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Radionuclide transport simulation in heterogeneous media using dual porosity model calibrated by particle swarm optimization method

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Radionuclide concentration predictions in aquifers play an important role in safety assessment of radioactive waste geological disposals. In particular, there is necessity of the safety assessment for historically existing underground disposal facilities of low- and intermediate-level liquid radioactive waste in heterogeneous deep geological formations. For flow and transport modelling in heterogeneous media the dual-porosity concept (Feehley, 2000) can be applied. This approach initially was introduced for fractured media and later has been proved to describe effectively flow and transport in highly heterogeneous media. Due to a lack of measured information (hydraulic heads, permeability, porosity, etc.) and phenomenological nature of the mass transfer coefficient the important step for a transport simulation using dual-porosity model is the calibration of model parameters.

It is well-known that manual parameter optimization for complex models often fails. It was also observed that deterministic optimization techniques for are not much better than manual ones performed by experts. Thus, here is an occasion for heuristic optimization approaches. In this work the Particle Swarm Optimization (Kennedy, 1995) is proposed as parameter calibration technique. This method is acknowledged as a fast converging and more efficient than deterministic optimization tools in various application ranges. It is inspired by birds' social behavior: each particle's search trajectory in the multi-dimensional parameter space is constructed using its local best known position, but is also influenced by the best known positions in the search-space, that are updated as better positions are found by other particles.

The dual-porosity flow and transport is performed by MODFLOW and MT3DMS software tools (Zheng, 2010), the optimization within the parameters' calibration (mobile and immobile porosities, mass-transfer rate, distribution coefficient of linear sorption isotherm) uses OSTRICH software toolkit (Matott, 2005). Calibration is based on normed monitoring data of the existing chemical and radionuclide contamination. The selected parameter estimation approach demonstrates a good performance on given data and fitted dual-porosity model allows more accurate description of radionuclide transport in heterogeneous geological media.

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