NEWTON STRATEGIES FOR IMPLICIT SIMULATIONS OF COUPLED TRANSPORT AND STANDARD CHEMISTRY

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In their simplest formulation, the standard equilibrium equations for chemistry consist of a system of linear equations (mass conservation) and linear equations for the logarithm of the concentrations (equilibrium laws). By nature, a linear and logarithmic scales are mixed and this strong non-linearity creates problem for the convergence of the Newton method. In this talk, we want to introduce two ideas that can be incorporated in a Newton solver to improve its robustness

The first idea originates from [2]. We will discuss the motivation but the outcome consists of using logarithmic variables and a special form of the mass conservation equations. In addition, we use natural physical bounds, as presented in [1]. The result is a solver showing good robustness properties on test cases that we will present.

Transport problems naturally mix components. For an implicit solver, we do not know - a priori - the elements that are present in a computation cell. This information will be given as the result of the computation of the solution of the nonlinear equations. However, to solve the chemical equations, this information is crucial, in particular when using logarithmic variables. Here, we present a strategy that can be used at each Newton step to estimate the appearance or disappearance of species. We will show some numerical experiments with calcite dissolution.

References

[1] J. Carrayrou, R. Mosé, and P. Behra, *New efficient algorithm for solving thermodynamic chemistry*, AIChE Journal, 48, pp. 894-904, 2002.

[2] T. W. Wall, D. Greening, and R. E.D Woolsey, *OR practice–solving complex chemical equilibria using a geometric-programming based technique*, Operations Research, 34, pp. 345-355, 1986.

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