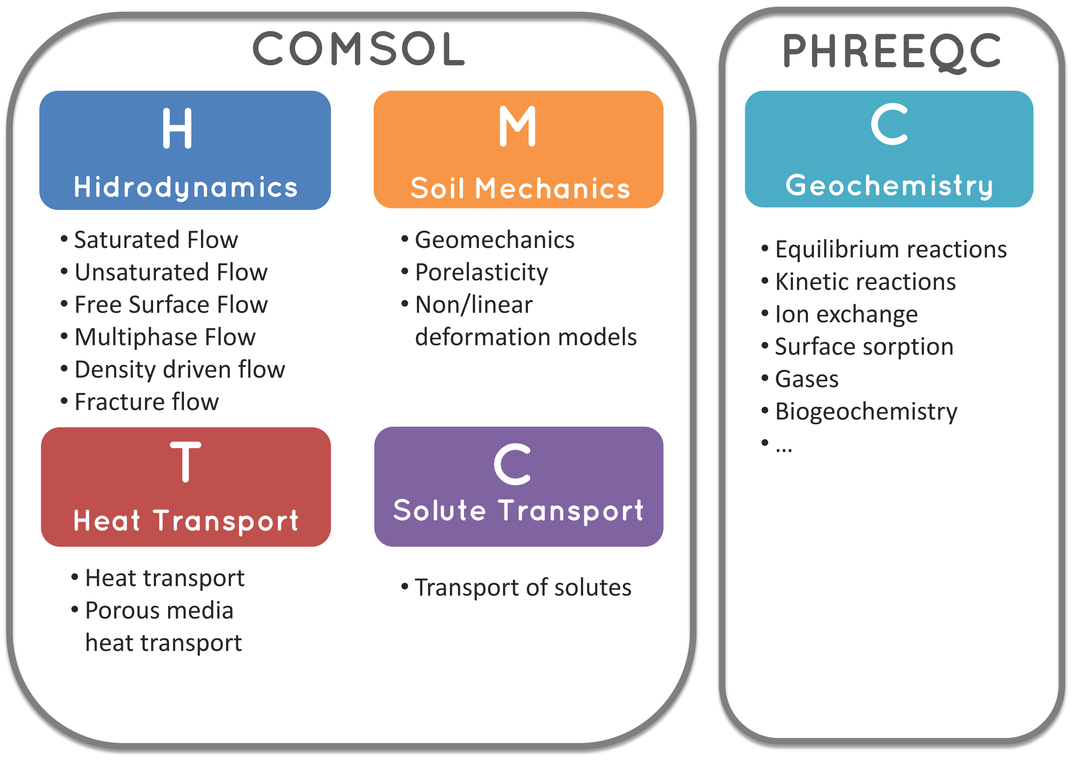
iCP 1.0: Stable release version of the interface COMSOL-PHREEQC

Albert Nardi, Luis Manuel de Vries, Álvaro Sáinz, Jorge Molinero
Amphos 21 Consulting

Introduction

iCP (Nardi et al, 2014) is a software that couples two standalone simulation programs: COMSOL Multiphysics® and the geochemical simulator PHREEQC (Parkhurst & Appelo, 2013). The main goal of the interface is to maximize the synergies between the aforementioned codes.

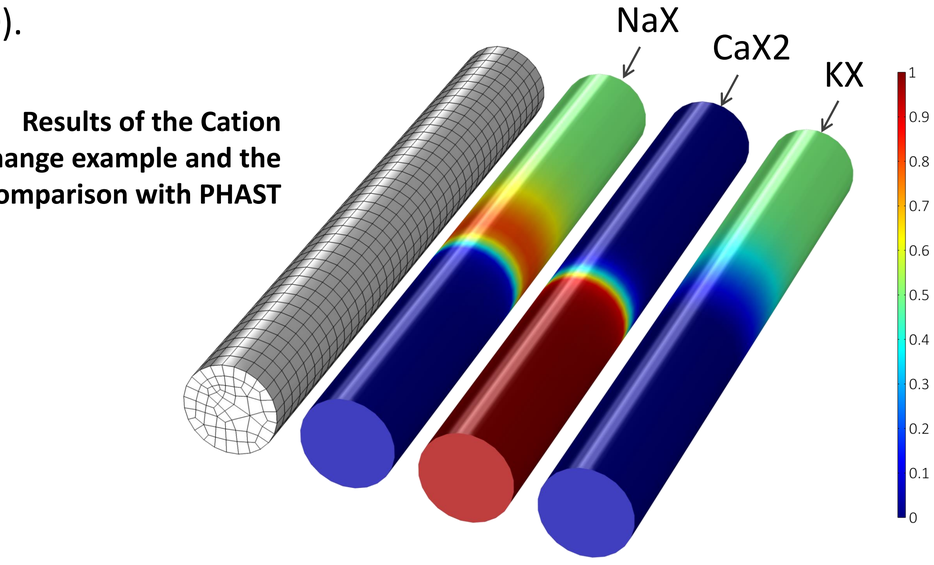
The tool is ideal for those interested to apply multiphysics and geochemistry to different fields of Earth Sciences. The flexibility and wide range of application of the two coupled codes result in an extensive list of possible modelling areas, covering most of the needs of the industry and offering good opportunities for R+D. An example of possible simulation combinations is represented in the following chart.

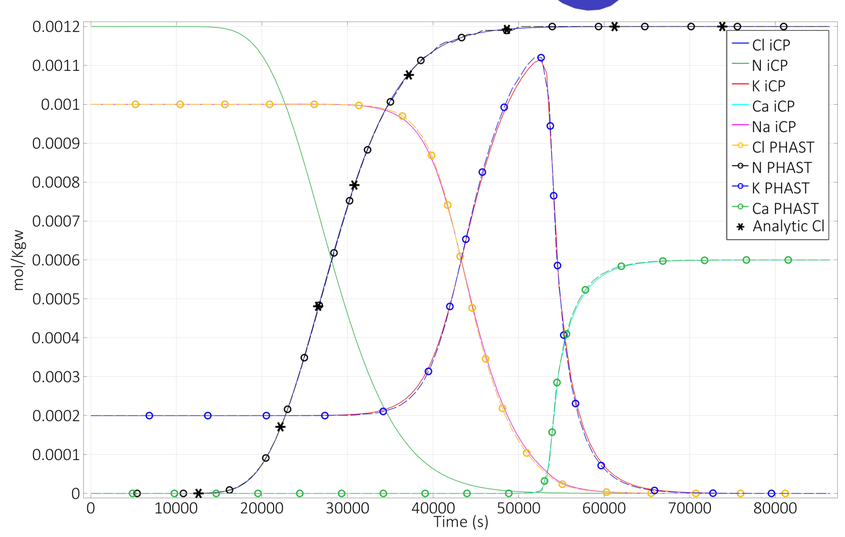


Benchmarking

The accuracy of iCP has been tested through a set of benchmark problems. These problems range from a 1D conservative transport problem to multidimensional problems with chemical reactions. Some of the benchmark problems are already described in the literature. The results have been compared with other codes such as PHREEQC, HP-1 (Simunek et al., 2006) or PHAST (Parkhurst et al., 2010).

Results of the Cation Exchange example and the comparison with PHAST





Code features

Easy friendly

- Easy GUI for launching the program
- The physics are completely defined in COMSOL and the chemistry in PHREEQC
- Whole post processing in COMSOL

Flexible couplings

- Possibility to link variables from COMSOL to PHREEQC and vice versa
- Any PUNCH expression from PHREEQC can be linked
- Links from PHREEQC to COMSOL are lagged in time

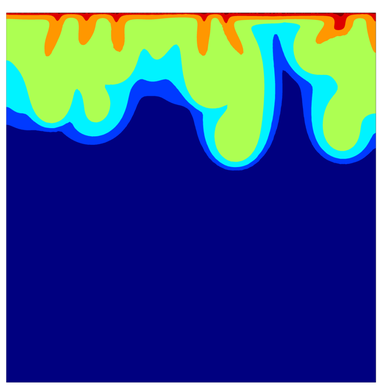
Chemistry step parallelized

- Ready to take profit on multicore machines
- Parallelized on multiple machines through MPI
- Possibility to slice complex chemical domains to avoid bottlenecks

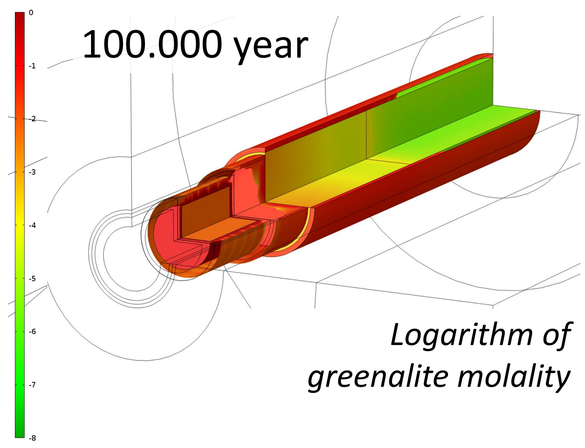
Application examples

Reactive CO2

pH distribution of acidic CO2 fingers



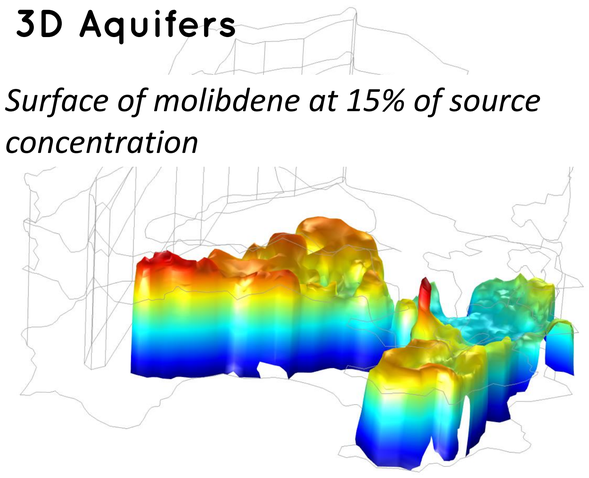
Engineering barriers



Logarithm of greenalite molality

3D Aquifers

Surface of molibdene at 15% of source concentration



References

Nardi, A., Idiart, A., Trinchero, P., de Vries, L. M. and Molinero, J., Interface Comsol-PHREEQC (iCP), an efficient numerical framework for the solution of coupled multiphysics and geochemistry, Computers & Geosciences, doi:10.1016/j.cageo.2014.04.011 (2014)

Parkhurst, D. L., and Appelo, C. A. J., Description of input and examples for PHREEQC version 3—A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations, U.S. Geological Survey Techniques and Methods, book 6, chap. A43, 497 p., available only at http://pubs.usgs.gov/tm/06/a43/ (2013).

Simunek, J., Jacques, D., van, M.T. & Mallants, D., 2006. Multicomponent geochemical transport modeling using HYDRUS-1 D and HP 1. Journal of the American Water Resources Association, 42(6), pp.1537-47.

Parkhurst, D.L., Kipp, K.L. & Charlton, S.R., 2010. PHAST Version 2—A program for simulating groundwater flow, solute transport, and multicomponent geochemical reactions. U.S. Geological Survey Techniques and Methods, 6–A35, p.235 p.

Excerpt from the Proceedings of the 2014 COMSOL Conference in Cambridge