

Algorithms for activity correction models for geochemical speciation and reactive transport modelling

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Abstract

Reactive transport codes are today one of the cornerstones of environmental research. They now contain multiphysics with very complex algorithms, including flow, transport, chemical and sometimes heat transport, mechanical and/or biological algorithms. Because of this complexity, some parts of these algorithms still have not been sufficiently studied. Here, we present a comparison of 3 algorithms for activity correction, a specific subset of equilibrium chemistry algorithms. We show that the most used algorithm (the inner fixed-point algorithm) or the most rigorous algorithm (the full Newton) might not be the most efficient, and we propose the outer fixed-point algorithm, which is more robust and faster than other algorithms.

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