How to characterise non-extractable residues (NER) in PBT assessment - development of a harmonised procedure to be used in routine testing

Microbial turnover of glyphosate to biomass: utilization as nutrient source, formation of AMPA and biogenic NER in an OECD 308 test

Predicting plant uptake of ionic chemicals: Redefining the dominant processes
Predicting the uptake of emerging organic contaminants in vegetables irrigated with treated wastewater - Implications for food safety assessment

Emerging organic contaminants (EOCs) undergoing incomplete removal during wastewater treatment may be found in treated wastewater (TWW) used for irrigation of agricultural products. Following uptake into edible plant parts, EOCs may eventually enter in the food chain, with associated human exposure. In the present study, we used a newly developed steady-state plant uptake model with added phloem transport to predict the uptake of four EOCs (carbamazepine, ibuprofen, ketoprofen and naproxen) into three varieties of lettuce. Input data were derived from an experimental study with vegetables grown in greenhouse and irrigated with TWW spiked with CBZ at 0, 30, 60, 120 and 210µg/L in each variety of lettuce. Predicted carbamazepine concentrations in leaves were on average 82% higher than in roots, with good agreement between measured and calculated data. We subsequently predicted the uptake of anti-inflammatory compounds ibuprofen, ketoprofen and naproxen, for which the chemical analysis could not provide concentrations above detection limit. These three substances are weak acids and predicted concentrations in roots were higher than in the edible leaves, mainly due to phloem transport downwards. The daily dietary intake of all four EOCs was estimated for consumption of leafy vegetables, being far below usual therapeutic doses.
experimentally discriminated: sequestered and entrapped residues (type I), containing either the parent substance or xenobiotic transformation products or both and having the potential to be released, which has indeed been observed. Type II NER are residues that are covalently bound to organic matter in soils or sediments or to biological tissue in organisms and that are considered being strongly bound with very low remobilization rates like that of humic matter degradation rates. Type III NER comprises biogenic NER (bioNER) after degradation of the xenobiotic chemical and anabolic formation of natural biomolecules like amino acids and phospholipids, and other biomass compounds. We developed the microbial turnover to biomass (MTB) model to predict the formation of bioNER based on the structural properties of chemicals. Further, we proposed an extraction sequence to obtain a matrix containing only NER. Finally, we summarized experimental methods to distinguish the three NER types. Type I NER and type II NER should be considered as potentially remobilizable residues in persistence assessment but the probability of type II release is much lower than that of type I NER, i.e., type II NER in soil are “operationally spoken” irreversibly bound and can be released only in minute amounts and at very slow rates, if at all. The potential of remobilization can be evaluated by chemical, physical and biological methods. BioNER are of no environmental concern and, therefore, can be assessed as such in persistence assessment. The general concept presented is to consider the total amount of NER minus potential bioNER as the amount of xenoNER, type I + II. If a clear differentiation of type I and type II is possible, for the calculation of half-life type I NER are considered as not degraded parent substance or transformation product(s). On the contrary, type II NER may generally be considered as (at least temporarily) removed. Providing proof for type II NER is the most critical issue in NER assessment and requires additional research. If no characterization and additional information on NER are available, it is recommended to assess the total amount as potentially remobilizable. We propose our unified approach of NER characterization and evaluation to be implemented into the persistence and environmental hazard assessment strategies for REACH chemicals and biocides, human and veterinary pharmaceuticals, and pesticides, irrespective of the different regulatory frameworks.
Classification and modelling of non-extractable residues (NER) formation from pesticides in soil

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, Helmholtz Centre for Environmental Research, RWTH Aachen University
Contributors: Kaestner, M., Nowak, K., Brock, A. L., Anja, M., Schaeffer, A., Trapp, S.
Number of pages: 1
Pages: 161
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Ratings: Web of Science (2018): Indexed yes
Original language: English
Source: FindIt
Source-ID: 2441553331
Research output: Contribution to journal › Conference abstract in journal – Annual report year: 2018 › Research › peer-review

How To Design for a Tailored Subcellular Distribution of Systemic Agrochemicals in Plant Tissues
Foliar-applied systemic agrochemicals require entrance into the plant vascular system or into specific subcellular compartments to reach their target in planta or to be imbibed by piercing/sucking pests. An inappropriate subcellular localization, like accumulation of aphicides in vacuoles, might lower the compound’s efficiency due to reduced exposure to the target. Permeabilities and mass distributions of 16 compounds covering a broad range of properties were measured across a pH gradient in a PAMPA (“parallel artificial membrane permeability assay”) system, providing experimental evidence for ion trapping of acids and bases in basic and acidic compartments, respectively. The results validated a predictive model which was then expanded to simulate a standardized plant cell (cytosol and vacuole) with a vascular system (phloem and xylem). This approach underlined that the absolute mass distribution across aqueous phases is defined by membrane retention, whereas the relative mass distribution is determined by the species (neutral, acidic, basic) of compounds. These processes depend largely on pK(a) and log K-ow of the test compounds, which subsequently determine the partitioning of the substances in plant cell compartments. The validated model can be used as a tool in agrochemistry research to tailor the subcellular distribution by chemistry design and to interpret biology results.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, Syngenta Crop Protection Münchwilen AG
Contributors: Hofstetter, S., Beck, A., Trapp, S., Buchholz, A.
Number of pages: 11
Pages: 8687-8697
Publication date: 2018
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Publication information
Journal: Journal of Agricultural and Food Chemistry
Volume: 66
Issue number: 33
ISSN (Print): 0021-8561
Improving risk assessment of agricultural reuse of wastewater through predictive plant uptake modeling of ionizable contaminants

General information
Publication status: Published
Organisations: Environmental Fate & Effect of Chemicals, Department of Environmental Engineering
Contributors: Jensen, C. K., Polesel, F., Trapp, S.
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Publisher: Technical University of Denmark (DTU)
Editors: C. M., K. M.
Article number: U-8
URLs:
http://www.sustain.dtu.dk/
Research output: Chapter in Book/Report/Conference proceeding – Annual report year: 2018 › Research › peer-review

Improving the interpretation of Non-Extractable Residues (NER) in degradation assessment

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Publication status: Published
Organisations: Environmental Fate & Effect of Chemicals, Department of Environmental Engineering, RWTH Aachen University, Helmholtz Centre for Environmental Research
Contributors: Schaeffer, A., Kästner, M., Trapp, S.
Pages: 343-344
Publication date: 2018

Host publication information
Title of host publication: SETAC Europe 28th Annual Meeting - Abstract book
Place of publication: Brussels, Belgium
Publisher: Society of Environmental Toxicology and Chemistry
Article number: WE061
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Abstract book
Research output: Chapter in Book/Report/Conference proceeding – Conference abstract in proceedings – Annual report year: 2018 › Research › peer-review

Interpretation of non-extractable residues (NERs) in the persistence assessment

General information
Publication status: Published
Organisations: Environmental Fate & Effect of Chemicals, Department of Environmental Engineering
Kinetic Modeling of Weak Base nAChR Ligand Selective Trapping within Intracellular Acidic Vesicles: Insights into Mechanisms Underlying Nicotine Addiction and Smoking Cessation

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, University of Chicago
Contributors: Liu, Y., Trapp, S., Green, W. N., Haddadian, E. J.
Pages: 630a-630a
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Publication information
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Volume: 114
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Article number: 3122-PosB330
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Scopus rating (2018): CiteScore 3.26 SJR 2.018 SNIP 1.049
Web of Science (2018): Impact factor 3.665
Web of Science (2018): Indexed yes
Original language: English
DOIs: 10.1016/j.bpj.2017.11.3404
Source: FindIt
Source-ID: 2396093806

Microbial growth yield estimation for incomplete degradation and macronutrient utilization – the case of glyphosate
Standardized simulation tests using isotope-labelled chemicals are carried out for persistency assessment. In these tests, formation of non-extractable residues (NER) is typically observed. Recent theoretical, experimental and analytical advances have helped deciphering the nature and composition of NER [1]. Among other types, biogenic NER is formed as the microorganisms use the test chemical as a source of carbon and energy, and methods for their prediction based on microbial yield estimations have been accordingly developed [2]. Evaluating and predicting biogenic NER formation still remains a challenge for test chemicals that (i) are utilized as a source of macronutrients (besides carbon); (ii) undergo incomplete degradation via multiple pathways, with formation of dead-end transformation products. In the present study, we addressed this challenge by (i) extending a recently developed microbial yield estimation method (MTB—Microbial Turnover to Biomass) by accounting for macronutrient limitation and incomplete degradation; and (ii) incorporating this method in a dynamic model to describe the fate of glyphosate and its main transformation product (AMPA) in a water-sediment simulation test. Glyphosate is known to be biodegraded via, at least, two pathways, one forming the recalcitrant metabolite AMPA [3]. For the assessment of model simulations, we used published data from turnover experiments using co-labelled 13C315N-glyphosate [4]. Determination of microbial yield for different degradation pathways required consideration of the flow of elements, energy and electrons. By adapting three parameters, namely the number of electrons and the number of C or N atoms that can be acquired in a transformation step, the MTB method could be used to predict the growth yield when either N or C are limiting growth. The results showed that the formation of AMPA reduces the growth yield (taken as g bacteria per mol of glyphosate metabolized) by more than threefold, and that glyphosate is a better source of nitrogen than of carbon. Dynamic model simulations adequately described the degradation of glyphosate and the formation of CO2 and AMPA in the water-sediment test. In particular, balancing 13C and 15N allowed
discriminating which macronutrient (carbon or nitrogen) limited microbial growth. Accordingly, the switch in glyphosate transformation pathway from full mineralization to the formation of AMPA could be explained by an initial nitrogen deficit, which during the experiment changed to nitrogen saturation and demand for carbon, thus affecting the formation of biogenic NER. These findings highlight the benefit of combining advanced prediction methods and experimental approaches to obtain deeper insights into microbial metabolism, chemical persistence and biogenic NER formation.

**General information**
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Organisations: Environmental Fate & Effect of Chemicals, Department of Environmental Engineering, Technical University of Munich, RWTH Aachen University, Helmholtz Centre for Environmental Research
Number of pages: 1
Publication date: 2018
Peer-reviewed: Yes
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Electronic versions:
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**Modelling the fate of organic microcontaminants in wastewater treatment and agricultural reuse – Experiences from two existing cases**

**General information**
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, Urban Water Systems, University of Murcia, Technical University of Denmark, Fondazione Politecnico di Milano
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Event: Abstract from XENOWAC II, Limassol, Cyprus.
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**Persistance assessment for a circular economy**

**General information**
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Organisations: Environmental Fate & Effect of Chemicals, Department of Environmental Engineering
Contributors: Trapp, S., Polesel, F., Brock, A. L.
Number of pages: 1
Publication date: 2018

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Publisher: Technical University of Denmark (DTU)
Editors: Melero, C., K. M.
Article number: U-4
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http://www.sustain.dtu.dk/

**Phytoscreening for vinyl chloride in groundwater discharging to a stream**
This study applies an optimized phytoscreening method to locate a chlorinated ethene plume discharging into a stream. To evaluate the conditions most suitable for successful phytoscreening, trees along the stream bank were monitored.
through different seasons with different environmental conditions and hence different uptake/loss scenarios. Vinyl chloride (VC) as well as cis-dichloroethylene (cis-DCE), trichloroethylene (TCE), and tetrachloroethylene (PCE) were detected in the trees, documenting that phytoscreening is a viable method to locate chlorinated ethene plumes, including VC, discharging to streams. The results reveal, that phytoscreening for VC is more sensitive to environmental conditions affecting transpiration than for the other chlorinated ethenes detected. Conditions leading to higher groundwater uptake by transpiration than contaminant loss by diffusion from the tree trunks are optimal (e.g., low relative humidity, plentiful hours of sunshine and an intermediate air temperature). Additionally, low precipitation prior to the sampling event is beneficial, as uptake of infiltrating precipitation dilutes the concentration in the trees. All chlorinated ethenes were sensitive to dilution by clean precipitation and in some months, this resulted in no detection of contaminants in the trees at all. Under optimal environmental conditions the tree cores allowed detection of chlorinated solvents and their metabolites in the underlying groundwater. Whereas, for less ideal conditions there was a risk of no detection of the more volatile VC. This study is promising for the future applicability of phytoscreening to locate shallow groundwater contamination with the degradation products of chlorinated solvents.

**General information**
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals
Contributors: Ottosen, C. B., Rønde, V. K., Trapp, S., Bjerg, P. L., Broholm, M. M.
Pages: 66-74
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Journal: Ground Water Monitoring & Remediation
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Scopus rating (2018): CiteScore 1.25 SJR 0.692 SNIP 0.929
Web of Science (2018): Impact factor 1.192
Web of Science (2018): Indexed yes
Original language: English
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Post_Print_Phytoscreening_for_vinyl_chloride_in_groundwater_discharging_to_a_stream.pdf. Embargo ended: 11/01/2019
DOIs:
10.1111/gwmr.12253
Research output: Contribution to journal › Journal article – Annual report year: 2018 › Research › peer-review

**Predicting the fate of pharmaceuticals during wastewater treatment and crop irrigation with reclaimed wastewater**

**General information**
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, University of Murcia
Contributors: González-García, M., Fernández-López, C., Polesel, F., Trapp, S.
Pages: 360-361
Publication date: 2018

**Host publication information**
Title of host publication: SETAC Europe 28th Annual Meeting - Abstract book
Place of publication: Brussels, Belgium
Publisher: Society of Environmental Toxicology and Chemistry
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Abstract_Mariano_Gonz_lez_v2.pdf
abstract_book_scientific_part_FINAL_cover_3_1_.pdf
Source: PublicationPreSubmission
Source-ID: 148017817
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2018 › Research › peer-review

**Prediction of the formation of biogenic non-extractable residues during degradation of environmental chemicals from biomass yields**
Degradation tests with radio or stable isotope labeled compounds enable the detection of the formation of non-extractable residues (NER). In PBT and vPvB assessment, remobilisable NER are considered as a potential risk while biogenic NER from incorporation of labeled carbon into microbial biomass are treated as degradation products. Relationships between yield, released CO2 (as indicator of microbial activity and mineralization) and microbial growth can be used to estimate the formation of biogenic NER. We provide a new approach for calculation of potential substrate transformation to microbial biomass (theoretical yield) based on Gibbs free energy and microbially available electrons. We compare estimated theoretical yields of biotechnological substrates and of chemicals of environmental concern with experimentally determined yields for validation of the presented approach. A five-compartment dynamic model is applied to simulate experiments of 13C-labeled 2,4-D and ibuprofen turnover. The results show that bioNER increase with time, and that most bioNER originate from microbial proteins. Simulations with pre-calculated input data demonstrate that pre-calculation of yields reduces the number of fit parameters considerably, increases confidence in fitted kinetic data and reduces the uncertainty of the simulation results.

**General information**
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, Helmholtz Centre for Environmental Research
Contributors: Trapp, S., Brock, A. L., Nowak, K. M., Kästner, M.
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Issue number: 2
ISSN (Print): 0013-936X
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Scopus rating (2018): CiteScore 7.38 SJR 2.514 SNIP 1.959
Web of Science (2018): Impact factor 7.149
Web of Science (2018): Indexed yes
Original language: English
Electronic versions:
acs.est.7b04275.pdf. Embargo ended: 12/12/2018
DOI: 10.1021/acs.est.7b04275
Source: FindIt
Source-ID: 2393963233
Research output: Contribution to journal  Journal article – Annual report year: 2018  Research  peer-review

**Predictive models to assess the uptake of organic micro contaminants and antibiotic resistant bacteria and genes by crops**

**General information**
Publication status: Published
Organisations: Environmental Fate & Effect of Chemicals, Department of Environmental Engineering
Contributors: Bayona, J. M., Trapp, S., Piña, B., Polesel, F.
Pages: 262-285
Publication date: 2018

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Publisher: CRC Press
Editors: del Carmen Durán-Domínguez-de-Bazúa, M., Enrique Navarro-Frómeta, A., Bayona, J. M.
ISBN (Print): 9781138739185
Research output: Chapter in Book/Report/Conference proceeding  Book chapter – Annual report year: 2018  Research  peer-review

**Simulation of the fate of co-labeled 13C3-15N-glyphosate in a water-sediment system and formation of biogenic non-extractable residues**

**General information**
Publication status: Published
Organisations: Environmental Fate & Effect of Chemicals, Department of Environmental Engineering, Technical University of Berlin, Technical University of Munich, Helmholtz Centre for Environmental Research
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Place of publication: Brussels, Belgium
Publisher: Society of Environmental Toxicology and Chemistry
Article number: WE059
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Abstract book
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2018 › Research › peer-review

Simulation of the fate of co-labeled $^{13}$C$_3$-$^{15}$N-glyphosate in a water-sediment system and formation of biogenic non-extractable residues

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, Technical University of Munich, RWTH Aachen University, Helmholtz Centre for Environmental Research
Contributors: Brock, A. L., Rein, A., Polesel, F., Nowak, K. M., Kästner, M., Trapp, S.
Number of pages: 1
Publication date: 2018
Peer-reviewed: Yes
Event: Abstract from SETAC Europe 28th Annual Meeting, Rome, Italy.
Electronic versions:
SETAC_2018_5.pdf
Source: PublicationPreSubmission
Source-ID: 148017773
Research output: Contribution to conference › Conference abstract for conference – Annual report year: 2018 › Research › peer-review

Toxicity of 2,3,5,6-tetrachlorophenol to willow trees (Salix viminalis)
Chlorinated phenols have been intensively investigated from an eco-toxicological point of view, however almost nothing is known about toxicity of tetrachlorophenol (TeCP) to higher terrestrial plants. This paper applied the willow tree acute toxicity test to study the toxicity of 2,3,5,6-TeCP to willows Salix viminalis (S. viminalis) at neutral and acidic conditions (roughly pH 7 and 4) with inhibition of transpiration as toxic endpoint. At neutral pH the EC50 was $>10$ mg L$^{-1}$ while the EC50 at acidic conditions was $0.32 \pm 0.17$ mg L$^{-1}$, clearly indicating that toxicity is exerted by the non-ionic chemical fraction. Standard tests running at neutral pH are therefore not capturing the full toxicity of weak acids and bases.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals
Corresponding author: Clausen, L. P. W.
Contributors: Clausen, L. P. W., Jensen, C. K., Trapp, S.
Pages: 941-948
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: Human and Ecological Risk Assessment
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BFI (2018): BFI-level 1
Scopus rating (2018): CiteScore 2.02 SJR 0.483 SNIP 0.758
Web of Science (2018): Impact factor 2.012
Web of Science (2018): Indexed yes
Original language: English
Keywords: Ecological Modeling, Pollution, Health, Toxicology and Mutagenesis, chlorinated phenols, ionizing compounds, phytotoxicity, tetrachlorophenol, willow
Untangling the biodegradation of hydrophobic chemicals in OECD and novel tests using a unified modelling approach

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, RWTH Aachen University, Helmholtz Centre for Environmental Research
Pages: 16-16
Publication date: 2018

Host publication information
Title of host publication: SETAC Europe 28th Annual Meeting - Abstract book
Place of publication: Brussels, Belgium
Publisher: Society of Environmental Toxicology and Chemistry
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1._Unified_model_for_OECD_test_prediction_FINAL.pdf
abstract_book_scientific_part_FINAL_cover_3_1_.pdf
Source: PublicationPreSubmission
Source-ID: 148017517
Research output: Chapter in Book/Report/Conference proceeding – Conference abstract in proceedings – Annual report year: 2018 › Research › peer-review

Acute and semi-chronic toxicity of vanadium tested on copepods of the species Temora longicornis

General information
Publication status: Published
Organisations: National Institute of Aquatic Resources, Section for Oceans and Arctic, Department of Environmental Engineering, Environmental Chemistry, Technical University of Denmark
Contributors: Kristiansen, M. H., Iversen, N. H., Koski, M., Trapp, S.
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Place of publication: Kgs. Lyngby, Denmark
Publisher: Technical University of Denmark (DTU)
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ABSTRACT BOOK
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Research output: Chapter in Book/Report/Conference proceeding – Conference abstract in proceedings – Annual report year: 2017 › Research › peer-review

Diffusion and sorption of organic micropollutants in biofilms with varying thicknesses

Solid-liquid partitioning is one of the main fate processes determining the removal of micropollutants in wastewater. Little is known on the sorption of micropollutants in biofilms, where molecular diffusion may significantly influence partitioning kinetics. In this study, the diffusion and the sorption of 23 micropollutants were investigated in novel moving bed biofilm reactor (MBBR) carriers with controlled biofilm thickness (50, 200 and 500 μm) using targeted batch experiments (initial concentration = 1 μg L−1, for X-ray contrast media 15 μg L−1) and mathematical modelling. We assessed the influence of biofilm thickness and density on the dimensionless effective diffusivity coefficient f (equal to the biofilm-to-aqueous diffusivity ratio) and the distribution coefficient Kd,eq (L g−1). Sorption was significant only for eight positively charged micropollutants (atenolol, metoprolol, propranolol, citalopram, venlafaxine, erythromycin, clarithromycin and roxithromycin), revealing the importance of electrostatic interactions with solids. Sorption equilibria were likely not reached within the duration of batch experiments (4 h), particularly for the thickest biofilm, requiring the calculation of the
distribution coefficient $K_{d,eq}$ based on the approximation of the asymptotic equilibrium concentration ($t > 4\ h$). $K_{d,eq}$ values increased with increasing biofilm thickness for all sorptive micropollutants (except atenolol), possibly due to higher porosity and accessible surface area in the thickest biofilm. Positive correlations between $K_{d,eq}$ and micropollutant properties (polarity and molecular size descriptors) were identified but not for all biofilm thicknesses, thus confirming the challenge of improving predictive sorption models for positively charged compounds. A diffusion-sorption model was developed and calibrated against experimental data, and estimated $f$ values also increased with increasing biofilm thickness. This indicates that diffusion in thin biofilms may be strongly limited ($f \approx 0.1$) by the high biomass density (reduced porosity).

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Water Technologies, Environmental Chemistry, Aarhus University, Veolia Water Technologies AB
Contributors: Torresi, E., Polesel, F., Bester, K., Christensson, M., Smets, B. F., Trapp, S., Andersen, H. R., Plósz, B. G.
Pages: 388-400
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Peer-reviewed: Yes

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Web of Science (2017): Indexed yes
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Source: FindIt
Source-ID: 2371503865
Research output: Contribution to journal › Journal article – Annual report year: 2017 › Research › peer-review

Ecological effects of scrubber water discharge on coastal plankton: Potential synergistic effects of contaminants reduce survival and feeding of the copepod Acartia tonsa
To meet the oncoming requirements for lower sulphur emissions, shipping companies can install scrubbers where the exhaust is sprayed with seawater and subsequently discharged to the sea. The discharge water has a pH around 3 and contains elevated concentrations of vanadium, nickel, lead and hydrocarbons. We investigated 1) the threshold concentrations of scrubber discharge water for survival, feeding and reproduction of the copepod Acartia tonsa, 2) whether the effects depend on the exposure route and 3) whether exposure to discharge water can be detected in field-collected organisms. A direct exposure to discharge water increased adult copepod mortality and reduced feeding at metal concentrations which were orders of magnitude lower than the lethal concentrations in previous single-metal studies. In contrast, reproduction was not influenced by dietary uptake of contaminants. Scrubber water constituents could have synergistic effects on plankton productivity and bioaccumulation of metals, although the effects will depend on their dilution in the marine environment.

General information
Publication status: Published
Organisations: National Institute of Aquatic Resources, Section for Oceans and Arctic, Department of Environmental Engineering, Environmental Chemistry
Contributors: Koski, M., Stedmon, C., Trapp, S.
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Publication date: 2017
Peer-reviewed: Yes

Publication information
Journal: Marine Environmental Research
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Ecological effects of scrubber water discharge on coastal plankton: Potential synergistic effects of contaminants reduce survival and feeding of the copepod *Acartia tonsa*

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Organisations: National Institute of Aquatic Resources, Section for Oceans and Arctic, Department of Environmental Engineering, Environmental Chemistry
Contributors: Koski, M., Stedmon, C., Trapp, S.
Number of pages: 1
Publication date: 2017

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Article number: A-9
Electronic versions:
*SustainAbstracts2017c.compressed_12.pdf*
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2017 › Research › peer-review

Environmental risk assessment of poorly soluble substances: Improved tools for assessing biodegradation, (de)sorption, and modeling (project RABIT)

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Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, RWTH Aachen University, German Federal Environment Agency
Contributors: Müller, M. E., Stibany, F., Polesel, F., Smith, K. E. C., Schulte, C., Trapp, S., Schäffer, A.
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Electronic versions:
*Müller_Poster_SETAC.pdf*
Source: PublicationPreSubmission
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Fate prediction and mass balances verification of pharmaceuticals compounds in Roldán-Balsicas WWTP (Murcia, Spain)

**General information**
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Murcia
Contributors: González-Garcia, M., Polesel, F., Trapp, S., Fernández-López (, C.
Number of pages: 1
Publication date: 2017
Peer-reviewed: Yes
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Microbial growth yield as a new parameter in environmental chemistry and risk assessment

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Organisations: Department of Environmental Engineering, Environmental Chemistry, Helmholtz Centre for Environmental Research
Contributors: Brock, A. L., Kästner, M., Trapp, S.
Number of pages: 1
Publication date: 2017
Peer-reviewed: Yes
Event: Abstract from 14th International Symposium on Persistent Toxic Substances, Nagoya, Japan.
Electronic versions: abstract_IS_PTS2017_Microbial_growth_yield_as_a_new_parameter_in_environmental_chemistry_and_riskassessment.pdf

Microbial growth yield estimates from thermodynamics and its importance for degradation of pesticides and formation of biogenic non-extractable residues

In biodegradation studies with isotope-labelled pesticides, fractions of non-extractable residues (NER) remain, but their nature and composition is rarely known, leading to uncertainty about their risk. Microbial growth leads to incorporation of carbon into the microbial mass, resulting in biogenic NER. Formation of microbial mass can be estimated from the microbial growth yield, but experimental data is rare. Instead, we suggest using prediction methods for the theoretical yield based on thermodynamics. Recently, we presented the Microbial Turnover to Biomass (MTB) method that needs a minimum of input data. We have estimated the growth yield of 40 organic chemicals (31 pesticides) using the MTB and two existing methods. The results were compared to experimental values, and the sensitivity of the methods was assessed. The MTB method performed best for pesticides. Having the theoretical yield and using the released CO2 as a measure for microbial activity, we predicted a range for the formation of biogenic NER. For the majority of the pesticides, a considerable fraction of the NER was estimated to be biogenic. This novel approach provides a theoretical foundation applicable to the evaluation and prediction of biogenic NER formation during pesticide degradation experiments, and may also be employed for the interpretation of NER data from regulatory studies.

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Sorption and diffusion of micropollutants on/in biofilms: experimental observations and a model-based interpretation

In this study we investigated the diffusion and sorption of 22 pharmaceuticals in/on nitrifying biofilms of different thickness. Experimental observations were subject to model-based interpretation and the assessment of a sorption coefficient $K_d$ and effective diffusivity coefficient $f$. Three biofilm depths were obtained by using Z-carriers (AnoxKaldnes) as support, which allows tight control of biofilm thickness. Biofilms of increasing thickness had increased porosity (and thus decreasing density). Sorption was significant for the positively charged compounds at experimental pH (with few exceptions) and $K_d$ increased with biofilm thickness. The effective diffusivity $f$ negatively correlated with biofilm density, suggesting that diffusion of micropollutants in thinner biofilms could be limited. Overall, this study elucidated how biofilm thickness can positively influence sorption of micropollutants on biofilm as well as how diffusion limitation is strongly impact by biofilm characteristics (density and porosity) and the specific chemical.

Test of aerobic TCE degradation by willows (Salix viminalis) and willows inoculated with TCE-cometabolizing strains of Burkholderia cepacia

Trichloroethylene (TCE) is a widespread soil and groundwater pollutant and clean-up is often problematic and expensive. Phytoremediation may be a cost-effective solution at some sites. This study investigates TCE degradation by willows (S. viminalis) and willows inoculated with three strains of B. cepacia (301C, PR1-31 and VM1330-pTOM), using chloride formation as an indicator of dehalogenation. Willows were grown in non-sterile, hydroponic conditions for 3 weeks in chloride-free nutrient solution spiked with TCE. TCE was added weekly due to rapid loss by volatilization. Chloride and TCE in solution were measured every 2-3 days and chloride and metabolite concentrations in plants were measured at test termination. Based on transpiration, no tree toxicity of TCE exposure was observed. However, trees grown in chloride-free solution showed severely inhibited transpiration. No or very little chloride was formed during the test, and levels of chloride in TCE-exposed trees were not elevated. Chloride concentrations in chloride containing TCE-free nutrient solution doubled within 23 days, indicating active exclusion of chloride by root cell membranes. Only traces of TCE-metabolites were detected in plant tissue. We conclude that TCE is not, or to a limited extent (less than 3%), aerobically degraded by the willow trees. The three strains of B. cepacia did not enhance TCE mineralization. Future successful application of rhizo- and phytodegradation of TCE requires measures to be taken to improve the degradation rates.
Toxicity of 56 substances to trees

Toxicity data of substances to higher plants is needed for the purpose of risk assessment, site evaluation, phytoremediation, and plant protection. However, the results from the most common phytotoxicity tests, like the OECD algae and Lemna test, are not necessarily valid for higher terrestrial plants. The willow tree toxicity test uses inhibition of transpiration (aside of growth and water use efficiency) of willow cuttings grown in spiked solutions or soils as end point to quantify toxicity. This overview presents results from 60 studies including 24 new unpublished experiments for 56 different chemicals or substrates. Highest toxicity (EC50 < 1 mg/L) was observed from exposure to heavy metals like copper and cadmium. Also, organotins and free cyanide showed very high toxicity. The toxic effect of chlorophenols on willows was comparable to that on duck weed (Lemna) and green algae, while volatile compounds like chlorinated solvents or benzene, toluene, ethylbenzene, and xylene had less effect on trees than on these aquatic plants, due to volatilization from leaves and test media. In particular low (g/L range) toxicity was observed for tested nanomaterials. Effects of pharmaceuticals (typically weak acids or bases) depended strongly of the solution pH. Like for algae, baseline toxicity was observed for willows, which is related to the water solubility of the compounds, with absolute chemical activity ranging from 0.01 to 0.1, but with several exceptions. We conclude that the willow tree toxicity test is a robust method for relating uptake, accumulation, and metabolism of substances to the toxicity to trees.
Analyzing tree cores to detect petroleum hydrocarbon-contaminated groundwater at a former landfill site in the community of Happy Valley-Goose Bay, eastern Canadian subarctic

This research examines the feasibility of analyzing tree cores to detect benzene, toluene, ethylbenzene, and m, p, o-xylene (BTEX) compounds and methyl tertiary-butyl ether (MTBE) in groundwater in eastern Canada subarctic environments, using a former landfill site in the remote community of Happy Valley-Goose Bay, Labrador. Petroleum hydrocarbon contamination at the landfill site is the result of environmentally unsound pre-1990s disposal of households and industrial solid wastes. Tree cores were taken from trembling aspen, black spruce, and white birch and analyzed by headspace-gas chromatography-mass spectrometry. BTEX compounds were detected in tree cores, corroborating known groundwater contamination. A zone of anomalously high concentrations of total BTEX constituents was identified and recommended for monitoring by groundwater wells. Tree cores collected outside the landfill site at a local control area suggest the migration of contaminants off-site. Tree species exhibit different concentrations of BTEX constituents, indicating selective uptake and accumulation. Toluene in wood exhibited the highest concentrations, which may also be due to endogenous production. Meanwhile, MTBE was not found in the tree cores and is considered to be absent in the groundwater. The results demonstrate that tree-core analysis can be useful for detecting anomalous concentrations of petroleum hydrocarbons, such as BTEX compounds, in subarctic sites with shallow unconfined aquifers and permeable soils. This method can therefore aid in the proper management of contamination during landfill operations and after site closures.

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A suggested minimum data list for documenting experimental plant uptake studies

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Bringing modelling to life: current research in an introductory MSc modelling course

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Environmental risk assessment of poorly soluble substances: Improved tools for assessing biodegradation, (de)sorption, and modeling

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Environmental risk assessment of poorly soluble substances: Improved tools for assessing biodegradation, (de)sorption, and modeling (project RABIT)

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Experiments and inverse modeling to plant uptake and degradation of eight emerging organic contaminants

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**How active ingredient localisation in plant tissues determines the targeted pest spectrum of different chemistries**

**BACKGROUND:**  
The efficacies of four commercial insecticides and of two research compounds were tested against aphids (Aphis craccivora and Myzus persicae), whiteflies (Bemisia tabaci) and red-spotted spider mites (Tetranychus urticae) in intrinsic (oral administration), curative (direct contact spray) and translaminar (arthropods infested on untreated leaf underside) assays. With a new translaminar model, the transport across the leaf cuticle and tissues and the electrochemical distribution of test compounds in cellular compartments and apoplast were calculated.

**RESULTS:**  
The comparison of both information sets revealed that the intracellular localisation of active ingredients determines the performance of test compounds against different target pests because of different feeding behaviours: mites feed on mesophyll, and aphids and whiteflies mostly in the vascular system. Polar compounds have a slow adsorption into leaf cells and thus a favourable distribution into apoplast and xylem sap. Slightly lipophilic bases get trapped in vacuoles, which is a less suited place to control hemipteran pests but appropriate to control mites. Non-favourable cellular localisation led to a strong reduction in translaminar efficacy against phloem feeders.

**CONCLUSION:**  
Prediction and optimisation of intracellular localisation of pesticides add valuable new information for targeted bioavailability and can indicate directions for improved pesticide design. © 2015 Society of Chemical Industry.

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Impact of bacterial activity on turnover of insoluble hydrophobic substrates (phenanthrene and pyrene)—Model simulations for prediction of bioremediation success

Many attempts for bioremediation of polycyclic aromatic hydrocarbon (PAH) contaminated sites failed in the past, but the reasons for this failure are not well understood. Here we apply and improve a model for integrated assessment of mass transfer, biodegradation and residual concentrations for predicting the success of remediation actions. First, we provide growth parameters for Mycobacterium rutuli and Mycobacterium palens growing on phenanthrene (PHE) or pyrene (PYR) degraded the PAH completely at all investigated concentrations. Maximum metabolic rates vmax and growth rates μ were similar for the substrates PHE and PYR and for both strains. The investigated Mycobacterium species were not superior in PHE degradation to strains investigated earlier with this method. Real-world degradation scenario simulations including diffusive flux to the microbial cells indicate: that (i) bioaugmentation only has a small, short-lived effect; (ii) Increasing sorption shifts the remaining PAH to the adsorbed/sequestered PAH pool; (iii) mobilizing by solvents or surfactants resulted in a significant decrease of the sequestered PAH, and (iv) co-metabolization e.g. by compost addition can contribute significantly to the reduction of PAH, because active biomass is maintained at a high level by the compost. The model therefore is a valuable contribution to the assessment of potential remediation action at PAH-polluted sites.

Inverse modeling of the biodegradation of emerging organic contaminants in the soil-plant system

Understanding the processes involved in the uptake and accumulation of organic contaminants into plants is very important to assess the possible human risk associated with. Biodegradation of emerging contaminants in plants has been observed, but kinetical studies are rare. In this study, we analyse experimental data on the uptake of emerging organic contaminants into lettuce derived in a greenhouse experiment. Measured soil, root and leaf concentrations from four contaminants were selected within the applicability domain of a steady-state two-compartment standard plant uptake model: bisphenol A (BPA), carbamazepine (CBZ), triclosan (TCS) and caffeine (CAF). The model overestimated concentrations in most cases, when no degradation rates in plants were entered. Subsequently, biodegradation rates were fitted so that the measured concentrations were met. Obtained degradation kinetics are in the order, BPA <CAF <TCS <CBZ in roots, and BPA < TCS <CBZ.
The utilisation of a given substrate leads to bacterial growth and the associated yield is normally determined experimentally. Different yield estimation methods exist based on knowledge of the Gibbs energy of reaction and the energy needed for synthesis of new biomass [1-4]. Estimating yield from thermodynamic considerations of stoichiometrically balanced reactions is typically done in biotechnology and wastewater treatment [5], an approach recently adopted by Helbling et al. [6]. More recent methods specifically incorporate detailed knowledge of the degradation pathway and bacterial metabolism to attain predictions closer to the experimentally observed yields [3]. However, this knowledge is seldom known for xenobiotics in the environment but is needed to assess the turnover leading to biomass production, i.e. for sludge production or biogenic residues. The objectives of the present study were thus to (i) formulate and use a simple quantitative structure-activity relationship to estimate a minimum growth yield under aerobic conditions and (ii) compare the estimations with experimental results from literature. We based our estimation method on the approach suggested by Diekert [2], requiring as input just the Gibbs energy of formation of the reactants and products and a limited amount of structural data (e.g., the number of carbon atoms in the substrate). To estimate the yield, the Gibbs energy of reaction was quantified from balanced mineralisation reactions as the difference between the Gibbs energy of formation of the products and reactants. The Gibbs energy of the mineralisation reaction can be regarded as the maximum...
energy released and partly captured by the biomass. The carbon present in the substrate is used for synthesis and oxidised to CO2 to yield energy for anabolism. We accounted for this by specifying how much of the energy can be used as a function of the chemical structure based on general rules of microbial turnover. Thus, we obtain a minimum yield from use of the substrate as a sole source of energy and carbon. In order to test the applicability of our estimation method, we evaluated it with both simple substrates (e.g. acetate, methanol, and glyoxylate) and xenobiotics (e.g 2,4-D, linuron, carbofuran, carbon tetrachloride, and toluene). Experimental data for the simple substrates were taken from [4], for xenobiotics from [6] and own experimental data. For simple substrates, our approach predicts yields close to experimental values and also for xenobiotics the yield predictions for most of the compounds are close to the experimentally obtained values. Overall, with our method we were able to obtain yield predictions close to experimental values with a minimum of input information. Mor

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Removal of Antibiotics in Biological Wastewater Treatment Systems—A Critical Assessment Using the Activated Sludge Modeling Framework for Xenobiotics (ASM-X)
Many scientific studies present removal efficiencies for pharmaceuticals in laboratory-, pilot-, and full-scale wastewater treatment plants, based on observations that may be impacted by theoretical and methodological approaches used. In this Critical Review, we evaluated factors influencing observed removal efficiencies of three antibiotics (sulfamethoxazole, ciprofloxacin, tetracycline) in pilot- and full-scale biological treatment systems. Factors assessed include (i) retransformation to parent pharmaceuticals from e.g., conjugated metabolites and analogues, (ii) solid retention time (SRT), (iii) fractions sorbed onto solids, and (iv) dynamics in influent and effluent loading. A recently developed methodology was used, relying on the comparison of removal efficiency predictions (obtained with the Activated Sludge Model for Xenobiotics (ASM-X)) with representative measured data from literature. By applying this methodology, we demonstrated that (a) the elimination of sulfamethoxazole may be significantly underestimated when not considering retransformation from conjugated metabolites, depending on the type (urban or hospital) and size of upstream catchments; (b) operation at extended SRT may enhance antibiotic removal, as shown for sulfamethoxazole; (c) not accounting for fractions sorbed in influent and effluent solids may cause slight underestimation of ciprofloxacin removal efficiency. Using tetracycline as example substance, we ultimately evaluated implications of effluent dynamics and retransformation on environmental exposure and risk prediction.

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Simulation and prediction of biomass turnover and soil organic matter formation

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Soil and Plant Contamination – Modelling and Simulation of Processes

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Toxicity testing with the willow tree transpiration test - 15 years of results

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Addressing the Chinese water challenges with hydroeconomic modelling

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Organisations: Department of Environmental Engineering, Water Resources Engineering, Environmental Chemistry, Chinese Academy of Sciences, University of Copenhagen
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Aerobic TCE degradation by willows and three root colonizing strains of B. cepacia

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Analysing half-lives for pesticide dissipation in plants
Overall dissipation of pesticides from plants is frequently measured, but the contribution of individual loss processes is largely unknown. We use a pesticide fate model for the quantification of dissipation by processes other than degradation. The model was parameterised using field studies. Scenarios were established for Copenhagen/Denmark and Shanghai/PR China, and calibrated with measured results. The simulated dissipation rates of 42 pesticides were then compared with measured overall dissipation from field studies using tomato and wheat. The difference between measured overall dissipation and calculated dissipation by non-degradative processes should ideally be contributable to degradation in plants. In 11% of the cases, calculated dissipation was above the measured dissipation. For the remaining cases, the non-explained dissipation ranged from 30% to 83%, depending on crop type, plant part and scenario. Accordingly, degradation is the most relevant dissipation process for these 42 pesticides, followed by growth dilution. Volatilisation was less relevant, which can be explained by the design of plant protection agents. Uptake of active compound from soil into plants leads to a negative dissipation process (i.e. a gain) that is difficult to quantify because it depends largely on interception, precipitation and plant stage. This process is particularly relevant for soluble compounds.

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Contributors: Jacobsen, R., Fantke, P., Trapp, S.
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Journal: S A R and Q S A R in Environmental Research
Biocides from façade coatings in urban surface waters: Estimating the leaching of biocides from render by polyacrylate-water partitioning constants?

Leaching of biocides from façade coatings attracts more and more attention within recent years. In-can as well as film preserving biocides are added to polymer resin based renders and paints in order protect from microbial spoilage. However, several studies revealed that biocides leach from the façade coating and are detectable in urban stormwater runoff. The present study focussed on the occurrence of biocides in the aqueous environment - both in urban water close to the sources as well as further away in fresh and marine waters. It could be shown that biocides are ubiquitous in the aqueous environment. They are detectable not only close to their sources in stormwater run-off but also further away in marine waters with concentrations up to 60 ng L⁻¹ (mecoprop up to 200 ng L⁻¹). Further work was done in order to estimate the leaching of biocides from building material. The possibility of using polyacrylate-water partition constants in comparison to render-water distribution constants was introduced for this purpose. The results showed that polyacrylate-water partition constants might serve as a useful and practical tool which would be closer to the reality than the commonly used water solubility and octanol-water partition constants.

Calibration of a Plant Uptake Model with Plant- and Site-Specific. Data for Uptake of Chlorinated Organic Compounds into Radish

The uptake of organic pollutants by plants is an important process for the exposure of humans to toxic chemicals. The objective of this study was to calibrate the parameters of a common plant uptake model by comparison to experimental results from literature. Radish was grown in contaminated soil (maximum concentration 2.9 mg/kg dw) and control plot. Uptake of HCHs, HCB, PCBs and DDT plus metabolites was studied (log Kow 3.66 to 7.18). Measured BCF roots-to-soil were near 1 g/g dw on the control plot and about factor 10 lower for the contaminated soil. With default data set, uptake into roots of most substances was under predicted up to factor 100. The use of site-specific data improved the predictions. Consideration of uptake from air into radish bulbs was relevant for PCBs. Measured BCF shoots ranged from <0.1 to >10 g/g dw and were much better predicted by the standard model. The results with default data and site-specific data were similar. Deposition from air was the major uptake mechanism into shoots. Transport from soil with resuspended particles was only relevant for the contaminated plot. The calculation results (in dry weight) were most sensitive to changes of the water content of plant tissue.
Classification and modelling of non-extractable residue (NER) formation from pesticides in soil

This presentation provides a comprehensive overview about the formation of nonextractable residues (NER) from organic pesticides and contaminants in soil and tries classifying the different types. Anthropogenic organic chemicals are deliberately (e.g. pesticides) or unintentionally (e.g. polyaromatic hydrocarbons [PAH], chlorinated solvents, pharmaceuticals) released in major amounts to nearly all compartments of the environment. Soils and sediments as complex matrices provide a wide variety of binding sites and are the major sinks for these compounds. Many of the xenobiotics entering soil undergo turnover processes and can be volatilised, leached to the groundwater, degraded by microorganisms or taken up and enriched by living organisms. Xenobiotic NER may be derived from parent compounds and primary metabolites that are sequestered (sorbed or entrapped) within the soil organic matter (type I) or can be covalently bound (type II). Both types may pose a considerably environmental risk of potential release. However, NER resulting from elevated biodegradation, which means the conversion of carbon (or nitrogen) from the compounds into microbial biomass molecules during microbial degradation (type III, bioNER), do not pose any risk. Experimental and analytical approaches to clearly distinguish between the types are provided and a model to prospectively estimate their fate in soil is proposed.

Comparison of Phytoscreening and Direct-Push- Based Site Investigation at a Rural Megasite Contaminated with Chlorinated Ethenes
The reliable characterization of subsurface contamination of spatially extended contaminated sites is a challenging task, especially with an unknown history of land use. Conventional technologies often fail due to temporal and financial constraints and thus hinder the redevelopment of abandoned areas in particular. Here we compare two site screening techniques that can be applied quickly at relatively low cost, namely Direct Push (DP)-based groundwater sampling and tree core sampling. The effectiveness of both methods is compared for a rural megasite contaminated with chlorinated hydrocarbons. Unexpected pollution hot spots could be identified using both of these methods, while tree coring even enabled the delineation of the contaminant plume flowing into an adjacent wetland inaccessible for DP units. Both methods showed a good agreement in revealing the spatial pattern of the contamination. The correlation between groundwater concentrations and equivalent concentrations in wood was linear and highly significant for trichloroethene. Correlation was less obvious for its metabolite cis-dichloroethylene, but still significant. As outcome of our study we recommend tree coring and for initial screening in combination with a DP sampling to retrieve quantitative data on groundwater pollutants in order to assess the contamination situation of a non- or only partly investigated site. The subsequent placement of monitoring wells for long-term monitoring of contamination levels is recommended. A combination of methods would achieve more relevant information at comparable or possibly even lower efforts in comparison to a conventional site investigation.

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Research output: Contribution to journal › Journal article – Annual report year: 2015 › Research › peer-review

Does intake of trace elements through urban gardening in Copenhagen pose a risk to human health?
This study investigates the potential health risk from urban gardening. The concentrations of the trace elements arsenic (As), cadmium (Cd), chromium (Cr), copper (Cu), lead (Pb), nickel (Ni), and zinc (Zn) in five common garden crops from three garden sites in Copenhagen were measured. Concentrations (mg/kg dw) of As were 0.002-0.21, Cd 0.03-0.25, Cr < 0.096-0.38, Cu 1.8e8.7, Ni < 0.23e0.62, Pb 0.05e1.56, and Zn 10e86. Generally, elemental concentrations in the crops do not reflect soil concentrations, nor exceed legal standards for Cd and Pb in food. Hazard quotients (HQs) were calculated from soil ingestion, vegetable consumption, measured trace element concentrations and tolerable intake levels. The HQs for As, Cd, Cr, Cu, Ni, and Zn do not indicate a health risk through urban gardening in Copenhagen. Exposure to Pb contaminated sites may lead to unacceptable risk not caused by vegetable consumption but by unintentional soil ingestion.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Copenhagen
Contributors: Warming, M., Hansen, M. G., Holm, P. E., Magid, J., Hansen, T. H., Trapp, S.
Pages: 17-23
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Environmental Pollution
Effective and reliable site investigation at large sites by the use of initial screening methods

Factors influencing sorption of ciprofloxacin onto activated sludge: Experimental assessment and modelling implications
From consumption to harvest: Environmental fate prediction of excreted ionizable trace organic chemicals

Excreted trace organic chemicals, e.g., pharmaceuticals and biocides, typically undergo incomplete elimination in municipal wastewater treatment plants (WWTPs) and are released to surface water via treated effluents and to agricultural soils through sludge amendment and/or irrigation with freshwater or reclaimed wastewater. Recent research has shown the tendency for these substances to accumulate in food crops. In this study, we developed and applied a simulation tool to predict the fate of three ionizable trace chemicals (triclosan-TCS, furosemide-FUR, ciprofloxacin-CIP) from human consumption/excretion up to the accumulation in soil and plant, following field amendment with sewage sludge or irrigation with river water (assuming dilution of WWTP effluent). The simulation tool combines the SimpleTreat model modified for fate prediction of ionizable chemicals in a generic WWTP and a recently developed dynamic soil-plant uptake model. The simulation tool was tested using country-specific (e.g., consumption/emission rates, precipitation and temperature) input data. A Monte Carlo-based approach was adopted to account for the uncertainty associated to physico-chemical and biokinetic model parameters. Results obtained in this study suggest significant accumulation of TCS and CIP in sewage sludge (1.4-2.8 mg kgDW-1) as compared to FUR (0.02-0.11 mg kgDW-1). For the latter substance, more than half of the influent load (60.1%-72.5%) was estimated to be discharged via WWTP effluent. Specific emission rates (g ha-1 a-1) of FUR to soil via either sludge application or irrigation were up to 300 times lower than for TCS and CIP. Nevertheless, high translocation potential to wheat was predicted for FUR, reaching concentrations up to 4.3 μg kgDW-1 in grain. Irrigation was found to enhance the relative translocation of FUR to plant (45.3%-48.9% of emission to soil), as compared to sludge application (21.9%-27.6%). A comparison with peer-reviewed literature showed that model predictions were close to experimental data for elimination in WWTP, concentrations in sewage and sludge and bioconcentration factors (BCFs) in plant tissues, which showed however a large variability. The simulation tool presented here can thus be useful for priority setting and for the estimation of human exposure to trace chemicals via intake of food crops.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Environmental Chemistry
Contributors: Polesel, F., Plósz, B. G., Trapp, S.
Pages: 85-98
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Water Research
Volume: 84
ISSN (Print): 0043-1354
Ratings:
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6.63 SJR 2.665 SNIP 2.476
Web of Science (2015): Impact factor 5.991
Web of Science (2015): Indexed yes
Original language: English
Keywords: Fate modeling, Ionizable organic trace chemicals, Wastewater treatment, Plant uptake, Agricultural sludge reuse, Irrigation
DOIs:
10.1016/j.watres.2015.06.033
Source: PublicationPreSubmission
Source-ID: 114520101
Research output: Contribution to journal › Journal article – Annual report year: 2015 › Research › peer-review

Hydroeconomic optimization of reservoir management under downstream water quality constraints
A hydroeconomic optimization approach is used to guide water management in a Chinese river basin with the objectives of meeting water quantity and water quality constraints, in line with the China 2011 No. 1 Policy Document and 2015 Ten-point Water Plan. The proposed modeling framework couples water quantity and water quality management and minimizes the total costs over a planning period assuming stochastic future runoff. The outcome includes cost-optimal reservoir releases, groundwater pumping, water allocation, wastewater treatments and water curtailments. The
optimization model uses a variant of stochastic dynamic programming known as the water value method. Nonlinearity arising from the water quality constraints is handled with an effective hybrid method combining genetic algorithms and linear programming. Untreated pollutant loads are represented by biochemical oxygen demand (BOD), and the resulting minimum dissolved oxygen (DO) concentration is computed with the Streeter-Phelps equation and constrained to match Chinese water quality targets. The baseline water scarcity and operational costs are estimated to 15.6 billion CNY/year. Compliance to water quality grade III causes a relatively low increase to 16.4 billion CNY/year. Dilution plays an important role and increases the share of surface water allocations to users situated furthest downstream in the system. The modeling framework generates decision rules that result in the economically efficient strategy for complying with both water quantity and water quality constraints.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Water Resources Engineering, Environmental Chemistry, Chinese Academy of Sciences, University of Copenhagen
Contributors: Davidsen, C., Liu, S., Mo, X., Holm, P. E., Trapp, S., Rosbjerg, D., Bauer-Gottwein, P.
Number of pages: 11
Pages: 1679-1689
Publication date: 2015
Peer-reviewed: Yes

Publication information
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Volume: 529
ISSN (Print): 0022-1694
Ratings:
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.54 SJR 1.686 SNIP 1.748
Web of Science (2015): Impact factor 3.043
Web of Science (2015): Indexed yes
Original language: English
Keywords: Hydroeconomic modeling, Integrated water resources management (IWRM), River basin, Stochastic dynamic programming (SDP), Water quality management, Water value, Biochemical oxygen demand, Costs, Dissolved oxygen, Dynamic programming, Genetic algorithms, Groundwater, Linear programming, Optimization, Quality management, Reservoir management, Reservoirs (water), Runoff, Stochastic models, Stochastic systems, Surface waters, Wastewater treatment, Water conservation, Water management, Water pollution, Water quality, Watersheds, Biochemical oxygen demands (BOD), Dissolved oxygen concentrations, Hydro-economic optimizations, Integrated Water Resources Management, Optimization modeling, River basins, Stochastic dynamic programming, Water resources
Electronic versions:
PostPrint_Davidsen_JoH.pdf. Embargo ended: 10/12/2016
DOIs:
10.1016/j.jhydrol.2015.08.018
Source: FindIt
Source-ID: 276431074
Research output: Contribution to journal › Journal article – Annual report year: 2015 › Research › peer-review

Modelling the Fate of Ionizable Trace Organic Chemicals from Consumption to Food Crops
In this study, we developed and applied a simulation tool to comprehensively predict the fate of three ionizable trace chemicals (triclosan—TCS, furosemide—FUR, ciprofloxacin—CIP) from human consumption/excretion up to the accumulation in wheat, following application of sewage sludge or irrigation with river water. Highest translocation to wheat (4.3 μg kgDW-1 in grain) was calculated for FUR, being more significant with irrigation (>45% of emission to soil) than with sludge application (<30%). The simulation tool presented here can be used for estimating human exposure to trace chemicals via food crop intake and for priority setting among emerging pollutants.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Water Technologies, Environmental Chemistry
Contributors: Polesel, F., Plósz, B. G., Trapp, S.
Number of pages: 2
Publication date: 2015
Peer-reviewed: Yes
Event: Abstract from 9th IWA Specialist Conference on Assessment and Control of Micropollutants and Hazardous Substances in Water, Singapore, Singapore.
Keywords: fate modelling of ionizable trace chemicals, plant uptake
Electronic versions:
Optimizing basin-scale coupled water quantity and water quality management with stochastic dynamic programming

Few studies address water quality in hydro-economic models, which often focus primarily on optimal allocation of water quantities. Water quality and water quantity are closely coupled, and optimal management with focus solely on either quantity or quality may cause large costs in terms of the other component. In this study, we couple water quality and water quantity in a joint hydro-economic catchment-scale optimization problem. Stochastic dynamic programming (SDP) is used to minimize the basin-wide total costs arising from water allocation, water curtailment and water treatment. The simple water quality module can handle conservative pollutants, first order depletion and non-linear reactions. For demonstration purposes, we model pollutant releases as biochemical oxygen demand (BOD) and use the Streeter-Phelps equation for oxygen deficit to compute the resulting minimum dissolved oxygen concentrations. Inelastic water demands, fixed water allocation curtailment costs and fixed wastewater treatment costs (before and after use) are estimated for the water users (agriculture, industry and domestic). If the BOD concentration exceeds a given user pollution threshold, the user will need to pay for pre-treatment of the water before use. Similarly, treatment of the return flow can reduce the BOD load to the river. A traditional SDP approach is used to solve one-step-ahead sub-problems for all combinations of discrete reservoir storage, Markov Chain inflow classes and monthly time steps. Pollution concentration nodes are introduced for each user group and untreated return flow from the users contribute to increased BOD concentrations in the river. The pollutant concentrations in each node depend on multiple decision variables (allocation and wastewater treatment) rendering the objective function non-linear. Therefore, the pollution concentration decisions are outsourced to a genetic algorithm, which calls a linear program to determine the remainder of the decision variables. This hybrid formulation keeps the optimization problem computationally feasible and represents a flexible and customizable method. The method has been applied to the Ziya River basin, an economic hotspot located on the North China Plain in Northern China. The basin is subject to severe water scarcity, and the rivers are heavily polluted with wastewater and nutrients from diffuse sources. The coupled hydro-economic optimization model can be used to assess costs of meeting additional constraints such as minimum water quality or to economically prioritize investments in wastewater treatment facilities based on economic criteria.
Phytoscreening and remediation of brownfield mega-sites

Phytotoxicity of Sodium Fluoride and Uptake of Fluoride in Willow Trees
The willow tree (Salix viminalis) toxicity test and a cress seed germination test (Lepidium sativum) were used to determine uptake and phytotoxicity of NaF. Concentrations in hydroponic solutions were 0-1000 mg F/L and 0-400 mg F/L in the preliminary and definitive test. A third test was done with soils collected from a fluoride-contaminated site at Fredericia, Denmark. The EC_{10}, EC_{20} and EC_{50} values for inhibition of transpiration were determined to 38.0, 59.6 and 128.7 mg F/L, respectively. The toxicity test with soil showed strong inhibition for the sample with the highest fluoride concentration (405 mg free F per kg soil, 75 mg F per L soil solution). The seed germination and root elongation test with cress gave EC_{10}, EC_{20} and EC_{50} values of 61.4, 105.0 and 262.8 mg F/L, respectively. At low external concentrations, fluoride was taken up more slowly than water and at high external concentrations at the same velocity. This indicates that an efflux pump becomes overloaded at concentrations above 210 mg F/L. Uptake kinetics were simulated with a non-linear mathematical model, and the Michaelis-Menten parameters were determined to half-saturation constant K_M near 2 g F/L and maximum enzymatic removal rate v_{max} at 9 g/(kg d).

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Aarhus University
Contributors: Clausen, L. P. W., Gosewinkel Karlson, U., Trapp, S.
Pages: 369-376
Publication date: 2015
Peer-reviewed: Yes

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Journal: International Journal of Phytoremediation
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Scopus rating (2015): CiteScore 2.17 SJR 0.702 SNIP 1.076
Web of Science (2015): Impact factor 2.085
Web of Science (2015): Indexed yes
Original language: English
DOIs:
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URLs:
http://www.tandfonline.com/doi/abs/10.1080/15226514.2014.910166#.VA7YgmPSqQo
Source: PublicationPreSubmission
Source-ID: 99723859
Research output: Contribution to journal › Journal article – Annual report year: 2014 › Research › peer-review

Regeneration of brownfield mega-sites - a review of existing and emerging technologies and their application for a test-site

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Water Resources Engineering, Institute for Ecology of Industrial Areas, University of Franche-Comté, Helmholtz Centre for Environmental Research
Contributors: Clausen, L. P. W., Bartke, S., Kalisz, M., Krupanek, J., Fatin-Rouge, N., Nielsen, M. A., Trapp, S.
Number of pages: 1
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Title of host publication: Book of abstracts - 13th International UFZ-Deltares Conference on sustainable Use and Management of Soil, Sediment and Water Resources (AquaConSoil) 2015
Electronic versions:
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Soil retention of hexavalent chromium released from construction and demolition waste in a road-base-application scenario

We investigated the retention of Cr(VI) in three subsoils with low organic matter content in laboratory experiments at concentration levels relevant to represent leachates from construction and demolition waste (C&DW) reused as unbound material in road construction. The retention mechanism appeared to be reduction and subsequent precipitation as Cr(III) on the soil. The reduction process was slow and in several experiments it was still proceeding at the end of the six-month experimental period. The overall retention reaction fit well with a second-order reaction governed by actual Cr(VI) concentration and reduction capacity of the soil. The experimentally determined reduction capacities and second-order kinetic parameters were used to model, for a 100-year period, the one-dimensional migration of Cr(VI) in the subsoil under a layer of C&DW. The resulting Cr(VI) concentration would be negligible below 7–70 cm depth. However, in rigid climates and with high water infiltration through the road pavement, the reduction reaction could be so slow that Cr(VI) might migrate as deep as 200 cm under the road. The reaction parameters and the model can form the basis for systematically assessing under which scenarios Cr(VI) from C&DW could lead to an environmental issue for ground- and receiving surface waters.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Residual Resource Engineering
Contributors: Butera, S., Trapp, S., Astrup, T. F., Christensen, T. H.
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Peer-reviewed: Yes

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Journal: Journal of Hazardous Materials
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ISSN (Print): 0304-3894
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Scopus rating (2015): CiteScore 5.54 SJR 1.633 SNIP 1.932
Web of Science (2015): Impact factor 4.836
Web of Science (2015): Indexed yes
Original language: English
Keywords: Leaching, Construction and demolition waste, Cr(VI) reduction, Cr(VI) migration, Road construction
DOIs: 10.1016/j.jhazmat.2015.06.025
Source: PublicationPreSubmission
Source-ID: 112913982
Research output: Contribution to journal > Journal article – Annual report year: 2015 > Research > peer-review

The Role of Dissipation Processes in Plants for Modeling Bioaccumulation

General information
Publication status: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Department of Environmental Engineering, Environmental Chemistry, ARC Arnot Research & Consulting Inc., Utah State University
Contributors: Fantke, P., Trapp, S., Arnot, J., Doucette, W.
Pages: 27-27
Publication date: 2015

Host publication information
Title of host publication: Abstract book : Buzzing with science
Publisher: SETAC
Electronic versions: Fantke_2015n.pdf
Research output: Chapter in Book/Report/Conference proceeding > Conference abstract in proceedings – Annual report year: 2015 > Research > peer-review
Tree Coring as a Complement to Soil Gas Screening to Locate PCE and TCE Source Zones and Hot Spots

Preliminary risk assessment for prioritisation of site investigations requires efficient screening to reveal type and level of contamination. The screening methods, tree coring and soil gas sampling were applied and compared at two forested sites contaminated with tetrachloroethylene (PCE) or trichloroethylene (TCE) to evaluate their ability to locate source zones and contaminant hot spots. One test site represented a relatively homogeneous sandy soil and aquifer, and the second a more heterogeneous geology with both sandy and less permeable clay till layers overlying a chalk aquifer. Tree cores from different tree species were sampled and analysed, and compared to soil gas measurements and existing soil gas data. Both methods were found useful as screening tools to locate hot spots of PCE and TCE in the shallow subsurface. Tree coring was found to be particularly beneficial as a complement to soil gas sampling at sites with low permeable soils, and where contamination was located in the capillary rise or shallow groundwater. The shorter time required for tree coring reduced the costs compared to soil gas sampling, but the sensitivity and precision of tree coring were lower. However, this did not affect the feasibility of using tree coring to locate the hot spots. Moreover, a combination of the two methods can help to focus any subsequent investigations like soil or groundwater sampling. The use of tree coring to complement soil gas sampling for pre-screening is expected to result in higher certainty for revealing hot spots and source zones at contaminated sites.
with tree cores; (ii) soil gas measurements for CH4, O2, and photoionization detector (PID); (iii) direct-push with membrane interface probe (MIP) and laser-induced fluorescence (LIF) sensors; (iv) direct-push sampling; and (v) sampling from soil and from groundwater monitoring wells. Phytoscreening and soil gas measurements are rapid and inexpensive pre-screening methods. Both indicated subsurface pollution and hot spots successfully. The direct-push sensors yielded 3D information about the extension and the volume of the subsurface plume. This study also expanded the applicability of tree coring to BTEX compounds and tested the use of high-resolution direct-push sensors for light hydrocarbons. Comparison of screening results to results from conventional soil and groundwater sampling yielded in most cases high rank correlation and confirmed the findings. The large-scale application of non- or low-invasive pre-screening can be of help in directing and focusing the subsequent, more expensive investigation methods. The rapid pre-screening methods also yield useful information about potential remediation methods. Overall, we see several benefits of a stepwise screening and site characterization scheme, which we propose in conclusion.

**General information**
Publication status: Published
Organisations: Department of Environmental Engineering, Water Resources Engineering, Environmental Chemistry, Institute for Ecology of Industrial Areas, SolGeo AG, Helmholtz Centre for Environmental Research, Fugro Consult GmbH
Contributors: Nielsen, M. A., Kalisz, M., Stalder, M., Martac, E., Krupanek, J., Trapp, S., Bartke, S.
Pages: 14673-14686
Publication date: 2015
Peer-reviewed: Yes

**Publication information**
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Scopus rating (2015): CiteScore 2.5 SJR 0.906 SNIP 1.059
Web of Science (2015): Impact factor 2.76
Web of Science (2015): Indexed yes
Original language: English
Keywords: Contamination, Tree core, Probe technologies, Brownfields, Phytoscreening, Direct-push, Soil gas, Site characterization

**Using pre-screening methods**

**What Makes a Good Compound against Sucking Petts?**

**General information**
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Syngenta Crop Protection, Syngenta Crop Protection Münchwilen AG
Contributors: Buchholz, A., O'Sullivan, A. C., Trapp, S.
Number of pages: 17
Pages: 93-109
Publication date: 2015

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Publisher: American Chemical Society
Editors: Maienfisch, P., Stevenson, T. M.
ISBN (Print): 9780841231023
ISBN (Electronic): 9780841231016
Keywords: Pesticide design, Intracellular localization, Vacuole trapping, Translaminar, Sucking pests
Source: PublicationPreSubmission
Classical and modelling of non-extractable residue (NER) formation of xenobiotics in soil - a synthesis
This review provides a comprehensive overview about NER formation and attempts to classify the various types. Xenobiotic NER derived from parent pesticides (or other environmental contaminants) and primary metabolites sorbed or entrapped within the soil organic matter (type I) or covalently bound (type II), are pose a considerably higher risk than those derived from productive biodegradation. However, bioNER (type III) resulting from conversion of carbon (or nitrogen) from the compounds into microbial biomass molecules do not pose any risk. Experimental approaches to clearly distinguish between the types are provided and a model to prospectively estimate bioNER formation in soil is proposed.

Comparative study of site investigation approaches and potential in situ remediation techniques: model-assisted evaluation of advantages and uncertainties
Site characterization is often time consuming and a financial burden for the site owners, which raises a demand for rapid and inexpensive (pre)screening methods. Phytoscreening by tree coring has shown to be a useful tool to detect subsurface contamination, especially of chlorinated solvents. However the application and dissemination of the method is still limited. On the other hand, soil gas sampling for mapping of volatile organic compounds in the subsurface is a common and commercially applied method. Both methods are semi-quantitative, low-invasive and inexpensive, which
makes them suitable as initial screening methods for site characterization.

The aim of this study is to compare tree coring and soil gas sampling to evaluate to which extent tree coring may supplement or substitute soil gas sampling as a site contaminant screening tool. And where both methods are feasible, evaluate when (with respect to compounds, soil properties, and locations) one method is preferred over the other.

Fields sampling was performed at European sites contaminated with fuel components or chlorinated solvents from former site activities (industrial production, gas stations, air base or gas plant) in fall 2012 and 2013. Samples from different tree species such as willow, asp, oak, birch and pine were collected and analyzed by headspace GC-MS. The soil gas measurements were conducted by consulting engineering firms as part of the site characterization prior to the tree core sampling events. Results obtained both by tree coring and soil gas sampling are compared and held up against quantitative results obtained by groundwater- and/or soil sample analysis.

Significant correlation between the methods is not always the case. However, both methods can detect contamination in the shallow subsurface and then identify high risk areas. The uptake of BTEX into trees varies to a greater extent with the tree species and the site conditions than chlorinated solvents, which lead to greater uncertainty. Both methods have their advantages and disadvantages. Hence, the methods supplement each other. Based on results from these initial screening methods, other more advanced/quantitative and cost-intensive methods can be focused, with the overall goal to make site characterization more complete and/or efficient.

**General information**
Publication status: Published  
Contributors: Nielsen, M. A., Stalder, M., Riis, C., Petersen, J., Kalisz, M., Krupanek, J., Trapp, S., Broholm, M. M.  
Number of pages: 1  
Publication date: 2014  
Peer-reviewed: Yes  
Event: Abstract from 11th International conference of Phytotechnologies, Heraklion, Crete, Greece.  
Electronic versions:  
Abstract_phyto2014_MANN_Submitted_final.pdf

**Bibliographical note**
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Source-ID: 104828068

Research output: Contribution to conference › Conference abstract for conference – Annual report year: 2015 › Research › peer-review

**Experimental Results and Integrated Modeling of Bacterial Growth on an Insoluble Hydrophobic Substrate (Phenanthrene)**
Metabolism of a low-solubility substrate is limited by dissolution and availability and can hardly be determined. We developed a numerical model for simultaneously calculating dissolution kinetics of such substrates and their metabolism and microbial growth (Monod kinetics with decay) and tested it with three aerobic phenanthrene (PHE) degraders: Novosphingobium pentaromativorans US6-1, Sphingomonas sp. EPA505, and Sphingobium yanoikuyae B1. PHE was present as microcrystals, providing non-limiting conditions for growth. Total PHE and protein concentration were tracked over 6-12 days. The model was fitted to the test results for the rates of dissolution, metabolism, and growth. The strains showed similar efficiency, with v(max) values of 12-18 g dw g(-1) d(-1), yields of 0.21 g g(-1), maximum growth rates of 2.5-3.8 d(-1), and decay rates of 0.04-0.05 d(-1). Sensitivity analysis with the model shows that (i) retention in crystals or NAPLs or by sequestration competes with biodegradation, (ii) bacterial growth conditions (dissolution flux and resulting chemical activity of substrate) are more relevant for the final state of the system than the initial biomass, and (iii) the desorption flux regulates the turnover in the presence of solid-state, sequestered (aged), or NAPL substrate sources.

**General information**
Publication status: Published  
Organisations: Department of Environmental Engineering, Environmental Chemistry, Helmholtz Centre for Environmental Research  
Contributors: Adam, I. K. U., Rein, A., Miltner, A., Fulgencio, A. C. D., Trapp, S., Kaestner, M.  
Number of pages: 10  
Pages: 8717-8726  
Publication date: 2014  
Peer-reviewed: Yes

**Publication information**
Journal: Environmental Science & Technology (Washington)  
Volume: 48  
Issue number: 15
Feasibility of phyto remediation of common soil and groundwater pollutants

This report is the deliverable D 4.3 and was done within the Timbre project WP4. It introduces into the various clean-up techniques that apply plants, evaluates the feasibility of phytoremediation of common soil and groundwater pollutants, and the knowledge collected for this purpose was applied to the two Timbre sites: Hunedoara (Romania) and Szprotawa (Poland). Phytoremediation is the technique to clean up (remediate) contaminated sites using plants, typically trees. The principles of the data were detailed, with focus on obstacles (phytotoxicity) and factors stimulating success (degradation). Application schemes were established. Quantitative data was collected and presented in tables. Kinetic models were established for later application at the test sites.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Water Resources Engineering
Contributors: Trapp, S., Rein, A., Clausen, L. P. W.; Nielsen, M. A.
Number of pages: 48
Publication date: 2014

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URLs:
Source: PublicationPreSubmission
Source-ID: 118090178
Research output: Book/Report › Report – Annual report year: 2015 › Commissioned › peer-review

Feasibility of phytoremediation of common soil and groundwater pollutants

This report is the deliverable D 4.3 and was done within the Timbre project WP4. It introduces into the various clean-up techniques that apply plants, evaluates the feasibility of phytoremediation of common soil and groundwater pollutants, and the knowledge collected for this purpose was applied to the two Timbre sites: Hunedoara (Romania) and Szprotawa (Poland). Phytoremediation is the technique to clean up (remediate) contaminated sites using plants, typically trees. The principles of the data were detailed, with focus on obstacles (phytotoxicity) and factors stimulating success (degradation). Application schemes were established. Quantitative data was collected and presented in tables. Kinetic models were established for later application at the test sites.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Water Resources Engineering
Contributors: Trapp, S., Rein, A., Clausen, L., Nielsen, M. A.
Number of pages: 48
Publication date: 2014

Publication information
How AI localisation in plant tissues determines the targeted pest spectrum of different chemistries

Many pests suck on the vascular system and/or cells of different plant tissues. The sucking target in the cell differs between pests such as Hemiptera (e.g., aphids and whiteflies) or Acari (mites). The agronomic control of sucking pests is most effective with pesticides taken up orally. The cuticle penetration as first crucial step can be modified by formulation whereas the active ingredient (AI) distribution within cells is usually solely determined by physicochemical properties. This passive AI distribution was calculated with the Fick-Nernst-Planck equation implemented in a cell model. The predictions were compared to the measured biological effects against three different arthropods. Test compounds differed in log P (-0.1 to 4.3) and pKa (4.1 to 10.7). Efficacies in different bioassays are discussed with the postulated cellular AI localisation and the individual feeding behaviour of the targeted pest.
Non-extractable residues (NER) from xenobiotics in soil: a new classification and relevance in the risk assessment

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, RWTH Aachen University, Helmholtz Centre for Environmental Research
Contributors: Nowak, K. M., Kästner, M., Miltner, A., Trapp, S., Schäffer, A.
Number of pages: 2
Publication date: 2014

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Non_extractable_residues_NER_from_xenobiotics_in_soil_a_new_classification_and_relevance_in_the_risk_assessment.pdf
Research output: Chapter in Book/Report/Conference proceeding > Conference abstract in proceedings – Annual report year: 2014 > Research > peer-review

Phytoremediation: A green solution

General information
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Organisations: Department of Environmental Engineering, Environmental Chemistry, Water Resources Engineering
Contributors: Clausen, L. P. W., Nielsen, M. A., Trapp, S.
Publication date: 2014
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Event information
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Location: Vigo, Spain
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Research output: Non-textual form > Sound/Visual production (digital) – Annual report year: 2014 > Research

Phytoscreening and phytoextraction of heavy metals at Danish polluted sites using willow and poplar trees

The main purpose of this study was to determine typical concentrations of heavy metals (HM) in wood from willows and poplars, in order to test the feasibility of phytoscreening and phytoextraction of HM. Samples were taken from one strongly, one moderately, and one slightly polluted site and from three reference sites. Wood from both tree species had similar background concentrations at 0.5 mg kg⁻¹ for cadmium (Cd), 1.6 mg kg⁻¹ for copper (Cu), 0.3 mg kg⁻¹ for nickel (Ni), and 25 mg kg⁻¹ for zinc (Zn). Concentrations of chromium (Cr) and lead (Pb) were below or close to detection limit. Concentrations in wood from the highly polluted site were significantly elevated, compared to references, in particular for willow. The conclusion from these results is that tree coring could be used successfully to identify strongly heavy metal-polluted soil for Cd, Cu, Ni, Zn, and that willow trees were superior to poplars, except when screening for Ni. Phytoextraction of HMs was quantified from measured concentration in wood at the most polluted site. Extraction efficiencies were best for willows and Cd, but below 0.5 % over 10 years, and below 1‰ in 10 years for all other HMs.
Phytoscreening of BTEX and chlorinated solvents by tree coring

Background/Objectives. Site characterization is often time consuming and a financial burden for the site owners, which raises a demand for rapid and inexpensive screening methods. Tree coring is a phytoscreening method useful for detection of contamination with organic compounds. The method takes advantage of the natural ability of trees to absorb water, nutrients and prospective contaminants from the soil pore water into their roots and upwards to the stem from where a core is sampled. Samples are then analyzed for the contaminants in the wood. The results give an impression of the contaminant level in the subsurface and plumes may be mapped. Various plants can be used for phytoscreening, however trees are preferable to smaller plants as their large root system can absorb chemicals from a broader and deeper area.

Approach/Activities. In this study tree coring is tested for fuel components and chlorinated solvents. The method was applied at various European sites contaminated with PCE/TCE or BTEXs due to former site activities (industrial production, gas stations, air base or gas plant). Tree core samples were collected in fall 2013 and analyzed by HS-GC/MS. Results were used to map the plume(s). The measured concentrations are also compared to concentrations detected in soil and/or groundwater. Furthermore, the two screening technologies Tree coring and Soil air sampling have been compared to evaluate the feasibility of the tree coring method.

Results/Lessons Learned. The method of tree coring can detect contamination with BTEX and chlorinated solvents in the shallow subsurface. The uptake of BTEX into trees varies to a greater extent with the site conditions and tree species than chlorinated solvents, which lead to greater uncertainty.

Tree coring is semi-quantitative, low-invasive and inexpensive, which makes it suitable as initial screening methods. The method is useful at large sites and at sites where conventional site characterization methods can be limited due to the sensitivity of the site (e.g. private land, moor, rocks and forest) or due to (former) activities at the site like explosive hazard which poses a risk when drilling. Phytoscreening by tree coring can be used to focus other more advanced and cost-intensive screening methods, with the overall goal to make site characterization more complete and/or efficient.
Phytoscreening of BTEX and chlorinated solvents by tree coring

General information
Publication status: Published
Contributors: Nielsen, M. A., Trapp, S., Kalisz, M., Krupanek, J., Stalder, M., Martac, E., Broholm, M. M.
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Publication date: 2014
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Event: Poster session presented at Ninth International Conference on Remediation of Chlorinated and Recalcitrant Compounds, Monterey, California, United States.
Electronic versions:
Monterey_Mann_Finally.pdf
Research output: Contribution to conference › Poster – Annual report year: 2015 › Research › peer-review

Phytotoxicity of Sodium Fluoride and Uptake of Fluoride to Willow Trees

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Aarhus University
Contributors: Clausen, L. P. W., Gosewinkel Karlson, U., Trapp, S.
Number of pages: 1
Publication date: 2014
Peer-reviewed: Yes
Event: Poster session presented at 11th International conference of Phytotechnologies, Heraklion, Crete, Greece.
Electronic versions:
Poster_Phytotoxicity_of_NaF_and_uptake_of_F_to_willow_trees.pdf
Research output: Contribution to conference › Poster – Annual report year: 2014 › Research › peer-review

Polyacrylate–water partitioning of biocidal compounds: Enhancing the understanding of biocide partitioning between render and water

In recent years, the application of polymer-based renders and paints for façade coatings of buildings has risen enormously due to the increased mounting of thermal insulation systems. These materials are commonly equipped with biocides - algaecides, fungicides, and bactericides - to protect the materials from biological deterioration. However, the biocides need to be present in the water phase in order to be active and, hence, they are flushed of the material by rain water. In order to increase the knowledge about the partitioning of biocides from render into the water phase, partition constants between the polymer - in this case polyacrylate - and water were studied using glass fibre filters coated with polyacrylate. The polyacrylate-water partition constants (logKAcW) of ten biocides used in construction material varied between 1.66 (isoproturon) and 3.57 (dichloro-N-octylisothiazolinone). The correlation of the polyacrylate-water partition constants with the octanol-water partition constants is significant, but the polyacrylate-water partition constants were predominantly below octanol-water partition constants (Kow). The comparison with render-water distribution constants showed that estimating the leaching of biocides from render based on polymer-water partitioning is a useful and practical tool.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Duisburg-Essen, Aarhus University
Contributors: Bollmann, U. E., Ou, Y., Mayer, P., Trapp, S., Bester, K.
Pages: 1021-1026
Predicting human exposure to pharmaceuticals and personal care products from plant tissue grown in biosolids-amended soil

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Guelph
Contributors: Prosser, R. S., Trapp, S., Sibley, P. K.
Number of pages: 1
Publication date: 2014

Host publication information
Title of host publication: Science Across Bridges, Borders and Boundaries: Programme Book
Place of publication: Basel, Switzerland
Publisher: SETAC-Europe
Electronic versions:
Predicting_human_exposure_to_pharmaceuticals_and_personal_care_products_from_plant_tissue_grown_in_biosolids_amended_soil.pdf

Bibliographical note
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Research output: Chapter in Book/Report/Conference proceeding > Conference abstract in proceedings – Annual report year: 2014 > Research > peer-review

Removal of pharmaceuticals in biological wastewater treatment systems: model generalisation and implications for environmental risk predictions

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Environmental Chemistry, Norwegian Institute for Water Research
Contributors: Polesel, F., Langford, K. H., Trapp, S., Thomas, K. V., Plósz, B. G.
Number of pages: 3
Publication date: 2014

Host publication information
Title of host publication: WWTmod 2014: Conference proceedings
Keywords: Pharmaceutical elimination, ASM-X, Model validation, Retransformation, Hospital WWTP
Electronic versions:
WWTmod2014 Generalization_final_submission_revised.pdf
Source: PublicationPreSubmission
Source-ID: 101935989
Research output: Chapter in Book/Report/Conference proceeding > Conference abstract in proceedings – Annual report year: 2014 > Research > peer-review
Removal of pharmaceuticals in sewage treatment plants: A model generalisation to international data

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Environmental Chemistry, Norwegian Institute for Water Research
Contributors: Polesel, F., Langford, K. H., Trapp, S., Thomas, K. V., Plósz, B. G.
Number of pages: 4
Publication date: 2014
Peer-reviewed: Yes
Keywords: Micropollutants removal, Retransformation of pharmaceuticals, ASM-X generalization
Electronic versions:
IWA_WWC_Generalization_abstract.pdf
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Research output: Contribution to conference › Conference abstract for conference – Annual report year: 2014 › Research › peer-review

Simulation and measurement of bacterial growth on low soluble phenanthrene substrate

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Helmholtz Centre for Environmental Research, Technical University of Munich
Contributors: Trapp, S., Adam, I., Rein, A., Miltner, A., da Socta Fulgencio, A., Kaestner, M.
Number of pages: 1
Publication date: 2014
Host publication information
Title of host publication: Science Across Bridges, Borders and Boundaries : Programme Book
Place of publication: Basel, Switzerland
Publisher: SETAC-Europe
Electronic versions:
Simulation_and_measurement_of_bacterial_growth_on_low_soluble_phenanthrene_substrate.pdf
Bibliographical note
TU228
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2014 › Research › peer-review

Simulation of pharmaceuticals in the environment

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry
Contributors: Trapp, S.
Number of pages: 2
Publication date: 2014
Host publication information
Title of host publication: Science Across Bridges, Borders and Boundaries : Programme Book
Place of publication: Basel, Switzerland
Publisher: SETAC-Europe
Electronic versions:
Simulation_of_pharmaceuticals_in_the_environment.pdf
Bibliographical note
Extended abstract
Source: PublicationPreSubmission
Source-ID: 92776702
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2014 › Research › peer-review
Tree Coring as an initial screening tool for typical pollutants in the subsurface
Previous guidelines report that tree coring is more or less useful for a variety of VOCs, such as BTEX, MTBE, trimethyl benzene, and chlorinated solvents (PCE, TCE, DCE, VC). This new guideline goes beyond the previous guidelines by including the use of a technique to screen for heavy metals, plus some new examples for BTEX. This update is based on field applications at sites contaminated with BTEX, chlorinated solvents, and/or heavy metals. The description of the method and its application covers sampling, chemical analysis, and data treatment, followed by a brief overview of current phytoscreening literature.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Water Resources Engineering, Environmental Chemistry
Contributors: Nielsen, M. A., Trapp, S.
Number of pages: 25
Publication date: 2014

Publication information
Original language: English
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Source: PublicationPreSubmission
Source-ID: 104754297
Research output: Book/Report › Report – Annual report year: 2015 › Research › peer-review

Activity-based fate modelling for risk assessment of three ionizable organic compounds (triclosan, furosemide, ciprofloxacin)

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Environmental Chemistry
Contributors: Polesel, F., Plósz, B., Trapp, S.
Number of pages: 2
Publication date: 2013
Peer-reviewed: Yes
Event: Abstract from Micropol & Ecohazard 2013, the 8th IWA Specialist Conference on Assessment and Control of Micropollutants/Hazardous Substances in Water, Zurich, Switzerland.

Electronic versions:
Abstract in Conference Proceedings.pdf

Bibliographical note
IWA-11677
Source: dtu
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Research output: Contribution to conference › Conference abstract for conference – Annual report year: 2013 › Research › peer-review

Activity-based fate modelling for risk assessment of three ionizable organic compounds (triclosan, furosemide, ciprofloxacin)

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Environmental Chemistry
Contributors: Polesel, F., Plósz, B., Trapp, S.
Number of pages: 1
Publication date: 2013
Peer-reviewed: Yes
Event: Poster session presented at Micropol & Ecohazard 2013, the 8th IWA Specialist Conference on Assessment and Control of Micropollutants/Hazardous Substances in Water, Zurich, Switzerland.

Electronic versions:
Comparing the desorption and biodegradation of low concentrations of phenanthrene sorbed to activated carbon, biochar and compost

Carbonaceous soil amendments are applied to contaminated soils and sediments to strongly sorb hydrophobic organic contaminants (HOCs) and reduce their freely dissolved concentrations. This limits biouptake and toxicity, but also biodegradation. To investigate whether HOCs sorbed to such amendments can be degraded at all, the desorption and biodegradation of low concentrations of 14C-labelled phenanthrene (5μgL−1) freshly sorbed to suspensions of the pure soil amendments activated carbon (AC), biochar (charcoal) and compost were compared. Firstly, the maximum abiotic desorption of phenanthrene from soil amendment suspensions in water, minimal salts medium (MSM) or tryptic soy broth (TSB) into a dominating silicone sink were measured. Highest fractions remained sorbed to AC (84±2.3%, 87±4.1%, and 53±1.2% for water, MSM and TSB, respectively), followed by charcoal (35±2.2%, 32±1.7%, and 12±0.3%, respectively) and compost (1.3±0.21%, similar for all media). Secondly, the mineralization of phenanthrene sorbed to AC, charcoal and compost by Sphingomonas sp. 10-1 (DSM 12247) was determined. In contrast to the amounts desorbed, phenanthrene mineralization was similar for all the soil amendments at about 56±11% of the initially applied radioactivity. Furthermore, HPLC analyses showed only minor amounts (<5%) of residual phenanthrene remaining in the suspensions, indicating almost complete biodegradation. Fitting the data to a coupled desorption and biodegradation model revealed that desorption did not limit biodegradation for any of the amendments, and that degradation could proceed due to the high numbers of bacteria and/or the production of biosurfactants or biofilms. Therefore, reduced desorption of phenanthrene from AC or charcoal did not inhibit its biodegradation, which implies that under the experimental conditions these amendments can reduce freely dissolved concentration without hindering biodegradation. In contrast, phenanthrene sorbed to compost was fully desorbed and biodegraded.

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Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Aarhus University
Pages: 1767–1778
Publication date: 2013
Peer-reviewed: Yes
Publication information
Journal: Chemosphere
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ISSN (Print): 0045-6535
Ratings:
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.92 SJR 1.721 SNIP 1.746
Web of Science (2013): Impact factor 3.499
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Original language: English
Keywords: Activated carbon, Charcoal, Compost, Phenanthrene, Desorption, Biodegradation
DOI: 10.1016/j.chemosphere.2012.07.048
Research output: Contribution to journal › Journal article – Annual report year: 2013 › Research › peer-review

Impact of activated carbon, biochar and compost on the desorption and mineralization of phenanthrene in soil

Sorption of PAHs to carbonaceous soil amendments reduces their dissolved concentrations, limiting toxicity but also potentially biodegradation. Therefore, the maximum abiotic desorption of freshly sorbed phenanthrene (≤5 mg kg−1) was measured in three soils amended with activated carbon (AC), biochar or compost. Total amounts of phenanthrene desorbed were similar between the different soils, but the amendment type had a large influence. Complete desorption was observed in the unamended and compost amended soils, but this reduced for biochar (41% desorbed) and AC (8% desorbed). Cumulative amounts mineralized were 28% for the unamended control, 19% for compost, 13% for biochar and 4% for AC. Therefore, the effects of the amendments in soil in reducing desorption were also reflected in the extents of mineralization. Modeling was used to analyze key processes, indicating that for the AC and charcoal treatments bacterial activity did not limit mineralization, but rather desorption into the dissolved phase.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Aarhus University
Modelling sorption of ciprofloxacin using the ASM-X framework – Evaluation of factors influencing activated sludge treatment and implications on environmental risk assessment

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Environmental Chemistry, RWTH Aachen University, Norwegian Institute for Water Research
Contributors: Polesel, F., Lehnberg, K., Dott, W., Trapp, S., Thomas, K. V., Plósz, B.
Number of pages: 1
Publication date: 2013
Peer-reviewed: Yes
Event: Poster session presented at 13th Nordic Wastewater Conference, Malmö, Sweden.
Electronic versions:
Fabio_Polesel_Ciprofloxacin.pdf
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Source-ID: u::8898
Research output: Contribution to conference » Poster – Annual report year: 2013 » Research » peer-review

Modelling sorption of ciprofloxacin using the ASM-X framework – Evaluation of factors influencing activated sludge treatment and implications on environmental risk assessment

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Environmental Chemistry, RWTH Aachen University, Norwegian Institute for Water Research
Contributors: Polesel, F., Lehnberg, K., Dott, W., Trapp, S., Thomas, K. V., Plósz, B.
Number of pages: 3
Publication date: 2013
Peer-reviewed: Yes
Electronic versions:
Pages_from_prod21383666330204.104_927_1_PB.pdf
Research output: Contribution to conference » Conference abstract for conference – Annual report year: 2013 » Research » peer-review

Modelling the fate of ciprofloxacin in activated sludge systems - The relevance of the sorption process
The sorption process can impact the removal of specific pharmaceuticals in municipal wastewater treatment plants (WWTPs). Ionic interactions (e.g., pH-driven equilibria and complexation), rather than hydrophobic interactions, are known to affect the sorption of zwitterionic pharmaceuticals. In a previous study [1], a daily systematic reduction of ciprofloxacin removal in a full-scale WWTP (Bekkelaget, Norway) was associated to deteriorated sorption. Therefore, in this study we further investigated the sorption of ciprofloxacin onto activated sludge at laboratory- and full-scale. Targeted batch
experiments were performed to estimate sorption model parameters using Freundlich isotherms under specific pH and iron salt dosing (used for chemical phosphorus removal) conditions. We used the previously tested activated sludge framework model for xenobiotic trace chemicals (ASM-X) to assess the fate of ciprofloxacin in a full-scale activated sludge system. Sorption was described by linear kinetics and, in an extended version of ASM-X, using a Freundlich-based submodel. In the latter case, Freundlich parameter values estimated from the batch experiments were used for model calibration. The prediction accuracy was statistically evaluated in the two cases by comparing the model output with measured data.

Batch experiments showed that maximum sorption capacity occurred at pH=7.4, corresponding to the isoelectric point of ciprofloxacin. A pH increase resulted in a significant reduction of sorption capacity as compared to the effect of the pH decrease applied in the experiment. Additionally, iron salt dosing was found to enhance sorption under both aerobic and anaerobic conditions. Using the extended ASM-X model, results obtained in scenario simulations – based on the batch experimental Freundlich parameters – suggest that pH conditions, rather than reduced salt dosing, can be responsible for the decrease of ciprofloxacin sorption in the full-scale WWTP. The most accurate predictions were obtained for Freundlich parameter values of K=0.01 (μg(1-1/n) L1/n mg-1) and 1/n=1.33. A pH increase was therefore estimated to cause reduced sorption in the anoxic and the aerobic reactors, possibly being a consequence of the lower sorption extent exhibited by the anionic ciprofloxacin species. Comparable prediction accuracy was obtained using linear sorption. A 20-fold decrease of the anoxic and aerobic KD values (1.1 and 0.42 L gXSS-1 under normal conditions, respectively) was estimated in the time interval when deteriorated sorption was hypothesized.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Environmental Chemistry, RWTH Aachen University, Norwegian Institute for Water Research
Contributors: Polesel, F., Lehnberg, K., Dott, W., Trapp, S., Thomas, K. H., Plósz, B.
Number of pages: 1
Publication date: 2013
Peer-reviewed: Yes
Event: Abstract from 14th EuCheMS International Conference on Chemistry and the Environment (ICCE 2013), Barcelona, Spain.
Electronic versions:
Fabio_Polesel_Modelling_fate_of_ciprofloxacin.pdf
Source: dtu
Source-ID: u::7793
Research output: Contribution to conference › Conference abstract for conference – Annual report year: 2013 › Research › peer-review

One-year measurements of chloroethenes in tree cores and groundwater at the SAP Mimoň Site, Northern Bohemia
Chlorinated ethenes (CE) are among the most frequent contaminants of soil and groundwater in the Czech Republic. Because conventional methods of subsurface contamination investigation are costly and technically complicated, attention is directed on alternative and innovative field sampling methods. One promising method is sampling of tree cores (plugs of woody tissue extracted from a host tree). Volatile organic compounds can enter into the trunks and other tissues of trees through their root systems. An analysis of the tree core can thus serve as an indicator of the subsurface contamination. Four areas of interest were chosen at the experimental site with CE groundwater contamination and observed fluctuations in groundwater concentrations. CE concentrations in groundwater and tree cores were observed for a 1-year period. The aim was to determine how the CE concentrations in obtained tree core samples correlate with the level of contamination of groundwater. Other factors which can affect the transfer of contaminants from groundwater to wood were also monitored and evaluated (e.g., tree species and age, level of groundwater table, river flow in the nearby Ploučnice River, seasonal effects, and the effect of the remediation technology operation). Factors that may affect the concentration of CE in wood were identified. The groundwater table level, tree species, and the intensity of transpiration appeared to be the main factors within the framework of the experiment. Obtained values documented that the results of tree core analyses can be used to indicate the presence of CE in the subsurface. The results may also be helpful to identify the best sampling period for tree coring and to learn about the time it takes until tree core concentrations react to changes in groundwater conditions. Interval sampling of tree cores revealed possible preservation of the contaminant in the wood of trees.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Czech University of Life Sciences Prague, AECOM CZ
Contributors: Wittlingerova, Z., Machackova, J., Petruzelkova, A., Trapp, S., Vlk, K., Zima, J.
Pages: 834-847
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Environmental Science and Pollution Research
Volume: 20
Simulation of the plant uptake of organophosphates and other emerging pollutants for greenhouse experiments and field conditions

The uptake of the organophosphates tris(2-chloroethyl) phosphate (TCEP), tris(1-chloro-2-propyl) phosphate (TCPP), tributyl phosphate (TBP), the insect repellent N,N-diethyl toluamide (DEET), and the plasticizer n-butyl benzenesulfonamide (NBBS) into plants was studied in greenhouse experiments and simulated with a dynamic physiological plant uptake model. The calibrated model was coupled to a tipping bucket soil transport model and a field scenario with sewage sludge application was simulated. High uptake of the polar, low-volatile compounds TCEP, TCPP, and DEET into plants was found, with highest concentrations in straw (leaves and stem). Uptake into carrot roots was high for TCPP and TBP. NBBS showed no high uptake but was rapidly degraded. Uptake into barley seeds was small. The pattern and levels of uptake could be reproduced by the model simulations, which indicates mainly passive uptake and transport (i.e., by the transpiration stream, with the water) into and within the plants. Also the field simulations predicted a high uptake from soil into plants of TCEP, TCPP, and DEET, while TBP is more likely taken up from air. The BCF values measured and calculated in the greenhouse study are in most cases comparable to the calculated values of the field scenario, which demonstrates that greenhouse studies can be suitable for predicting the behavior of chemicals in the field. Organophosphates have a high potential for bioaccumulation in crops and reach agricultural fields both via sewage sludge and by atmospheric deposition.

General information
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Organisations: Department of Environmental Engineering, Environmental Chemistry, Norwegian Institute for Agricultural and Environmental Research
Contributors: Trapp, S., Eggen, T.
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ISSN (Print): 0944-1344
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BFI (2013): BFI-level 1
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Web of Science (2013): Impact factor 2.757
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Original language: English
Keywords: Bioaccumulation, Emerging contaminants, Modeling, Organophosphates, Flame inhibitors, Detergents, Consumer products, Plant uptake
DOI:
10.1007/s11356-012-1238-9
Source: dtu
Source-ID: u::5820
Research output: Contribution to journal › Journal article – Annual report year: 2012 › Research › peer-review
A method to simultaneously determine reduction in PAH dissolved concentrations and bioaccessibility in carbon amended soils

General information
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Organisations: Environmental Chemistry, Department of Environmental Engineering, Aarhus University
Number of pages: 1
Pages: 385
Publication date: 2012

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Title of host publication: Abstract Book : 6th SETAC World Congress/SETAC Europe 22nd Annual Meeting
Publisher: Society of Environmental Toxicology and Chemistry
Electronic versions:
Marchal_etal_2012b_SETAC.pdf
URLs:
http://berlin.setac.eu/scientific_programme/download_the_abstracts_book/?contentid=582&pr_id=403&last=435
Source: dtu
Source-ID: u::4101
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report
year: 2012 › Research › peer-review

Combined modeling of plant uptake and leaching of heavy metals and organic compounds

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry
Contributors: Rein, A., Legind, C. N., Trapp, S.
Number of pages: 1
Pages: 174
Publication date: 2012

Host publication information
Title of host publication: Grundwasserschutz und Grundwassernutzung : FH-DGG-Tagung
Place of publication: Dresden (SDGG; No. 78).
Source: dtu
Source-ID: u::4096
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report
year: 2012 › Research › peer-review

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

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering, Aarhus University, Helmholtz Centre for Environmental Research
Number of pages: 1
Pages: 158
Publication date: 2012

Host publication information
Title of host publication: Abstract Book : 6th SETAC World Congress/SETAC Europe 22nd Annual Meeting
Publisher: Society of Environmental Toxicology and Chemistry
Electronic versions:
4.pdf
URLs:
http://berlin.setac.eu/scientific_programme/download_the_abstracts_book/?contentid=582&pr_id=403&last=435
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report
year: 2012 › Research › peer-review
Coupled modelling of plant uptake, soil water balance and soil solute transport for estimating the fate of cadmium and lead in amended agrosystems

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Veolia Environnement, National Institute for Agronomic Research
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Pages: 38-39
Publication date: 2012

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Publisher: Society of Environmental Toxicology and Chemistry
Electronic versions:
2.pdf
URLs:
http://berlin.setac.eu/scientific_programme/download_the_abstracts_book/?contentid=582&pr_id=403&last=435
Research output: Chapter in Book/Report/Conference proceeding ▶ Conference abstract in proceedings ▶ Annual report year: 2012 ▶ Research ▶ peer-review

Critical evaluation and further development of methods for testing ecotoxicity at multiple pH using Daphnia magna and Pseudokirchneriella subcapitata
To meet the requirements of risk assessment legislature regarding the ecotoxicity of ionizing compounds, the present study attempts to establish easy, robust methods for testing ecotoxicity at various pH levels. An overview is given of the buffering methods found in the literature. This is supplemented by a series of experiments where toxicity and ability to stabilize pH of seven common buffering compounds was tested on Daphnia magna and Pseudokirchneriella subcapitata.
We consider a buffer applicable at a given concentration if the pH drift is below 0.2 pH units, and if there are no toxic effects. Twenty-four- and 48-h acute toxicity tests with D. magna were carried on a series of organic buffers with pH monitoring. Based on the experimental results it is possible to give recommendations for buffer concentrations for use in toxicity testing with D. magna at pH levels in the range of pH 6.0-7.8 for 48 h exposure, and pH 6.0-9.5 for 24 h exposure. Forty-eight- and 72-h growth inhibition tests with P. subcapitata were carried out, and recommendations for buffer concentrations at pH 7.5 and 8.0 are made for both 48 and 72 h of exposure. Environ. Toxicol. Chem. 2012; 31: 1843-1852. © 2012 SETAC.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry
Contributors: Rendal, C., Trapp, S., Kusk, K. O.
Pages: 1843-1852
Publication date: 2012
Peer-reviewed: Yes

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Journal: Environmental Toxicology and Chemistry
Volume: 31
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ISSN (Print): 0730-7268
Ratings:
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.81 SJR 1.639 SNIP 1.105
Web of Science (2012): Impact factor 2.618
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Original language: English
Keywords: Buffer, Daphnia magna, Ionization, Pseudokirchneriella subcapitata, Toxicity
DOIs:
10.1002/etc.1883
Source: dtu
Source-ID: n:oai:DTIC-ART:pubmed/366937879::18237
Research output: Contribution to journal ▶ Journal article ▶ Annual report year: 2012 ▶ Research ▶ peer-review
Dynamic passive dosing for studying microbial PAH degradation: a comparison of experimental and model results

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering, Aarhus University
Contributors: Smith, K. E. C., Rein, A., Trapp, S., Gosewinkel Karlson, U.
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year: 2012 › Research › peer-review

Dynamic Passive Dosing for Studying the Biotransformation of Hydrophobic Organic Chemicals: Microbial Degradation as an Example

Biotransformation plays a key role in hydrophobic organic compound (HOC) fate, and understanding kinetics as a function of (bio)availability is critical for elucidating persistence, accumulation, and toxicity. Biotransformation mainly occurs in an aqueous environment, posing technical challenges for producing kinetic data because of low HOC solubilities and sorptive losses. To overcome these, a new experimental approach based on passive dosing is presented. This avoids using cosolvent for introducing the HOC substrate, buffers substrate depletion so biotransformation is measured within a narrow and defined dissolved concentration range, and enables high compound turnover even at low concentrations to simplify end point measurement. As a case study, the biodegradation kinetics of two model HOCs by the bacterium Sphingomonas paucimobilis EPA505 were measured at defined dissolved concentrations ranging over 4 orders of magnitude, from 0.017 to 658 μg L⁻¹ for phenanthrene and from 0.006 to 90.0 μg L⁻¹ for fluoranthene. Both compounds had similar mineralization fluxes, and these increased by 2 orders of magnitude with increasing dissolved concentrations. First-order mineralization rate constants were also similar for both PAHs, but decreased by around 2 orders of magnitude with increasing dissolved concentrations. Dynamic passive dosing is a useful tool for measuring biotransformation kinetics at realistically low and defined dissolved HOC concentrations.

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Contributors: Smith, K. E. C., Rein, A., Trapp, S., Mayer, P., Karlson, U. G.
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Pollutant plume delineation from tree core sampling using standardized ranks

There are currently contradicting results in the literature about the way chloroethene (CE) concentrations from tree core sampling correlate with those from groundwater measurements. This paper addresses this issue by focusing on groundwater and tree core datasets in CE contaminated site, Czech Republic. Preliminary analyses revealed strongly and positively skewed distributions for the tree core dataset, with an intra-tree variability accounting for more than 80% of the total variability, while the spatial analyses based on variograms indicated no obvious spatial pattern for CE concentration. Using rank transformation, it is shown how the results were improved by revealing the initially hidden spatial structure for both variables when they are handled separately. However, bivariate analyses based on crosscovariance functions still failed to indicate a clear spatial correlation between groundwater and tree core measurements. Nonetheless, tree core sampling and analysis proved to be a quick and inexpensive semi-quantitative method and a useful tool.

Simultaneous simulations of uptake in plants and leaching to groundwater of cadmium and lead for arable land amended with compost or farmyard manure.

The water budget of soil, the uptake in plants and the leaching to groundwater of cadmium (Cd) and lead (Pb) were simulated simultaneously using a physiological plant uptake model and a tipping buckets water and solute transport model for soil. Simulations were compared to results from a ten-year experimental field study, where four organic amendments were applied every second year. Predicted concentrations slightly decreased (Cd) or stagnated (Pb) in control soils, but increased in amended soils by about 10% (Cd) and 6% to 18% (Pb). Estimated plant uptake was lower in amended plots, due to an increase of K(d) (dry soil to water partition coefficient). Predicted concentrations in plants were close to measured levels in plant residues (straw), but higher than measured concentrations in grains. Initially, Pb was mainly predicted to deposit from air into plants (82% in 1998); the next years, uptake from soil became dominating (30% from air in 2006), because of decreasing levels in air. For Cd, predicted uptake from air into plants was negligible (1-5%).
Uptake and fate of organic contaminants in plants of constructed wetlands

General information
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Organisations: Department of Environmental Engineering
Contributors: Rein, A., Legind, C. N., Nielsen, M. A., Trapp, S.
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Use-Dependent Inhibition of Synaptic Transmission by the Secretion of Intravesicularly Accumulated Antipsychotic Drugs

Tischbirek et al. find that weak-base antipsychotic drugs are accumulated in synaptic vesicles and are secreted upon exocytosis, leading to increased extracellular drug concentrations following neuronal activity. The secretion of the drugs in turn inhibits synaptic transmission in a use-dependent manner.

General information
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Organisations: Department of Environmental Engineering, Environmental Chemistry, Friedrich-Alexander University Erlangen-Nürnberg, Oslo University Hospital, European Neuroscience Institute Göttingen
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Application of passive dosing to study the biotransformation and biodegradation of hydrophobic compounds

Achieving well-defined and constant dissolved concentrations of hydrophobic compounds is challenging due to volatilization or sorptive losses. With passive dosing, continual partitioning into the test medium of compound(s) loaded in a polymer compensates for losses, and provides defined and constant dissolved concentrations. Passive dosing can be used for studying biotransformation/degradation. Here, the polymer HOC reservoir also compensates for losses due to the bio-transformation/degradation process itself. Furthermore, a large mass of test compound is introduced so that compound turnover is significant even at low dissolved concentrations thus facilitating measurement of the relevant endpoint (e.g., metabolic products in biotransformation or growth in biodegradation). This study details two applications of passive dosing for studying bio-transformation/degradation. A format has been developed to study the biodegradation of phenanthrene and fluoranthene by the bacterial strain EPA 505, allowing degradation rates to be quantified at defined freely dissolved concentrations from mg/L down to ng/L levels. Passive dosing was also applied for quantifying the mutagenicity of benzo(a)pyrene metabolites produced after activation by the liver S9 mix in the in vitro Ames II assay. Compared to the case with spiking, responses from passive dosing were shifted by a factor 100-1000 to lower concentrations, and were also more reproducible between repeated tests. This difference in apparent sensitivity cannot solely be explained by partitioning, and is due to slow dissolution kinetics as well as massdepletion of the spiked benzo(a)pyrene. Therefore, passive dosing is a useful tool for the study of hydrophobic compound bio-transformation/degradation at well-defined dissolved concentrations down to very low levels. Important advantages include studying process kinetics at precisely defined dissolved concentrations and allowing increased compound turnover even at constant and low concentrations.

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Atmospheric fate of non volatile and ionizable compounds

A modified version of the Multimedia Activity Model for Ioniics MAMI, including two-layered atmosphere, air–water interface partitioning, intermittent rainfall and variable cloud coverage was developed to simulate the atmospheric fate of ten low volatility or ionizable organic chemicals. Probabilistic simulations describing the uncertainty of substance and environmental input properties were run to evaluate the impact of atmospheric parameters, ionization and air–water (or air–ice) interface enrichment. The rate of degradation and the concentration of OH radicals, the duration of dry and wet periods, and the parameters describing air–water partitioning (KAW and temperature) and ionization (pKa and pH) are the key parameters determining the potential for long range transport. Wet deposition is an important removal process, but its efficiency is limited, primarily by the duration of the dry period between precipitation events. Given the underlying model assumptions, the presence of clouds contributes to the higher persistence in the troposphere because of the capacity of cloud water to accumulate and transport non-volatile (e.g., 2,4-D) and surface-active chemicals (e.g., PFOA). This limits the efficiency of wet deposition from the troposphere enhancing long-range transport.

General information
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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Department of Environmental Engineering, Environmental Chemistry, Unilever, University of Michigan, Ann Arbor
Contributors: Franco, A., Hauschild, M. Z., Jolliet, O., Trapp, S.
Can clouds enhance long-range transport of low volatile, ionizable and surface-active chemicals?

Atmospheric partitioning and transport of low volatile organic compounds is strongly influenced by the presence of water (e.g. clouds) and its deposition velocity (e.g. rainfall, snow). It was identified that the assumption of continuous rainfall underestimates the residence time and the transport potential of non-volatile substances. The liquid water content of clouds and the high specific surface of frozen or liquid cloud droplets can significantly contribute to the total activity capacity (i.e. the capacity to sorb chemicals) of the atmosphere for non-volatile, ionizable and surface active substances. A modified version of the regional multimedia activity model for ionics MAMI, including twolayered atmosphere with atmospheric boundary layer (ABL) and lower/middle troposphere (LMT), interface partitioning, intermittent rainfall and variable cloud coverage was applied to a selection of ten low volatile or ionizable chemicals to investigate the potential of clouds to enhance the atmospheric transport potential. Probability density functions were derived for input substance properties and environmental parameters to quantify uncertainty and variability and probabilistic simulations at steady state were run for a constant emission to the atmospheric boundary layer to identify key model inputs. The degradation rate, the duration of dry and wet periods and the parameters describing air-water bulk partitioning (KAW and T) and ionization (pKa and pH) determine the residence time in the ABL. In the LMT, however, the residence time depends also on the water content of clouds and on interface partitioning. In some cases the residence time and its variability range is similar in the two compartments, while some compounds (e.g. diazinon, 2,4-D, perfluorooctanoic acid) are more persistent in the LMT. The longer residence time predicted for some compounds in the LMT is due to the capacity of clouds to sorb non-volatile molecules in the liquid water and at the interface of cloud droplets. The efficiency of wet deposition to remove low volatile organic pollutants from the atmosphere is limited primarily by the duration of the dry interval between precipitation events. During dry periods persistent non-volatile chemicals can be transported to the troposphere. Here, the high capacity of of tropospheric clouds to sorb non-volatile and surface active chemicals limits oxidation and wet deposition rates and increases the potential for long-range transport.
bodies from the impact of CBs. The efficiency and seasonal variability of monochlorobenzene (MCB), 1,4-dichlorobenzene (1,4-DCB) and 1,2-dichlorobenzene (1,2-DCB) removal, the impact of planting, and gaseous MCB emissions from the filter surface were investigated over the course of 1 year in both a vegetated pilot-scale CW and an unplanted reference plot (UR). Annual mean concentration decreases of MCB and 1,4-DCB were observed; however, annual mean 1,2-DCB removal was seen only in the upper filter layer. Planting (Phragmites australis) had a statistically significant beneficial effect on removal. The CB removal efficiency in the CW generally decreased with depth, and seasonal variations of removal were evident, with less concentration decrease during summer. Load removal efficiencies of 59–65% (282–358 mg m⁻² d⁻¹) for MCB, 59–69% (4.0–5.1 mg m⁻² d⁻¹) for 1,4-DCB and 29–42% (0.6–2.1 mg m⁻² d⁻¹) for 1,2-DCB were observed in June and July. Volatilization of MCB from the filter surface accounted for 2–4% of the total amount removed. Simple cover layers of organic materials on the filter surface were suitable for MCB emission reduction. Model calculations were carried out to estimate the MCB removal potential attributable to microbial degradation, volatilisation, and plant uptake in the CW and UR. Microbial degradation was the dominating process. The observed positive impact of plants on MCB removal was caused by improved oxygen supply (due to root oxygen release into the rhizosphere and enhanced water table fluctuations), and direct plant uptake.

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Dynamic plant uptake model applied for drip irrigation of an insecticide to pepper fruit plants.
BACKGROUND: Drip application of insecticides is an effective way to deliver the chemical to the plant that avoids off-site movement via spray drift and minimizes applicator exposure. The aim of this paper is to present a cascade model for the uptake of pesticide into plants following drip irrigation, its application for a soil-applied insecticide and a sensitivity analysis of the model parameters. RESULTS: The model predicted the measured increase and decline of residues following two soil applications of an insecticide to peppers, with an absolute error between model and measurement ranging from 0.002 to 0.034 mg kg fw⁻¹. Maximum measured concentrations in pepper fruit were approximately 0.22 mg kg fw⁻¹. Temperature was the most sensitive component for predicting the peak and final concentration in pepper fruit, through its influence on soil and plant degradation rates. CONCLUSION: Repeated simulations of pulse inputs with the cascade model adequately describe soil pesticide applications to an actual cropped system and reasonably mimic it. The model has the potential to be used for the optimization of practical features, such as application rates and waiting times between applications and before harvest, through the integrated accounting of soil, plant and environmental influences. Copyright © 2011 Society of Chemical Industry

General information
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Organisations: Environmental Chemistry, Department of Environmental Engineering, DuPont, Waterborne Environmental Inc.
Contributors: Legind, C. N., Kennedy, C. M., Rein, A., Snyder, N., Trapp, S.
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Publication date: 2011
Dynamic plant uptake modelling and mass flux estimation

Plants significantly influence contaminant transport and fate. Important processes are uptake of soil and groundwater contaminants, as well as biodegradation in plants and their root zones. Models for the prediction of chemical uptake into plants are required for the set-up of mass balances in environmental systems at different scales. Feedback mechanisms between plants and hydrological systems can play an important role. However, they have received little attention to date. Here, a new model concept for dynamic plant uptake models applying analytical matrix solutions is presented, which can be coupled to groundwater transport simulation tools. Exemplary simulations of plant uptake were carried out in order to estimate chemical concentrations in the soil–plant–air system and the influence of plants on contaminant mass fluxes from soil to groundwater.

Identification of Novel Functional Inhibitors of Acid Sphingomyelinase

We describe a hitherto unknown feature for 27 small drug-like molecules, namely functional inhibition of acid sphingomyelinase (ASM). These entities named FIASMAs (Functional Inhibitors of Acid SphingoMyelinAse), therefore, can be potentially used to treat diseases associated with enhanced activity of ASM, such as Alzheimer’s disease, major depression, radiation-and chemotherapy-induced apoptosis and endotoxic shock syndrome. Residual activity of ASM measured in the presence of 10 μM drug concentration shows a bimodal distribution; thus the tested drugs can be classified into two groups with lower and higher inhibitory activity. All FIASMAs share distinct physicochemical properties in showing lipophilic and weakly basic properties. Hierarchical clustering of Tanimoto coefficients revealed that FIASMAs occur among drugs of various chemical scaffolds. Moreover, FIASMAs more frequently violate Lipinski’s Rule-of-Five than compounds without effect on ASM. Inhibition of ASM appears to be associated with good permeability across the blood-brain barrier. In the present investigation, we developed a novel structure-property-activity relationship by using a random forest-based binary classification learner. Virtual screening revealed that only six out of 768 (0.78%) compounds of natural products functionally inhibit ASM, whereas this inhibitory activity occurs in 135 out of 2028 (6.66%) drugs licensed for medical use in humans.
Influence of non-hydrophobic factors on the sorption of ionizable xenobiotics to solids

It is well known that xenobiotics sorb to solid phases like soil and sediment, depending on their inherent properties and environmental conditions. Traditionally it was accepted, that the hydrophobicity of the chemical, i.e. the log KOW, as well as the solid's content of organic carbon (OC) were the parameters describing the extent of sorption. Realizing that ionizable chemicals like weak acids and bases not always sorb according to their hydrophobicity, a correcting factor has been suggested. Correcting the hydrophobic sorption according to the Henderson-Hasselbalch equation has recently shown to improve the predicted sorption of weak acids significantly, however, weak bases do still show discrepancies compared with experimental data. In this investigation it was studied how a range of electrostatic parameters have influence on the sorption of weak bases to solid phases. Besides log KOW, pH and OC content of the solids, this investigation also included parameters like clay, silt and sand content, cation exchange capacity, zeta potential and other properties of the solids, and the impact on the sorption of weak bases to solids. Weak bases with pKa-values differing about half a unit in the range 4-9, resulting in ionization within an environmental relevant pH range, are selected for the study. Literature is searched for data on distribution coefficients (log KD) where also information about the experimental conditions regarding electrostatic parameters was reported. Taking the above mentioned parameters into consideration, predictions and regressions of the distribution to solids shall be improved.

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Integrated testing strategies (ITS) for bioaccumulation: hierarchical scheme of chemistry-driven modules and definition of applicability domains

The efficient assessment of the bioaccumulation potential of chemicals under REACH with integrated test strategies (ITS) requires multiple tools. Existing data have to be searched and information from chemical structures and physico-chemical properties need to be evaluated prior to considering to conduct in-vivo experiments with vertebrates. The OSIRIS inventory of chemistry-driven and in-silico BCF modules for ITS compiles:

- Sources of existing data
- Computational methods - B/nonB classification models - QSARs - Physiological models - Exposure models - Read across
- in-vitro tools
- 3R (Refine, Reduce, Replace) modules

The ITS components for bioaccumulation listed in the ECHA Guidance on information requirements and chemical safety assessment [1,2] have been extended with new knowledge generated in OSIRIS and complemented with feedback from stakeholders on the actual problems in using ITS for chemical registration. The alternative ITS modules share three major objectives to save time and money by reducing the number of experimental animals required to come to a conclusion about the bioaccumulation potential of chemicals under REACH:

- Classification of non-B/B/vB-compounds
- Omission of BCF studies, that are scientifically unnecessary or technically not feasible
- Waiving of BCF studies, that provide no risk-relevant information


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Modeling experimental findings on sorption and biodegradation of PAHs
Polycyclic aromatic hydrocarbons (PAHs) in the environment are to a major degree bound to organic matter or soot particles. It is disputed whether and to which extent the adsorbed fraction of PAH in soil and sediment can be attacked by microbial enzymes, or whether dissolution in aqueous media is required. In that case, the degradation depends critically on the bioavailability, or better the bioaccessibility of PAH for microbes. The increasing non-accessibility of PAH with time (‘aging’) may explain the formation of a residual fraction, which has been observed in remediation projects. A unified model for sorption, sequestration and degradation of neutral organic compounds in soils and sediments has been developed and tested (see also Trapp et al. session J01). Adsorption was considered as a two-phase process, with rapid and slow adsorption rates. Calculated or experimental sorption rates and kinetic data for growth and metabolism of PAH-degrading bacteria were obtained as input parameters. The model simulations were compared to existing solutions (such as the Best equation) and to experimental results. With this new model approach, a range of experimental observations available in literature could be simulated, encompassing various soil types and PAHs, and different bacterial strains. Own experiments are currently performed on phenantrene, fluoranthene and other PAHs and on ad/desorption as well as on biodegradation. The results shall be used to calibrate and verify the new model approach. The model was also used to simulate typical scenarios of adsorption (aging) and microbial degradation, in order to identify sensitive parameters and processes. Furthermore, the impact of dissolved organic matter and various types of amendments was studied, which potentially enhance diffusive mass transfer and biodegradation performance. The final goal is to optimize remediation options.

General information
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Organisations: Environmental Chemistry, Department of Environmental Engineering, Aarhus University
New concepts for dynamic plant uptake models

Models for the prediction of chemical uptake into plants are widely applied tools for human and wildlife exposure assessment, pesticide design and for environmental biotechnology such as phytoremediation. Steady-state considerations are often applied, because they are simple and have a small data need. However, often the emission pattern is non-steady. Examples are pesticide spraying, or the application of manure and sewage sludge on agricultural fields. In these scenarios, steady-state solutions are not valid, and dynamic simulation is required. We compared different approaches for dynamic modelling of plant uptake in order to identify relevant processes and timescales of processes in the soil–plant–air system. Based on the outcome, a new model concept for plant uptake models was developed, approximating logistic growth and coupling transpiration to growing plant mass. The underlying system of differential equations was solved analytically for the inhomogenous case, i.e. for constant input. By superposition of the results of n periods, changes in emission and input data between periods are considered. This combination allows to mimic most input functions that are relevant in practice. The model was set up, parameterized and tested for uptake into growing crops. The outcome was compared with a numerical solution, to verify the mathematical structure.

Optimal choice of pH for toxicity and bioaccumulation studies of ionizing organic chemicals

It is recognized that the pH of exposure solutions can influence the toxicity and bioaccumulation of ionizing compounds. The present study investigates whether it can be considered a general rule that an ionizable compound is more toxic and more bioaccumulative when in the neutral state. Three processes were identified to explain the behavior of ionizing compounds with changing pH: the change in lipophilicity when a neutral compound becomes ionized, electrical attraction, and the ion trap. The literature was screened for bioaccumulation and toxicity tests of ionizing organic compounds performed at multiple pH levels. Toxicity and bioconcentration factors (BCFs) were higher for acids at lower pH values, whereas the opposite was true for bases. The effect of pH was most pronounced when pH-pKa was in the range of -1 to 3
for acids, and -3 to 1 for bases. The factor by which toxicity and BCF changed with pH was correlated with the lipophilicity of the compound (logKOW of the neutral compound). For both acids and bases, the correlation was positive, but it was significant only for acids. Because experimental data in the literature were limited, results were supplemented with model simulations using a dynamic flux model based on the Fick-Nernst-Planck diffusion equation known as the cell model. The cell model predicts that bases with delocalized charges may in some cases show declining bioaccumulation with increasing pH. Little information is available for amphoteric and zwitterionic compounds; however, based on simulations with the cell model, it is expected that the highest toxicity and bioaccumulation of these compounds will be found where the compounds are most neutral, at the isoelectric point. © 2011 SETAC.
The effect of pH on the uptake and toxicity of the bivalent weak base chloroquine tested on Salix viminalis and Daphnia magna

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Organisations: Department of Environmental Engineering, Environmental Chemistry
Contributors: Rendal, C., Kusk, K. O., Trapp, S.
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Research output: Contribution to journal › Journal article – Annual report year: 2011 › Research › peer-review

The neutral species of the weak base trimethoprim is more toxic to willow trees (Salix viminalis) than the cation

The acute toxicity of the veterinary antibiotic trimethoprim (TMP) to willow trees was tested at three different pH levels in hydroponic solutions with TMP concentrations of 1, 10, 100 or 1000 mg/L. The pH variation was achieved by using ammonium (pH 4.3, low) or nitrate (pH 6.4, medium) as nitrogen source, and by additional tritration with KOH (pH 8.15, high). TMP is a weak base that dissociates at pKa 7.2. A statistically significant higher toxicity of the neutral form was observed, i.e. a higher toxicity at medium and high pH than at low pH. A toxic effect of the neutral form was observed at an external concentration of 100 mg/L, while the toxicity of the cation appeared only at the concentration of 1000 mg/L. The result of the study shows that the toxicity of TMP to willow trees is low, but also that the toxicity of weak bases varies with pH.

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Organisations: Environmental Chemistry, Department of Environmental Engineering, Masaryk University
Contributors: Mikes, O., Trapp, S.
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Unified model for sorption, sequestration and degradation in soils and sediments

The objective of this study is to combine ad/desorption models for organic compounds with the growth and degradation kinetics of microbes in a mathematical simulation model. The goal is to interpret and predict observed effects, such as increasing persistence with time, decreasing degradation rates with concentration, and effects of amendments on sorption and degradation. A second objective is the mathematical definition of the terms "persistence", "bioavailability" and "bioaccessibility". A numerical model was set up that combines ad/desorption, microbial metabolism and the formation of non-extractable residues (NER). It contains the compartments non-aqueous phase liquids or solids (N), dissolved compound (D), adsorbed (A) and sequestered (S) compound, bacterial mass (X) and biotic as well as abiotic NER. The exchange between these compartments is expressed by rates. Bacterial growth follows Monod kinetics minus decay (maintenance) rate, degradation is due to bacterial maintenance or growth. The evolving non-linear differential equations are solved numerically. The model is formulated in activity notation and implemented in Matlab. Comparison to the analytical Best equation gave (for suitable scenarios) full agreement, which is a verification of the model structure, mathematics and implementation of the numerical model. Validation by comparison to experimental studies is underway (see Rein et al., this session). The unified model allows the simulation of sorption, sequestration, bacterial growth and degradation processes simultaneously and coupled together. By this, we hope to get a better understanding of aging and persistence in soil and of the formation of bound residues (better: non-extractable residues), but the goal is also the optimization of amendments, such as DOC, compost or charcoal. Acknowledgement - The authors thank the European Commission for funding by the FP 7 grant No. 245226 MAGICPAH”Molecular Approaches and MetaGenomic Investigations for optimizing Clean-up of PAH contaminated sites, and the Research School of Environmental Chemistry, Microbiology and Toxicology (RECETO) for funding the project PUB - Prediction of persistence of soil pollutants under various conditions of bioavailability.
Activity-Based Concept for Transport and Partitioning of Ionizing Organics

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Acute Toxicity of the Dissociating Veterinary Antibiotics Trimethoprim to Willow Trees at Varying pH

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A Multimedia activity model for ionizable compounds - Validation study with 2,4-Dichlorophenoxyacetic acid, aniline and trimethoprim

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An unexpected challenge: Ionizable compounds in the REACH chemical space

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Source-ID: 268490
Research output: Contribution to journal › Journal article – Annual report year: 2010 › Research › peer-review

Comparison of prediction methods for the uptake of As, Cd and Pb in carrot and lettuce
The New Model Framework (NMF) for uptake into crops is based on particle deposition and Transfer factors from soil to plant calculated from the BÂse de donnÃ¨es sur les teneurs en Elments Traces mttaliques de Plantes Potagres (BAPPET) database. Besides NMF, approaches developed by the National Institute of Public Health and the Environment (RIVM), Hough, and the United States Environmental Protection Agency (US EPA), and the Contaminated Land Exposure Assessment (CLEA) approach were tested. Experimental data were assembled from the BAPPET database and Danish background data of As, Cd and Pb in soil, air and crops was collected. None of the models proved able to estimate the measured concentrations in plants from the BAPPET database with an absolute normalized error smaller than 70%. On average, the predictions had an error of 80-250%. However, when applying the models to the rural Danish background scenario, the NMF and other models predicted the concentrations in carrot and lettuce within the range of measured values. Regressions considering soil pH, organic matter and clay content were not superior to simple transfer factors. The transfer from air to plant is significant, at least under background conditions, and should be considered in the prediction methods.

General information
Coupling of Groundwater Transport and Plant Uptake Models

Plants significantly influence contaminant transport and fate. Important processes are uptake of soil and groundwater contaminants, as well as biodegradation in plants and their root zones. Models for the prediction of chemical uptake into plants are required for the setup of mass balances in environmental systems at different scale. Feedback mechanisms between plants and hydrological systems can play an important role, however having received little attention to date. Here, a new model concept for dynamic plant uptake models applying analytical matrix solutions is presented, which can be coupled to groundwater transport simulation tools. Exemplary simulations of plant uptake were carried out, in order to estimate concentrations in the soil-plant-air system and the influence of plants on contaminant mass fluxes from soil to groundwater.

Dynamic models to predict the uptake and fate of organic compounds in plants

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Rein, A., Legind, C. N., Kennedy, A., Trapp, S., Franco, A.
Publication date: 2010

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Publisher: SETAC Europe Office
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http://www.eventure-online.com/eventure/publicAbstractView.do?id=116589&congressId=3358
Effect of pH and dissociation on the fate and exposure of ionizable chemicals

Ionizable organic chemicals comprise an important fraction of pharmaceuticals, pesticides as well as industrial chemicals. It has been estimated that 33% of the preregistered REACH substances is mostly ionized at pH 7. To extend the applicability of existing exposure models, a Multimedia Activity Model for Ionics (MAMI) was recently developed and tested. In the present study, the impact of the parameters describing ionization was assessed by performing the sensitivity and the uncertainty analysis on MAMI for the acids 2,4-D, pentachlorophenol, bisphenol-A, perfluorooctanoic acid and the bases aniline, 4-chloroaniline and trimethoprim. A realistic emission scenario was simulated for each test chemical. First, a sensitivity analysis was performed to assess the influence of individual input parameters on the results. Then, probability density functions were derived for the most sensitive input parameters. The sensitivity analysis showed that the parameters describing ionization, pH and the dissociation constant (pKa), are among the most sensitive model parameters. The uncertainty analysis, however, indicated that these parameters are not the major source of uncertainty, which statistically justifies the use of species-specific models for ionics. The water content in air is a sensitive parameter for the PEC in air of molecules with negligible air-water partition coefficient, such as ions. The uncertainty of the QSARs for solid-water sorption significantly affects the PECs in soils and sediments. In most cases, the uncertainty of PECs and of persistence is largely explained by the uncertainty of (bio)degradation rates, which may be caused by model assumptions, experimental or estimation errors or by the environmental variability, including the effect of pH.

Lipophilic Cationic Drugs Increase the Permeability of Lysosomal Membranes in a Cell Culture System
New model concepts for dynamic plant uptake and mass flux estimates in the soil-plant-air system

Plants significantly influence contaminant transport and fate. Important processes are uptake of soil and groundwater contaminants, as well as biodegradation in plants and their root zones. Models for the prediction of chemical uptake into plants are required for the setup of mass balances in environmental systems at different scales. Feedback mechanisms between plants and hydrological systems can play an important role. However, they have received little attention to date. Here, a new model concept for dynamic plant uptake models applying analytical matrix solutions is presented, which can be coupled to groundwater transport simulation tools. Exemplary simulations of plant uptake were carried out in order to estimate chemical concentrations in the soil-plant-air system and the influence of plants on contaminant mass fluxes from soil to groundwater.

Pesticide exposure assessment in flowing waters – results for predicted environmental concentrations in some brooks in Germany

The "Georisk"- project of the German Federal Environmental Agency forms the scientific basis for an integration of more realistic landscape based scenarios into the process of pesticide registration. Here, first results of geodata-based simulations are presented. The objective of the simulations was to predict initial environmental concentrations in flowing water bodies after spray drift exposure. Based on this the downstream development of these concentrations over space and time with regard to dispersion processes was simulated (PECtwa, Time over Threshold). An adequate GIS-based software-environment and a functional workflow have been developed which make use of high and medium resolution geodata (water bodies, application areas, mitigating vegetation) and implement results of the relevant scientific work. The observed spatial entity here, as a first step, is a brook in the Hallertau Region, Germany. The analysis was carried out with two different data bases: (i) a mesoscale dataset from the German ATKIS (official landuse data), and (ii) a high resolution (HR) landscape classification derived from digital ortho-images. The results show a continuous downstream increase of ToTh and a downstream increasing TWA strongly correlated to the neighbouring application areas. Differences between the databases can be stated: PECtwa(1h) at 3150 m from the source simulated on ATKIS data amounts to 18 µg/l (Max: 18.5 µg/l at 6000 m), whereby the value calculated on HR-data is 11.7 µg/l (Max: 18 µg/l at 4250 m). The plot for TWA on Hr-basis shows a stronger variability due to a higher spatial resolution of the data. ToTh at 3150 m based on ATKIS lasts 2 h 49 min (Max: 5 h 10 m at 6000 m), the value based on HR-data is 1 h 48 min (Max: 4 h 50 m at 6000 m).
Removal of 4-chlorobenzoic acid from spiked hydroponic solution by willow trees (Salix viminalis)

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Deavers, K., Macek, T., Karlson, U., Trapp, S.
Pages: 1355-1361
Publication date: 2010
Peer-reviewed: Yes

Publication information
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Volume: 17
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Scopus rating (2010): SJR 1.148 SNIP 1.127
Web of Science (2010): Impact factor 2.87
Web of Science (2010): Indexed yes
Original language: English
DOIs: 10.1007/s11356-010-0321-3

Standardized rank for tree core sampling on chlorinated ethenes contamination site

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Wahyudi, A., Bogaert, P., Trapp, S., Machackova, J.
Number of pages: 215
Publication date: 2010

Host publication information
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Volume: Abstracts of presentations
Publisher: UFZ

The pH dependent toxicity and bioaccumulation of chloroquine tested on S. viminalis (basket willow)
It is known that the uptake and accumulation of electrolytes is very sensitive to pH owing to the slower diffusion of charged compounds across membranes, and other factors such as the Nernst effect and the ion trap effect. However, the significance of pH to the bioaccumulation of electrolytes has only been investigated sparingly in practical laboratory experiments leaving limited data with which to confirm the accuracy of current modeling efforts in the area. The aim of this study was to examine the effects of pH on the bioaccumulation and toxicity of the malaria drug chloroquine (a divalent weak base) on S. viminalis (basket willow). The transpiration of sprouted S. viminalis cuttings was monitored under the exposure of increasing concentrations (1, 10, 20, and 40 mg/L) of chloroquine at pH levels of 6, 7, 8, and 9. Solutions were buffered with phosphate (pH 6 and 7) and TRIS (hydroxymethyl) – aminomethane (pH 8 and 9). Concentrations were determined with spectrophotometer. Toxicity was derived from calculations of normalized transpiration over time, and RCF (root concentration factor) values were calculated. Increasing BCF values were found for increasing pH levels, and the toxicity was likewise seen to increase with increasing pH. These trends were in good agreement with the expected, and
with the findings from other studies where uptake has been examined at various pH.

The value and adaptation of plant uptake models in international trade of produce treated with crop protection products

Crop Protection Product (CPP) national registrations and/or international trade require magnitude and decline of residue data for treated produce. These data are used to assess human dietary risk and establish legal limits (Maximum Residue Limits, MRLs) for traded produce. The ability to predict residues based on limited data sets affords business value by enabling informed product development decisions about the likelihood for MRL compliance for varied product use scenarios. Predicted residues can additionally support the design and conduct of time-constrained interdependent studies required for product registrations. While advances in predicting residues for the case of foliar applications of CPPs have been achieved, predictions for the case of soil applications of CPPs provide additional challenge. The adaptation of a newly developed dynamic model to CPP product use scenarios will be explored with respect to the accuracy required to derive business value.

Tree Core Sampling for Screening of Toxic Elements in Soils: Poster J2

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Nielsen, M. A., Rein, A., Legind, C. N., Trapp, S.
Publication date: 2010
Peer-reviewed: No
Tree core sampling for the screening of heavy metal contamination in the subsurface

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Aarhus University, Norwegian Institute for Agricultural and Environmental Research
Contributors: Rein, A., Karlson, U., Amundsen, C., Trapp, S.
Number of pages: 111
Publication date: 2010

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Title of host publication: Grundwasser für die Zukunft, FH-DGG Tagungen
Place of publication: Neustadt
Publisher: Geschäftsstelle der Fachsektion Hydrogeologie in der Deutschen Gesellschaft für Geowissenschaften e.V. (SGG).
Source: orbit
Source-ID: 262934
Research output: Chapter in Book/Report/Conference proceeding » Conference abstract in proceedings – Annual report
year: 2010 » Research

Trees as indicators of subsurface pollution

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Rein, A., Nielsen, M., Karlson, U., Amundsen, C., Trapp, S.
Number of pages: 213
Publication date: 2010

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Title of host publication: ConSoil 2010
Publisher: UFZ
Source: orbit
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year: 2010 » Research » peer-review

Bioaccumulation of pharmaceuticals: Extended Abstract PH02A-4

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Trapp, S., Franco, A.
Publication date: 2009

Host publication information
Title of host publication: SETAC Europe 19th Annual Meeting Göteborg, Sweden 31 May - 4 June 2009. Protecting ecosystem health: facing the challenge of a globally changing environment
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Place of publication: Brussels
Publisher: SETAC Europe Office
Source: orbit
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Research output: Chapter in Book/Report/Conference proceeding » Conference abstract in proceedings – Annual report
year: 2009 » Research » peer-review

Bioaccumulation of polar and ionizable compounds in plants

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Trapp, S.
Brug af trækerneprøver til screening for chlorerede opløsningsmidler

Contaminant uptake into plants: consideration of dynamic processes: Abstract Org P57

Finding activity feasible: a multimedia model for ionizable compounds. Test results for 2,4-D and aniline: Extended Abstract CH05A-3
Influence of soil pH on the sorption of ionizable chemicals: modeling advances

The soil-water distribution coefficient of ionizable chemicals (K-d) depends on the soil acidity, mainly because the pH governs speciation. Using pH-specific K-d values normalized to organic carbon (K-OC) from the literature, a method was developed to estimate the K-OC of monovalent organic acids and bases. The regression considers pH-dependent speciation and species-specific partition coefficients, calculated from the dissociation constant (pK(a)) and the octanol-water partition coefficient of the neutral molecule (log P-n). Probably because of the lower pH near the organic colloid-water interface, the optimal pH to model dissociation was lower than the bulk soil pH. The knowledge of the soil pH allows calculation of the fractions of neutral and ionic molecules in the system, thus improving the existing regression for acids. The same approach was not successful with bases, for which the impact of pH on the total sorption is contrasting. In fact, the shortcomings of the model assumptions affect the predictive power for acids and for bases differently. We evaluated accuracy and limitations of the regressions for their use in the environmental fate assessment of ionizable chemicals.

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Franco, A., Fu, W., Trapp, S.
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Peer-reviewed: Yes

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Scopus rating (2009): SJR 1.616 SNIP 1.053
Web of Science (2009): Indexed yes
Original language: English
Keywords: Sorption, Organic carbon-water partition coefficient
Source: orbit
Source-ID: 238371

Insignificant acute toxicity of TiO2 nanoparticles to willow trees

Manufactured nanoparticles (MNP) are expected to increase in production in near future. In response, their environmental fate and effects are intensively studied. Phytotoxicity of some types of nanoparticles has been observed for annual species in the seed germination and root elongation test. Yet, no results of toxicity tests with trees have been reported. Woody species, dominant in many ecosystems, may be vulnerable in particular due to the large porous wood compartment. This study tests the toxicity of TiO2 nanoparticles on trees with the short-term willow tree transpiration test. TiO2 particles with 25- and 100-nm diameter were suspended in distilled water at concentrations of 0, 1, 10, and 100 mg/L (first test) and 0, 10, 20, and 50 mg/L (second test). Effects on transpiration, growth, and water use efficiency of exposed willow cuttings were monitored. The concentration of nanoparticles was measured by spectrophotometry. None of the measured effect parameters (growth, transpiration, and water use efficiency) showed any significant change during the test. Particles were rapidly lost from solution, probably due to sedimentation as a result of aggregation and also due to adsorption to roots. The loss of nanoparticles from solution was faster for particles with larger diameter and in the presence of trees. Willow trees were not sensitive to short-term exposure to TiO2 nanoparticles. Similar results were obtained for other plant species. Effects of nanoparticles were observed for zinc and zinc oxide particles, but these effects were probably due to heavy metal toxicity and not nanosize specific. In summary, we came to the conclusion that woody species are not in particular vulnerable to nanosized TiO2 particles in the conditions, concentrations, and time periods used in this study. The preliminary results of this study should be confirmed with other types of MNP, other plant species, experiments in soil and experiments combining longer duration, and low exposure concentrations before a final conclusion in this issue can be made.

General information
Methods for estimating the bioconcentration factor of ionizable organic chemicals

General information
Publication status: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Environmental Chemistry, Department of Environmental Engineering
Contributors: Fu, W., Franco, A., Trapp, S.
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Peer-reviewed: Yes

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Scopus rating (2009): SJR 1.616 SNIP 1.053
Web of Science (2009): Indexed yes
Original language: English
DOIs:
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Source: orbit
Source-ID: 244891
Research output: Contribution to journal › Journal article – Annual report year: 2009 › Research › peer-review

Microbial degradation of PCB congener related to their bioavailability

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry
Contributors: Rein, A., Fernqvist, M., Mayer, P., Trapp, S., Karlson, U.
Number of pages: 26
Publication date: 2009
Modelling the exposure of children and adults via diet to chemicals in the environment with crop-specific models

Exposure to chemicals via diet is a major uptake pathway for many compounds but is often estimated in a rather generic way. We use a new model framework (NMF) with crop-specific models to predict the dietary intake by 4–5-year-old children and 14–75-year-old women of three environmental compounds from their background concentrations in soil and air. Calculated daily intakes of benzo(a)pyrene and 2,3,7,8-TCDD are in good agreement with measured results from diet studies. The major source of both compounds in human diet is deposition from air. Inhalation of air and ingestion of soil play a minor role. Children take up more than twice the amount than adults per kg bodyweight, due to higher consumption per kg bodyweight. Contrary, the methods for indirect human exposure suggested in the Technical Guidance Document (TGD) for chemical risk assessment in the EU lead to overprediction, due to unrealistic consumption data and a false root model.

Modelling the indirect human exposure to chemicals in soil and air with crop-specific models: Extended Abstract TE01-1

Modelling the indirect human exposure to chemicals in soil and air with crop-specific models: Extended Abstract TE01-1

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Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Legind, C. N., Trapp, S.
Publication date: 2009

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Place of publication: Brussels
Publisher: SETAC Europe Office
Source: orbit
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Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2009 › Research › peer-review
Monitoring of heavy metal subsurface contamination using trees

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Rein, A., Karlson, U., Amundsen, C., Trapp, S.
Publication date: 2009

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Title of host publication: GreenRemediation. Incorporating Sustainable Approaches in Site Remediation, International Conference, Copenhagen, Denmark, 9-10 November 2009 : Proceedings
Volume: CD-ROM
Place of publication: Allerød
Publisher: Niras
Source: orbit
Source-ID: 253058
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2009 › Research

Role of pH for the bioconcentration of ionizable organic compounds
The role of pH for the bioconcentration of ionizable organic compounds was investigated using measured bioconcentration factor (BCF) data of monovalent acids and bases collected from literature. Only studies where BCF was measured at more than one pH were considered. The measured BCF-values were highly correlated to the log D, external pH (except acids in fish) and pKa of the test substances. Existing regressions (Veith and Fu for fish and Briggs RCF for plant cells) with log D (apparent octanol-water partition coefficient) as input parameter were tested for their capability to predict BCF-values determined at different pH. As second tool, a dynamic cell model based on the Fick-Nernst-Planck equation was tested. For the BCF fish of monovalent acids and bases, the BCF regressions and the cell model performed similar. For the BCF of water plants and plant roots, the regression failed to predict the BCF for low log D values. The cell model had higher accuracy and precision for both acids and bases. The results indicate that for the BCF data in fish, lipophilic sorption of neutral molecule and ion are the dominating process. For the BCF in plant cells, the ion trap often led to an increase in accumulation. An ion trap is pH dependent and occurs when the molecule permeates the cell membrane in a neutral state but dissociates inside. For measurements of BCF-values of acids and bases it is recommended to use a low pH for acidic compounds and a high pH for alkaline compounds.

Uptake of polychlorinated biphenyls and organochlorine pesticides from soil and air into radishes (Raphanus sativus)
Uptake of organochlorine pesticides and polychlorinated biphenyls from soil and air into radishes was measured at a heavily contaminated field site. The highest contaminant concentrations were found for DDT and its metabolites, and for beta-hexachlorocyclohexane. Bioconcentration factor (BCF, defined as a ratio between the contaminant concentration in the plant tissue and concentration in soil) was determined for roots, edible bulbs and shoots. Root BCF values were constant and not correlated to log K-OW. A negative correlation between BCF and log K-OW was found for edible bulbs. Shoot BCF values were rather constant and varied between 0.01 and 0.22. Resuspended soil particles may facilitate the transport of chemicals from soil to shoots. Elevated POP concentrations found in shoots of radishes grown in the control plot support the hypothesis that the uptake from air was more significant for shoots than the one from soil. The uptake of POPs from air was within the range of theoretical values predicted from log K-OA.
Using tree core samples to monitor natural attenuation and plume distribution of pollutants in groundwater

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Trapp, S.
Number of pages: 16
Publication date: 2009

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Publisher: Helmholtz Centre for Environmental Research - UFZ
Source: orbit
Source-ID: 244097
Research output: Chapter in Book/Report/Conference proceeding > Conference abstract in proceedings – Annual report year: 2009 > Research

Adapting environmental fate models to ioniable compounds: Abstract TUPC1-7

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Franco, A., Fu, W., Trapp, S.
Publication date: 2008

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Volume: Abstract book
Place of publication: Brussels
Publisher: SETAC
Source: orbit
Source-ID: 220631
Research output: Chapter in Book/Report/Conference proceeding > Conference abstract in proceedings – Annual report year: 2008 > Research > peer-review

Coupled mother-child model for bioaccumulation of POPs in nursing infants

General information
Publication status: Published
Direct measurement of VOC diffusivities in tree tissues: Impacts on tree-based phytoremediation and plant contamination

Recent discoveries in the phytoremediation of volatile organic compounds (VOCs) show that vapor-phase transport into roots leads to VOC removal from the vadose zone and diffusion and volatilization out of plants is an important fate following uptake. Volatilization to the atmosphere constitutes one fundamental terminal fate processes for VOCs that have been translocated from contaminated soil or groundwater, and diffusion constitutes the mass transfer mechanism to the plant–atmosphere interface. Therefore, VOC diffusion through woody plant tissues, that is, xylem, has a direct impact on contaminant fate in numerous vegetation–VOC interactions, including the phytoremediation of soil vapors and dissolved aqueous-phase contaminants. The diffusion of VOCs through freshly excised tree tissue was directly measured for common groundwater contaminants, chlorinated compounds such as trichloroethylene, perchloroethene, and tetrachloroethane and aromatic hydrocarbons such as benzene, toluene, and methyl tert-butyl ether. All compounds tested are currently being treated at full scale with tree-based phytoremediation. Diffusivities were determined by modeling the diffusive transport data with a one-dimensional diffusive flux model, developed to mimic the experimental arrangement. Wood–water partition coefficients were also determined as needed for the model application. Diffusivities in xylem tissues were found to be inversely related to molecular weight, and values determined herein were compared to previous modeling on the basis of a tortuous diffusion path in woody tissues. The comparison validates the predictive model for the first time and allows prediction for other compounds on the basis of chemical molecular weight and specific plant properties such as water, lignin, and gas contents. This research provides new insight into phytoremediation efforts and into potential fruit contamination for fruit-bearing trees, specifically establishing diffusion rates from the transpiration stream and modeling volatilization along the transpiration path, including the trunk and branches. This work also has importance in other plant–VOC interactions, such as potential uptake from the atmosphere for hydrophobic compounds and also uptake from vapor-phase soil contaminants.
Distribution and bioconcentration of organochlorine pesticides (OCPs) and polychlorinated biphenyl's (PCBs) in the soil/plant/air system using radishes (Raphanus sativus): Abstract TU 134

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Mikes, O., Cupr, P., Trapp, S., Klanova, J.
Number of pages: 131
Publication date: 2008

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Volume: Abstract book
Place of publication: Brussels
Publisher: SETAC
Source: orbit
Source-ID: 220612
Research output: Chapter in Book/Report/Conference proceeding – Annual report year: 2008 › Research › peer-review

Estimation of the soil-water partition coefficient normalized to organic carbon for ionizable organic chemicals
The sorption of organic electrolytes to soil was investigated. A dataset consisting of 164 electrolytes, composed of 93 acids, 65 bases, and six amphoters, was collected from literature and databases. The partition coefficient log KOW of the neutral molecule and the dissociation constant pKa were calculated by the software ACD/Labs®. The Henderson-Hasselbalch equation was applied to calculate dissociation. Regressions were developed to predict separately for the neutral and the ionic molecule species the distribution coefficient (Kd) normalized to organic carbon (KOC) from log KOW and pKa. The log KOC of strong acids (pKa <4) was not correlated to these parameters. The regressions derived for weak acids and bases (undissociated at environmental pH) were similar. The highest sorption was found for strong bases (pKa > 7.5), probably due to electrical interactions. Nonetheless, their log KOC was highly correlated to log KOW. For bases, a nonlinear regression was developed, too. The new regression equations are applicable in the whole pKa range of acids, bases, and amphoters and are useful in particular for relatively strong bases and amphoters, for which no predictive methods specifically have been developed so far.

General information
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Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Franco, A., Trapp, S.
Pages: 1995-2004
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Source: orbit
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Research output: Contribution to journal › Journal article – Annual report year: 2008 › Research › peer-review
Multidisciplinary characterization of chloroethene subsurface contamination in sedimentary bedrock

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Machackova, J., Wittlingerova, Z., Trapp, S., Larsen, M.
Pages: F-008
Publication date: 2008

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Volume: CD-ROM
Place of publication: Columbus, OH
Publisher: Battelle Memorial Institute
Source: orbit
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Research output: Chapter in Book/Report/Conference proceeding → Article in proceedings – Annual report year: 2008

Multidisciplinary Characterization of Chloroethene Subsurface Contamination in Sedimentary Bedrock

General information
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Organisations: Environmental Chemistry, Department of Environmental Engineering, AECOM CZ, Czech University of Life Sciences Prague
Contributors: Machackova, J., Wittlingerova, Z., Trapp, S., Larsen, M.
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Research output: Contribution to conference → Conference abstract for conference – Annual report year: 2008

Phytotoxicity of salt and plant salt uptake: Modeling ecohydrological feedback mechanisms

General information
Publication status: Published
Organisations: Residual Resource Engineering, Department of Environmental Engineering, Environmental Chemistry
Contributors: Bauer-Gottwein, P., Rasmussen, N., Feificova, D., Trapp, S.
Pages: 1-14
Publication date: 2008
Peer-reviewed: Yes

Publication information
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Scopus rating (2008): SJR 1.814 SNIP 1.562
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Original language: English
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Pagination: W04418/1-W04418/14
**Plant uptake of NaCl in relation to enzyme kinetics and toxic effects**

**General information**
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering, Residual Resource Engineering
Contributors: Trapp, S., Feificova, D., Rasmussen, N., Bauer-Gottwein, P.
Pages: 1-7
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Peer-reviewed: Yes

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Ratings:
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- Scopus rating (2008): SJR 0.963 SNIP 1.51
- Web of Science (2008): Indexed yes
Original language: English
DOIs:
10.1016/j.envexpbot.2008.05.001

**Quantitative modeling of selective lysosomal targeting for drug design**
Lyposomes are acidic organelles and are involved in various diseases, the most prominent is malaria. Accumulation of molecules in the cell by diffusion from the external solution into cytosol, lysosome and mitochondrium was calculated with the Fick–Nernst–Planck equation. The cell model considers the diffusion of neutral and ionic molecules across biomembranes, protonation to mono- or bivalent ions, adsorption to lipids, and electrical attraction or repulsion. Based on simulation results, high and selective accumulation in lysosomes was found for weak mono- and bivalent bases with intermediate to high log $K_{ow}$. These findings were validated with experimental results and by a comparison to the properties of antimalarial drugs in clinical use. For ten active compounds, nine were predicted to accumulate to a greater extent in lysosomes than in other organelles, six of these were in the optimum range predicted by the model and three were close. Five of the antimalarial drugs were lipophilic weak dibasic compounds. The predicted optimum properties for a selective accumulation of weak bivalent bases in lysosomes are consistent with experimental values and are more accurate than any prior calculation. This demonstrates that the cell model can be a useful tool for the design of effective lysosome-targeting drugs with minimal off-target interactions.

**General information**
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Trapp, S., Rosania, G., Horobin, R., Kornhuber, J.
Pages: 1317-1328
Publication date: 2008
Peer-reviewed: Yes

**Publication information**
Journal: European Biophysics Journal
Volume: 37
Issue number: 8
ISSN (Print): 0175-7571
Ratings:
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.311 SNIP 0.823
- Web of Science (2008): Indexed yes
Original language: English
DOIs:
10.1007/s00249-008-0338-4
Uptake, removal, accumulation and phytotoxicity of 4-chlorophenol in willow trees: Abstract WE 129

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Ucisik, A. S., Trapp, S.
Number of pages: 167
Publication date: 2008

Host publication information
Title of host publication: World under stress: scientific and applied issues in environmental toxicology and chemistry.
SETAC Europe annual meeting, 18, 25-29 May 2008
Volume: Abstract book
Place of publication: Brussels
Publisher: SETAC
Source: orbit
Source-ID: 220613

Uptake, removal, accumulation, and phytotoxicity of 4-chlorophenol in willow trees
4-chlorophenol (4-CP) is a well-known hazardous chlorinated compound and a precursor for the synthesis of the herbicide 2,4-dichlorophenoxyacetate. The relation between uptake, accumulation, toxicity, and removal of 4-CP in willow trees (Salix viminalis) was determined. In addition, the feasibility of implementing phytoremediation as a treatment method for 4-CP contamination was investigated. Willows were exposed to 4-CP levels ≤79.9 mg/L in hydroponic solution. The transpiration of the trees was used to determine toxic effects. Almost no inhibition of transpiration was detected at concentrations ≥15 mg/L. For concentrations ≥37.3 mg/L, transpiration decreased to ≤50%, and the trees wilted. Trees exposed to 79.9 mg/L wilted and eventually died. For concentrations of 79.9 mg/L, a significantly higher amount of 4-CP remained at the end of experiments in the test system compared with the amount remaining at all other concentrations. The loss of chemical from the system in experiments with trees was high, ≤99.5%. In treeless experiments, the mass loss of 4-CP was only 6% to 10%. The results indicated that degradation in the root zone is the main reason for the removal of 4-CP from the media. Phytoremediation of 4-CP in willow trees seems to be a remediation option, especially at concentrations

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Contributors: Ucisik, A. S., Trapp, S.
Pages: 619-627
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Archives of Environmental Contamination and Toxicology
Volume: 54
Issue number: 4
ISSN (Print): 0090-4341
Ratings:
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.162 SNIP 1.012
Web of Science (2008): Indexed yes
Original language: English
DOIs:
10.1007/s00244-007-9065-6
Source: orbit
Source-ID: 220828

Research output: Contribution to journal › Journal article – Annual report year: 2008 › Research › peer-review
Using tree core samples to monitor natural attenuation and plume distribution

General information
Publication status: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Publication date: 2008
Peer-reviewed: Yes
Event: Abstract from ConSoil 3-6 : The 10th international UFZ-Deltares/TNO conference on soil-water systems, Milano, Italy.
Electronic versions:
ENV2008-098.pdf
Source: orbit
Source-ID: 220626
Research output: Contribution to conference › Conference abstract for conference – Annual report year: 2008 › Research › peer-review

Using tree core samples to monitor natural attenuation and plume distribution after a PCE spill
The potential of using tree core samples to detect and monitor natural attenuation of perchloroethene (PCE) in groundwater was investigated at a PCE-contaminated site. In the area of the known plume with PCE concentrations between 0.004 and >40 mg/L, cores were collected from tree trunks at a height of about 1 m above ground surface. Tree sampling of the site was completed in under six hours. Chlorinated ethenes were analyzed by headspace GC/MS. PCE (0.001 to 7 mg/kg) and natural attenuation products, TCE

Bioakkumulation polarer Stoffe in pflanzlichen Nahrungsmitteln

Bioakkumulation polarer Stoffe in pflanzlichen Nahrungsmitteln

Bioakkumulation polarer Stoffe in pflanzlichen Nahrungsmitteln

Bioakkumulation polarer Stoffe in pflanzlichen Nahrungsmitteln

Bioakkumulation polarer Stoffe in pflanzlichen Nahrungsmitteln
Degradation of PCB congeners by bacterial strains

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Helmholtz Centre for Environmental Research, Aarhus University
Contributors: Rein, A., Fernqvist, M., Mayer, P., Trapp, S., Bittens, M., Karlson, U.
Pages: 469-481
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Applied Microbiology and Biotechnology
Volume: 77
Issue number: 2
ISSN (Print): 0175-7598
Ratings:
Scopus rating (2007): SJR 1.037 SNIP 1.015
Web of Science (2007): Indexed yes
Original language: English
Keywords: Bacteria, Cometabolism, Genetically modified, Biodegradation, Modelling, Monod kinetics, PCB, Rhizoremediation, Soil contamination, Willow
Electronic versions:
Rein_etal_AMB_revised.pdf
DOIs:
10.1007/s00253-007-1175-6
URLs:
http://www.springerlink.com/content/100457/
Source: orbit
Source-ID: 207359
Research output: Contribution to journal › Journal article – Annual report year: 2007 › Research › peer-review

Diffusion of PAH in potato and carrot slices and application for a potato model
A method for quantifying the effect of medium composition on the diffusive mass transfer of hydrophobic organic chemicals through thin layers was applied to plant tissue. The method employs two silicone disks, one serving as source and one as sink for a series of PAHs diffusing through thin layers of water, potato tissue, and carrot tissue. Naphthalene, phenanthrene, anthracene, and fluoranthene served as model substances. Their transfer from source to sink disk was measured by HPLC to determine a velocity rate constant proportional to the diffusive conductivity. The diffusive flux through the plant tissue was modeled using Fick's first law of diffusion. Both the experimental results and the model suggest that mass transfer through plant tissue occurs predominantly through pore water and that, therefore, the mass transfer ratio between plant tissue and water is independent of the hydrophobicity of the chemical. The findings of this study provide a convenient method to estimate the diffusion of nonvolatile organic chemicals through various plant materials. The application to a radial diffusion model suggests that "growth dilution" renders the concentration of highly hydrophobic chemicals in potatoes below their equilibrium partitioning level. This is in agreement with field results for the bioconcentration of PAHs in potatoes.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Technical University of Denmark, Catholic University of the Sacred Heart, Aarhus University
Contributors: Trapp, S., Cammarano, A., Capri, E., Reichenberg, F., Mayer, P.
Pages: 3103-3108
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Environmental Science & Technology (Washington)
Volume: 41
Issue number: 9
Effect of temperature on the uptake and metabolism of cyanide by weeping willows

Plants’ uptake and metabolism of cyanide in response to changes in temperature was investigated. Pre-rooted weeping willows (Salix babylonica L.) were exposed to hydroponic solution spiked with potassium cyanide for 2–3 d. Ten different temperatures were used, ranging from 11°C to 32°C. Cyanide in water, plant tissue, and air was analyzed spectrophotometrically. The results revealed that significant amounts of the applied cyanide were removed from the aqueous solutions in the presence of plants. Small amounts of free cyanide were detected in plant materials in all treatments, but there was no clear trend that showed an increase or decrease in the accumulation in plant material with temperature. The highest cyanide metabolism rate for weeping willows was found at 32°C with a value of 2.78 mg CN/(kg·d), whereas the lowest value was 1.20 mg CN/(kg·d) at 11°C. The temperature coefficient, Q10, which is the ratio of metabolism rates at a 10°C difference, was determined for weeping willows to be 1.46. In conclusion, changes in temperature have a substantial influence on the uptake and metabolism of cyanide by plants, but cyanide accumulation does not increase with temperature.

Enhanced diffusion of polycyclic aromatic hydrocarbons in artificial and natural aqueous solutions

Uptake of hydrophobic organic compounds into organisms is often limited by the diffusive transport through a thin boundary layer. Therefore, a microscale diffusion technique was applied to determine the diffusive mass transfer of 12 polycyclic aromatic hydrocarbons through water, air, surfactant solutions, humic acid solutions, aqueous soil and horse manure extracts, digestive fluid of a deposit-feeding worm, and root exudates from willow plants. In most cases the
Diffusive mass transfer of PAHs was much higher through the tested media than through water, and the enhancement factors increased with increasing hydrophobicity of the PAHs. The diffusive flux of benzo[a]pyrene was for instance enhanced 74 times through gut fluid of a deposit-feeding worm when compared to water. These findings demonstrate that a wide variety of dissolved organic carbon (DOC) at environmental levels can enhance diffusive mass transfer in various transport scenarios. The diffusive uptake of PAHs into sediment dwelling organisms is particularly efficient within the gut and at direct contract with the sediment matrix. Bioremediation might be enhanced by the addition of auxiliary agents that enhance diffusive mass transfer. Enhanced diffusion needs also to be considered in dynamic transport models and for the operation and calibration of passive sampling techniques.
Mitochondriotropics: A review of their mode of action, and their applications for drug and DNA delivery to mammalian mitochondria

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Horobin, R., Trapp, S., Weissig, V.
Pages: 125-136
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Journal of Controlled Release
Volume: 121
ISSN (Print): 0168-3659
Ratings:
Scopus rating (2007): SJR 2.168 SNIP 1.81
Web of Science (2007): Indexed yes
Original language: English
DOIs:
10.1016/j.jconrel.2007.05.040
Source: orbit
Source-ID: 202034
Research output: Contribution to journal › Journal article – Annual report year: 2007 › Research › peer-review

Monitoring von Schadstoffen in Boden und Grundwasser mit Bäumen

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Karlson, U.
Number of pages: 129
Publication date: 2007

Host publication information
Place of publication: Frankfurt am Main
Publisher: Gesellschaft Deutscher Chemiker
Source: orbit
Source-ID: 203117
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2007 › Research › peer-review

Pesticide residue legal standards for beverages: risk regulation and public perception
Exposure to pesticide residues in dietary sources is a major concern of Europeans. Meanwhile, drinking water and food safety authorities establish and implement maximum residue levels (MRLs) for pesticides in drinking water and food. This study compares MRLs between EU, US and Codex authorities for both drinking water and other beverages, i.e. milk, juice and wine, investigating differences between authorites as well as
between beverage types. These results were confronted with public perceptions towards pesticide residues in beverages, based on a consumer survey conducted in Copenhagen, Denmark. Seven frequently-occurring pesticides were selected for this study. Results show that since no specific MRLs for juice and wine exist, MRLs for the raw products were used instead. Furthermore, established MRLs are significantly greater for pesticides in beverages when compared to legal standards for drinking water. Maximum levels in drinking water, if available, are generally low (0.0001 mg/L in the EU), while MRLs for pesticides in milk, juice and wine range from 0.05 to 60 mg/L. At the same time, questionnaire participants were equally concerned about their exposure to pesticide residues in drinking water and other beverage types. These findings reveal some inconsistencies in setting legal maximum concentrations for pesticide residues in different dietary sources as well as between different drinking water and food safety authorities.

General information
Publication status: Submitted
Organisations: Department of Environmental Engineering, Environmental Chemistry
Contributors: Grieger, K. D., Trapp, S.
Number of pages: 50
Publication date: 2007

Quantitative Modeling of Selective Lysosomal Targeting by Passive Diffusion of Xenobiotic Compounds: Model Development and Simulations for Single Cells
A model for prediction of accumulation of molecules in lysosomes by diffusive transport processes was developed. The model is based on an analytical solution of the Fick-Nernst-Planck-equation for a single cell, capturing drug transport from an external solution into various intracellular compartments: cytosol, lysosome and mitochondrion, and also lipids in these organelles. The model considers the diffusion of neutral and ionic molecules across membranes, dissociation to mono- or bivalent ions, dissolution in lipids and/or other adsorbing structures, and electrical attraction or repulsion. Input data of the chemical are log Kow, pKa(s) and valency. Based on simulation results, high and selective accumulation in lysosomes was found for lipophilic mono- and in particular bivalent bases with pKa values near 8. The model also indicates that lipophilic strong acids show moderate accumulation in lysosomes, by electrical attraction. Modeling intracellular transport may be a useful complement to molecular target-driven screening assays for facilitating design of lysosome-targeting drugs with minimal off-target interactions.

Keywords:

General information
Publication status: Submitted
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Glasgow, Department of Psychiatry and Psychotherapy, University of Michigan, Ann Arbor
Contributors: Trapp, S., Rosania, G., Horobin, R. W., Kornhuber, J.
Publication date: 2007
Peer-reviewed: No

Publication information
Journal: The Journal of Medicinal Chemistry
ISSN (Print): 0022-2623
Ratings:
Scopus rating (2007): SJR 2.085 SNIP 1.648
Web of Science (2007): Indexed yes
Original language: English
Research output: Contribution to journal › Journal article – Annual report year: 2007 › Research

The role of plants and bacteria in phytoremediation: kinetics aspects

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Ucisik, A. S., Romano, P., Larsen, M.
Pages: 41-49
Publication date: 2007

Host publication information
Title of host publication: Bioremediation of soils contaminated with aromatic compounds: Proceedings of the NATO advanced research workshop, Tartu, Estonia, 1-3 July 2004
Toxicity of tributyltin to willow trees

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Ciucani, G., Sismilich, M.
Pages: 517-517
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Environmental Science and Pollution Research
Volume: 14
Issue number: 7
ISSN (Print): 0944-1344
Ratings:
Scopus rating (2007): SJR 0.814 SNIP 0.991
Web of Science (2007): Indexed yes
Original language: English
Keywords: willows, tributyltin, toxicity, organotin, plants, (TBT), pH, cash crops
DOIs:
10.1007/BF02979647
Source: orbit
Source-ID: 214165
Research output: Contribution to journal › Journal article – Annual report year: 2007 › Research › peer-review

Transport und Akkumulation von elektrisch geladenen Stoffen in lebenden Zellen

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S.
Number of pages: 125
Publication date: 2007

Host publication information
Place of publication: Frankfurt am Main
Publisher: Gesellschaft Deutscher Chemiker
Source: orbit
Source-ID: 203118
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2007 › Research › peer-review

Uptake, accumulation, phytotoxicity and removal of 2,4-dichlorophenol in willow trees

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Ucisik, A. S., Trapp, S., Kusk, K. O.
Pages: 1165-1171
Publication date: 2007
Peer-reviewed: Yes

Publication information
Ammonium persulfate for the persulfate oxidation of aqueous Cr(III) as a function of oxidant and pH. Abstr. P770

Although the specific mechanisms are not completely understood, plant uptake of most xenobiotic organic compounds is believed to be a passive process related at least in part to the lipophilicity of the compound. The transpiration stream concentration factor (TSCF), a ratio of xylem to root-zone solution concentrations, is one of the most widely used descriptors in plant uptake modeling. Unfortunately, experimentally determined TSCF values are extremely limited and TSCF values used in modeling efforts are often estimated from empirically derived bell-shaped curves that relate TSCF to the log octanol/water partition coefficient (Kow). The shape of the curve implies that there is an optimal lipophilicity for uptake and translocation and compounds that are highly polar are not expected to be significantly translocated. However, recent experimental uptake data generated for highly water-soluble and water miscible compounds (e.g., sulfolane, 1,4-dioxane, MTBE) suggest that this relationship may not be appropriate. An alternative TSCF-log Kow relationship in combination with a refined model for predicting uptake and accumulation in edible fruits.

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Doucette, W., Trapp, S.
Number of pages: 165
Publication date: 2006

Host publication information
Title of host publication: SETAC North America 27th annual meeting: Global environment and sustainability - sound science in a world of diversity. 5-9 November 2006. Montreal, Canada
Place of publication: Pensacola, FL
Publisher: SETAC
Source: orbit
Source-ID: 195545
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2006 › Research › peer-review
Monitoring natural attenuation with trees

Phytoremediation of phenol and its uptake, accumulation and phytotoxicity

Response of weeping willows to linear alkylbenzene sulfonate
Setting standards - water versus wine: WE3/EU/P08

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Grieger, K.
Number of pages: 240
Publication date: 2006

Host publication information
Title of host publication: Controversies and solutions in environmental sciences : SETAC Europe 16th annual meeting, The Hague, The Netherlands, 7-11 May 2006
Volume: Abstracts
Place of publication: Brussels
Publisher: SETAC
Source-ID: 189259

Research output: Chapter in Book/Report/Conference proceeding – Annual report year: 2006 › Research › peer-review

Trees as indicators of subsurface degradation of chlorinated solvents: Poster P.T00.8

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Karlson, U., Trapp, S., Larsen, M., Burken, J., Machakova, J.
Publication date: 2006
Peer-reviewed: Yes
Event: Poster session presented at Integrating Microbial Knowledge into Human Life : FEMS Congress of European Micorbiologists, Madrid, July 4-8, .
Source-ID: 190423

Research output: Contribution to conference › Poster – Annual report year: 2006 › Research › peer-review

Uptake of iron cyanide complexes into willow trees

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Larsen, M., Trapp, S.
A predictive model for the selective accumulation of chemicals in tumor cells

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Horobin, R.
Pages: 959-966
Publication date: 2005
Peer-reviewed: Yes

Publication information
Journal: European Biophysics Journal
Volume: 34
ISSN (Print): 0175-7571
Ratings:
Scopus rating (2005): SJR 0.918 SNIP 0.72
Web of Science (2005): Indexed yes
Original language: English
DOIs: 10.1007/s00249-005-0472-1
Source: orbit
Source-ID: 182557
Research output: Contribution to journal › Journal article – Annual report year: 2005 › Research › peer-review

Chromium release from waste incineration air-pollution-control residues

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Astrup, T., Rosenblad, C., Trapp, S., Christensen, T. H.
Pages: 3321-3329
Publication date: 2005
Peer-reviewed: Yes

Publication information
Journal: Environmental Science and Technology
Volume: 23
ISSN (Print): 1382-3124
Ratings:
Web of Science (2005): Indexed yes
Original language: English
DOIs: 10.1021/es049346q
Source: orbit
Source-ID: 181489
Research output: Contribution to journal › Journal article – Annual report year: 2005 › Research › peer-review
Crop-specific human exposure assessment for polycyclic aromatic hydrocarbons in Czech soils

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Kulhánek, A., Trapp, S., Sismilich, M., Janku, J., Zimova, M.
Pages: 71-80
Publication date: 2005
Peer-reviewed: Yes

Publication information
Journal: Science of the Total Environment
Volume: 339
Issue number: 1-3
ISSN (Print): 0048-9697
Ratings:
Scopus rating (2005): SJR 1.439 SNIP 1.509
Web of Science (2005): Indexed yes
Original language: English
DOI:
10.1016/j.scitotenv.2004.08.003
Source: orbit
Source-ID: 181060
Research output: Contribution to journal › Journal article – Annual report year: 2005 › Research › peer-review

ESPR - A journal for our time

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Young, A., Holder, J., Lammel, G., Luthardt, P., McCutcheon, S., Trapp, S.
Pages: 61
Publication date: 2005
Peer-reviewed: Unknown

Publication information
Journal: Environmental Science and Pollution Research
Volume: 12
Issue number: 2
ISSN (Print): 0944-1344
Ratings:
Scopus rating (2005): SJR 0.595 SNIP 0.929
Web of Science (2005): Indexed yes
Original language: English
DOI:
10.1065/espr2005.02.001
Source: orbit
Source-ID: 180674
Research output: Contribution to journal › Journal article – Annual report year: 2005 › Communication

Estimation of transpiration stream concentration factor (TSCF), A phytoremediation parameter, for methyl tert-butyl ether (MTBE)

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Xiaozhang, Y., Trapp, S.
Pages: 235-238
Publication date: 2005
Peer-reviewed: No

Publication information
Journal: Yingyong Yu Huanjing Shengwu Xuebao
Volume: 9
Growth of plants on TBT-contaminated harbour sludge and effect on TBT removal

**General information**
- **Publication status:** Published
- **Organisations:** Department of Environmental Engineering
- **Contributors:** Novak, J., Trapp, S.
- **Pages:** 332-341
- **Publication date:** 2005
- **Peer-reviewed:** Yes

**Publication information**
- **Journal:** Environmental Science and Pollution Research
- **Volume:** 12
- **Issue number:** 6
- **ISSN (Print):** 0944-1344
- **Ratings:**
  - Scopus rating (2005): SJR 0.595 SNIP 0.929
  - Web of Science (2005): Indexed yes
- **Original language:** English
- **DOIs:** 10.1065/espr2005.08.282

Method for improving phytoremediation treatment of a contaminated medium

**General information**
- **Publication status:** Published
- **Organisations:** Unknown
- **Contributors:** Lelie, D. V. D., D'Haene, S., Dowling, D. N., Karlson, U., Moore, E. R., Taghavi, S., Trapp, S., Vangronsveld, J.
- **Publication date:** 2005

**Publication information**
- **Country:** Denmark
- **Patent number:** US 2005/015003
- **Filing date:** 07/07/2005
- **Original language:** English

Modelling organic contaminant transfer from soil into plants

**General information**
- **Publication status:** Published
- **Organisations:** Department of Environmental Engineering
- **Contributors:** Trapp, S.
- **Publication date:** 2005
- **Peer-reviewed:** No
- **Event:** Paper presented at COST Action 631- Understanding and modelling plant-soil interactions in the rhizosphere environment UMPIRE: Rhizosphere management in soils contaminated with organic and inorganic pollutants. 5th Joint meeting of management committee and working groups, Krakow-Tomaszowice, Poland 12-14 May.
- **Source:** orbit
- **Source-ID:** 181268

Research output: Contribution to conference › Paper – Annual report year: 2005 › Research
Monitoring of subsurface pollution by use of vegetation samples

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Karlson, U., Pieper, D.
Number of pages: 28
Publication date: 2005

Host publication information
Title of host publication: 2nd European conference on natural attenuation, soil and groundwater risk management, May 18-20, 2005, DECHEMA-House, Frankfurt am Main: Book of abstracts
Place of publication: Frankfurt am Main
Publisher: DECHEMA
Source: orbit
Source-ID: 181267
Research output: Chapter in Book/Report/Conference proceeding > Conference abstract in proceedings – Annual report year: 2005 > Research

Phytotoxicity of cyanide to weeping willow trees

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Yu, X., Trapp, S., Zhou, P.
Pages: 109-113
Publication date: 2005
Peer-reviewed: Yes

Publication information
Journal: Environmental Science and Pollution Research
Volume: 12
ISSN (Print): 0944-1344
Ratings:
Scopus rating (2005): SJR 0.595 SNIP 0.929
Web of Science (2005): Indexed yes
Original language: English
DOIs: 10.1065/espr2005.02.237
Source: orbit
Source-ID: 181576
Research output: Contribution to journal > Journal article – Annual report year: 2004 > Research > peer-review

Plant uptake of iron cyanide complexes

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Larsen, M., Trapp, S.
Number of pages: 24
Publication date: 2005

Host publication information
Title of host publication: COST Action 859 - Phytotechnologies to promote sustainable land use and improve food safety: 1st Scientific workshop and Management Committee meeting 14-16 June 2005, Pisa, Italy. Abstract Book
Place of publication: Pisa
Publisher: Institute of Ecosystem Study - Department of Soil chemistry - CNR
Source: orbit
Source-ID: 181457
Research output: Chapter in Book/Report/Conference proceeding > Conference abstract in proceedings – Annual report year: 2005 > Research
Quantifying the effect of medium composition on the diffusive mass transfer of hydrophobic organic chemicals through unstirred boundary layers

Unstirred boundary layers (UBLs) often act as a bottleneck for the diffusive transport of hydrophobic organic compounds (HOCs) in the environment. Therefore, a microscale technique was developed for quantifying mass transfer through a 100-μm thin UBL, with the medium composition of the UBL as the controllable factor. The model compound fluoranthene had to (1) partition from a contaminated silicone disk (source) into the medium, (2) then diffuse through 100 μm of medium (UBL), and finally (3) partition into a clean silicone layer (sink). The diffusive mass transfer from source to sink was monitored over time by measuring the fluoranthene content of the source and sink disks. The diffusive flux of fluoranthene was slightly higher for air than for water. Cyclodextrin, humic acids, and micelles of sodium dodecyl sulfate (SDS) enhanced the diffusive flux of fluoranthene in water by more than 1 order of magnitude. These results demonstrate that medium constituents, which normally are believed to bind hydrophobic organic chemicals, actually can enhance the diffusive mass transfer of HOCs in the vicinity of a diffusion source (e.g., contaminated soil particles). The technique can be used to evaluate the effect of natural fluids on diffusive mass transfer, as it integrates the different processes, partitioning and diffusion, in one laboratory model.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Danish Centre for Environment and Energy
Contributors: Mayer, P., Karlson, U., Christensen, P., Johnsen, A., Trapp, S.
Pages: 6123-6129
Publication date: 2005
Peer-reviewed: Yes

Publication information
Journal: Environmental Science & Technology
Volume: 39
Issue number: 16
ISSN (Print): 0013-936X
Ratings:
Scopus rating (2005): SJR 2.608 SNIP 1.994
Web of Science (2005): Indexed yes
Original language: English
DOIs:
10.1021/es050556s
Source: orbit
Source-ID: 182061
Research output: Contribution to journal › Journal article – Annual report year: 2005 › Research › peer-review

The effect of temperature on the rate of cyanide metabolism of two woody plants

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Pages: 1099-1104
Publication date: 2005
Peer-reviewed: Yes

Publication information
Journal: Chemosphere
Volume: 59
ISSN (Print): 0045-6535
Ratings:
Scopus rating (2005): SJR 1.479 SNIP 1.551
Web of Science (2005): Indexed yes
Original language: English
DOIs:
Source: orbit
Source-ID: 181059
Research output: Contribution to journal › Journal article – Annual report year: 2005 › Research › peer-review
Uptake, metabolism, accumulation and toxicity of cyanide in willow trees

Chemicals taken up into plants may be accumulated so leading to toxic effects. Uptake and phytotoxicity of free cyanide was determined with the willow-tree transpiration test. Willow sets were grown in sand and irrigated with varying levels of cyanide (CN). Toxicity was determined by measuring transpiration. At CN concentrations below 10 mg/L, no toxic effects were observed. At 20 mg/L, transpiration was reduced to approximately 50% after 96 h. With 30, 40 and 50 mg/L, the transpiration decreased with a similar rate to < 20% of the initial transpiration within 96 h. Accumulation of cyanide in plant tissue was observed at 40 and 50 mg/L. The kinetics of metabolism of cyanide by roots, stems and leaves of willows was determined by the closed-bottle metabolism test. The Michaelis–Menten parameters $v_{\text{max}}$ and $K_M$ (maximal metabolic velocity and half-saturation constant, respectively) were determined by nonlinear regression. Estimates of uptake and metabolism were balanced using a nonlinear mathematical model. The model predicted that at low doses (<10 mg/L), the cyanide would be rapidly metabolized. At higher doses, uptake would be faster than metabolism and consequently cyanide would accumulate in the plant tissue. This relation between external dose and internal accumulation is nonlinear and explains the toxic effects observed.

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Larsen, M., Ucisik, A. S., Trapp, S.
Pages: 2135-2142
Publication date: 2005
Peer-reviewed: No

Publication Information
Journal: Environmental Science and Technology
Volume: 39
Issue number: 7
ISSN (Print): 1382-3124
Ratings:
Web of Science (2005): Indexed yes
Original language: English
DOIs: 10.1021/es048799s
Source: orbit
Source-ID: 180866
Research output: Contribution to journal › Journal article – Annual report year: 2005 › Research

Uptake, metabolism, accumulation and toxicity of cyanide in willow trees

Biodegradation of toxic compounds by plants or by associated bacteria

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Larsen, M.
Number of pages: 43
Publication date: 2005

Host publication information
Title of host publication: COST Action 859 - Phytotechnologies to promote sustainable land use and improve food safety : 1st Scientific workshop and Management Committee meeting 14-16 June 2005, Pisa, Italy. Abstract Book
Place of publication: Pisa
Publisher: Institute of Ecosystem Study - Department of Soil chemistry - CNR
Source: orbit
Source-ID: 181458
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2005 › Research

Biodegradation of toxic compounds by plants or by associated bacteria

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S.
Publication date: 2004

Host publication information
Title of host publication: 39th Midwest Regional American Chemical Society Meeting, October 20-22, 2004, Kansas State University, Manhattan, KS : Program and Abstracts
Degradation of organic pollutants by plant-colonising bacteria

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Number of pages: 35
Publication date: 2004

Host publication information
Title of host publication: COST 859 working group 4 meeting: Integration and application of phytotechnologies, October 28-29, 2004 Leipzig, Germany. Abstracts
Place of publication: Leipzig
Publisher: BioPlanta GmbH
Source: orbit
Source-ID: 135538
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2004 › Research

Determination of Michaelis-Menten kinetics for the removal of cyanide by plants

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Larsen, M., Trapp, S.
Number of pages: 1
Publication date: 2004

Host publication information
Title of host publication: Environmental science solutions: A Pan-European perspective: SETAC Europe 14th annual meeting
Place of publication: Brussels
Publisher: SETAC
Source: orbit
Source-ID: 135540
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2004 › Research

Effect of molecular properties on the selective accumulation of chemicals in tumor cells

General information
Publication status: Published
Growth of plants in harbour sludge and effect on TBT degradation

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Novak, J.
Number of pages: 34
Publication date: 2004

Host publication information
Title of host publication: COST 859 working group 4 meeting: Integration and application of phytotechnologies, October 28-29, 2004 Leipzig, Germany. Abstracts
Place of publication: Leipzig
Publisher: BioPlanta GmbH
Source: orbit
Source-ID: 135553
Research output: Chapter in Book/Report/Conference proceeding > Conference abstract in proceedings – Annual report year: 2004 > Research

JSS-Quiz: Six mental exercises to check your fitness in soil chemistry

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S.
Pages: 210
Publication date: 2004
Peer-reviewed: Unknown

Publication information
Journal: Journal of Soils and Sediments
Volume: 4
Issue number: 3
ISSN (Print): 1439-0108
Ratings:
Scopus rating (2004): SJR 0.553 SNIP 0.623
Web of Science (2004): Indexed yes
Original language: English
Source: orbit
Source-ID: 90503
Research output: Contribution to journal > Journal article – Annual report year: 2004 > Communication

Metabolism of cyanide by Chinese vegetation

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Pages: 121-126
Publication date: 2004
Phytoremediation of TBT-contaminated Harbour Sediment: Draft report for the TBT CLEAN project

This sub-project of the TBT CLEAN project investigated the feasibility of growing plants on dredged harbour sediments and the influence of vegetation on TBT degradation. The toxicity of TBT to vascular plants was determined with the willow tree transpiration test. Compared to other species, the toxicity of TBT to willows was very low. In a field study from 2003, however, willows did not survive in fresh harbour sludge. A plausible reason is the salt content of the substrate: willows have a low salt tolerance. Besides, the structure of the soil resulting from the sludge was not supporting plant growth. It was therefore decided to lagoon the sediments before bringing plants out.

In a laboratory growth test, seeds of several plants were sown into fresh sediments, lagooned sediments, garden soil and in garden soil irrigated with salt water. Barley (Hordeum vulgare) performed best in these studies. The sediment was characterized as clay loam/sandy clay loam with a high content of nutrients and neutral pH. Fresh sediments were highly saline, with electrical conductivities up to 14 mS/cm, but upon lagooning, the salinity dropped to moderate levels of 3.7 mS/cm.

In the outdoor growth test, fresh and lagooned sludge with high (around 33 mg/kg) and low TBT (about 3 mg/kg) content were used. Several plant species were growing excellently in this substrate, particularly barley (9 to 10 tons/ha dry weight) and sorghum (10 to 13 tons/ha dry weight). The TBT content had no negative influence on the growth of plants. Many species grew better on the highly contaminated sludge.

Samples were taken below vegetation and below unvegetated blanks in a depth of 5 – 15 cm and 50 cm and analyzed for TBT and its degradation products. Below barley, the degradation was significantly enhanced. However, resulting concentrations were far above the target value (0.007 mg/kg) of the OSPAR convention. No measurable uptake of TBT and metabolites was found for barley (corn), whereas TBT, DBT and MBT were taken up in the other two investigated crops, reed and clover/grass.

It was concluded that the dredged sediment is – after lagooning – a good substrate for plant growth. Although plants support the degradation of TBT, phytoremediation is a slow process which will take several years. The transfer of TBT into crops does not allow an agricultural use of the substrate. Non-food production, such as rape-seed for biodiesel or barley for alcohol, might be an alternative.
Removal of cyanide by woody plants

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Larsen, M., Trapp, S., Pirandello, A.
Pages: 325-333
Publication date: 2004
Peer-reviewed: Yes

System for the Reduction of Substances in Reject Water from Reed-Bed Sludge Mineralization Plants

The invention is a system for the reduction of substances in reject water from reed-bed sludge mineralization plants (also referred to as sludge dewatering reed-beds). The systems utilizes the composition of substances in reject water from reed-beds and that of sludge to reduce substance mass from the reject water via recirculation into a mixed reactor and back onto the reed-beds. The mixed reactor consists of a container in which sludge (that is typically loaded directly on to reed-beds) is mixed with recirculated reject water from reed-beds. The sludge mixture has a definable hydraulic retention time within the container. The solution is then applied to the reed-beds, which dewater, converts, and partially mineralize the sludge mixture. The reject water from the reed-beds is split where up to 100% of the reject water is recirculated back to the mixed reactor and the remaining usually disposed of by sending it back to the head of a wastewater treatment plant. The system has proven to reduce the mass of nitrogen, COD, and water in the reject water, and can possibly reduce phosphorus and other substances. The overall effect is a reduction in the substance recycle within a wastewater treatment plant, and a decrease in the overall treatment demand.

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Urban Water Engineering
Contributors: Maret, D., Trapp, S., Henze, M., Petersen, G.
Publication date: 2004
The role of plants and bacteria in phytoremediation

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Ücisik, A., Romano, P., Larsen, M.
Number of pages: 7
Publication date: 2004

Host publication information
Title of host publication: Bioremediation of soils contaminated with aromatic compounds: Effects of rhizosphere, bioavailability, gene regulation and stress adaptation, Tartu, Estonia, 1-3 July 2004 : International NATO advanced research workshop
Place of publication: Tartu, Estonia
Publisher: University of Tartu
Source: orbit
Source-ID: 135554
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2004 › Research

Toxicity of tributyltin into willow trees

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Ciucani, G., Sismilich, M.
Pages: 327-330
Publication date: 2004
Peer-reviewed: Yes

Publication information
Journal: Environmental Science and Pollution Research
Volume: 11
ISSN (Print): 0944-1344
Ratings:
Scopus rating (2004): SJR 0.807 SNIP 1.007
Web of Science (2004): Indexed yes
Original language: English
Source: orbit
Source-ID: 43989
Research output: Contribution to journal › Journal article – Annual report year: 2004 › Research › peer-review

Uptake of tributyltin into willow trees

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Ciucani, G., Mosbæk, H., Trapp, S.
Pages: 267-272
Publication date: 2004
Peer-reviewed: Yes

Publication information
Journal: Environmental Science and Pollution Research
Volume: 11
Issue number: 4
ISSN (Print): 0944-1344
Ratings:
Scopus rating (2004): SJR 0.807 SNIP 1.007
Web of Science (2004): Indexed yes
Original language: English
DOIs:
http://dx.doi.org/10.1065/espr2004.05.201
Applicazione di modelli matematici per la registrazione dei prodotti fitosanitari: assorbimento radicale e trasporto xilematico di elettroliti deboli

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Ciucani, G., Capri, E., Trevisan, M., Trapp, S.
Publication date: 2003

Publication information
Place of publication: Pavia, Italy
Publisher: La Goliardica Pavese Edizioni
Original language: Italian
Source: orbit
Source-ID: 43453

Can global biomass influence global chemical cycles?

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S.
Pages: 235-237
Publication date: 2003
Peer-reviewed: Yes

Publication information
Journal: Stochastic Environmental Research and Risk Assessment
Volume: 17
ISSN (Print): 1436-3240
Ratings:
Scopus rating (2003): SJR 0.45 SNIP 0.599
Web of Science (2003): Indexed yes
Original language: English
DOIs:
10.1007/s00477-003-0136-6
Source: orbit
Source-ID: 43984

Determination of Michaelis-Menten kinetics for the removal of cyanide by plants

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Larsen, M., Trapp, S.
Number of pages: 23
Publication date: 2003

Host publication information
Title of host publication: International symposium biochemical interactions of microorganisms and plants with technogenic environmental pollutants, Saratov, Russia, 28-30 July 2003, Abstract Book
Place of publication: Saratov
Publisher: Saratov University Publishing House
Source: orbit
Source-ID: 135578
Research output: Chapter in Book/Report/Conference proceeding – Conference abstract in proceedings – Annual report year: 2003 – Research
Endophytic degrader bacteria for improving phytoremediation of organic xenobiotics: Final Report DRAFT

This project represented a completely new approach towards improving the technology of phytoremediation of soil and groundwater contaminated with water soluble and volatile compounds. It endeavoured to tackle the problem of inefficient degradation of these compounds during phytoremediation by improving their degradation during transport in the plant vascular system. Introducing endophytic degrader bacteria into the plants' vascular system was proposed as a tool to achieve this goal.

As a scientific necessity, the project comprised the thorough ecological and genetic investigation of endophytic bacteria, and the isolation of a large number of natural endophytic strains. The project delivered on this goal by providing a large collection of 150 novel characterized endophytic bacteria from poplar and willow, two plant species commonly used for phytoremediation, and from Flag Iris, a plant used for the novel technology of constructed wetlands. Several of these bacteria were engineered to degrade specific organic contaminants, including BTX, TCE, 2,4-D and naphthalene.

Central to the whole project was the goal to reveal the potential of endophytic inoculants for improving phytoremediation in terms of

- plant survival (decreased phytotoxicity of the pollutant) and contaminant removal (bacterial degradation), resulting in reduced accumulation of contaminants, their metabolites (misrouting products), or their release in the environment via plant transpiration.

Work completed with the Yellow Lupin / Burkholderia cepacia / toluene model demonstrates clearly that the inoculated endegrader (endophytic bacterial degrader) protects the plant from chemical toxicity, by degrading the toxic compound (the phytoprotection aspect of the “ENDEGRADE concept”),

- the inoculated endegrader strongly reduces the emission of the chemical from the test system, by a more complete degradation of the compound (the environmental remediation aspect of the “ENDEGRADE concept”),

- the observed effects are not due to rhizosphere colonising or soil inhabiting bacteria.

Thereby the project delivered on its central goal, and confirmed the somewhat daring project hypothesis, for which there had been only scarce evidence at the time the project was conceived.

As an unexpected result of the project, now we better understand the limitations of phytoremediation:

- TBT does not get taken up by plants,
- TCE and toluene do not get degraded by plant tissues.

These findings explain some of the hitherto inexplicable problems that phytoremediation researchers have had with these two compounds.

A spin-off of the project was the unexpected transfer of a mathematical uptake model, developed for intact plants, to human tissues and cancer cells. It appears that—as a byproduct of this project—the design of new chemotherapeutic drugs can be accelerated significantly, because using a mathematical uptake model will avoid lengthy screening steps with human tumor cell cultures. This invention was not patented and can be utilised free of charge.

Another potential spin-off of the project was the unexpected generation of constitutive TCE degraders, i.e., bacteria that do not require toluene or phenol for induction of cometabolic TCE degradation. Genetic engineering methods were not involved in the generation of this metabolic trait. The business potential of this new biotechnology is under evaluation.

General information
Publication status: Published
Organisations: Department of Environmental Science and Engineering, Danish Centre for Environment and Energy, Flemish Institute for Technological Research, Macaulay Land Use Research Institute, Hasselt University, Institute of Technology Carlow, DEME Environmental Contractors
Number of pages: 71
Publication date: 2003

Publication information
Original language: English
URLs:
http://endegrade.dmu.dk

Bibliographical note
Confidential.

ENDEGRADE EU project QLK3-2000-00164 1.jan 2001 - 31.dec. 3003.
Research output: Book/Report › Report – Annual report year: 2003 › Research

Feasibility of cyanide elimination using plants. Technical note

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Larsen, M., Pirandello, A., Danquah-Boakye, J.
Apples and other fruits are frequently cultivated in gardens and are part of our daily diet. Uptake of pollutants into apples may therefore contribute to the human daily intake of toxic substances. In current risk assessment of polluted soils, regressions or models are in use, which were not intended to be used for tree fruits. A simple model for uptake of neutral organic contaminants into fruits is developed. It considers xylem and phloem transport to fruits through the stem. The mass balance is solved for the steady-state, and an example calculation is given. The Fruit Tree Model is compared to the empirical equation of Travis and Arms (T&A), and to results from fruits, collected in contaminated areas. For polar compounds, both T&A and the Fruit Tree Model predict bioconcentration factors fruit to soil (BCF, wet weight based) of > 1. No empirical data are available to support this prediction. For very lipophilic compounds (log K-OW > 5), T&A overestimates the uptake. The conclusion from the Fruit Tree Model is that the transfer of lipophilic compounds into fruits is not relevant. This was also found by an empirical study with PCDD/F. According to the Fruit Tree Model, polar chemicals are transferred efficiently into fruits, but empirical data to verify these predictions are lacking.
Harmonized European Assessment for the Transfer of Chemicals from Soil into Food

Exposure routes of chemical compounds from soil into plants need to be known to assess the risk of food contamination. Each EU member state so far uses or develops its own assessment methods. This is inefficient and may lead to non-optimal solutions. An expression of interest was sent to the EC, proposing an initiative within the 6th EU framework programme, which aims at harmonizing the assessment methods for the transfer of chemicals into food. Existing and new methods shall be evaluated and compared in close accordance with the administrative needs. Gaps of knowledge will be identified and filled. An assessment tool (multilingual) for the EU member states based on the best available knowledge will be implemented and made available.

Modelling of Accumulation of Organic Substances in Plants and Fruit

Modelling of Accumulation of Organic Substances in Plants and Fruit

Persistence of Methyl Tertiary Butyl Ether (MTBE) against Metabolism by Danish Vegetation
Remediation technology and risk assessment

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Samsoe-Petersen, L.
Pages: 253
Publication date: 2003
Peer-reviewed: Yes

Publication information
Journal: Journal of Soils and Sediments
Volume: 3
ISSN (Print): 1439-0108
Ratings:
- Scopus rating (2003): SJR 0.625 SNIP 1.199
- Web of Science (2003): Indexed yes
Original language: English
Source: orbit
Source-ID: 43988
Research output: Contribution to journal › Journal article – Annual report year: 2003 › Research › peer-review

Results from a rapid test of acute toxicity to trees

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Sismilich, M., Suwannaetana, S., Larsen, M., Trapp, S.
Publication date: 2003
Peer-reviewed: No
Event: Poster session presented at Achievements and Prospects of Phytoremediation in Europe, Vienna, Austria.
Source: orbit
Source-ID: 135587
Research output: Contribution to conference › Poster – Annual report year: 2003 › Research

Review of plant uptake models

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S.
Pages: 397-407
Publication date: 2003

Host publication information
Title of host publication: Proceedings of the XII Symposium Pesticide Chemistry June 4-6, 2003 Piacenca, Italy
Place of publication: Piacenca, Italy
Publisher: Università Cattolica del Sacro Cuore
Source: orbit
Source-ID: 135739
Research output: Chapter in Book/Report/Conference proceeding › Article in proceedings – Annual report year: 2003 › Research
Risk assessment of cyanide contaminated gas work soil

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Larsen, M., Trapp, S.
Number of pages: 203
Publication date: 2003

Host publication information
Title of host publication: Understanding the complexity of environmental issues. A way to sustainability : SETAC Europe 13th annual meeting, Hamburg, Germany 27 April - 1 May 2003. Abstracts
Place of publication: Brussels
Publisher: SETAC
Source: orbit
Source-ID: 135579
Research output: Chapter in Book/Report/Conference proceeding › Conference abstract in proceedings – Annual report year: 2003 › Research › peer-review

Assorbimento e tossicità di tributilstagno su piante di salice

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Ciucani, G., Capri, E., Trevisan, M., Trapp, S.
Publication date: 2002
Peer-reviewed: No
Event: Poster session presented at XX Convegno Nazionale SICA (Società Italiana Chimica Agraria), Padova, Italy.
Source: orbit
Source-ID: 135601
Research output: Contribution to conference › Poster – Annual report year: 2002 › Research

Die Bedeutung biologischer Verfahren zur Bodenreinigung wird zunehmend erkantet, Bakterien, Pilze aber auch Pflanzen verfügen über Mechanismen, toxische Stoffe zu entgiften, Noch ist die Anwendung biologischer In-Situ-Verfahren wenig verbreitet

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Karlson, U.
Pages: 72-75
Publication date: 2002
Peer-reviewed: No

Publication information
Journal: Regina
Issue number: September
ISSN (Print): 0355-841X
Original language: German
Source: orbit
Source-ID: 43977
Research output: Contribution to journal › Journal article – Annual report year: 2002 › Research

Dynamic root uptake model for neutral lipophilic organics
In current European risk assessment, an equilibrium approach is used to estimate chemical uptake from soil into root vegetables. Here a dynamic model for uptake of neutral lipophilic compounds from soil into roots is presented. Using experimental results, it is compared with the equilibrium approach. Very lipophilic compounds (e.g., DDT) diffuse very slowly into plant tissue, so they are likely to remain in the peel of root vegetables. In addition, a dynamic (steady-state) flux model for uptake with transpiration water into thick roots is presented. The model considers input from soil and output to stem with the transpiration stream plus first-order metabolism and dilution by exponential growth. For chemicals with low or intermediate lipophilicity (log Kow , 2), there was no relevant difference between dynamic model and equilibrium approach. For lipophilic compounds, the dynamic model gave concentrations far below the thermodynamic equilibrium. The approach was tested against experimental uptake data of benzo[a]pyrene, polychlorinated biphenyls (PCBs), and
chlorobenzenes from soil into carrots. Measured concentrations in carrot peels were up to 100 times higher than in the core. The equilibrium approach can predict concentrations in the peels, but for carrot cores and for the whole carrot, the flux model is superior and should be preferred for a more realistic risk assessment.

**General information**
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S.
Pages: 203-206
Publication date: 2002
Peer-reviewed: Yes

**Measurement of xylem translocation of weak electrolytes with the pressure chamber technique**
Xylem translocation and root uptake of weak electrolytes were investigated with the pressure chamber technique (PCT) using de-topped soybean plants. Two compounds were organic bases (fenpropimorph and imazalil) and four were organic acids (bentazone, primisulfuron-methyl, rimsulfuron and triasulfuron). The compounds covered a wide range of log K-OW and pK(a) values. Concentrations in external solution and in xylem sap were measured by HPLC at pH values in external solution of 4.5, 6.5 and 8.5. For weak bases, translocation was higher at low pH and the transpiration stream concentration factors (TSCF) were in the range 0.31-0.95. At pH 8.5, the concentrations in leaking xylem sap were very low for fenpropimorph, and steady-state was probably not reached. For weak acids, TSCF values derived with external pH from 4.5 to 8.5 were in the range 0.55-1.50 for primisulfuron-methyl, 0.64-1.35 for rimsulfuron, 0.81-0.93 for triasulfuron and 0.69-0.92 for bentazone. The variation of TSCF of the weak electrolytes was much smaller in these PCT experiments than in recent experiments with intact plants. The likely reason is that de-topped soybean plants in the pressure chamber seemed to be unable to regulate their xylem sap pH, which was almost identical to the pH in external solution. Without pH differences, the ion-trap process, which is responsible for accumulation or exclusion of weak acids and bases in the xylem of living plants, does not take place. Model simulations carried out for intact and de-topped plants supported this hypothesis. By variation of the pH of the xylem sap, good agreement between measurements and simulations could be achieved. (C) 2002 Society of Chemical Industry.

**Endegrade: Endophytic bacteria for improving phytoremediation**
Xylem translocation and root uptake of weak electrolytes were investigated with the pressure chamber technique (PCT) using de-topped soybean plants. Two compounds were organic bases (fenpropimorph and imazalil) and four were organic acids (bentazone, primisulfuron-methyl, rimsulfuron and triasulfuron). The compounds covered a wide range of log K-OW and pK(a) values. Concentrations in external solution and in xylem sap were measured by HPLC at pH values in external solution of 4.5, 6.5 and 8.5. For weak bases, translocation was higher at low pH and the transpiration stream concentration factors (TSCF) were in the range 0.31-0.95. At pH 8.5, the concentrations in leaking xylem sap were very low for fenpropimorph, and steady-state was probably not reached. For weak acids, TSCF values derived with external pH from 4.5 to 8.5 were in the range 0.55-1.50 for primisulfuron-methyl, 0.64-1.35 for rimsulfuron, 0.81-0.93 for triasulfuron and 0.69-0.92 for bentazone. The variation of TSCF of the weak electrolytes was much smaller in these PCT experiments than in recent experiments with intact plants. The likely reason is that de-topped soybean plants in the pressure chamber seemed to be unable to regulate their xylem sap pH, which was almost identical to the pH in external solution. Without pH differences, the ion-trap process, which is responsible for accumulation or exclusion of weak acids and bases in the xylem of living plants, does not take place. Model simulations carried out for intact and de-topped plants supported this hypothesis. By variation of the pH of the xylem sap, good agreement between measurements and simulations could be achieved. (C) 2002 Society of Chemical Industry.
Phytotoxicity of polycyclic aromatic hydrocarbons to willow trees

The toxicity of PAH to willow trees (Salix alba, S. viminalis, S. viminalis x schwerinii) was investigated. Willow cuttings were grown in PAH-saturated hydroponic solution (naphthalene NAP, phenanthrene PHEN and benzo(a)pyrene BaP). Toxicity was related to aqueous solubility and was highest for NAP. PHEN did not show significant effects, except in one case. Exposure of trees to BaP showed no effect in two cases, but increased transpiration and growth in two others. High dosages of NAP were fatal for the trees, the lowest dosage significantly stimulated growth. Soil samples were taken from several PAH contaminated sites, among them gas works sites and a former sludge basin. The PAH contents ranged from 1.76 mg/kg to 1451 mg/kg. None of the soils was lethally toxic to the trees, and difference between growth in control soils and growth in PAH contaminated soils was not apparent. Growth and water use efficiency were positively, but not significantly correlated to the PAH content of the soils. Outdoor growth of willows and poplars on the former sludge basin in Valby was monitored, with willows growing faster than poplars (Populus trichocarpa). Phytotoxic effects could be observed at some willows at the Valby sludge basin, but it is not sure whether these effects can be contributed to PAH.

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Thygesen, R., Trapp, S.
Pages: 77-82
Publication date: 2002
Peer-reviewed: Yes
Rensning af olieførenet jord ved hjælp af planter

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Karlson, U., Nielsen, M., Trapp, S.
Pages: 45-48
Publication date: 2002
Peer-reviewed: Unknown

TBT uptake and transport in willow trees

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Ciucani, G., Capri, E., Trapp, S.
Publication date: 2002

Waste related emissions scenarios for risk assessment of chemicals. Report to Danish Environmental Protection Agency

General information
Publication status: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Residual Resource Engineering, Quantitative Sustainability Assessment, Department of Management Engineering
Publication date: 2002
Aspects of phytoremediation of organic pollutants

Phytoremediation is a quite novel technique to clean polluted soils using plants. In theory, phytoremediation methods are cheap, are accepted by the public and, compared to physical or chemical approaches, are ecologically advantageous. Until today, however, there are only a few examples of successful applications. One reason is that the processes involved are complex, and a full clean up may require many years. Plants affect the water balance of a site, they change redox potential and pH, and stimulate microbial activity of the soil. These indirect influences may accelerate degradation in the root zone or reduce leaching of compounds to groundwater. Compounds taken up into plants may be metabolised, accumulated, or volatilised into air. Based on these processes, several phytoremediation methods have been developed: phytoextraction, rhizofiltration, phytostabilisation, rhizo and phytodegradation, pump and tree, land farming, phytovolatilisation, hydraulic control and more. Already in use are plants (and here willow, poplar and grass) for the degradation of petroleum products, aromatic hydrocarbons (BTEX), chlorinated solvents, explosives and cyanides. However, phytotoxicity and pollutant mass balances were rarely documented. Often, the success of the projects was not controlled, and only estimates can be made about the applicability and the potential of phytoremediation. This lack of experience about possibilities and limitations seems to be a hindrance for a broader use of these techniques.

General information
Publication status: Published
Organisations: Department of Environmental Engineering
Contributors: Trapp, S., Karlson, U.
Pages: 37-43
Publication date: 2001
Peer-reviewed: Yes

Publication information
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Aufnahme von Cyanid in Pflanzen: Risiko oder Chance für die Phytoremediation?
Cyanides are waste products from the pyrolysis of coal and are frequent soil pollutants in cities nowadays. Prussic acid (HCN) is a fast acting, highly toxic poison, but iron-complexed cyanides in soil are far less toxic. The phytotoxicity of free CN to basket willows (Salix viminalis) was determined with the tree transpiration test. The EC10 for t = 72 h is 0.76 mg KCN (0.3 mg CN) per liter, the EC50 is 4.47 mg/l. 5 mg/l KCN are ultimately lethal. Balsam poplars (Populus trichocarpa) can survive concentrations of up to 2500 mg/l ferroferricyanide (Prussian blue), although with reduced growth. Willows survived in gas work soils with up to 452 mg/kg total CN. More CN was taken up from nutrient solution than from the soil. Complexed cyanide is probably translocated into the leaves as well. Free CN was readily eliminated from Erlenmeyers with plants growing in nutrient solution. Planting appropriate vegetation might be a suitable solution for many former gas work and mining sites.

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Organisations: Department of Environmental Engineering, Technische Universität Berlin, TeamProtection A/S
Contributors: Trapp, S., Koch, I., Christiansen, H.
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Publication information
Journal: Umweltwissenschaften und Schadstoff-Forschung
Volume: 13
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Bepflanzung einer Tankstelle mit Weiden

In Axelved, Denmark, an abandoned gas filling station serves as a test field for phytoremediation. Laboratory studies accompany the project. The toxicity of fresh and weathered gasoline and diesel to willow and poplar trees was studied by use of a tree transpiration toxicity test. The correlation between diesel content in soil and decrease in willow tree transpiration (Salix viminalis x schwerinii) was highly significant ($r^2 = 0.81$, $n = 19$). The EC50 (50% inhibition of transpiration) for the sum of hydrocarbons (HC) was determined to be 3910 mg/kg (95% confidence interval from 2900 to 5270 mg/kg). The EC10 was 810 mg/kg (95% confidence interval 396 to 1660 mg/kg). The results were verified with artificially mixed diesel and gasolinel contaminated soils and two willow and one poplar species (S. viminalis, S. alba and Populus nigra). The degradation of radiolabeled m-xylene was studied with and without willows. The compound was readily degraded. Willow trees accelerated the elimination, but mainly due to the volatilization of m-xylene. Model studies provided the result that biodegradation in soil is the fastest elimination process at the site, but it is limited by the availability of electron acceptors. The pollutants are almost persistent in the groundwater, but in aerated soil, 10000 mg/kg hydrocarbons at 1 m depth are degraded within 13 years. The main effect of willows on the pollutants' persistence is that willows transpire water, lower the groundwater level and aerate the soil, hereby speeding up biodegradation.
Bioaccumulation of weak acids and bases

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Organisations: Department of Environmental Engineering
Contributors: Trapp, S.
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Eliminating Cyanide, Reducing Heavy Metals, and Harvesting Gold from Mining Waste with Plants

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Contributors: Trapp, S.
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Endegrade: Endophytic degrader bacteria for improving phytoremediation of organic xenobiotics

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Contributors: Karlson, U., Trapp, S., Moore, E., Vangronsveld, J., Dowling, D., d'Haene, S., van der Lelie, D.
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Experimente zum Verbleib von Cyanid nach Aufnahme in Pflanzen

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Fytoremediering af forurening med olie- og tjæreprodukter

Dette projekt er udført under Teknologiudviklingsprogrammet for jord- og grundvandsforurening. Projektet omhandler en gennemgang og vurdering af den publicerede litteratur om emnet. Fytoremediering er en teknologi til at oprense lokaliteter for forurening ved hjælp af planter. Der er dels lagt vægt på at udrede begreber og redegøre for relevante processer, og dels er der lagt vægt på at opdage de seneste års udvikling på området og de resultater, der er opnået. Der beskrives både laboratorieforsøg og feltforsøg.

Projektet omhandler olie- og tjæreprodukter. Således er der medtaget afsnit om PAH, BTEX, alkaner og desuden et mindre afsnit om MTBE, da dette stof også er en problematisk bestanddel i benzin. Denne fokusering i projektet betyder ikke, at man kun bruger fytoremediering til oprensning af organisk forurening, da teknologien ligeledes er forsøgt anvendt til at oprense uorganiske forbindelser herunder tungmetal. Det er også bevidst undladt at fokusere på oprensning af andre organiske stoffer, så som pesticider, selvom teknologien er anvendelig til formålet. Sidst i projektet opridser perspektiverne for den fremtidige forskning og der redegøres dermed også for, hvor der er huller i den nuværende viden.

Arbejdet med dette projekt er et samarbejde mellem Afdeling for Mikrobiel Økologi og Bioteknologi på Danmarks Miljøundersøgelser og Institut for Miljøteknologi på Danmarks Tekniske Universitet. Tak til Steward Strand, University of Washington, for hjælp med afsnitt om MTBE.

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Contributors: Karlson, U., Nielsen, M., Trapp, S.
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Phytooprensning på Søllerød Gasværk

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Contributors: Zambrano, K. C., Larsen, L., Trapp, S., Christiansen, H.
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Phytotoxicity of fresh and weathered diesel and gasoline to willow and poplar trees
The toxicity of fresh and weathered gasoline and diesel fuel to willow and poplar trees was studied using a tree transpiration toxicity test. Soils were taken from an abandoned filling station. Concentrations in the samples were measured as the sum of hydrocarbons from C5 to C10 (gasoline) and C12 to C28 (diesel). Concentrations ranged from 145 to 921 mg/kg gasoline and 143 to 18231 mg/kg diesel. The correlation between log soil concentration and toxicity to willows (Salix viminalis x schwerinii) was highly significant for the diesel fraction (r²=0.81, n=19) and for the sum of hydrocarbons (r²=0.84, n=19). The EC50 (50% inhibition of transpiration) for the sum of hydrocarbons was determined at 3910 mg/kg (95% C.I., 2900 to 5270 mg/kg) and followed a log-normally distributed sigmoidal curve. The EC10 was 810 mg/kg (95% C.I., 396 to 1660 mg/kg). The results were verified with artificially mixed diesel and gasoline contaminated soils, and two willow and one poplar species (S. viminalis, S. alba and Populus nigra). Fresh diesel at about 1000 mg/kg showed no effect on S. alba, although P. nigra was more sensitive. 10000 mg/kg seriously affected the transpiration of all species, silver willow (S. alba) being the least sensitive. Free phase diesel killed all trees within six weeks. Fresh gasoline at 1000 mg/kg was deadly for all trees, hence was more toxic than weathered gasoline. Survival of poplars and willows planted at the abandoned filling station was compared to the laboratory findings. There was some correlation, but in the field, trees also suffered from other stress factors than fuel pollution.

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Sorption of lipophilic organic compounds to wood and implications for their environmental fate

The sorption from water to wood (KWood) of 10 organic chemicals (logKOW, 1.48-6.20) was experimentally determined for oak (Quercus robur) and basket willow (Salix viminalis). Linear regression yielded log KWood = -0.27 ((0.25) + 0.632 ((0.063)log KOW for oak (r = 0.90, n = 27) and log KWood = -0.28 ((0.40) + 0.668 ((0.103)log KOW for willow (r = 0.79, n = 27). According to an equilibrium-partitioning model, wood should be an important storage compartment for lipophilic environmental chemicals, but this is contrary to analytical results. Diffusive uptake from air into wood was estimated to be a relevant transport process only for chemicals with a high KAW. Uptake of chemicals from soil via xylem into stem was simulated with a dynamic one-compartment model. This pathway seems to be important for chemicals with low and intermediate lipophilicity. In large trees, the chemicals are retained for a long time. If metabolism inside the stem occurs, wood can serve as a “safe sink” for environmental chemicals. This might be of use in phytoremediation.

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Contributors: Trapp, S., Miglioranza, S., Mosbæk, H.
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Validierung von Umweltexpositionsmodellen und in Modellen verwendeten Parametern

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Contributors: Berding, V., Schwartz, S., Trapp, S., Matthies, M.
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A phytotoxicity test using transpiration of willows

A short-term acute toxicity assay for willow trees growing in contaminated solution or in polluted soil was developed and tested. The test apparatus consists of an Erlenmeyer flask with a prerooted tree cutting growing in it. Growth and reduction of transpiration are used to determine toxicity. Transpiration is closely related to photosynthesis and growth, but is easier and faster to measure and can be measured without disturbance of the test system. Plants are grown for 24 h in uncontaminated nutrient solution before the toxicant is added to determine the initial transpiration. The loss of weight is expressed as % decrease after 48 and 72 h or longer compared to the initial transpiration, divided by the transpiration of control plants. More toxicity parameters are growth and water use efficiency of the plants. The sensitivity of the test was evaluated with 3,5-dichlorophenol. EC50 values between 5.8 and 9.6 mg/L were found. This is similar to the results from algal growth rate tests. The willow tree toxicity test may be useful for determining the site-specific toxicity of polluted soils and for terrestrial risk assessment of new chemicals and pesticides.
Aspekte der Phytoremediation organischer Schadstoffe
Phytoremediation is the quite novel technique of cleaning polluted sites through the use of plants. Phytoremediation methods are comparatively cheap, are accepted by the public and are ecologically advantageous, compared to common technological approaches. Until today, there have been only a few examples for successful applications. One reason is that the processes occurring are complex, and a full clean up may require many years. Plants have an influence on the water balance of a site, they change redox potential and pH, and stimulate microbial activity of the soil. These indirect influences may accelerate degradation in the root zone or reduce the leaching of compounds into the groundwater. Compounds taken up into plants may be metabolised, accumulate, or volatilise into air. Based on these processes, several phytoremediation methods have been developed: Phytoextraction, rhizofiltration, phytostabilisation, rhizound phytodegradation, pump and tree, land farming, phytovolatilisation, hydraulic control and even more. Already in use are plants (and here mainly willows, poplars and grasses) for the degradation of petroleum products, aromatic hydrocarbons (BTEX), chlorinated solvents, explosives and cyanides. Phytotoxicity and pollutants mass balance have rarely been documented carefully. Often, the success of the projects was not controlled, and only estimates can be made about the applicability and the potential of phytoremediation. This lack of experience about possibilities and limitations seems to be a hindrance for a broader use of these techniques.

Ein Fließgewässer im urbanen Umfeld. Analyse des ökologischen Zustandes des unteren Belmer Baches (Osnabrück, Niedersachsen) anhand des Makrozoobenthos
Ein Fließgewässer im urbanen Umfeld. Analyse des ökologischen Zustandes des unteren Belmer Baches (Osnabrück, Niedersachsen) anhand des Makrozoobenthos
The organic pollution of the lower Belmer Bach can be attributed to its agriculturally intensively used drainage area. Already before entering the urbanized region, the macrozoobenthos is poor in species due to saprobic pollution and the structural poverty of the waterbed and the banks. When comparing the species numbers of a reference sampling plot located before the urban region and a sampling plot situated within this region, hardly any differences could be ascertained. The longitudinal isolation and the rise in temperature of 1 °C in the urban brook section negatively influence its fauna; this, however, is compensated by the varied riparian vegetation and the greater structural diversity of the waterbed due to hydraulic engineering. A rise in temperature of 5 °C and a continuous inflow of suspended matter from a sewageworks reduce the macrozoobenthos to few dominant taxa.

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Modelling uptake into roots and subsequent translocation of neutral and ionisable organic compounds
A study on uptake of neutral and dissociating organic compounds from soil solution into roots, and their subsequent translocation, was undertaken using model simulations. The model approach combines the processes of lipophilic sorption, electrochemical interactions, ion trap, advection in xylem and dilution by growth. It needs as input data, apart from plant properties, log KOW, pKa and the valency number of the compound, and pH and chemical concentration in the soil solution. Equilibrium and dynamic (steady-state) models were tested against measured data from several authors, including non-electrolytes as well as weakly acidic and weakly basic compounds. Deviations from the measured values led to further development of the model approach: sorption in the central cylinder may explain the small transpiration stream concentration factor of lipophilic compounds. For non-electrolytes, the model predicted uptake and translocation with high accuracy. For acids and bases, the tendency of the results was satisfactory. The dynamic model and the equilibrium approach gave similar results for the root concentration factor. The calculation of the transpiration stream concentration factor was more accurate with the dynamic model, but still gave deviations up to factor of ten or more. The dominating process for monovalent weak electrolytes was found to be the ion trap effect. C 2000 Society of Chemical Industry

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Proposals to overcome limitations in the EU chemical risk assessment scheme

The notification of new chemicals in the European Union requires a risk assessment. A Technical Guidance Document (TGD) was prepared for assistance. The TGD proposes QSARs, regressions and models from various sources. Each method has its own range of applicability and its own restrictions. Regressions used in the assessment of indirect human exposure have a common regression range from log $K_{OW} \pm 4.6$. Most models are compartment models, which do not consider a spatial distribution of the chemical, and were originally developed for non-dissociating, lipophilic persistent chemicals with measurable vapor pressure. Taking this into account, the TGD is only applicable for a minority of chemical classes. Dissociating compounds, ions, polar and very non-polar compounds do not belong to them. The effect of mixtures cannot be considered, except for hydrocarbons. Using the example of plant uptake, it is shown that in certain cases uptake is underestimated by the model due to processes not considered. This may lead to a wrong security in risk assessment. To overcome these limitations, a set of alternative models with different application ranges should be developed. When no applicable method is available, it might be better not to use a model at all instead of an inadequate model, and look for other sources of information. © 2000 Elsevier Science Ltd. All rights reserved.
Soil Water Dynamics In Central Europe and Brazil

Georeferenced fate modelling of LAS in the Itter stream
For the simulation of spatial concentration patterns of 'down-the-drain' chemicals mathematical models were coupled with a Geographic Information System (GIS) to predict concentrations in the receiving surface waters, using the detergent chemicals Linear Alkylbenzenesulfonate (LAS) and Boron and the Itter stream, a small tributary to the Rhine, as an example. In order to estimate the release of the aforementioned chemicals into the Itter two different model concepts have been implemented and evaluated. The first concept shows that mainly the connectivity to the STPs and the elimination processes taking place in them influence the predicted concentrations. In the second concept, concentrations in various stretches of the Itter are calculated based on the release via point sources (STPs). The second concept, accompanied by statistical analyses, shows a high correlation between the half-life of LAS in the riverine water and the water quality parameters TOC and ammonium. This study is closely linked to the ongoing project GREAT-ER. (C) 1999 Elsevier Science Ltd. All rights reserved.
Limitations of the applicability of the European risk assessment scheme. (Abstract No. 2p/003)

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