

OPTIMIZATION PROBLEMS IN GEOCHEMISTRY

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Geochemistry involves aqueous reactions and mineral precipitation or dissolution. Quantities of solute species are assumed to be strictly positive, whereas those of minerals can vanish. The mathematical model is expressed as the minimization of Gibbs energy subject to positivity of mineral quantities and conservation of mass. Optimality conditions lead to a complementarity problem.

We show that, in the case of a dilute solution, this problem can also be considered as optimality conditions of another minimization problem, subject to inequality constraints. This new problem is easier to handle, both from a theoretical and a practical point of view.

Then we define a partition of the total quantities in the mass conservation equation. This partition builds a precipitation diagram such that a mineral is either precipitated or dissolved in each subset. We propose a symbolic algorithm to compute this diagram.

Simple numerical examples illustrate our methodology.

References

- [1] J. Erhel and T. Migot, *Characterizations of Solutions in Geochemistry: Existence, Uniqueness and Precipitation Diagram*, Computational Geosciences, (2018), online.