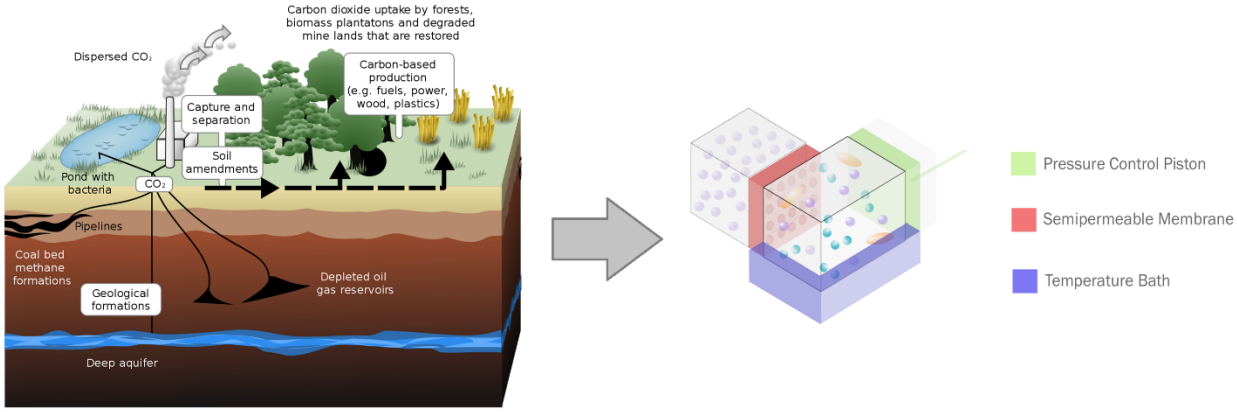
State Function-Based Flash Specifications for Open Systems: Application to CO_2 Underground Geological Storage

Phase equilibrium calculations subject to chemical potential specifications are very common in Geochemistry. Several of the scenarios analyzed in this field consist of a system that can exchange mass with reservoirs of given species at a fixed temperature, pressure and composition, and therefore chemical potential [1]. An important application of such calculations is in the underground geological storage (UGS) of carbon dioxide. The fate of the CO_2 injected in mineral formations, such as saline aquifers or depleted oil reservoirs, can be better understood by simulating the phase equilibrium behavior of brines when in contact with reservoirs of carbon dioxide at injection conditions, as done by Marini [2].

Phase equilibrium algorithms for open systems are well-established in Geochemistry. Mainstream programs in the field such as PHREEQC or EQ3/EQ6 have built-in algorithms based on root-finding procedures for this purpose. Other programs (GEM-Selektor or Reaktoro), which are based on state function minimization, do not present this feature. In this presentation, the development of algorithms for open systems based on state function minimization is discussed. They are derived from fundamental thermodynamic theory on state functions, with the aid of Legendre transforms [3]. The methodology followed here is an extension of Michelsen's Q-function approach [4]. By using such methodology, the family of RAND algorithms for reactive systems can be applied to chemical potential specifications. With those algorithms at hand, phase equilibrium calculations in the context of CO_2 UGS in saline aquifers can be performed in a more robust and efficient way.

References:

[1] C. M. Bethke, Geochemical and Biogeochemical Reaction Modeling. 2ed. Cambridge University Press; 2007.
[2] L. Marini, Geological Sequestration of Carbon Dioxide – Thermodynamics, Kinetics, and Reaction Path Modeling. 1ed Elsevier, 2007.
[3] Medeiros, F. A., Stenby, E. H. and Yan W., State Function-Based Flash Specifications for Open Systems in the Absence or Presence of Chemical Reactions, submitted to AIChE Journal.
[4] Michelsen ML. State function based flash specifications. Fluid Phase Equilibria, 1999; 158-160: 617–626.



CO2 Sequestration and Storage Scheme

Schematic Representation as an Open Flash Calculation

Figure 1 - Graphical Abstract