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Making fate and exposure models for freshwater ecotoxicity in life cycle assessment suitable for organic acids and bases

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HIGHLIGHTS

- ▶ We provide freshwater fate and exposure factors for acids and bases.
- ▶ pK_a and pH dependency of ionic chemicals are now included in the model.
- ▶ Predicted factors were compared to predictions of a neutrals model version.
- ▶ New fate factors were up to 2.0×10^4 larger compared to the neutral model.
- ▶ Differences in fate and exposure factors were larger for bases than for acids.

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ABSTRACT

Freshwater fate and exposure factors were determined for organic acids and bases, making use of the knowledge on electrical interaction of ionizing chemicals and their sorption to particles. The fate factor represents the residence time in the environment whereas exposure factors equal the dissolved fraction of a chemical. Multimedia fate, exposure, and effect model USES–LCA was updated to take into account the influence of ionization, based upon the acid dissociation constant (pK_a) of a chemical, and the environmental pH. Freshwater fate (FF) and exposure (XF) factors were determined for 415 acids and 496 bases emitted to freshwater, air, and soil. The relevance of taking account of the degree of ionization of chemicals was tested by determining the ratio (R) of the new vs. fate and exposure factors determined with USES–LCA suitable for neutral chemicals only. Our results show that the majority of freshwater fate and exposure factors of chemicals that are largely ionized in the environment are larger with the ionics model compared to the factors determined with the neutrals model version. R_{FF} ranged from 2.4×10^{-1} to 1.6×10^{1} for freshwater emissions, from 1.2×10^{-2} to 2.0×10^{4} for soil emissions and from 5.8×10^{-2} to 6.0×10^{3} for air emissions, and R_{XF} from 5.3×10^{-1} to 2.2×10^{1}. Prediction of changed solid–water partitioning, implying a change in runoff and in removal via sedimentation, and prediction of negligible air–water partition coefficient, leading to negligible volatilization were the main contributors to the changes in freshwater fate factors.

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1. Introduction

Life cycle assessment (LCA) is a tool to assess the environmental impact of products and services, considering their entire life cycles (Guinée et al., 1993; Finnveden et al., 2009). One part of this process is the life cycle impact assessment (LCIA), valued concerning their environmental burden for various impact categories, such as human toxicity and ecotoxicity (Consoli et al., 1993; Udo de Haes et al., 1999). In LCIA, characterization factors (CFs) are used to express the magnitude of the impact of a unit mass released. Characterization factors are specified for all combinations of emission- and receptor compartments. CFs for freshwater ecotoxicity are calculated from multimedia fate, exposure and effect models. They combine fate factors (FF in days), which express the change in steady-state mass (kg) of a chemical due to a change in emission (kg d^{-1}), exposure factors (XF (–)), which express the dissolved concentration resulting from the total concentration, and effect factors (EF in yr kg^{-1}), which express the effect per unit concentration (Rosenbaum et al., 2008; Van Zelm et al., 2009; Henderson et al., 2011).

Being directly related to the multimedia model used, FFs echo the model input data on transport and removal processes, which

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determine the total concentration in a specific environmental compartment upon an emission. The XF then takes the part of the chemical that is in the dissolved state and therefore assumed bioavailable (McKone, 1993; Huijbregts et al., 2005b; Rosenbaum et al., 2008). The EF expresses the effect of the emitted substance and is derived from human and ecological toxicity data (Pennington et al., 2004; Huijbregts et al., 2005a).

Current LCIA models have a limited applicability domain, i.e. they are optimized for neutral hydrophobic organic chemicals (Rosenbaum et al., 2008). However, it is estimated that of the pre-registered REACH chemicals (143 000 in 2010), about one third is mostly ionized at pH 7 (Franco et al., 2010). Examples of widely used ionizing chemicals can be found among detergents, pesticides and pharmaceuticals. For ionizing chemicals, electrical interaction and sorption to particles is to a high degree dependent on the acid dissociation constant (pK_a) of a chemical and the pH of the environment (Franco and Trapp, 2008; Franco et al., 2009) and these processes need therefore to be taken into account in LCIA models.

Advances have been made in modeling the partitioning behavior for acids and bases. Franco and Trapp (2010) implemented newly derived rules for partitioning of ionic species in their multimedia model MAMI. This model is able to determine the concentration of monovalent acids, bases and amphoters after an emission into the environment. Csiszar et al. (2011) adapted the aquivalence approach to explicitly treat neutral and ionizing interconverting forms of a chemical and described the fate of four pharmaceutical chemicals. However, the models were applied to a small dataset only and no models are currently available that can calculate characterization factors of ionizable chemicals used for LCIA.

The goal of the current research is therefore twofold: (1) to implement calculation routines for partitioning of ionizing substances that include pK_a and pH dependency in the multimedia fate, exposure and effects model USES–LCA 2.0 to enable it to more reliably calculate fate and exposure factors for ionics; and (2) to provide fate and exposure factors for a number of acids and bases. Subsequently, the outcomes of the adaptations are discussed, as well as the relevance and applicability in LCIA.

2. Methodology

Freshwater fate and exposure factors were determined with the multimedia fate, exposure and effects model USES–LCA 2.0 (Van Zelm et al., 2009), adapted here for ionic substances. The fate and exposure factors reflect the change in dissolved mass due to a change in emission (days). The fraction of a chemical transferred from emission compartments air and agricultural soil to freshwater determine the fate and exposure factors for these emission compartments (Henderson et al., 2011). Fate and exposure factors were determined for emissions to freshwater, agricultural soil, and air.

2.1. Model adaptations

Chemical fate can be modeled when sufficient information is available on the chemical and environmental characteristics. Partition coefficients that depend on these characteristics influence the magnitude of the transport processes within and between environmental compartments.

Acids and bases exist in neutral or ionized forms. The ratio between these ionic and neutral forms depends on the pK_a of the chemical and the pH of the environment (Henderson, 1908). Ionic species have different physical–chemical properties than their neutral equivalents, which results in changed behavior regarding transport and removal processes (Kah and Brown, 2007; Franco and Trapp, 2008; Franco et al., 2009). Transport processes within and between, and removal processes from each environmental compartment can be affected since ionization takes place in water, which is present in all environmental compartments.

The magnitude of the air–water partition coefficient (K_{aw}) depends on the vapor pressure of the chemical; ions have no measurable vapor pressure and therefore do not volatilize, resulting in a K_{aw} of zero for the ionic fraction (Trapp et al., 2010). When the ionization of an acid or base increases, volatilization flow is expected to decrease. The K_{aw} is used to estimate the gas exchange rates between air and earth surface and to estimate other partition coefficients, for example the aerosol–air partition coefficient.

The solid–water partition coefficient normalized to organic carbon (K_{oc}) is dependent on interactions between the chemical and the soil. For neutral chemicals, hydrophobic interactions are considered dominant and the K_{oc} can be predicted by the molecular structure or octanol–water partition coefficient (K_{ow}) and organic carbon content of the soil (e.g. Meylan et al., 1992; Sabljic et al., 1995; Schüürmann et al., 2006). For ions, however, electrostatic forces play a role and the pH of the soil can influence the distribution of the chemical (Franco and Trapp, 2008; Franco et al., 2009). The K_{oc} has to be determined for the mixture of the neutral and ionic species. Appropriate regressions to determine the K_{oc} for monovalent acids and bases that more accurately describe the partitioning behavior for this group of chemicals were established by Franco and Trapp (2008). Recommendations from Franco and Trapp (2010) were followed regarding the choice of regressions (see Appendix A). These regressions suggest that also for the neutral fraction of an acid or base, the partitioning between solid matter and water differs from that of non-ionizing organic chemicals. The chosen pH for each environmental compartment can be found in Table A1 of the Appendix.

The solid–water partition coefficient is used for many regressions in fate and exposure modeling, a.o. to determine specific soil–water and sediment–water partition coefficients and transport processes such as runoff from soil to water, sedimentation, desorption flow from sediment to water, and leaching. K_{oc} decreases with ionization for acids; more of the chemical is present in the water phase (Franco and Trapp, 2008). This will increase the transport due to runoff to water and decrease transport due to sedimentation from water. For bases, decrease of K_{oc} with increasing ionization is less clear (Franco and Trapp, 2008).

The regressions used for calculating the K_{oc} for the electrolytes are suited for acids within the pK_a range 0–12 and with a log K_{ow} between -2.18 and 8.50. For bases the pK_a needs to be above 2 and log K_{ow} is between -1.66 and 7.03 (Franco and Trapp, 2008). A complete list of model adaptations can be found in the Supporting Information.

2.2. Data input

To calculate freshwater fate and exposure factors, the substance database of the USEtox model (Rosenbaum et al., 2008) was included in USES–LCA 2.0. The USEtox substance database contains 3073 organic chemicals, of which 1683 ionics; 415 acids and 496 bases qualified for the application domain and the data requirements for ionics in the adapted version of USES–LCA (i.e. pK_a and K_{ow} ranges for which the regressions were suitable).

Physico-chemical properties in the USEtox database were gathered from the EPISuite 4.0 software package (USEPA, 2009). EPISuite provides experimental data when available and, additionally, EPISuite can be used to estimate chemical parameters when experimental data are not available. Missing experimental pK_a values for acids and bases were determined with SPARC (USEPA, http://archemcalc.com/sparc/) (Huijbregts et al., 2010). Original K_{oc} values were obtained from EPISuite 4.0 (USEPA, 2009), based on QSAR

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