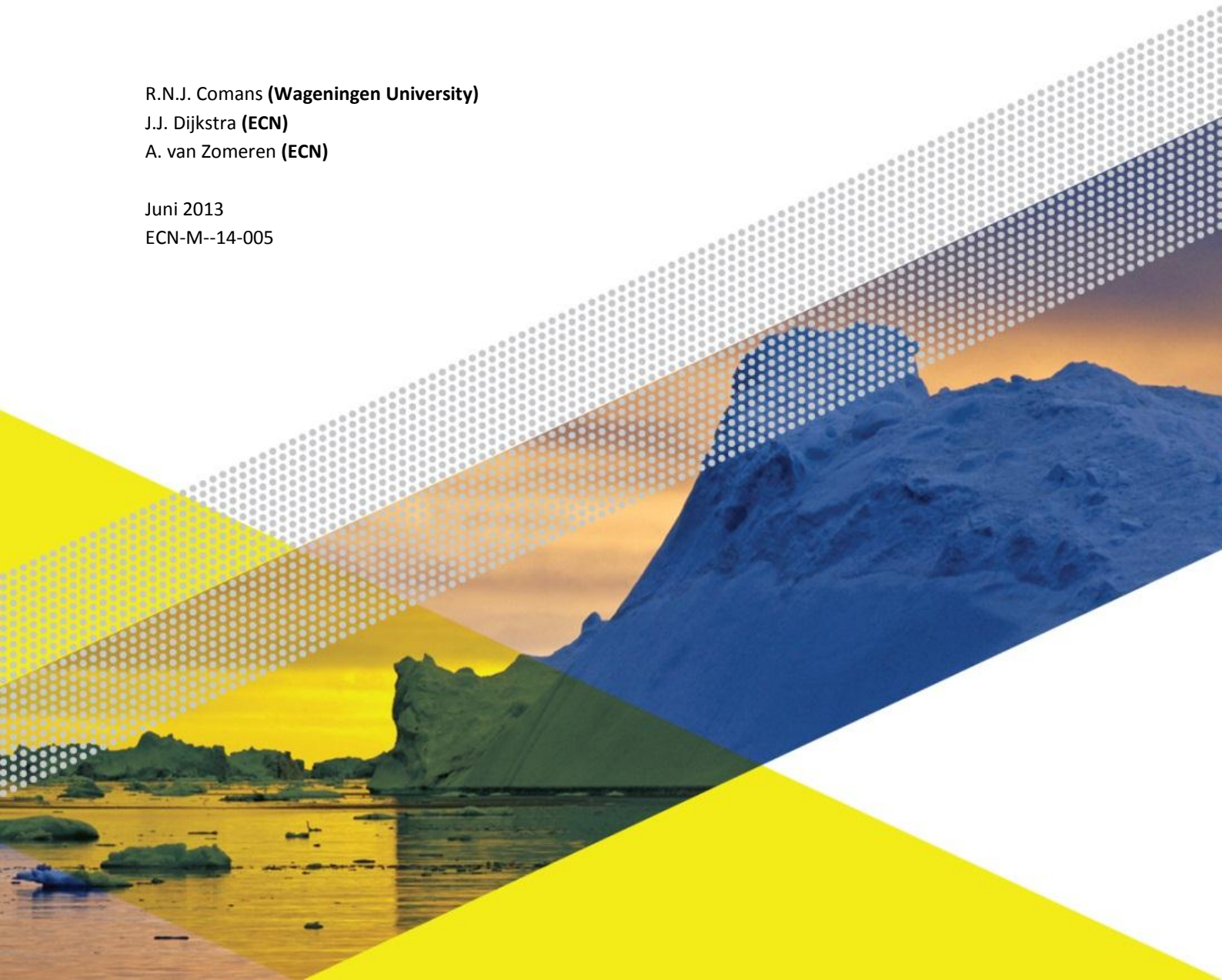
Generic geochemical modelling approach for the leaching of elements from waste materials and soils

R.N.J. Comans **(Wageningen University)**
J.J. Dijkstra **(ECN)**
A. van Zomeren **(ECN)**

Juni 2013
ECN-M--14-005



Generic geochemical modelling approach for the leaching of elements from waste materials and soils

Rob N.J. Comans[1], Joris J. Dijkstra[2], Andre van Zomeren[2]
[1]*Department of Soil Quality, Wageningen University, The Netherlands, rob.comans@wur.nl;*
[2]*Energy research Centre of the Netherlands (ECN), Petten, The Netherlands*

ABSTRACT: Geochemical modelling is increasingly being used in both scientific research and risk assessment regarding the environmental properties of contaminated materials. The performance and reliability of model predictions are strongly determined by the specific modelling approach, as well as by the applied methodologies to estimate the necessary model parameters. This presentation will give an overview of our development of a generic multi reactive surface model, including methodologies for its parameterisation and testing. The approach is being developed to describe the speciation and solid/liquid partitioning (leaching) of a wide range of elements in both soils and waste materials, on the basis of the notion that the reactive organic and mineral surfaces that are being considered in this modelling approach, play a generic and determining role in the speciation and leaching of elements in these different materials.

The multi-reactive surface model relies on individual adsorption models for which generic binding parameters have been developed and published for a wide range of elements. It includes reactions for aqueous speciation and (selected) mineral solubility, in combination with sorption to organic matter (NICA-Donnan model), Fe/Al-(hydr)oxides (Generalized Two-Layer Model) and clay (Donnan model). As such, the model is fully based on published generic thermodynamic parameters for these different types of processes and used without any parameter fitting. Model parameters are obtained with standard methods for the estimation of the potentially available/reactive fraction of the elements of interest, and the available amount of the above reactive surfaces. Particular attention is given to estimation of the reactive fractions of (particulate and dissolved) organic matter, using a recently developed rapid batch fractionation procedure [1]. The performance of the model has been tested for a range of different contaminated materials, particularly by comparing measurements and model predictions of the solid/liquid partitioning of elements over a wide pH range.

We have found in different studies that the binding properties of the reactive surfaces that are being considered in this modelling approach play a generic role in the speciation and leaching of elements among very different waste and soil materials. As an example, the approach has been successfully applied to different soils [2], amended soils [3], municipal incinerator bottom ash [4], steel slag [5, 6], bauxite residues [7], recycled concrete aggregate [8], and RDF incineration and gasification bottom ash [9]. We will present examples from these different model applications, illustrate similarities and differences in controlling processes and element speciation in these materials and provide an outlook on current work and ambitions to further develop and improve this generic multi-reactive surface model.

References:

[1] van Zomeren, A. & Comans, R.N.J. (2007) Measurement of humic and fulvic acid concentrations and dissolution properties by a rapid batch procedure. Environ. Sci. Technol. 41, 6755-6761.
[2] Dijkstra, J. J.; Meeussen, J. C. L.; Comans, R. N. J. (2009) Evaluation of a generic multi-surface sorption model for inorganic soil contaminants. Environ. Sci. Technol., 43, 6196-6201.

[3] Carter, C. M.; Van der Sloot, H. A.; Cooling, D. (2009) pH dependent extraction of soils and soil amendments to understand the factors controlling element mobility - New approach to assess soil and soil amendments. Eur. J. Soil Sci. 60, 622-637.
[4] Dijkstra, J. J.; Van Zomeren, A.; Meeussen, J. C. L.; Comans, R. N. J. (2006) Effect of Accelerated Aging of MSWI Bottom Ash on the Leaching Mechanisms of Copper and Molybdenum. Environ. Sci. Technol. 40, 4481-4487.
[5] Apul, D. S.; Gardner, K. H.; Eighmy, T. T.; Fallman, A.; Comans, R. N. J. (2005) Simultaneous application dissolution/precipitation and surface complexation/surface precipitation modeling to contaminant leaching. Environ. Sci. Technol. 39, 5736-5741.
[6] Huijgen, W. J. J.; Comans, R. N. J. (2006) Carbonation of steel slag for CO2 sequestration: leaching of products and reaction mechanism. Environ. Sci. Technol. 40, 2790-2796.
[7] Carter, C. M.; Van der Sloot, H. A.; Cooling, D.; Van Zomeren, A.; Matheson, T. (2008) Characterization of untreated and neutralized bauxite residue for improved waste management. Environ. Eng. Sci. 25, 475-489.
[8] Engelsen, C. J.; Van der Sloot, H. A.; Wibetoe, G.; Petkovic, G.; Stoltenberg-Hansson, E.; Lund, W. (2009) Release of major elements from recycled concrete aggregates and geochemical modelling. Cement and concrete research 39, 446-459.
[10] Rocca, S., van Zomeren, A., Costa, G., Dijkstra, J.J., Comans, R.N.J., Lombardia, F. (2012) Characterisation of major component leaching and buffering capacity of RDF incineration and gasification bottom ash in relation to reuse or disposal scenarios. Waste Management 32, 759-768.

ECN
Westerduinweg 3
1755 LE Petten
The Netherlands

P.O. Box 1
1755 LG Petten
The Netherlands

T +31 88 515 4949
F +31 88 515 8338
info@ ecn.nl
www.ecn.nl