD}), hydrolysis (HV_{HYD}) and bioconcentration (HV_{BCF}).

The algorithm to assess the total hazard (tHV) by CHEMS-1 algorithm is multiplication of the sum of hazards related to toxicity by hazards related to exposure factors (Swanson et al., 1997)

$$tHV=(HV_{ORAL} + HV_{INH} + HV_{CAR} + HV_{HE} + HV_{ORAL} + HV_{FA} + HV_{FC})*(HV_{BOD} + HV_{HYD} + HV_{BCF})$$

The main exposure pathway when solvents are applied in analytical laboratories is inhalation. The original scoring algorithm does not have any term related to exposure via inhalation. The hazard value related to exposure via inhalation could be calculated based on boiling point (BP) or vapour pressure. Both parameters are easily accessible (Mackay et al., 2006) but the operation with boiling points seem to be more convenient. Very volatile solvents (BP < 50 °C) are scored by 2.5 while semi-volatile solvents (BP > 200 °C) are scored by 1 hazard value. The hazard value, related to the volatility (HV_{VOL}), was calculated with the following formulas:

$$HV_{VOL} = 3–0.01*BP \quad \text{for } 50°C \le BP < 200\ °C$$
$$HV_{VOL} = 1 \quad \text{for } BP \ge 200\ °C$$
$$HV_{VOL} = 2.5 \quad \text{for } BP < 50\ °C$$

The algorithm of total analytical hazard value (taHV) calculation is like follows:

$$taHV=(HV_{ORAL} + HV_{INH} + HV_{CAR} + HV_{HE} + HV_{ORAL} + HV_{FA} + HV_{FC})*(HV_{BOD} + HV_{HYD} + HV_{BCF} + HV_{VOL})$$

Original algorithm included the possibility of weighting hazard values (Swanson et al., 1997). In this study, however, we apply no weights, as we assume each hazard is equally important. Weighting of hazard values can be applied if there is one dominating exposure pathway or some data are significantly more or less reliable than other.

3. Results and discussion

3.1. Scoring of solvents

The algorithm was run for 34 different solvents, characterised by different physiochemical properties, that are commonly used in analytical chemistry laboratories. They find application as extraction solvents in different modes of liquid extraction, auxiliary solvents and mobile phases in liquid chromatography. Table 1 shows the scoring of solvents with original and modified CHEMS-1.

The values of total hazard and total analytical hazard values are the highest for benzene and chlorinated solvents. These compounds posses high oral, inhalation and aquatic toxicities, are categorised as carcinogens and possess other specific human health effects. Moreover their exposure factor is high as they are relatively persistent in the environment. Boiling points of investigated compounds are mainly below 100 °C, so their analytical exposure factor is also high. In analytical laboratories they are usually used as extraction solvents in various modes of liquid–liquid extraction or solid–liquid extraction.

The least hazardous organic solvents used in analytical laboratories are polar ones, like short chain alcohols, ethers, acetone and ethyl acetate. Their toxicities are comparatively low and they are readily biodegradable, hydrolysable and non-bioaccumulative. In analytical laboratories polar organic solvents are mainly used as

Table 1
The results of total hazard values (tHV) and total analytical hazard values (taHV) calculation.

	Compound name	CAS number	tHV	taHV
Hydrocarbons	Pentane	109-66-0	23.4	36.4
	Hexane	110-54-3	53.8	81.4
	Cyclohexane	110-82-7	57.9	79.8
	Heptane	142-82-5	15.2	20.9
	Isooctane	540-84-1	57.1	79.2
	Benzene	71-43-2	84	122
	Toluene	108-88-3	43.9	60.5
	Xylenes	1330-20-7	51.5	68.2
Alcohols	Methanol	67-56-1	8.8	15.7
	Ethanol	64-17-5	4.1	7.2
	Isopropanol	67-63-0	3.9	6.8
	Heptanol	111-70-6	22.9	28.6
	Octanol	111-87-5	38.3	45.7
	Nonanol	143-08-8	39.8	46.7
	Benzyl alcohol	100-51-6	45.2	55.1
Ethers	Diethyl ether	60-29-7	8.7	16
	Methyl tert-butyl ether	1634-04-4	2.7	3.8
	Tetrahydrofuran	109-99-9	9.1	14.9
Aldehydes	Furfural	98-08-1	47.7	69.2
	Benzaldehyde	100-52-7	56.9	77.5
Ketones	Acetone	67-64-1	1.5	2.6
Organic acids	Formic acid	64-18-6	25.8	43
	Acetic acid	64-19-7	1.3	2.1
	Propionic acid	79-19-4	27	41.2
Esters	Ethyl acetate	141-78-6	5	7.3
Chlorinated hydrocarbons	Dichloromethane	75-09-2	39.3	59.8
	Chloroform	67-66-3	70.7	103.8
	Carbon tetrachloride	56-23-5	80	109.7
	Trichloroethylene	79-01-6	90.9	125.1
	Tetrachloroethylene	127-18-4	82.7	107.7
	1.1.1-Trichloroethane	71-55-6	34.7	49
	1.1.2.2-Tetrachloroethane	79-34-5	76.9	97.3
	Chlorobenzene	108-90-7	58	75.9
Others	Acetonitrile	75-05-8	18.8	26.8
	Carbon disulphide	75-15-0	61.6	89.6

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