On coupling variable porosity and water activity with two-phase flow in reactive transport modelling

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Introduction

In the recent years, multi-phase flow has been on the rise within reactive transport simulators and has become an important tool for different applications. Meanwhile, dealing with variable porosity has always been a challenge for the reactive transport community. Furthermore, in some applications, water plays a key role in the chemical equilibrium and its amount can become a limiting factor. An accurate coupling of the two-phase flow problems with variable porosity requires new resolution schemes for the reactive transport algorithm. We present these modifications for the reactive transport code Hytec.

Algorithms limitations and modifications

Hytec is a reactive transport code with a modular algorithm. First, Hytec solves the flow (saturated / unsaturated / biphasic), for which a compressible multicomponent two-phase flow was integrated [1].

Second, the reactive transport is solved based on a sequential iterative approach, coupling a hydrodyanmics module (R2D2) and a geochemical module (CHESS). The geochemical equilibrium is based on the conservation of the basis-species concentration , and computes the porosity based on the mineral concentrations when the equilibrium is reached[2].

The initial structure of the code is represented in figure 1. There is a weak coupling between the flow and chemistry : since the gas density is subject to significant change based on its composition, gaseous transport is considered in the two-phase flow solver.

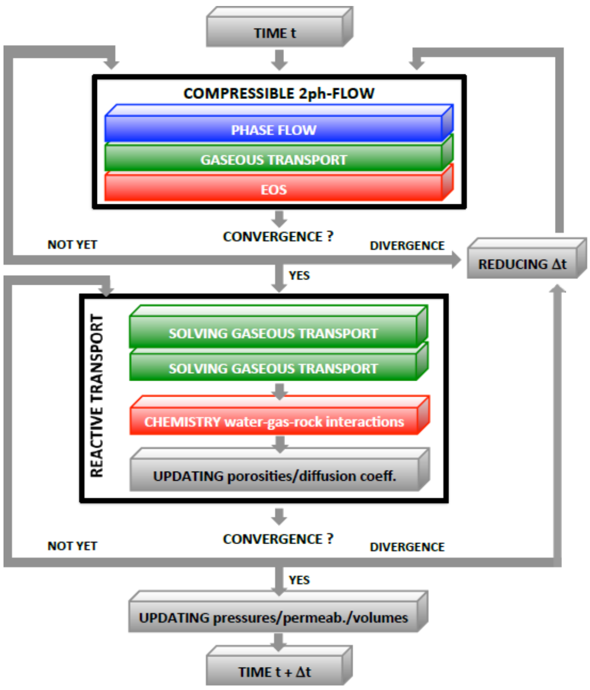

Figure 1: Hytec algorithm

However, applying the latter algorithm when dealing with variable porosity might prove to be insuficient. An accurate simulation needs to compute the exact amount of water and porosity. As these variables will intrinsically modify the concentration of basis and secondary species, the CHESS algorithm leads to an error.

To overcome this, the structure of the CHESS algorithm has been modified, in order to implicitly solve the porosity and solvent mass as a primary variables. To increase the accuracy of the calculation, CHESS solves the conservation of the total absolute amount of basis species (in moles), instead of total molality. This also leads to a higher numerical efficiency.

However, the solved geochemical system sees its volume evolve as the volume occupied by the mineral and the solvent is not constant. This can be dealt with by adding a source-term in the flow, or a gas-volume in the case of a two-phase flow. This leads to an increased coupling between the reactive transport and the 2-phase flow.

The case of the atmospheric carbonation of concrete

The atmospheric carbonation of concrete is a problem which illustrates this effect. The drying and CO_2 gas migration inside the material is a two-phase flow problem. The gas dissolution in the concrete pore-solution leads to the formation of carbonates and, in fine, reacts with calcium to form calcite. The consumption of calcium in the pore solution also leads to the dissolution of the cement pate solid minerals (Portlandite, C-S-H). The evolution of the pore structure and the transport properties is significant [3]. Furthemore, as water plays an active role in these reactions, its activity might differ from one.

The atmospheric carbonation of concrete is considered to be an important degradation in the context of radioactive waste management. Its simulation by means of reactive transport modelling requires an accurate coupling between the different occurring phenomenons which have been challenging for the reactive transport community.

References

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