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Benchmark of reactive transport models within CEBAMA
Application to a concrete / clay interface

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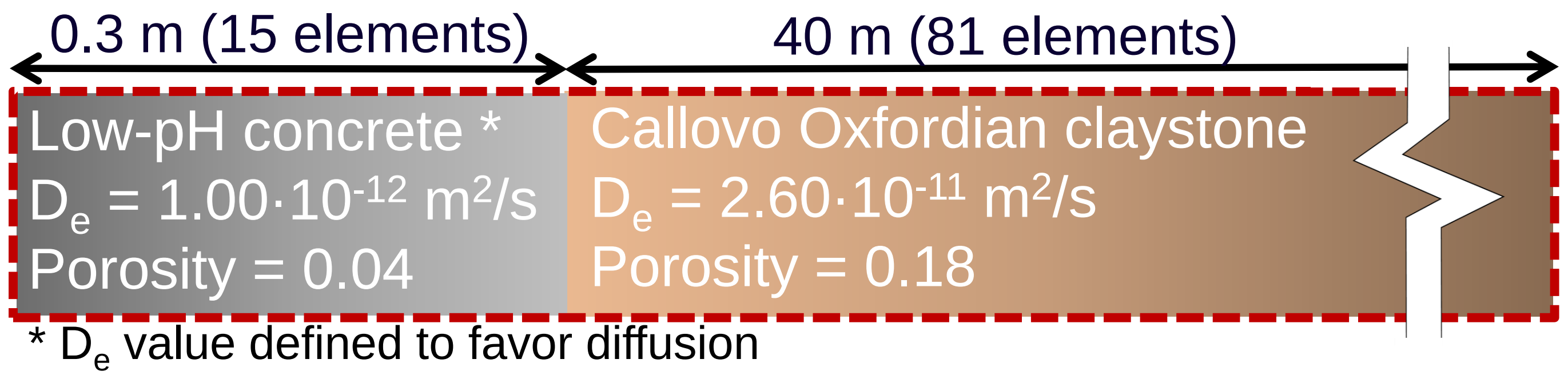
Introduction and objectives

A benchmark modelling study of interactions between low-pH concrete and clay rock is presented here, conducted within the framework of the EC Horizon 2020 CEBAMA [1]. The concrete composition corresponds to the reference low-pH concrete manufactured and characterized in CEBAMA as an experimental benchmark [2]. Different modelling approaches were used for modelling and interpretation of experimental data generated within CEBAMA, with focus on reactive transport processes that can impact the physical properties of cementitious materials and their interface with clayey systems. Model and experimental results were satisfactorily compared [3]. A common modelling task was conducted to build confidence in the consistency of the different modelling approaches. The work aimed at benchmarking the capabilities of reactive transport codes to simulate physical and chemical processes governing long-term interactions at the concrete-clay interface. The benchmark also considered a set of sensitivity cases to test the effect of key parameters on the results. The main outcomes of the collaborative study are described in detail in [4] and presented here.

Methodology and description 1D reactive transport model setup

The studied system considers a generic concrete structure in contact with a clayey host rock under isothermal (25ºC) and saturated conditions. Solute transport by Fickian diffusion and a simulation time of 100 kyr is considered. Several models of increasing complexity have been implemented and simulated, including a set of sensitivity cases.



0.3 m (15 elements)

40 m (81 elements)

Low-pH concrete *
$D_e = 1.00 \cdot 10^{-12}$ m²/s
Porosity = 0.04

Callovo Oxfordian claystone
$D_e = 2.60 \cdot 10^{-11}$ m²/s
Porosity = 0.18

* D_e value defined to favor diffusion

Partner	Modelling tool
AMPHOS 21 (A21)	iCP
KIT	iCP
JUELICH	OGS (OpenGeoSys-GEM)
PSI	OGS
NRG	ORCHESTRA
UDC	CORE2D
ANDRA	MIN3P

ID	Description of simulation cases
P1	Preliminary 1: diffusion of a tracer from concrete into the clay rock
P2	Preliminary 2: diffusion, cation exchange and aqueous speciation reactions
P3	Preliminary 3: idem case P2, and adding mineral reactions in equilibrium
FRC	Full Reference Case: full chemical description, including kinetics
S1	Sensitivity 1: different porosity-diffusion couplings considered
S2	Sensitivity 2: effective diffusivity of concrete reduced by 1 order of magnitude
S3	Sensitivity 3: electrochemical coupling (i.e. Nernst-Planck equations)
S4	Sensitivity 4: use of a different thermodynamic database (TDB)

Processes	P1	P2	P3	FRC	S1	S2	S3	S4
Tracer diffusion	×	×	×	×	×	×	×	×
Aqueous species + cation exchange		×	×	×	×	×	×	×
Minerals in equilibrium			×	×	×	×	×	×
Reaction kinetics				×	×	×	×	×
Chemical/Porosity couplings					×			
Lower diffusion coefficient in concrete						×		
Multicomponent diffusion							×	
Use of different TDB								×

Results

As an example, results of the FRC are presented and compared to the case P3 in terms of mineralogical evolution of the system (Fig. 1), as well as pH and porosity changes (Fig. 2) after 100,000 years of interaction. Very good agreement is observed between the different reactive transport models and between the FRC and P3 cases (differing in the incorporation or not of kinetically-controlled mineral reactions).

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Results - continued

Concrete degrades significantly over half of its thickness, with substantial dissolution of C-S-H, decreasing pH, and increasing porosity. Precipitation of calcite and brucite clogs the concrete porosity close to the interface. The high-pH plume into the claystone is negligible, also shown by the negligible dissolution of montmorillonite.

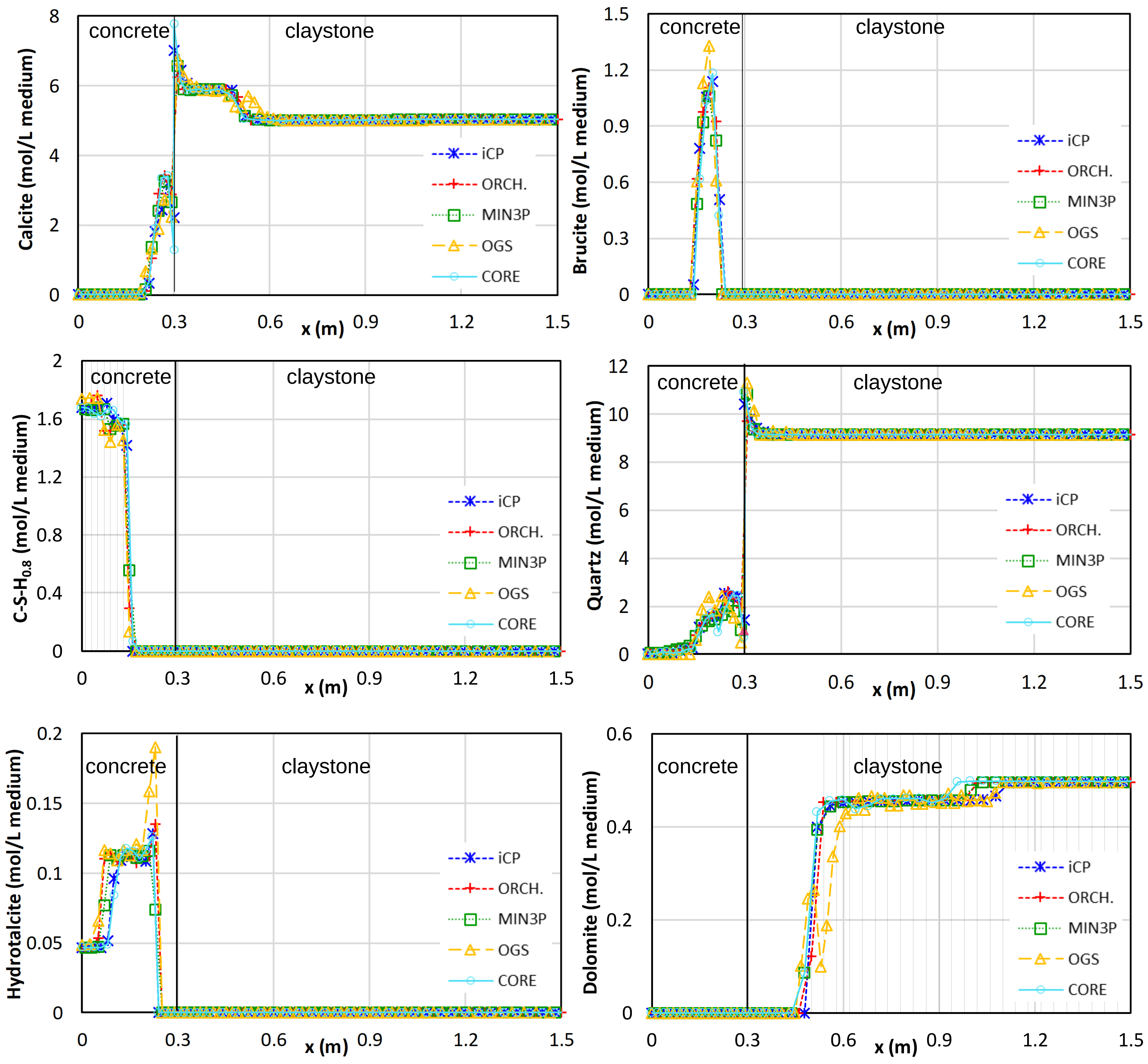

Fig. 1. Results comparison: mineral phases (in mol/L medium) in the concrete and clay domains at 100,000 years obtained with iCP, ORCHESTRA, and MIN3P for the FRC, and OGS and CORE for case P3.

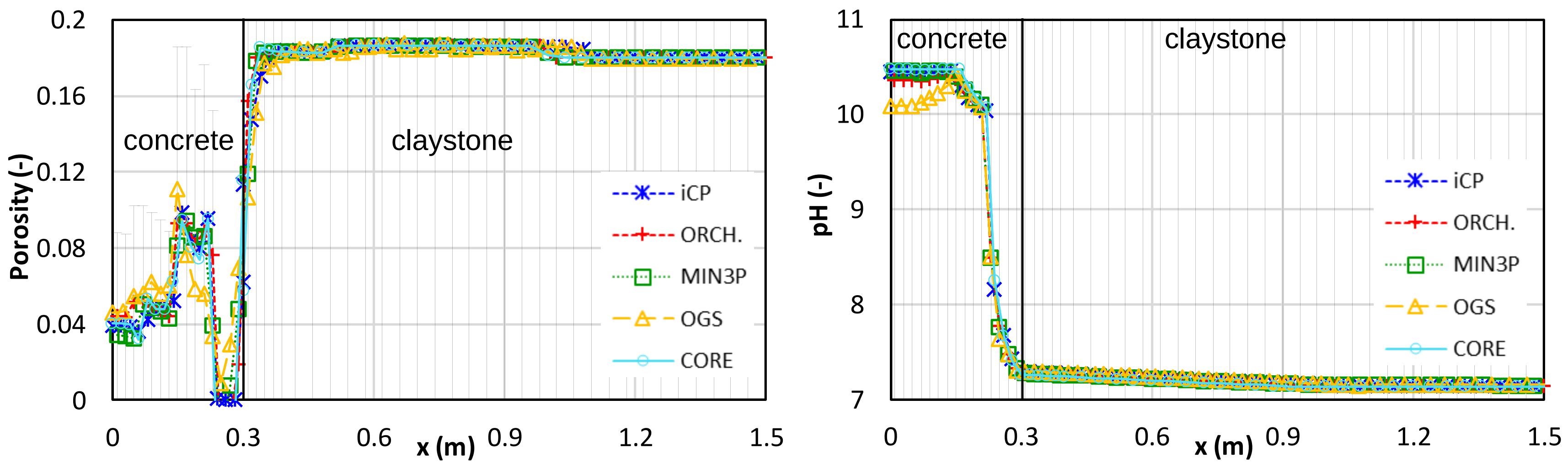

Fig. 2. Results comparison: pH and porosity profiles in concrete and clay at 100,000 years (iCP, ORCHESTRA, MIN3P: FRC / OGS, CORE: P3).

Conclusions

Within the CEBAMA project, the common modelling task has served to build confidence on the representation of cement-clay complex systems with reactive transport modelling tools when simulating the long-term behaviour of low-pH cementitious systems interfaced with a clayey host rock. The impacts of key parameters, such as diffusion coefficients, thermodynamic data or couplings between geochemical and transport parameters, have also been assessed.

The results show not only the high level of understanding of the governing processes but also the good agreement obtained with different codes, which is essential to demonstrate the applicability of reactive transport modelling to support the safety assessments.

References

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Acknowledgement: The research leading to these results has received funding from the European Union's European Atomic Energy Community's Horizon 2020 Programme (NFRP-2014/2015) under grant agreement, 662147 - Cebama