

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

D. Negro¹, D. Sampietro¹, A. Sainz-Garcia², E. Coene¹, E. Abarca¹, M. Laviña¹, O. Silva¹, J. Molinero¹, A. Idiart¹

¹Amphos 21 Consulting S.L., Barcelona, Spain

²Amphos 21 Consulting S.L., Barcelona, Spain & Université Toulouse III, Toulouse, France

Abstract

Reactive transport models (RTM) that couple physical and chemical processes are commonly used to solve a large variety of problems in the environmental industry. There are a series of codes designed to solve this kind of problems. However, their use requires typically much effort due to their non-user-friendly interface and their large learning curve. This work presents an application to solve RTM problems with iCP taking advantage of COMSOL Multiphysics® and its Application Builder. iCP (Nardi et al., 2014) is a software that couples COMSOL Multiphysics® and the geochemical simulator PHREEQC (Parkhurst & Appelo, 2013). Its flexibility and wide range of applicability make iCP suitable for many modeling challenges in various fields of Earth Sciences (Sainz-Garcia et al., 2017, Karimzadeh et al., 2017); covering most of the needs of the industry and offering good opportunities for R+D (Figure 1).

iCP Apps have been developed integrating the capabilities of iCP and COMSOL Applications. They inherit all the benefits from COMSOL Applications, adding the capabilities to solve complex chemical problems. iCP Apps allow the modification of iCP and COMSOL parameters and the visualization of the model results from a single application. The capacity of COMSOL Applications to embed third-party Java libraries and to call APIs, provides a foolproof base platform to run iCP models. iCP Apps provide an easy and user-friendly interface to solve challenges, making accessible reactive transport models to a broader public.

Figures used in the abstract

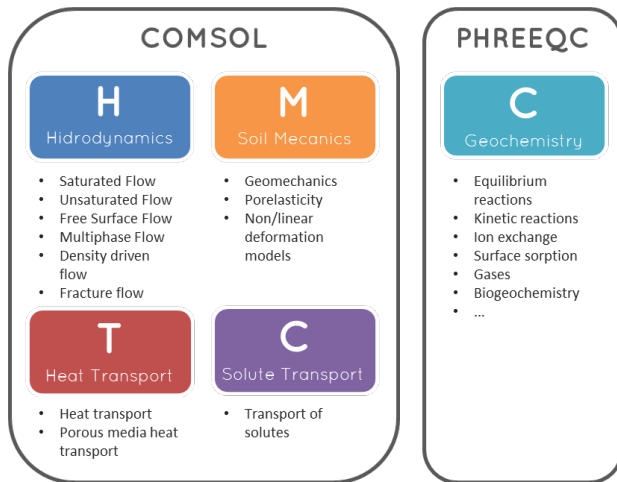


Figure 1: Physics that can be solved with iCP Apps.