

# Environmental Science Processes & Impacts

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## IN THIS ISSUE

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See Matthew MacLeod *et al.*, pp. 10–11.  
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**Inside cover**  
See Keri C. Hornbuckle *et al.*, pp. 210–219.  
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## EDITORIAL

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### Modeling in environmental chemistry

Matthew MacLeod,\* Todd Gouin and Thomas E. McKone

Guest editors Matthew MacLeod, Todd Gouin and Thomas McKone introduce the Modeling in Environmental Chemistry themed issue of *Environmental Science: Processes & Impacts*.



Matthew MacLeod



Todd Gouin



Thomas McKone

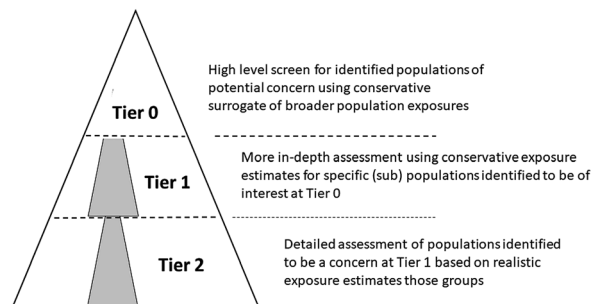
## PERSPECTIVES

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### Improving the relevance and efficiency of human exposure assessments within the process of regulatory risk assessment

Chris Money

The article explores how tiered and targeted information acquisition can improve the effectiveness of the human exposure assessment process.



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# Environmental Science Processes & Impacts

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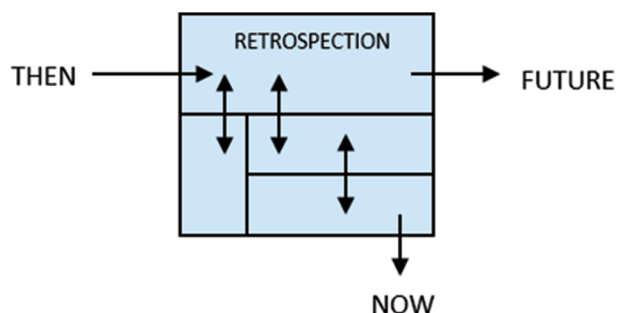


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## Fate and exposure modeling in regulatory chemical evaluation: new directions from retrospection

Mark A. Bonnell,\* Angelika Zidek, Adam Griffiths and Don Gutzman

A regulatory perspective on the application of fate and exposure modeling in the past and for the future.

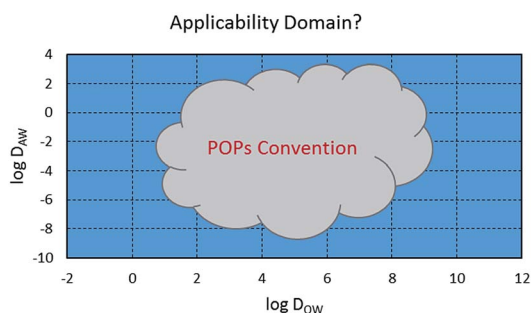


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## Can the Stockholm convention address the spectrum of chemicals currently under regulatory scrutiny? Advocating a more prominent role for modeling in POP screening assessment

Michael S. McLachlan

Applying POP screening to a large chemical domain requires less reliance on individual criteria and more on integrated assessment with models.

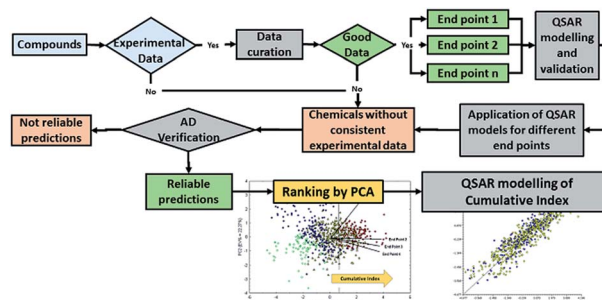


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## QSAR modeling of cumulative environmental end-points for the prioritization of hazardous chemicals

Paola Gramatica,\* Ester Papa and Alessandro Sangion

Indexes for the prioritization of potential hazardous chemicals can be derived and modelled by combining PCA and QSAR models.

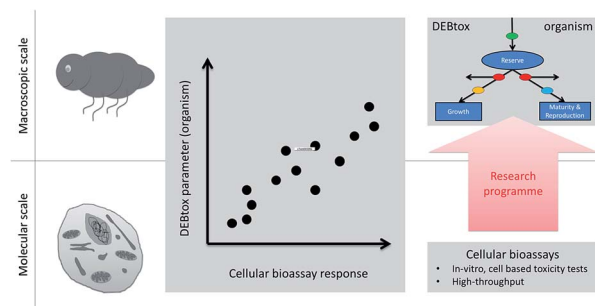


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## Physiological modes of action across species and toxicants: the key to predictive ecotoxicology

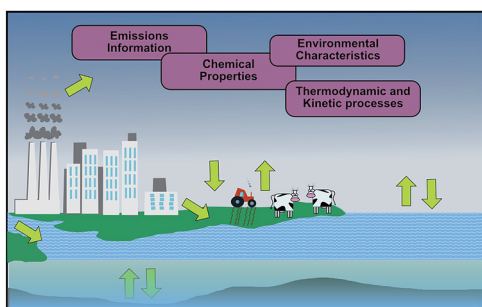
Roman Ashauer\* and Tjalling Jager

We outline a research strategy that will deliver more effective theory and models for environmental risk assessment of chemicals.



## CRITICAL REVIEW

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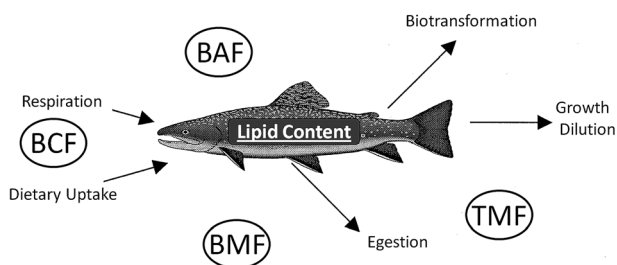
### Environmental fate and exposure models: advances and challenges in 21<sup>st</sup> century chemical risk assessment

Antonio Di Guardo, Todd Gouin, Matthew MacLeod and Martin Scheringer\*

Twenty-five years of progress in modeling the environmental fate and exposure of organic contaminants is reviewed, and a strategy for more rapidly adopting scientific progress into regulatory models is proposed.

## PAPERS

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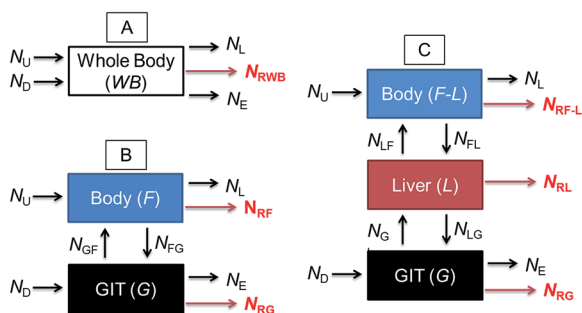


### Bioconcentration, bioaccumulation, biomagnification and trophic magnification: a modelling perspective

Donald Mackay, Alena K. D. Celsie,\* David E. Powell and J. Mark Parnis

The uptake and output processes and lipid content for an aquatic organism affects BCF, BAF, BMF, and TMF values.

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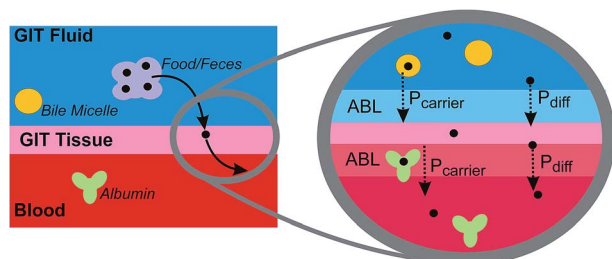


### The influence of chemical degradation during dietary exposures to fish on biomagnification factors and bioaccumulation factors

Jon A. Arnot\* and Donald Mackay

The chemical dietary absorption efficiency ( $E_D$ ) quantifies the amount of chemical absorbed by an organism relative to the amount of chemical an organism is exposed to following ingestion.

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### Modelling oral up-take of hydrophobic and super-hydrophobic chemicals in fish

Wolfgang Larisch\* and Kai-Uwe Goss\*

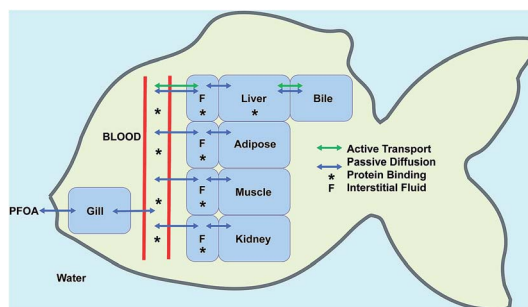
PbTk simulations with hydrophobic chemicals have revealed that diffusive transport through aqueous boundary layers in the gastro-intestinal tract and in the blood is the limiting process for oral uptake scenarios. This process can only be modelled correctly if transport facilitated by albumin and bile micelles through these boundary layers is accounted for.

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### Evaluating parameter availability for physiologically based pharmacokinetic (PBPK) modeling of perfluorooctanoic acid (PFOA) in zebrafish

Manoochehr Khazaei and Carla A. Ng\*

Physiologically based pharmacokinetic (PBPK) models are considered useful tools to describe the absorption, distribution, metabolism and excretion of xenobiotics.

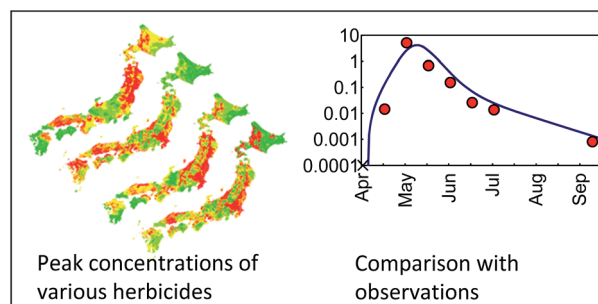


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### Development and validation of a simulation method, PeCHREM, for evaluating spatio-temporal concentration changes of paddy herbicides in rivers

Yoshitaka Imaizumi,\* Noriyuki Suzuki, Fujio Shiraishi, Daisuke Nakajima, Shigeko Serizawa, Takeo Sakurai and Hiroaki Shiraishi

A model simulating high-resolution concentration changes of various herbicides in Japan was developed and validated.

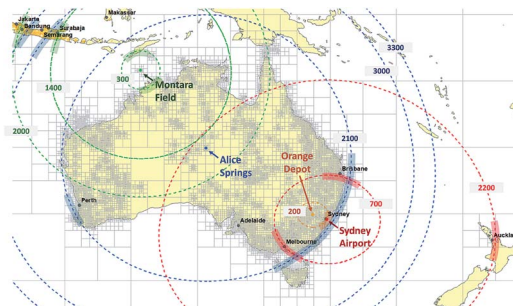


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### Source-to-exposure assessment with the Pangea multi-scale framework – case study in Australia

Cedric Wannaz,\* Peter Fantke, Joe Lane and Olivier Jolliet

Global multi-scale modeling platform for spatial analysis of population intake and multimedia source apportionment of 4000+ Australian emission sources.

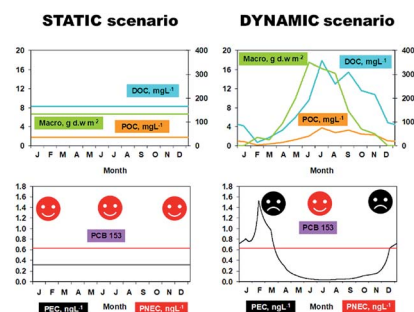


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### Do environmental dynamics matter in fate models? Exploring scenario dynamics for a terrestrial and an aquatic system

Melissa Morselli, Elisa Terzaghi and Antonio Di Guardo\*

Most of the currently used risk assessment scenarios are based on steady scenario conditions which may not reflect environmental variations in time and space.



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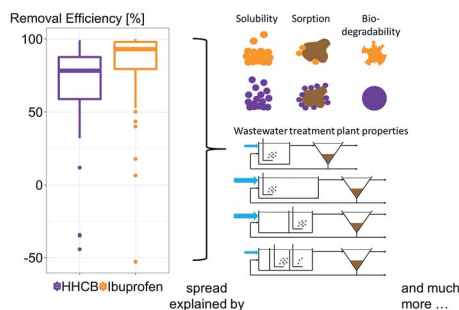


### Quantitative structure–activity relationships for primary aerobic biodegradation of organic chemicals in pristine surface waters: starting points for predicting biodegradation under acclimatization

Tom M. Nolte,\* Kevin Pinto-Gil, A. Jan Hendriks, Ad M. J. Ragas and Manuel Pastor

Microbial biomass and acclimation can affect the removal of organic chemicals in natural surface waters.

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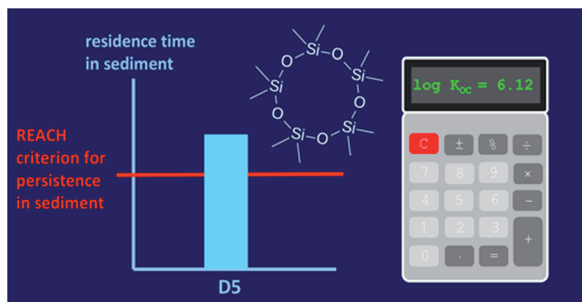


### Quantifying variability in removal efficiencies of chemicals in activated sludge wastewater treatment plants – a meta-analytical approach

Mélanie Douziech,\* Irene Rosique Conesa, Ana Benítez-López, Antonio Franco, Mark Huijbregts and Rosalie van Zelm

A meta-analysis summarises the removal of fragrances, surfactants, and pharmaceuticals and identifies the main influencing parameters.

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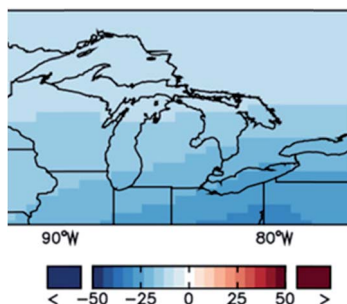


### A critical assessment of the environmental fate of linear and cyclic volatile methylsiloxanes using multimedia fugacity models

Dimitri Panagopoulos\* and Matthew MacLeod

Modeled residence times of volatile methyl siloxanes exceed several persistence criteria in aquatic environments.

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### Responses of deposition and bioaccumulation in the Great Lakes region to policy and other large-scale drivers of mercury emissions

J. A. Perlinger,\* N. R. Urban, A. Giang, N. E. Selin, A. N. Hendricks, H. Zhang, A. Kumar, S. Wu, V. S. Gagnon, H. S. Gorman and E. S. Norman

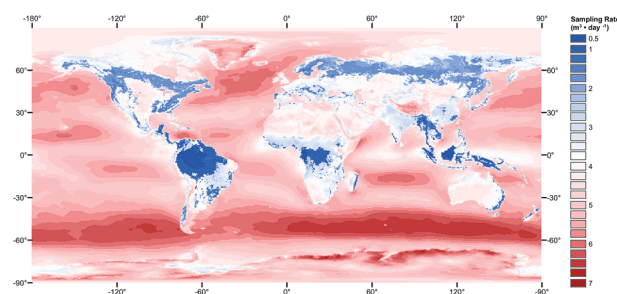
The effect of policy on fish mercury levels varies spatially, even within the Great Lakes Basin.

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## Calibration and evaluation of PUF-PAS sampling rates across the Global Atmospheric Passive Sampling (GAPS) network

Nicholas J. Herkert, Scott N. Spak, Austen Smith, Jasmin K. Schuster, Tom Harner, Andres Martinez and Keri C. Hornbuckle\*

Here we present and evaluate a method to determine PUF-PAS sampling rates ( $R_S$ ), and the effective sampling volume ( $V_{\text{eff}}$ ), for gas-phase chemical compounds deployed anywhere in the world.

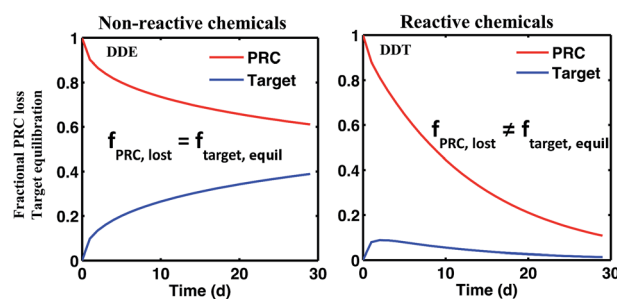


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## Passive sampling of DDT, DDE and DDD in sediments: accounting for degradation processes with reaction–diffusion modeling

A. Patricia Tcaciuc,\* Raffaella Borrelli, Luciano M. Zaninetta and Philip M. Gschwend

Applying passive sampling to reactive species may be a way to obtain information about *in situ* reactivity of compounds in sediments that occur on timescales of days to months.

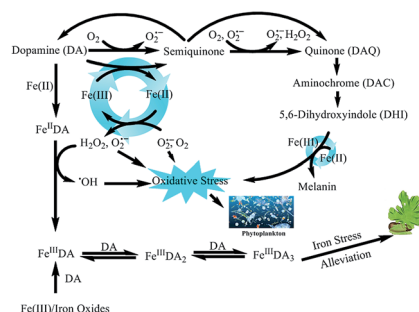


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## Effect of release of dopamine on iron transformations and reactive oxygen species (ROS) generation under conditions typical of coastal waters

Yingying Sun, A. Ninh Pham and T. David Waite\*

Release of dopamine by *Ulvaria obscura* var. *blyttii* may, allelopathically, assist *Ulvaria* growth by  $\text{H}_2\text{O}_2$  generation and benefit the bloom region through alleviation in iron stress and by mitigating the effects of other oxidative metabolites.



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## Is secondary organic aerosol yield governed by kinetic factors rather than equilibrium partitioning?

Chen Wang, Frank Wania and Kai-Uwe Goss\*

The concept of differential SOA yield and a consideration of kinetic processes are important when modelling SOA formation under atmospherically relevant conditions.

