iCP Apps to Readily Solve Reactive Transport Simulations in COMSOL Multiphysics®

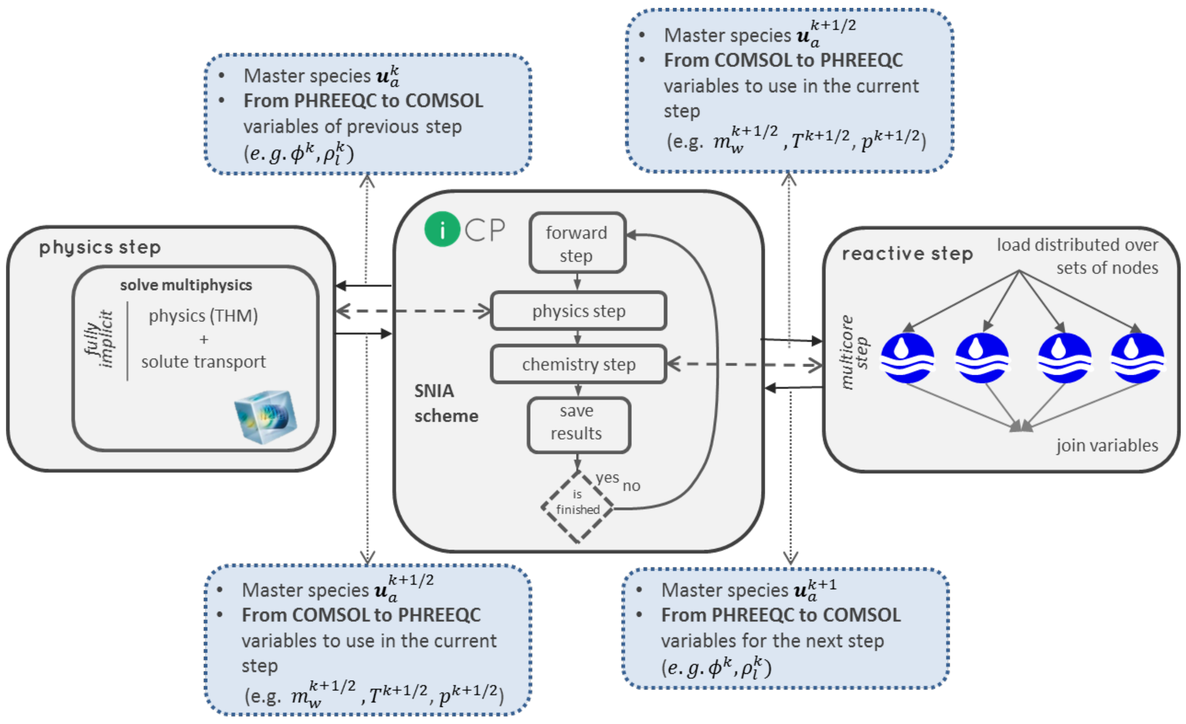
D. Negro[(1)], A. Sáinz-García[(1)], D. Sampietro[(1)], E. Coene[(1)], E. Abarca[(1)], A. Idiart[(1)], M. Laviña[(1)], O. Silva[(1)], J. Molinero[(1)].

[(1)]*Amphos 21 Consulting S.L., Barcelona, Spain.*
https://image-modelling.net/project/view/1/iCP

Introduction

Many natural phenomena involve coupled systems where multiple physical and chemical processes interact. To model such systems in the subsurface environment, multidimensional codes able to reproduce complex coupled THMC processes are needed.

iCP (Nardi et al., 2014) is a software that couples two standalone programs: COMSOL Multiphysics® and the geochemical simulator PHREEQC (Parkhurst & Appelo, 2013). iCP maximizes the synergies between both codes; being of great benefit in applications where geochemistry is linked to other physical processes. Its flexibility and wide range of applicability make iCP suitable for many modelling challenges in various fields of Earth Sciences. It has been successfully applied to model complex natural and engineered environments (Sainz-Garcia et al., 2017; Karimzadeh et al., 2017); covering most of the needs of the industry and offering an excellent framework for complex R+D projects.

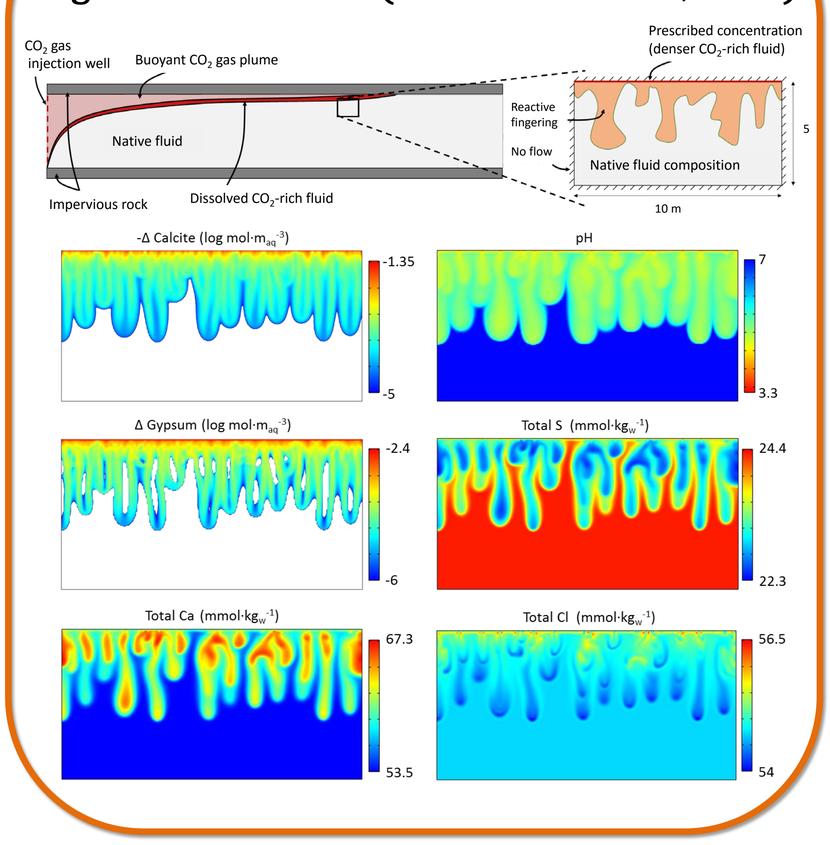


iCP Apps and other examples

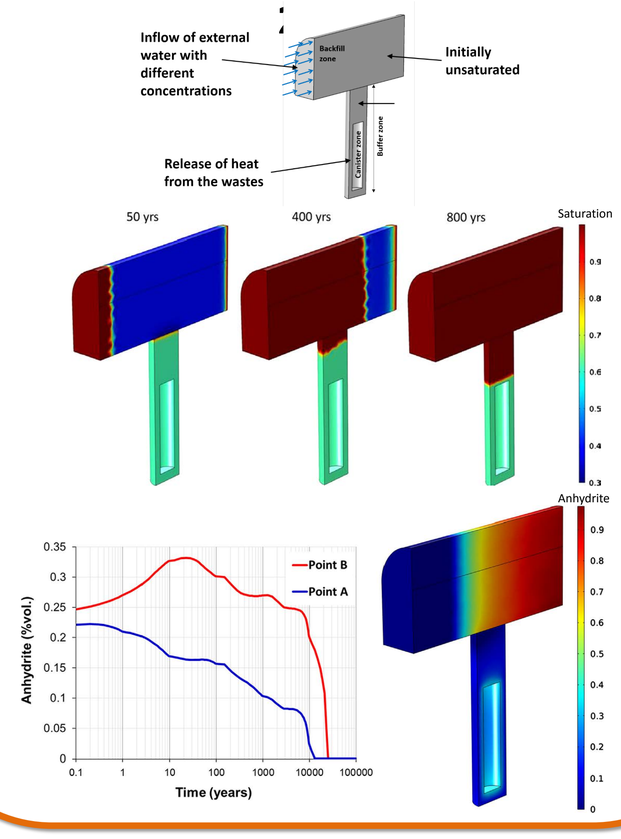
iCP Apps have been developed using the COMSOL Application Builder. These user-friendly Apps are tailored for specific physical configurations in which the chemical system can be adapted. iCP Apps allow the users to focus on the aspects that matter without requiring a high level numerical computation foreknowledge.

iCP Apps run simulations, pre- and post-process an iCP model from a COMSOL Application. iCP Apps allow the modification of iCP and COMSOL parameters.

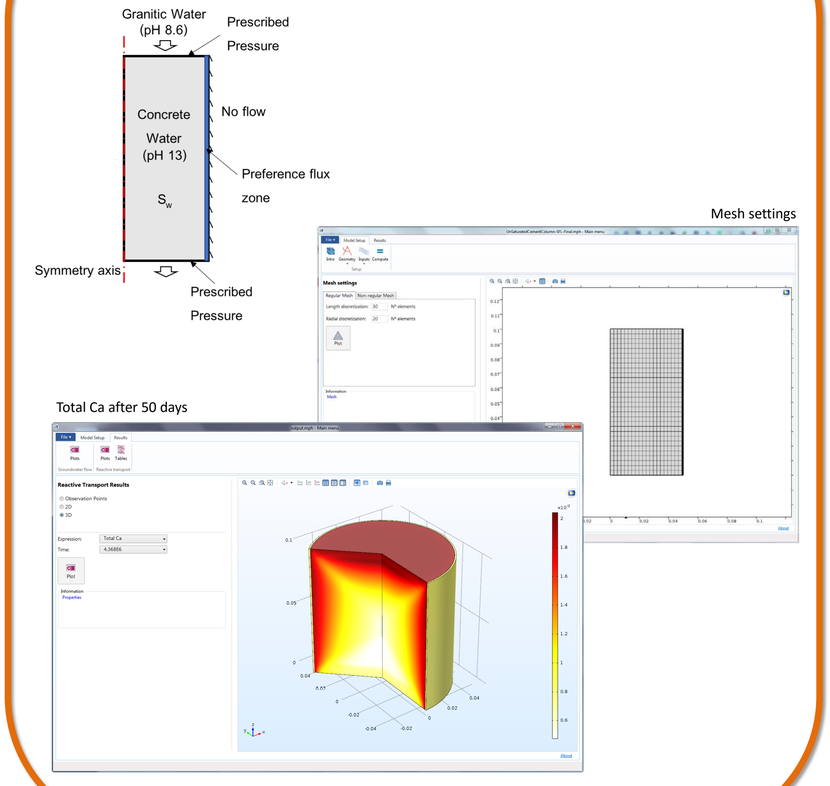
Reactive density-driven convective mixing fingers in carbonates (Sainz-Garcia et al., 2017)



THC model of bentonite for nuclear waste geological disposal (Nardi et al.,



Column experiment of concrete degradation - iCP App



References

Nardi, A., Idiart, A., Trinchero, P., de Vries, L. M., and J. Molinero. Interface COMSOL-PHREEQC (iCP), an efficient numerical framework for the solution of coupled multiphysics and geochemistry. Computers & Geosciences 69 (2014) 10-21.

Parkhurst, D. L., and Appelo, C. A. J. (2013) 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.

Sainz-Garcia, A; Abarca, E; Nardi, A; Grandia,F; Oelkers,E.H. (2017) Convective mixing fingers and chemistry interaction in carbon storage International Journal of Greenhouse Gas Control 58, 52–61.

Karimzadeh, L., Lippmann-Pipke, J., Franke, K., Lippold, H, (2017) Mobility and transport of copper (II) influenced by the microbial siderophore DFOB: Column experiment and modelling, Chemosphere 173, 326-329.

Excerpt from the Proceedings of the 2017 COMSOL Conference in Rotterdam