Optimal solution methods for aqueous speciation problems

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Expressed in terms of mathematical formalisms, chemical speciation in aquatic systems leads to a multi-dimensional system of non-linear algebraic equations for which, unfortunately, no robust resolution algorithm exists. Yet, a very accurate solution of the problem is required for complex systems. If coupled with hydrodynamic (flow) models, efficiency becomes a key-issue as well. Different approaches are proposed in the literature to combine both accuracy and efficiency. The most promising approaches will be outlined, emphasizing their advantages and inconveniences.

Secondly, we will focus on additional features, required for many realistic chemical systems, including surface complexation with electrostatic effects, colloid formation and reaction kinetics. The mixed equilibrium-kinetic approach is interesting but has severe implications on the numerics involved and overall resolution efficiency. An optimal approach will be outlined, based on an amended Newton-Raphson method with the kinetic reactions included in an analytically solved Jacobian matrix.