Reactive transport processes at a low-pH concrete / clay interface: a benchmark modelling study

A Idiart[1*], M Laviña[1], E Coene[1], V Montoya[2], G Kosakowski[3], B Cochepin[4], I Munier[4], J Samper[5], A Mon[5], J Meeussen[6], G Deissmann[7], S Rohmen[7], J Poonoosamy[7], D Vopálka[8]

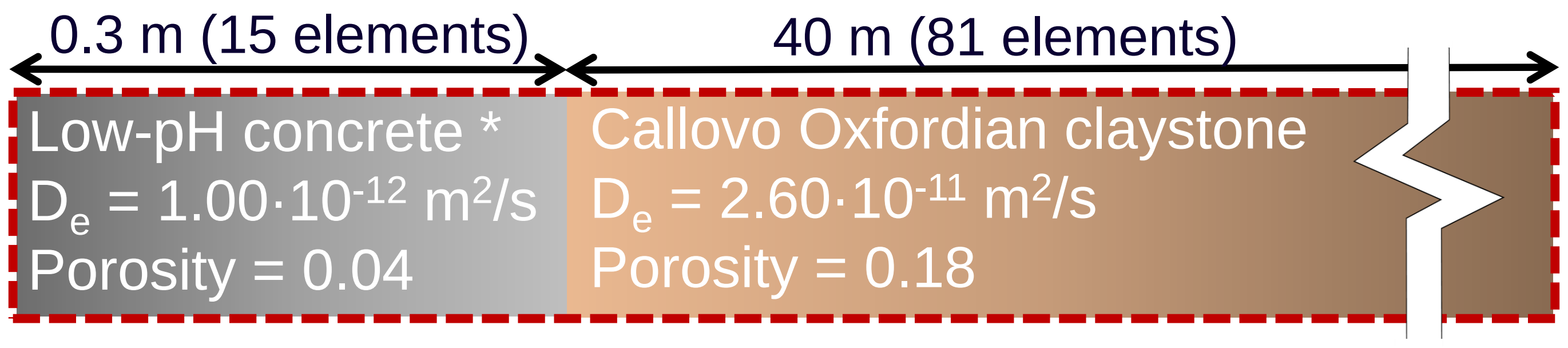
[1]Amphos 21 Consulting S.L., Spain; [2]KIT-INE, Germany; [3]Paul Scherrer Institute, Switzerland; [4]Andra, France; [5]Univ. A Coruña, Spain; [6]Nuclear Res. Consultancy Group, The Netherlands; [7]Forschungszentrum Jülich GmbH, IEK-6, Germany; [8]Czech Technical Univ., Czech Republic

Introduction and Objectives

Within the framework of the EC Horizon 2020 **Cebama** (Cement-based materials, properties, evolution, barrier functions [1; 2]), a benchmark modelling study of interactions between low-pH concrete and clay rock is being conducted. One of the main goals of Cebama is to improve our level of understanding of interaction processes between cementitious and clayey systems. Part of the work is devoted to the modelling and interpretation of experimental data generated within the project. Different modelling approaches are used, with focus on reactive transport processes that can impact the physical properties of cementitious materials and their interface with clayey systems. The objective of the benchmark modelling study that is currently on-going is to build confidence in the consistency of the different modelling approaches in use within Cebama.

1D reactive transport model benchmark – setup

The models consider isothermal (25ºC) and saturated conditions and solute transport by Fickian diffusion with a simulation time of 100 kyr


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

- 7 research teams
- 5 numerical codes
- 11 simulation cases

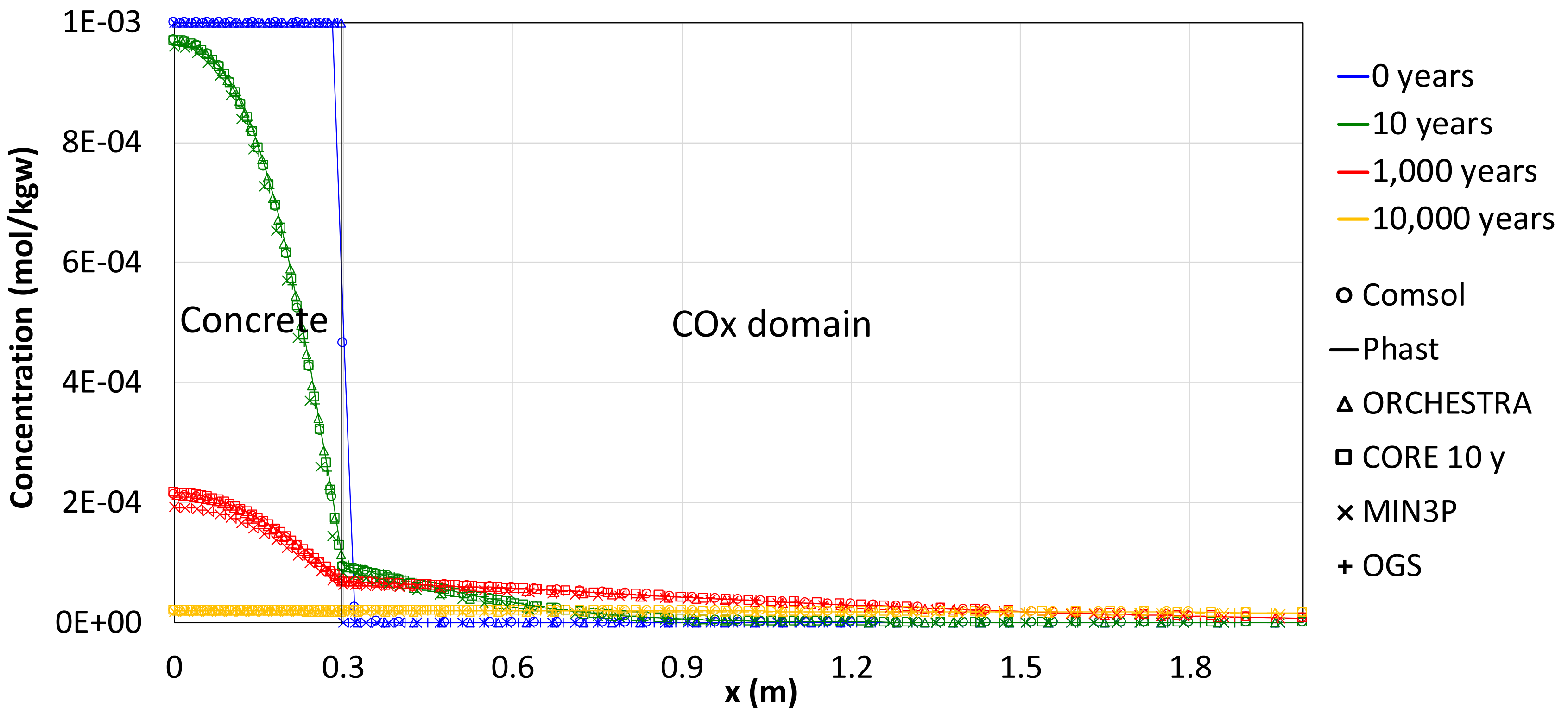
Team	Code
A21	iCP
NRG	ORCHESTRA
ANDRA	MIN3P
UDC	CORE
JULICH	iCP
KIT	iCP
PSI	OGS/NPS

Preliminary Cases	
P1	Tracer diffusion
P2	Cation exchange
P3	Minerals in equilibrium
Full Reference Case	
FRC	Complete chemical setup
Sensitivity Cases	
S1	Simple porosity coupling
S2	Advanced porosity coupling
S3	Lower concrete De
S4	Multicomponent diffusion
S5	Use of different TDB's
S6	Hydration coupling
S7	Set of 2ry minerals

Low-pH concrete				COx domain			
Primary minerals volume fraction (%)							
$C\text{-}S\text{-}H_{0.8}$	9.962			Calcite	18.605		
Calcite	0.032			Celestite	0.574		
Ettringite	0.842			Dolomite	3.194		
Ferrihydrite	0.228			Pyrite	0.457		
Hydrotalcite	1.065			Siderite	0.582		
Magnetite	$8.90 \cdot 10^{-5}$			Illite	26.981		
Strätlingite	1.033			Montmorillonite	6.558		
Quartz	3.967			Microcline	2.682		
Silica fume	1.394			Quartz	20.772		
Inert Solids	77.477			Ripidolite	1.564		
Exchanger fraction (%)							
X_2Ca	38.24			X_2Ca	45.19	XK	3.74
XK	47.53			X_2Mg	31.25	X_2Sr	1.13
XNa	14.53			XNa	18.42	X_2Fe	0.27
Initial porewater composition (mol/kg water)							
pH	10.68	pe	-0.46	pH	7.06	Pe	-2.84
Al	$1.4 \cdot 10^{-4}$	Mg	$3.7 \cdot 10^{-7}$	Al	$8.5 \cdot 10^{-8}$	Mg	$5.2 \cdot 10^{-3}$
C	$1.5 \cdot 10^{-5}$	Na	$1.9 \cdot 10^{-2}$	C	$3.8 \cdot 10^{-3}$	Na	$4.0 \cdot 10^{-2}$
Ca	$5.2 \cdot 10^{-3}$	S	$3.1 \cdot 10^{-2}$	Ca	$7.6 \cdot 10^{-3}$	S	$1.1 \cdot 10^{-2}$
Cl	$1 \cdot 10^{-10}$	Si	$2.0 \cdot 10^{-3}$	Cl	$4.1 \cdot 10^{-2}$	Si	$1.8 \cdot 10^{-4}$
Fe	$5.4 \cdot 10^{-8}$	Sr	$1 \cdot 10^{-10}$	Fe	$4.4 \cdot 10^{-5}$	Sr	$2.4 \cdot 10^{-4}$
K	$3.4 \cdot 10^{-2}$	Tra	$1.0 \cdot 10^{-3}$	K	$5.1 \cdot 10^{-4}$	Tra	$1.0 \cdot 10^{-6}$

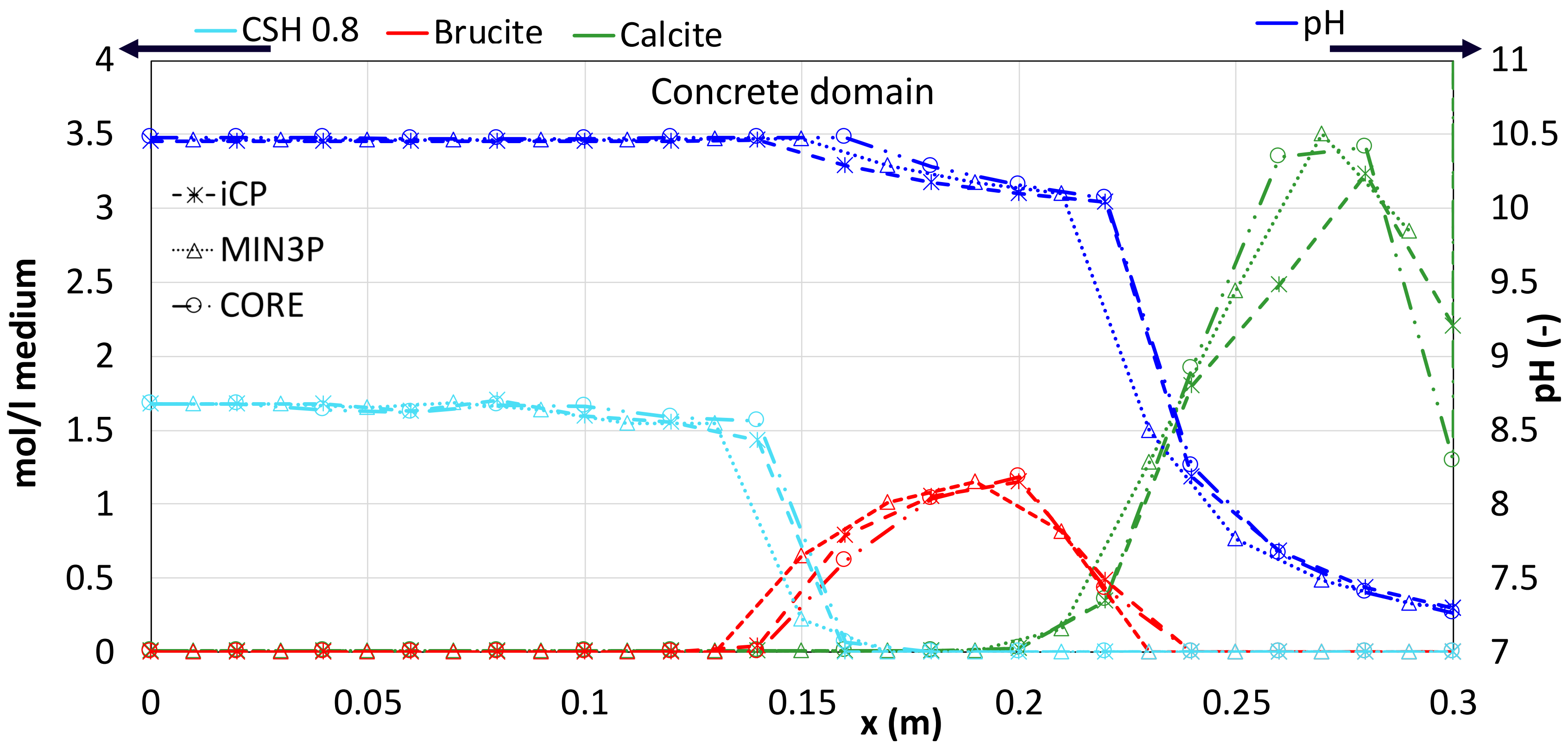
Results

P1: Tracer diffusion



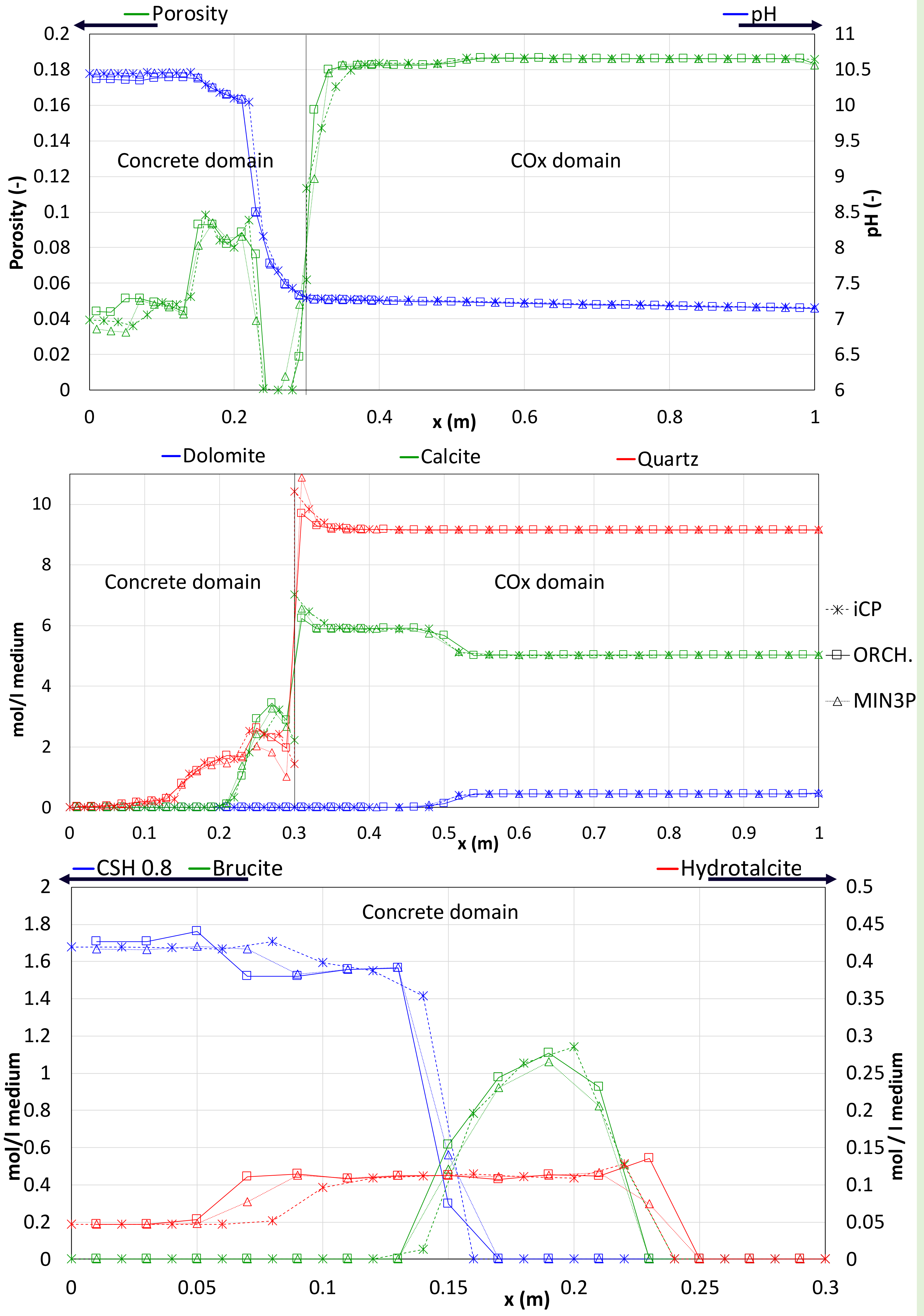
Comparison between 6 different codes computing tracer diffusion

P3: Aqueous + Exchanger + Equilibrium phases



Results comparison for pH and main minerals in concrete after 100 kyr

FRC: Complete chemical setup



Porosity, pH values and mineral concentration spatial distributions after 100 kyr. Results for 3 different codes: iCP, ORCHESTRA and MIN3P

Conclusions

- (P1) Very good agreement of diffusion with the different codes.
- (P2) Cation exchange formulation needs to be homogenized.
- (P3) Good agreement when including minerals in equilibrium.
- (FRC) Good agreement of results for 3 codes after 100 kyr of concrete-clay interaction. Porosity clogging and important changes in pH are obtained for the first 5cm on the concrete side.
- On-going work aims at completing the simulation cases and comparison exercise. The results and outcomes will be published.

References

[1] Altmaier M, Montoya V, Duro L, Valls A. (2017). Proceedings of the First Annual Workshop of the HORIZON 2020 CEBAMA Project. KIT-SR 7734, Karlsruhe, Germany. www.cebama.eu

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**** Corresponding author e-mail: andres.idiart@amphos21.com***

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