

Technical University of Denmark



Towards a more robust fate modeling of metals' long-term emissions in an LCIA context

Bakas, Ioannis; McKone, T.E. ; Astrup, Thomas Fruergaard; Hauschild, Michael Zwicky; Rosenbaum, R.K.

Publication date:
2014

[Link back to DTU Orbit](#)

Citation (APA):

Bakas, I., McKone, T. E., Astrup, T. F., Hauschild, M. Z., & Rosenbaum, R. K. (2014). Towards a more robust fate modeling of metals' long-term emissions in an LCIA context. Poster session presented at SETAC Europe 24th Annual Meeting, Basel, Switzerland.

DTU Library

Technical Information Center of Denmark

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Towards a more robust fate modeling of metals' long-term emissions in an LCIA context

Ioannis Bakas¹, T.E. McKone², T.F. Astrup³, M.Z. Hauschild¹, R.K. Rosenbaum⁴

1: Division for Quantitative Sustainability Assessment, DTU Management Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark
 2: Lawrence Berkeley National Laboratory, Berkeley, California, USA
 3: Department of Environmental Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark
 4: irstea, National Research Institute of Science and Technology for Environment and Agriculture. Montpellier, France

AIM

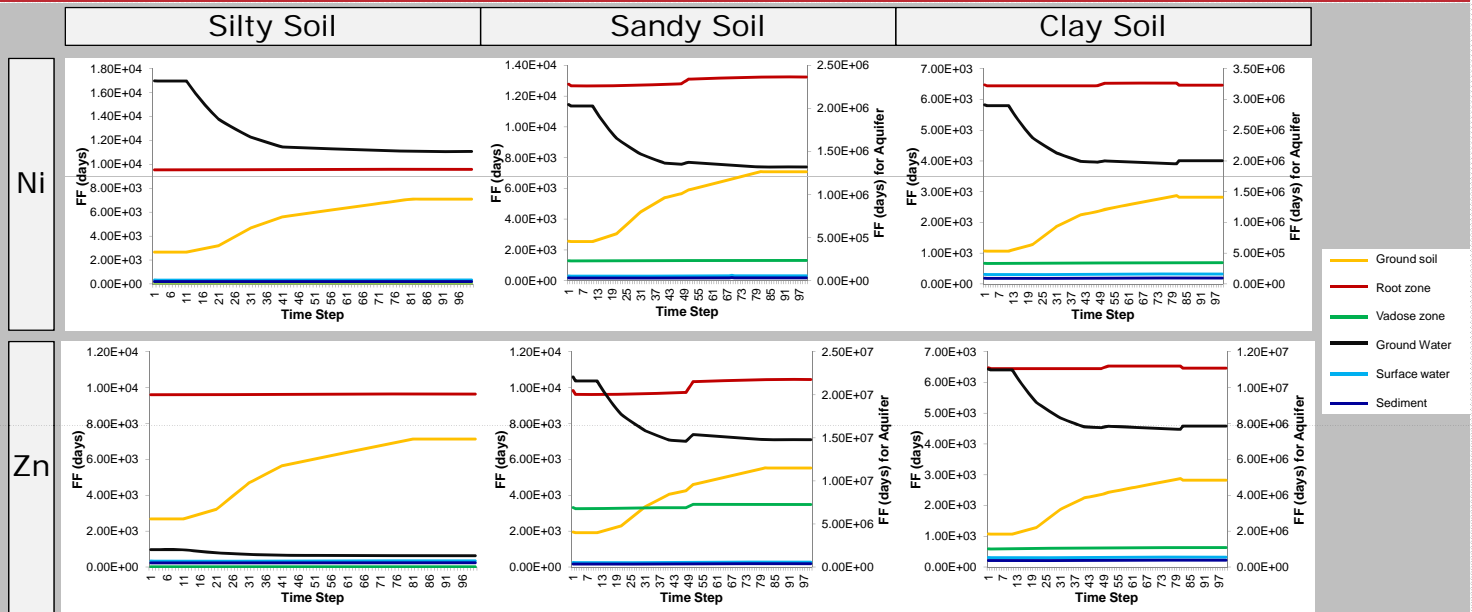
Develop dynamic fate factors for long-term emissions of selected heavy metals

- based on the evolution of soil parameters
- by respecting the individual characteristics of selected metals
- by taking into account spatial variations

CONCLUSIONS

- Similar patterns of fate factors development for all soil types for each metal
- Residence times in the upper soil layer and in saturated zone change over time
- Residence times in all other compartments remain relatively stable over the modeled time period
- The soil layers' thickness: most influential parameter for determining the metals' fate

RESULTS



METHOD

Modeling the evolution of soil for 100,000 years

1. Select influential parameters that determine fate of Ni, Zn, Cd, Pb emissions to soil
2. Model the development of parameters over the next 100,000 years based on literature models and soil chemistry
3. Select soil types: Sandy, Silty, Clay
4. Model each soil type for 100 time steps (1,000 years each) with changing soil parameters in CalTOX multimedia model
5. Obtain fate factors for 100 time steps for each metal and soil type
6. Perform sensitivity analysis in order to pinpoint the most crucial parameters for fate calculations as check of the selection of step 1

Parameter	Correlation with	Calculated for	Reference
Annual average precipitation	Temperature	Full time period	IPCC, 2013; Kuhl and Litt, 2003
Thickness of the ground soil layer	Physical and chemical weathering and translocation processes	Full time period	Salvador-Blanes et al., 2007
Soil particle density	Sand/Silt/Clay content	Full time period	Salvador-Blanes et al., 2007
Water content in surface soil	n.r.	Only initial conditions	Batjes, 2008
Erosion of surface soil	n.r.	Only initial conditions	Montgomery, 2007
Thickness of the root-zone soil	Physical and chemical weathering and translocation processes	Full time period	Salvador-Blanes et al., 2007
Water content of root-zone soil	n.r.	Only initial conditions	Batjes, 2008
Thickness of the vadose-zone soil	Physical and chemical weathering and translocation processes	Full time period	Salvador-Blanes et al., 2007
Water content; vadose-zone soil	n.r.	Only initial conditions	Batjes, 2008
Ambient environmental temperature	n.r.	Full time period	IPCC, 2013; Kuhl and Litt, 2003
Organic carbon fraction in upper soil zone	Temperature, annual average precipitation, evapotranspiration	Full time period	Parton et al., 1987
Organic carbon fraction in vadose zone	Temperature, annual average precipitation, evapotranspiration	Full time period	Parton et al., 1987
Partition coefficient in ground/root soil layer	pH	Only initial conditions	Janssen et al., 1997
Partition coefficient in vadose-zone soil layer	pH	Only initial conditions	Janssen et al., 1997

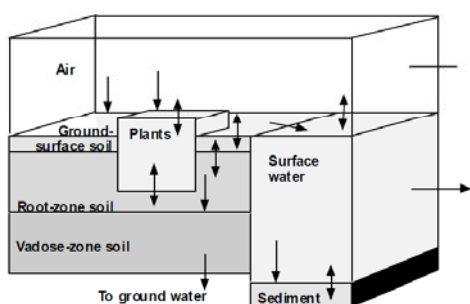


Figure 1: The CalTOX environmental compartments