ORCHESTRA is a computer program for calculating chemical speciation and reactive transport.

ORCHESTRA includes various advanced models for ion binding. It includes the NICA-Donnan model for ion binding to dissolved and particulate organic matter and the Generalized Two Layer Model (GTLM) and the CD-MUSIC model for ion binding to iron (hydr)oxides. The program includes databases with default model parameters for a large set of cations for the NICA-Donnan model and default parameters for cations and anions for the GTLM model. For inorganic speciation in solution the Minteq V4 database is included. With the graphical user interface of the program chemical equilibrium calculations can be set up by selecting the elements and sorption models. ORCHESTRA is written in Java and runs on Windows, Linux and Apple OSX. A special feature of ORCHESTRA in comparison with other chemical speciation programs is the possibility for users to add (mathematical) expressions and models in text format.

ORCHESTRA can be downloaded free from: www.orchestra.meeussen.nl
This website also provides further information on how to get started with the program and includes various examples

Deriving model parameters with PEST-ORCHESTRA
To be able to derive model-parameters for the sorption models from experimental data the model ORCHESTRA can be used in combination with the freely available parameter estimation program PEST. The coupling of ORCHESTRA with PEST to derive model parameters is described in the publication "PEST-ORCHESTRA, a tool for optimizing advanced ion-binding model parameters: derivation of NICA-Donnan model parameters for humic substances reactivity". The examples provided in this publication will help users to set up their own parameter estimation calculations for the NICA-Donnan model and all other sorption models implemented in ORCHESTRA. The ORCHESTRA and PEST files of these examples can be downloaded here:

Examples PEST-ORCHESTRA

PEST can be downloaded free from www.pesthomepage.org
This website also provides the manual of PEST

For further information contact Bert-Jan Groenenberg bertjan.groenenberg@wur.nl