A Kinetic Environmental Fate Model for the Risk Assessment of Engineered Nanomaterials

Jenny Perez Holmberg
(University of Gothenburg, Sweden)

Rute F. Domingos, Claus Svendsen, Egon Dumont, Marianne Matzke, Ralph Vanhauten, Stephen Lofts, Virginie Keller, and Geert Cornelis

SETAC Europe - 26th Annual Meeting
Nantes, 23 May 2016

European Union's Seventh Framework Programme (FP7/2007-2013)
and Horizon 2020 (EU Framework Programme for Research and Innovation)

Outline

- Project background
- Model overview and key features
- (I will complete this slide last)

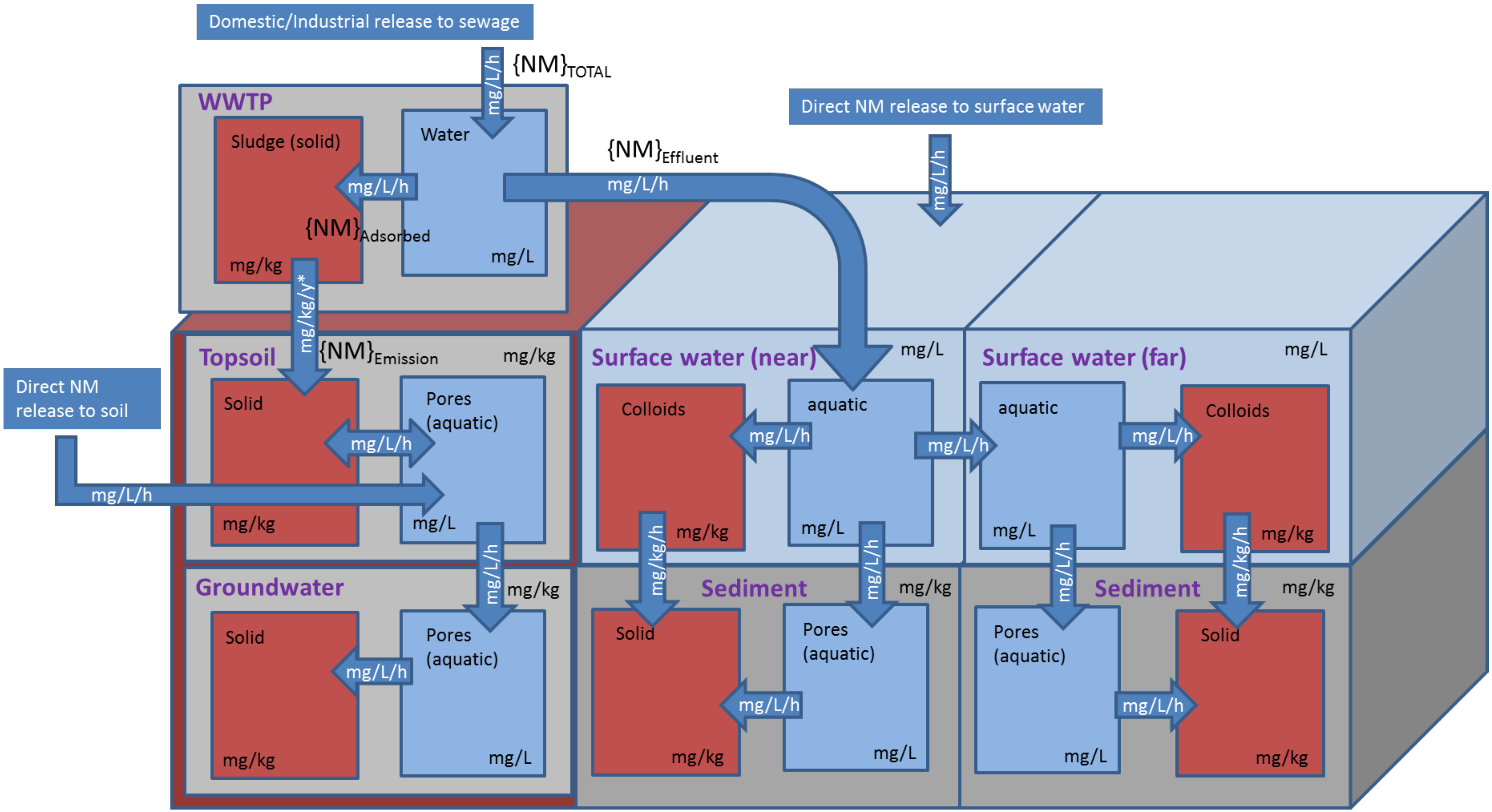
GUIDEnano and NanoFASE

- GUIDEnano (EU FP7)
  - Evaluate and manage human and environmental health risks of nano-enabled products
  - Web-based Guidance Tool for industry
  - www.guidenano.eu
- NanoFASE (Horizon 2020)
  - Integrated Exposure Assessment Framework
  - www.nanofase.eu
- Both projects require the development of computational exposure models – eventually linking to hazard

Key features of the fate model

- Model world
  - Compartments: surface water, sediment, soil and WWTP
- Kinetic
  - NM flows as mass fluxes
  - Incorporates reaction and transport rates
- Bioavailability
  - Mobility and spatial distribution over time are critical
- Compromise between mechanistical accuracy and operational simplicity
  - Use of fate descriptors such as attachment and distribution coefficients

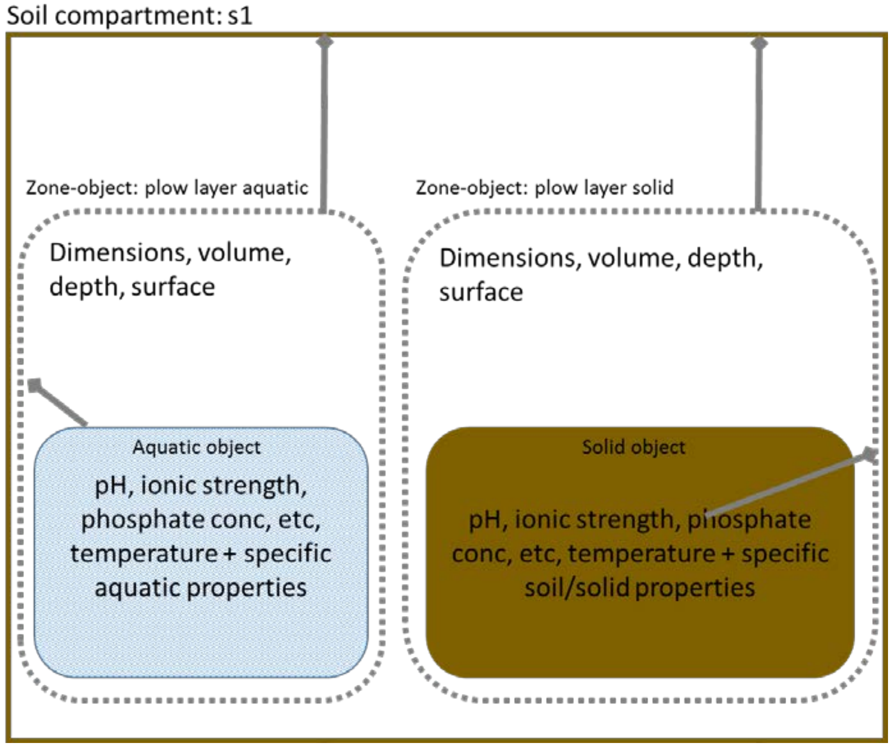
Environmental compartments



Model approach and terminology

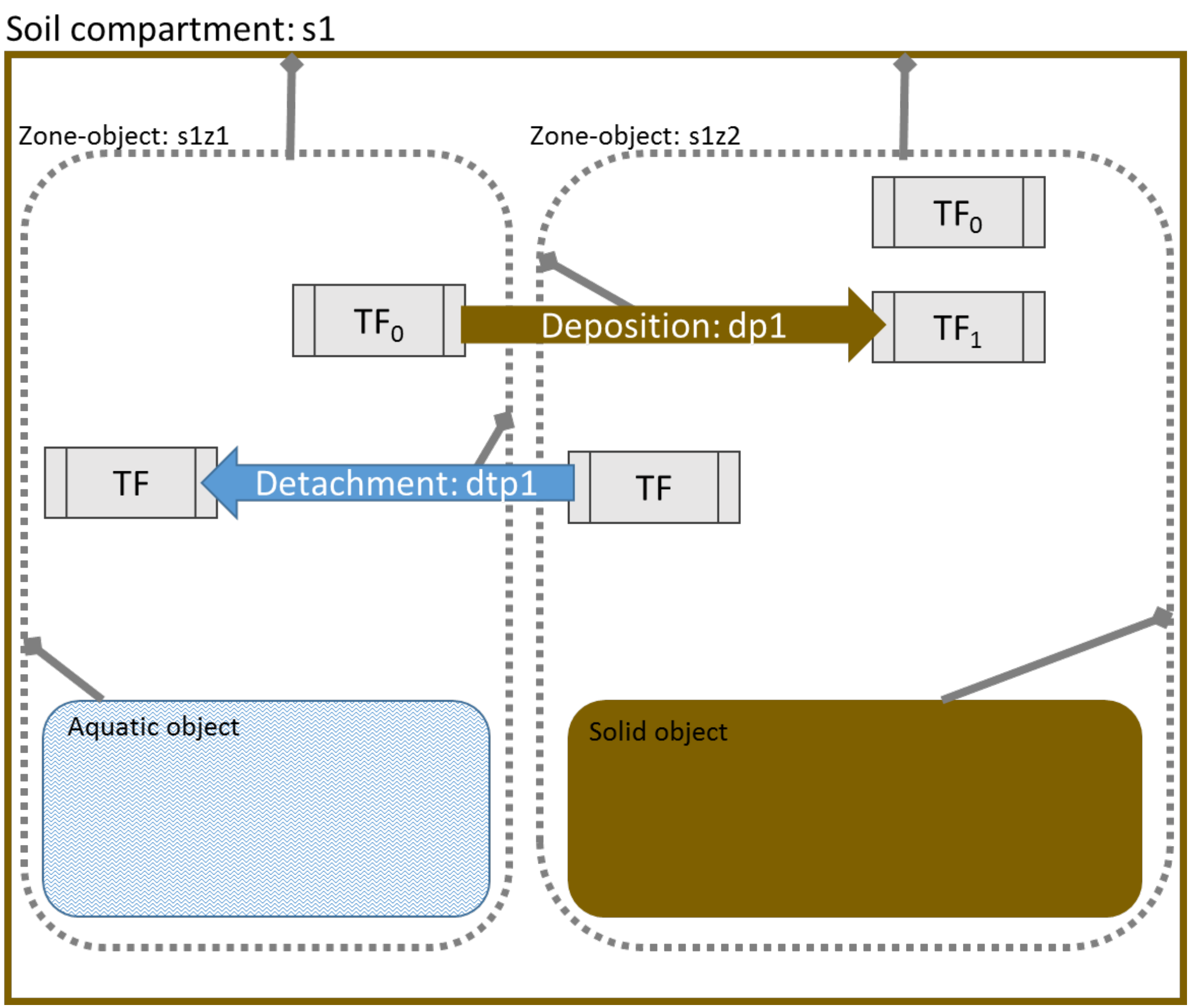
- Web-based tool – object-oriented
  - Compartments
  - Zones – aquatic and solid
  - Processes (transformation and transport)
  - Activities – human-initiated events
  - Timeframes

- Sources of information
  - Existing literature
  - Experimental validation

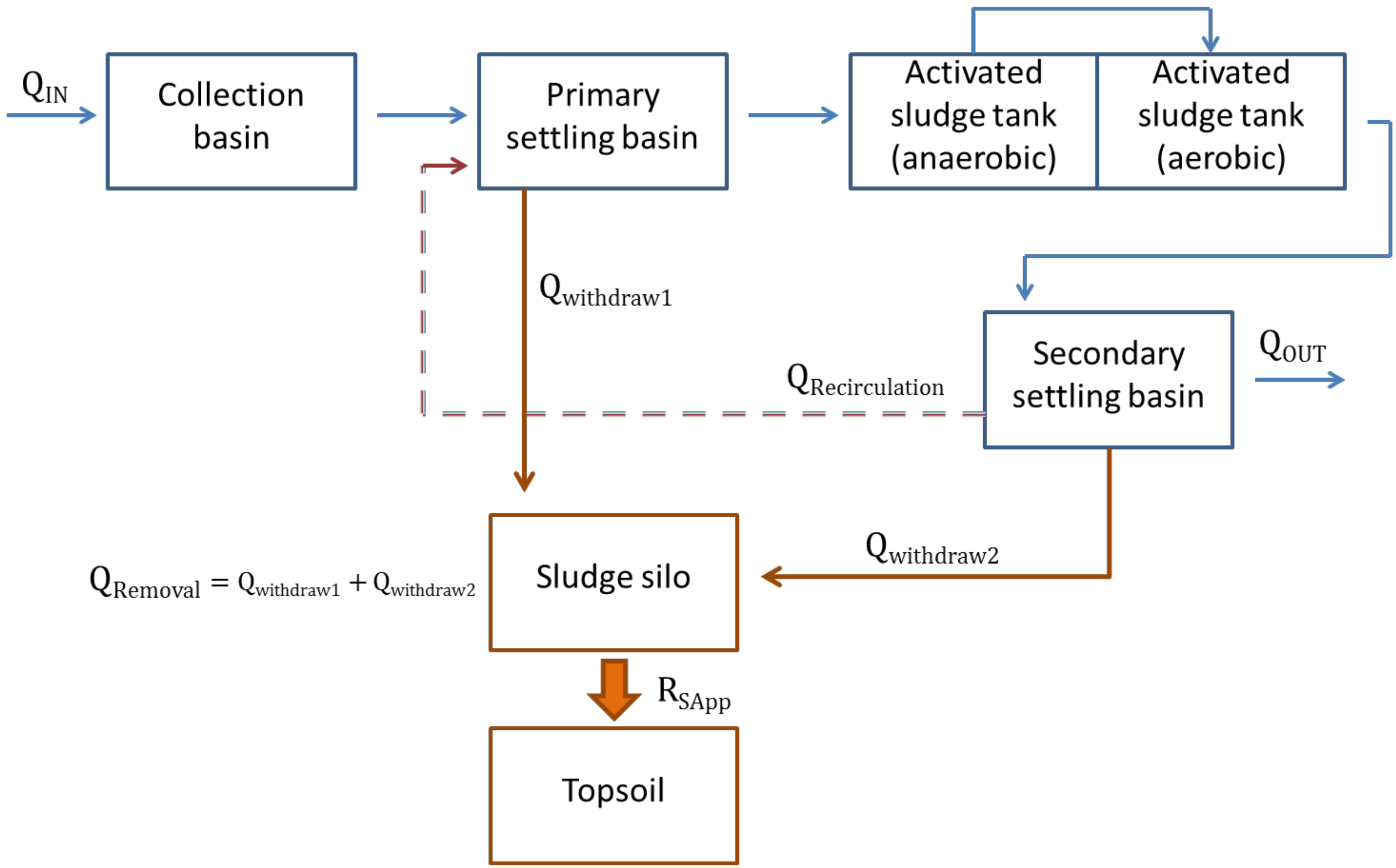


- Three zone composition classes
  - Aquatic
  - Solid (Soil)
  - Air (Gaseous)

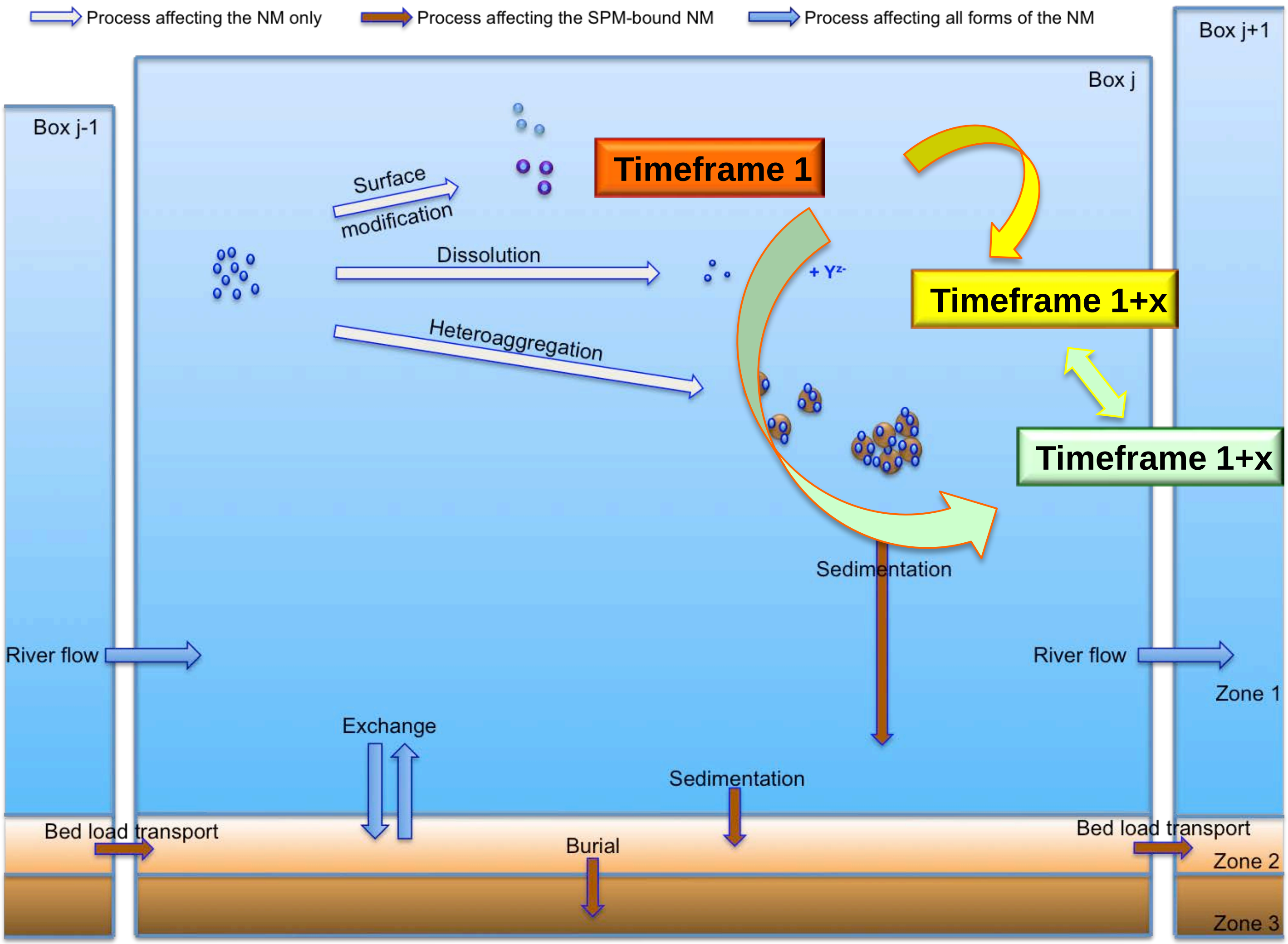
Timeframes and processes



Waste water treatment plant (WWTP)

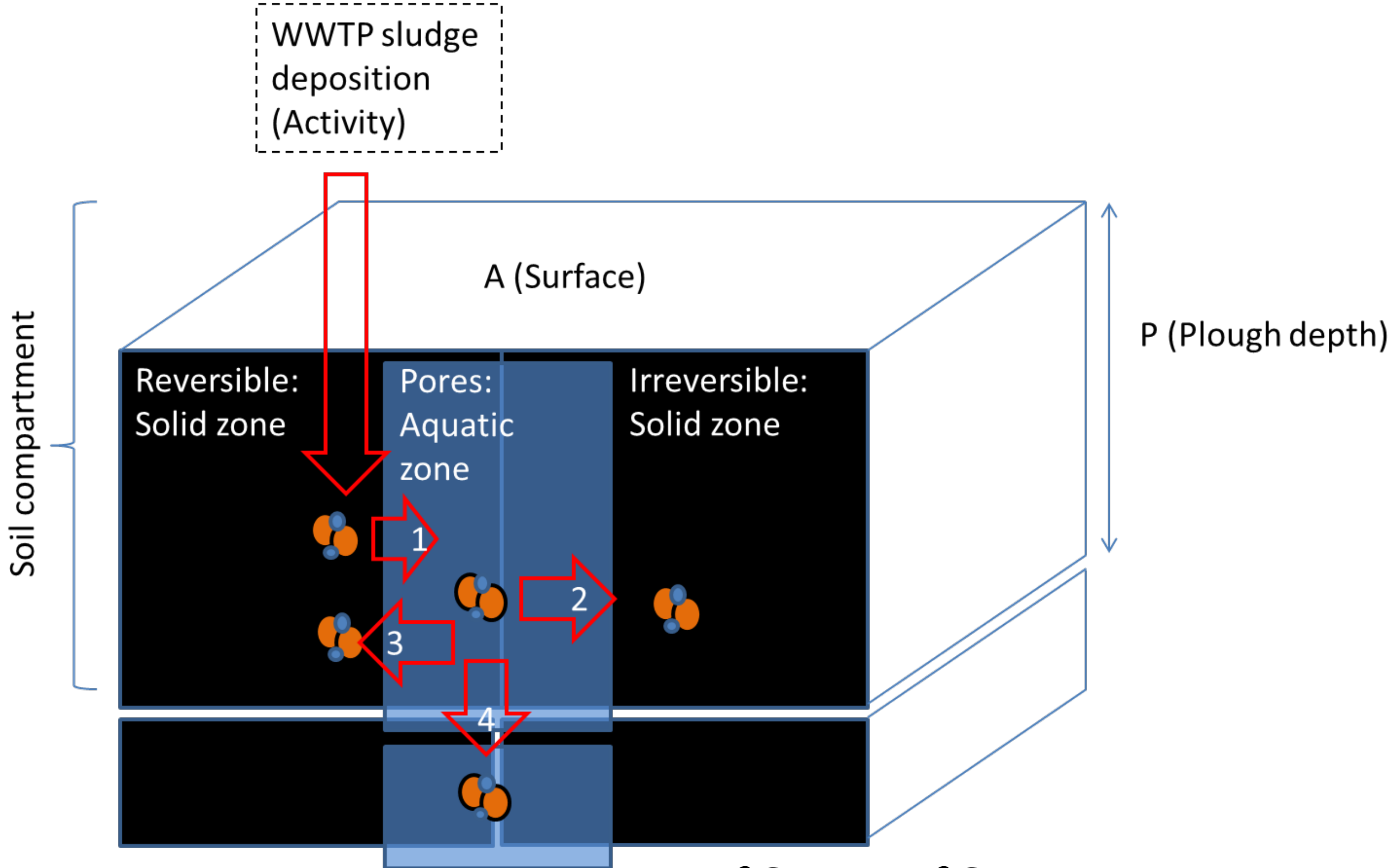


Rivers and sediment



Adapted from: Praetorius, et al. (2012) *Environ. Sci. & Tech.* **46**, 6705−6713

Soil

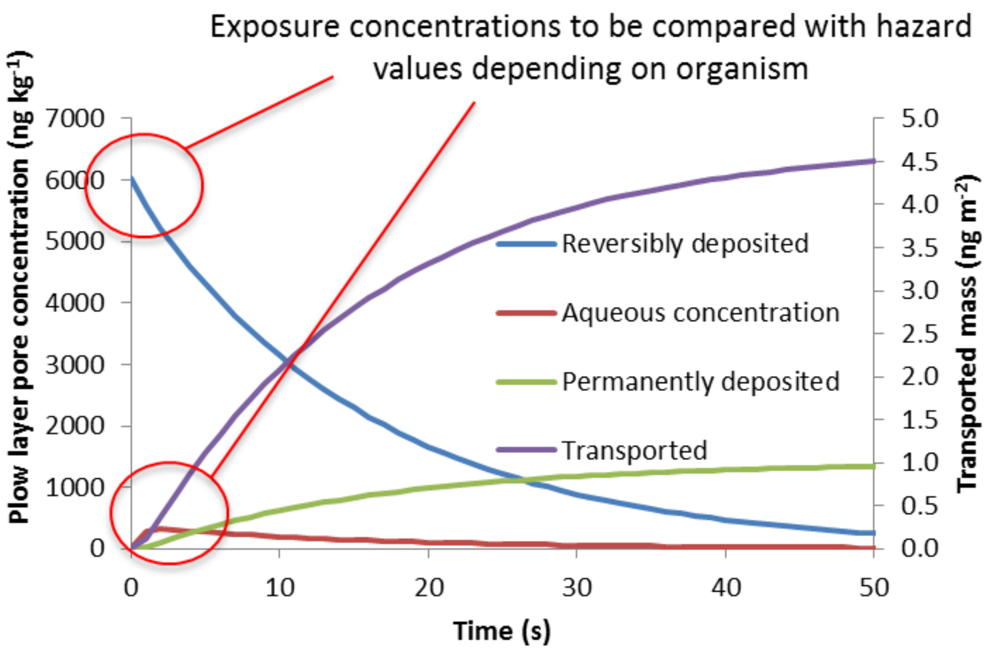


$$\theta \frac{\partial C}{\partial t} = -u\theta \frac{\partial C}{\partial z} - k_{det}\rho S - k_{att}\theta C - k_{transf}\theta C$$

Kinetic approach to concentrations in soil

Differential equation: $$\theta \frac{\partial c}{\partial t} = -u\theta \frac{\partial c}{\partial z} - k_{det}\rho S - k_{att}\theta C - k_{transf}\theta C$$

Analytical solution:



Speciation and bioavailability: link to hazard

Based on the EC50s

Options

The EC50 is compared with the modelled *t*-dependent exposure concentration integrated over time *t*.

The EC50 is compared with the maximum modelled *t*-dependent exposure concentration.

The EC50 is compared with the average modelled *t*-dependent exposure concentration.

Independently of the option it should be argued the limitations regarding:

i) The static values for the EC50 and the dynamic modelled exposure.

ii) The media used in each which will be inevitably different.

Case study: Ag nanoparticles

Ongoing work

- Experimental validation
- Descriptors for transformation and transport (attachment/detachment, sedimentation)

Conclusions and Outlook

Acknowledgements

- University of Gothenburg – Department of Chemistry and Molecular Biology

UNIVERSITY OF GOTHENBURG

Vetenskapsrådet