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Modern thermodynamic databases: storing model parameters and model code in one place

JOHANNES C L MEEUSSEN

Nuclear Research and Consultancy Group, Petten, Delft University of Technology

Presenting Author: meeussen@nrg.eu

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Johannes C.L. Meeussen

NRG (Nuclear Research and Consultancy Group), 1755 ZG Petten, The Netherlands.

Department of Civil Engineering and Geosciences, Delft University of Technology , 2628 CN Delft

Geochemical speciation and reactive transport codes such as PHREEQC, GEMS, MINTEQ, PFlotran, ECOSAT, GWB, ORCHESTRA and others are widely used to predict long term migration behavior of (nuclear) contaminants within the context of performance assessment calculations. Such calculations depend on databases with thermodynamic parameters for substances and reactions. Traditionally, these databases only contain numerical input parameters for different model types, while the calculation recipes, in the form of expressions and equations, are defined within the speciation code executables.

This separation of data and code is not a problem in case of “standard” aqueous equilibrium reactions which are implemented in the same way in the different speciation codes, but this becomes progressively problematic in case of more sophisticated chemical (adsorption) models which are implemented in different ways within these codes. This leads to different interpretation of reaction or adsorption “constants” in a database by different speciation codes, resulting in different calculations while using the same database. Several papers have been published on how different codes calculate multi-dentate adsorption models internally.

We demonstrate here how this issue can be solved by storing not only numerical parameters, but also complete model calculation recipes, in the form of object classes, in the same database that is read as input during run-time. Storing this information in a single place automatically ensures consistency between model and parameters and also makes model calculations accessible and transparent by end-users, which can be important to assure the quality of performance assessment calculations.

Apart from the advantages of storing code and parameters together in thermodynamic databases we also discuss what special model requirements are necessary to make this possible, and what effects this approach has on calculation efficiency.

Although the ORCHESTRA framework is used here to demonstrate the approach, the principles are generic and can be used in the design and development of next generation geochemical speciation codes.