Combined modelling of PAH biodegradation, soil sorption and dissolution from organic phases

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partitioning from the outer into the inner membrane. The model was calibrated to two data sets which were merged: uptake efficiency of environmental pollutants measured in different mammals during feeding studies, and a pharmaceutical data set with human oral absorption efficiencies.

The new model estimated uptake efficiency for compounds with logKOW ranging from -10 to +8, and estimation was improved for polar compounds by accounting for the bilayer structure of the membrane. Including the inner membrane resistance improved RMSE especially for the compounds with KOW<0 from 28.3 to 18.3, while also overall performance improved from 18.4 to 14.0. Therefore, the new model provides a tool to estimate uptake efficiency for new compounds based on sound mechanistic processes.

MO 063

A standardized contact transfer method for assessing soil-to-clothing exposure to soil-sorbed chemicals


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Exposure to chemicals, including chemical warfare agents (CWA), can present a potential Contact Hazard even when the compounds are sorbed onto soil. Previous studies have investigated levels of CWA transferred from contaminated surfaces utilizing a malleable latex material (dental dam; DD) as transfer substrate; however DD is typically inconsistent in compositions, and may not be representative of other contact substrates. Therefore, a malleable material (4”-diameter circular swatch of ACU material was selected, similar to surface areas that may contact soil at knee or elbow locations; standard contact was created by placing the ACU material on top of the swatch for 5 minute duration, then covering the swatch with a 4”-diameter Plexiglass disk to distribute force from a centrally-placed standard mass. Contact Transfer of CWA was determined by solvent extraction of swatches, with subsequent analyses by GC/GC-MS or HPLC/HPLC-MS. Masses 0.250, 0.500, 1.000, 1.500 kg, resulted in significantly greater CWA transfer (p ≤0.05) at ≥0.500kg compared to 0.250kg; therefore the 1-kg standard mass was selected for this study.

A standardized contact transfer method for assessing soil-to-clothing exposure to soil-sorbed chemicals can be used to parametrize and calibrate the proposed model for PAH bioaccumulation and depuration in mussel species.

MO 066

Thermodynamic modelling of PAH bioaccumulation in Mytilus galloprovincialis with a three-compartment model

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Polycyclic aromatic hydrocarbons (PAH) are a class of compounds used in the manufacture of coal tar and pitch, used extensively in industry. They can dissolve in soil organic matter and can contaminate the environment via agriculture and industrial processes. PAHs are present in soil, water, and air and are bioaccumulated by aquatic organisms such as mussels (Mytilus galloprovincialis).

The model was calibrated to two data sets which were merged: uptake efficiency of environmental pollutants measured in different mammals during feeding studies, and a pharmaceutical data set with human oral absorption efficiencies. First order kinetic equations were used for the description of accumulation and depuration of selected PAHs in mussel tissues. Data were obtained from experiments performed with selected PAHs under constant conditions. In the model, three compartments were defined: (1) mussels, (2) surrounding environment (seawater), and (3) algae (Phaeodactylum tricornutum) as food source for the mussels. During the bioaccumulation period, the mussels take up the contaminants both from seawater and with PAHs applied on algae. Thus, the model considers dynamic exchange of PAHs between algae and seawater. Experimental data were used to parametrize and calibrate the proposed model for benzo(a)anthracene and phenanthrene.

The application of the DynANet model to the case study allowed to compile a preliminary mass balance for HHCB and AHTN and to predict concentration changes under environmental phenomena such as precipitations events, temperature variations, soil use, etc. The measured concentrations and simulated results were compared to the prediction of existing models such as GREATER.