FE² Multiscale Modelling of Chloride Ions Transport in Recycled Aggregates Concrete

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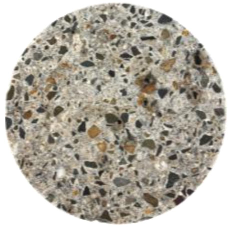
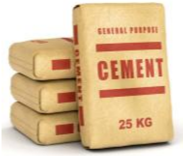
Context



Concrete
(2400kg/m³)

Water
(150kg/m³)



Cement
(300kg/m³)

Sand
(650kg/m³)

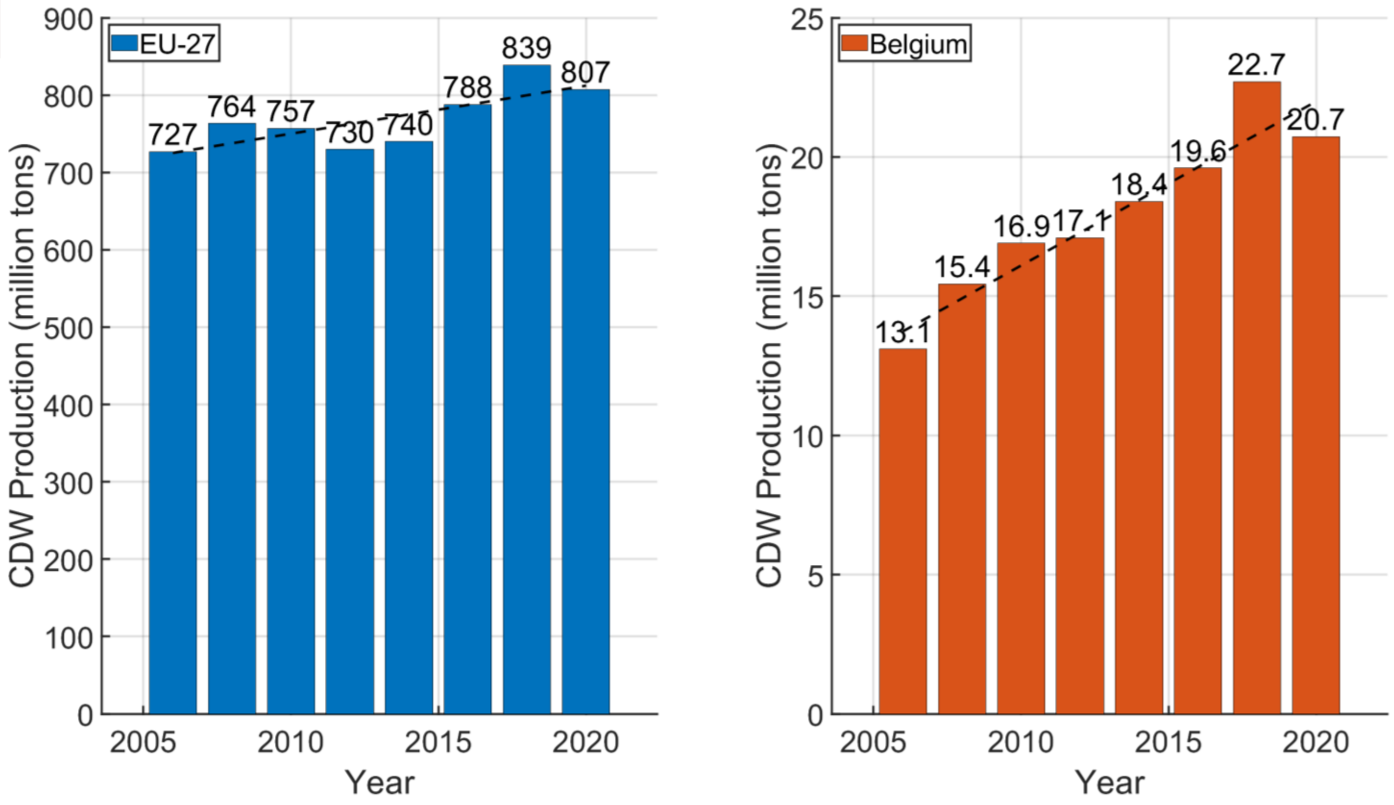
Aggregates
(1300kg/m³)
50% vol.

- Natural Aggregates (NA)
- Industrial Aggregates
- Recycled Aggregates (RCA)

- 1.2 billion tons of concrete produced in 2019 in the EU-27 [CEMBUREAU,2021] vs. 0.16 billions tons of steel in 2018 [EUROFER,2019]
- 2.55 billion tons of NA extracted in 2019 in the EU-27 [UEPG,2021]
- 327 million tons of recycled and reused aggregates in 2019 in the EU-27, 21% of vol. in Belgium [UEPG,2020]

Context

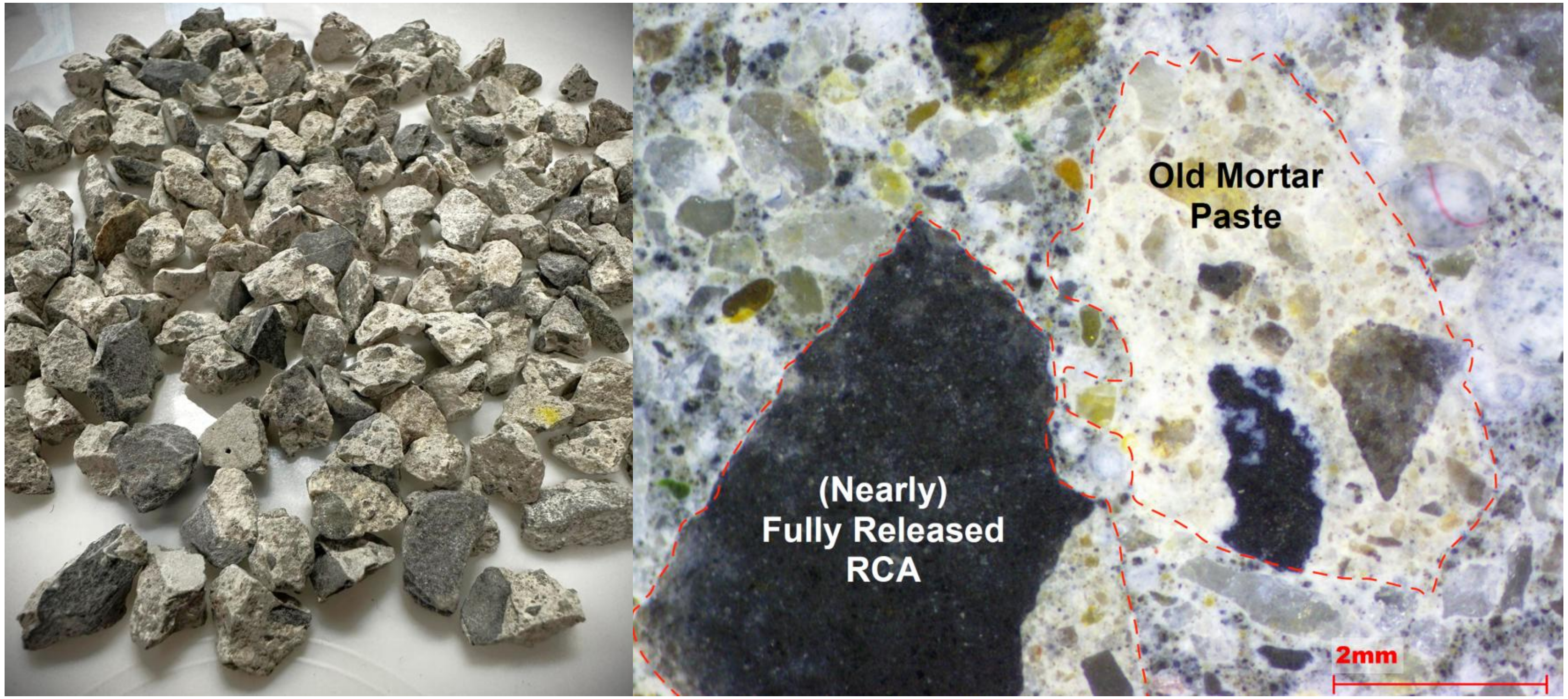
Generation of Construction and Demolition Waste (CDW) [EUROSTAT,2023]



- 807 million tons of CDW generated in 2020 in the EU-27, 20.7 million for Belgium [EUROSTAT,2023]
- CDW are heterogeneous and contain concrete, brick, glass, wood and gypsum
- Concrete makes up between 32% and 75% of CDW volume [Meyer,2008,Zhao et al., 2020]

Context

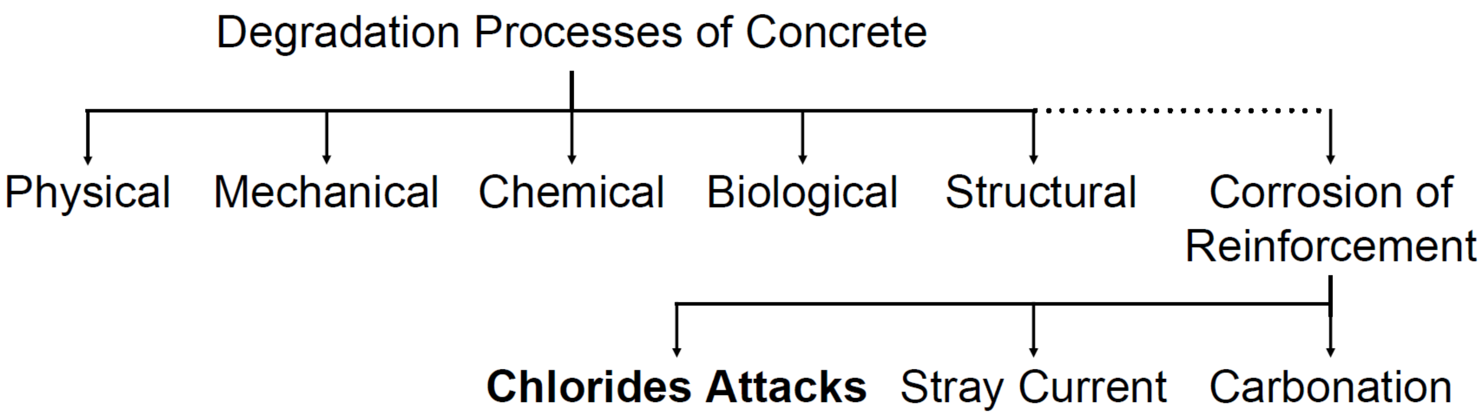
- EU Waste Framework Directive (2008/98/EC) Article 11(2)(b): members of the EU must take appropriate actions to ensure that **70% of non-hazardous CDW** are prepared for **re-use, recycling and other material recovery** (…) using waste as a substitute for other materials, by 2020 [EU, 2008]
- Recycled Concrete Aggregates (RCA) are being studied as a replacement for Natural Aggregates (NA) in new concrete materials.



Context

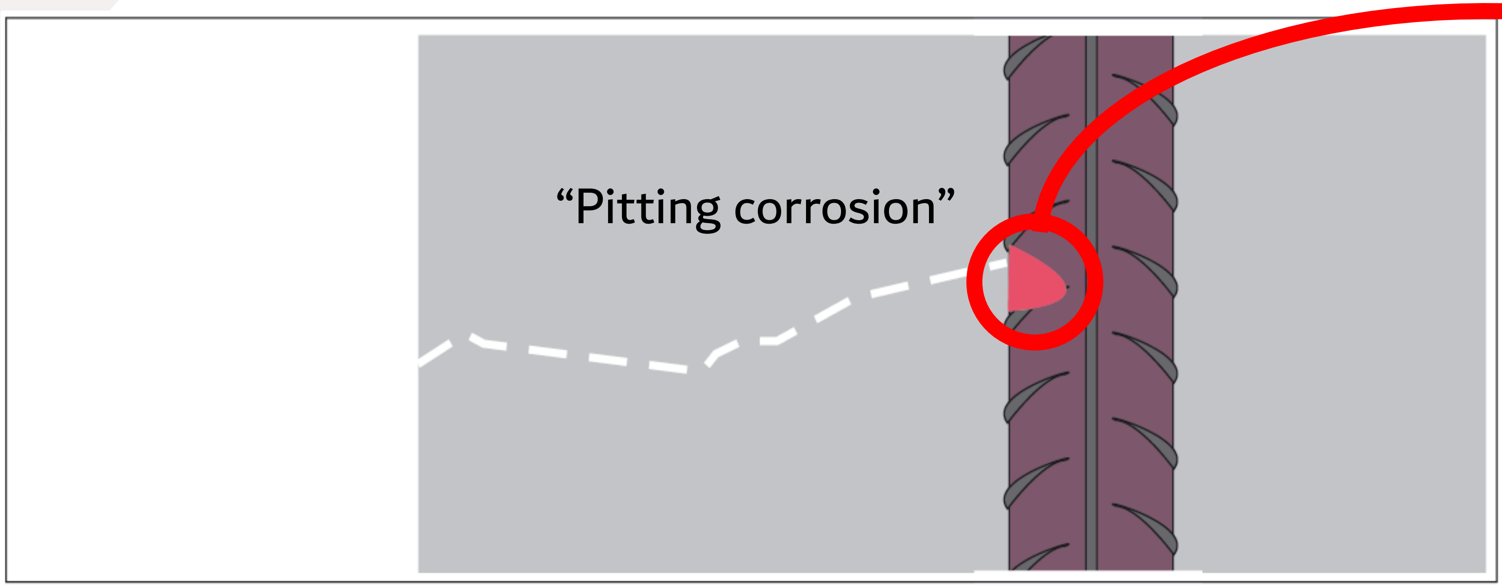
RCA are said to decrease the durability of concrete due to their adherent mortar content. [Debieb et al., 2010]

The **durability** of concrete refers to its ability to **withstand external aggressive agents** over an extended period **without compromising** its intended performance.

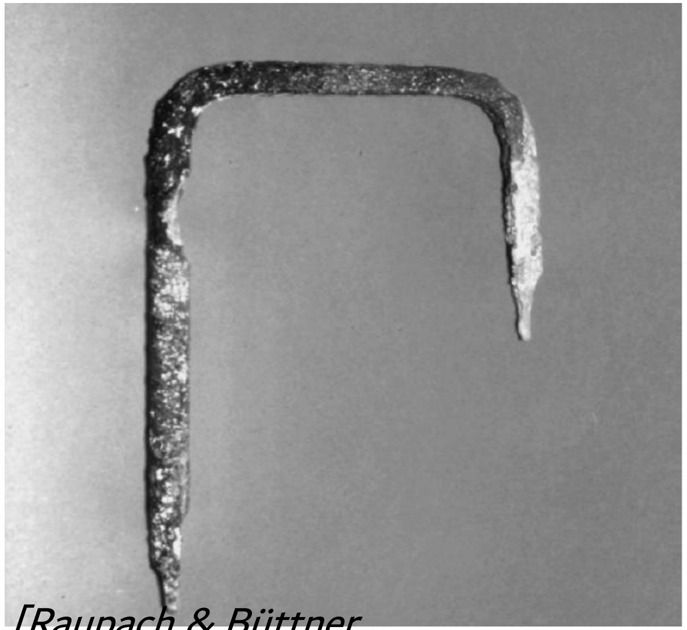


Context

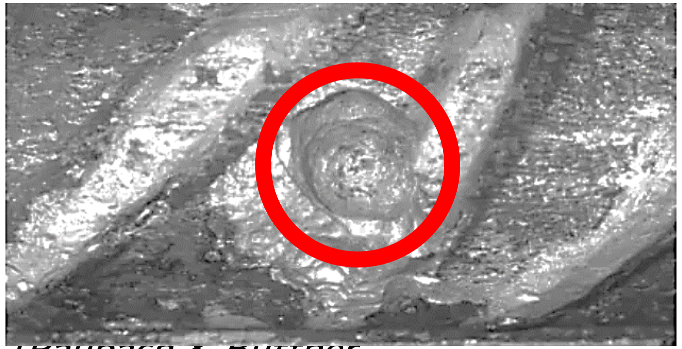
- Chloride attacks is one of the main cause of degradation near roads or coastal areas.



[Ployaert, 2008]



[Raupach & Büttner, 2014]



[Raupach & Büttner, 2014]

Context

“ How does the incorporation of Recycled Concrete Aggregates affect the durability of concrete in terms of chloride attacks? ”

- Experimental approach:
  - Concrete made from 100% NA or RCA produced in the laboratory, as well as a mortar and a cement pastes;
  - Several experiments are performed to obtain intrinsic properties of water and chloride ions transfer.
- Numerical approach:
  - Development of a multi-scale multi-physics model using the Finite Element Square (FE^2) method;
  - Advection and diffusion of chloride ions in both saturated and unsaturated conditions;
  - Validated analytically, experimentally, numerically;
  - Simulation of an application with realistic conditions.

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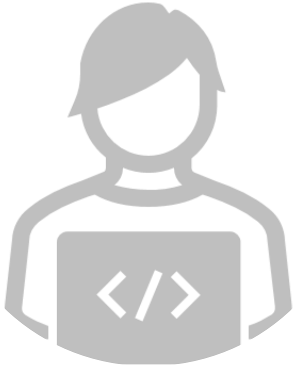
Context

What are Recycled Concrete Aggregates and how do they impact chloride ingress in concrete?

Experimental Approach

Results of the experimental campaign on our materials.



Numerical Approach

Development of the FE² model and results of the performed simulations.

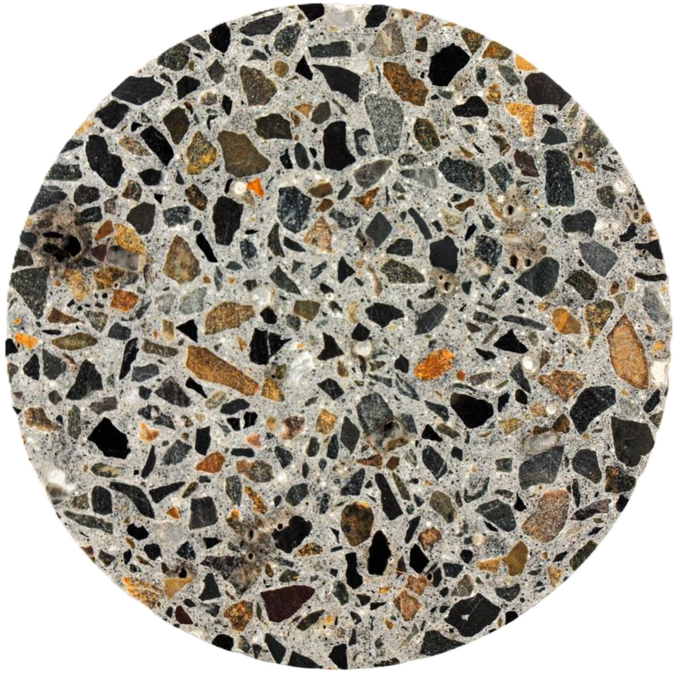
Conclusion

Conclusions of this work and perspectives for future research.

Experimental Compositions

1. NAC: A micro-concrete comprising 2/8 natural aggregates of limestone origin;
2. RAC: A micro-concrete comprising 2/8 recycled concrete aggregates (from SeRaMCo) (same PSD and volume fraction than NAC);
3. E-M: A mortar composed of natural 0/2 Rhine sand with C.E.M. method;
4. E-CP: A plain cement paste made of CEM I 42.5N with C.E.M. method.

Constant effective W/C



Experimental plan

- Water transfer properties
  - Water Absorption by Immersion (WAI)
  - Intrinsic Water Permeability experiment
  - Static Sorption and Desorption experiment
- Chloride ions transfer properties
  - Chloride diffusion under steady-state
  - Chloride diffusion under unsteady-state

Experimental plan

- Water transfer properties
  - Water Absorption by Immersion (WAI)
  - Intrinsic Water Permeability experiment
  - **Static Sorption and Desorption experiment**
    - Water retention curves
    - Vapour control method
    - 100x100x10mm square plates.

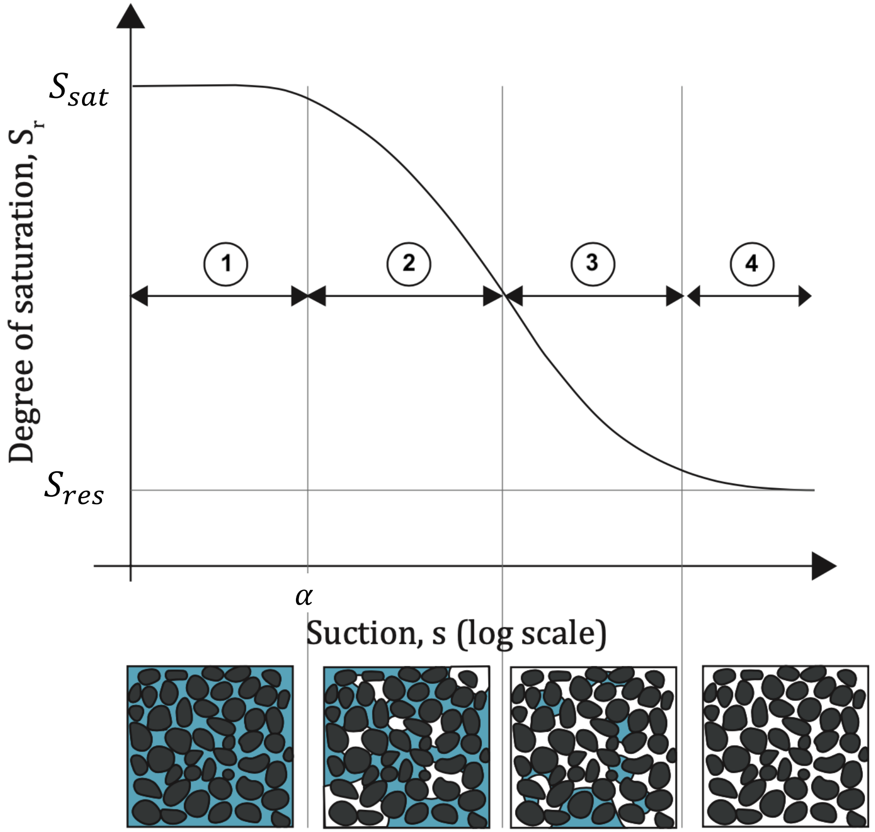
Figure 4.3: Left: Chambers used for the static sorption and desorption experiment, with the RH and temperature probe and the samples inside. Right: sensor housing displaying the measures for the four probes used.

Chamber id.	Saline solution	Target RH [%]	Target suction [MPa]
1 and 1'	KCl	90	-14.3
2 and 2'	$NaCl$	75	-39.1
3 and 3'	$Ca(NO_3)_2$	56	-78.7
4 and 4'	$MgCl_2$	35	-142.5
5 and 5'	Silica salt	0	∞

Table 4.4: Saline solutions used for the static sorption and desorption experiments.

Static Sorption and Desorption

- The suction is related to the amount of water (water content or degree of saturation) stored in a porous medium by the water retention curves.



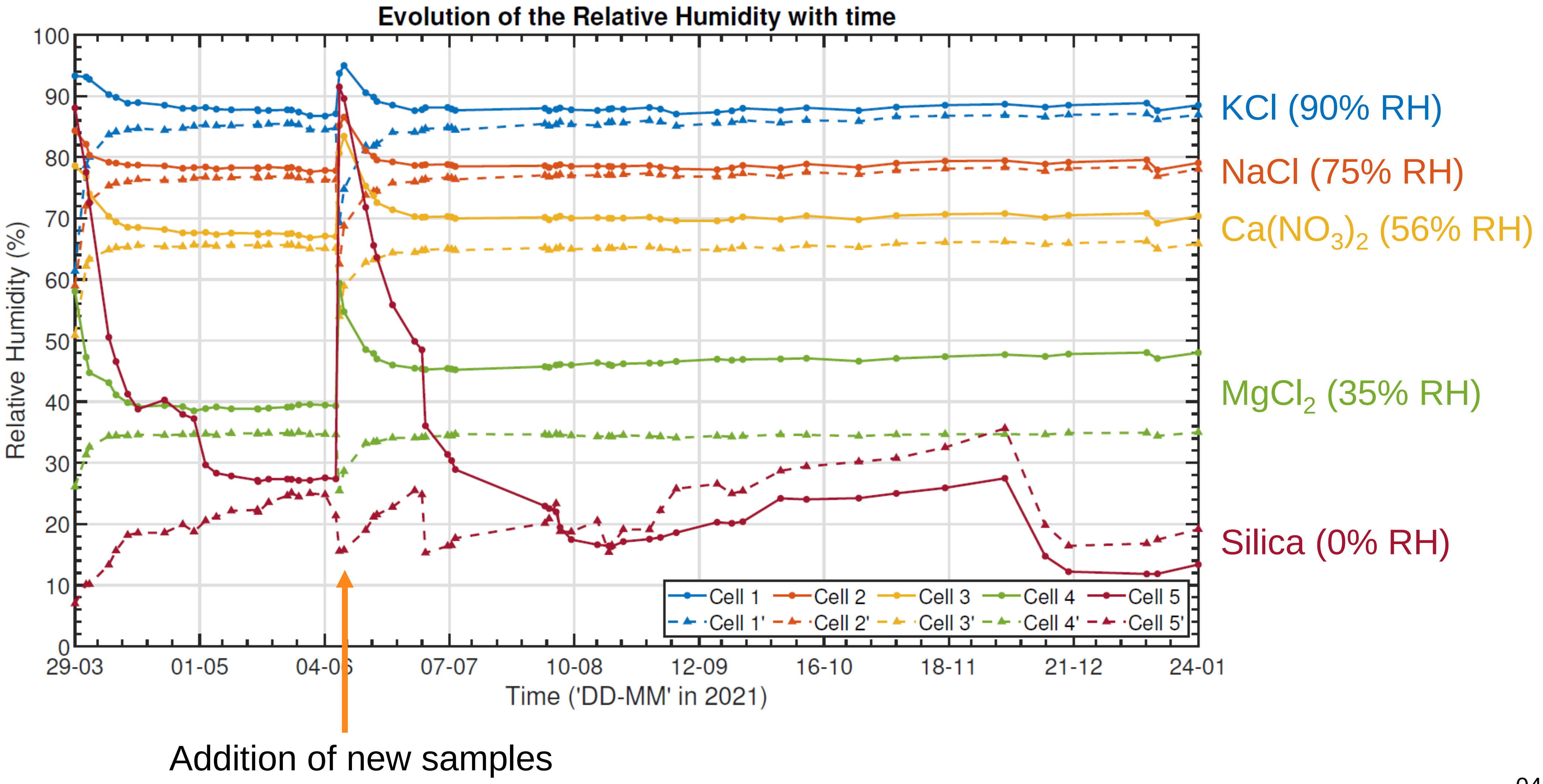
- Suction (Kelvin's law):

$$s = \frac{\rho_w RT}{M} \ln(RH)$$

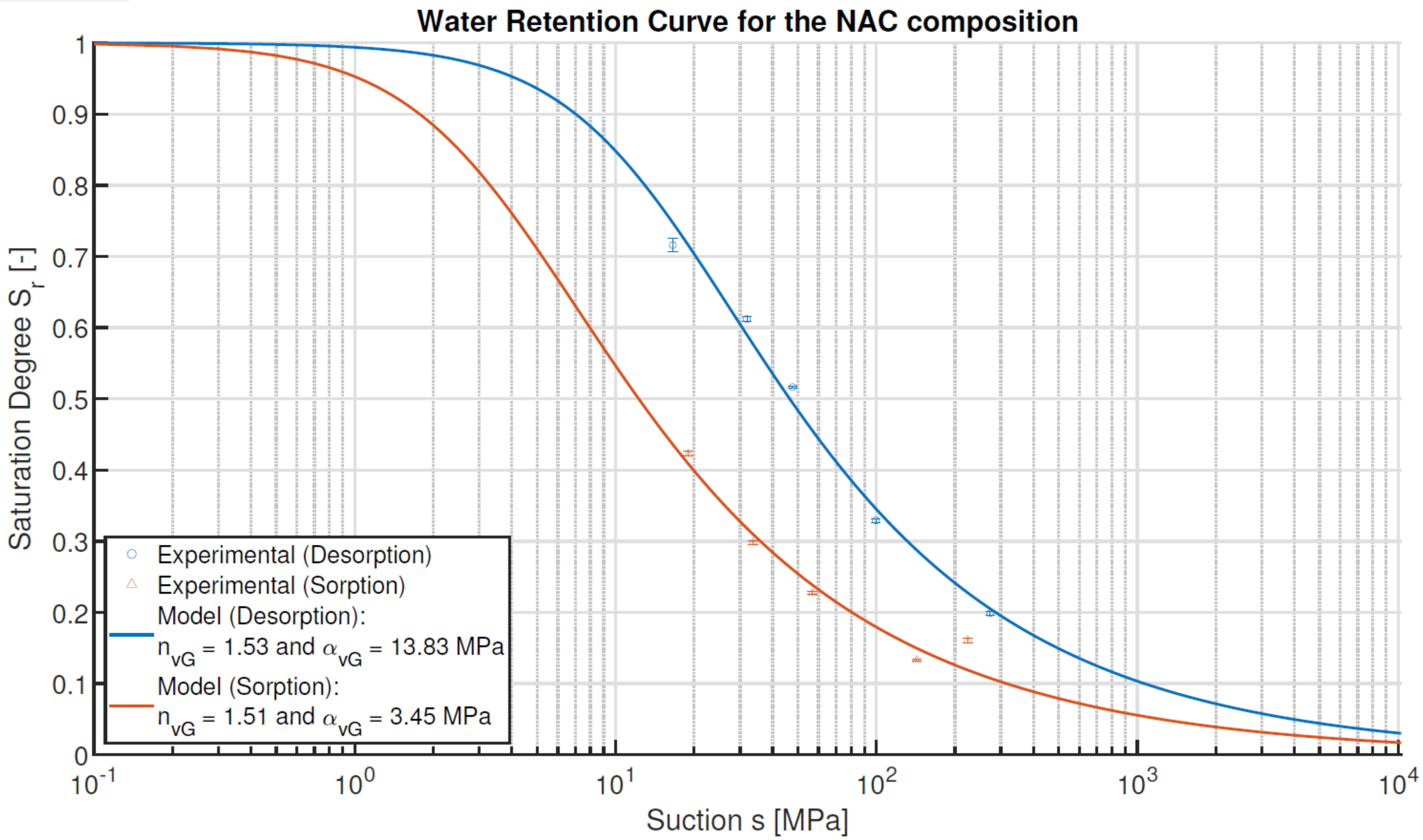
- Saturation degree (Van Genuchten model):

$$S_r = S_{res} + (S_{sat} - S_{res}) \left(1 + \left(\frac{s}{\alpha}\right)^n\right)^{-m} \text{ with } m = 1 - \frac{1}{n}$$

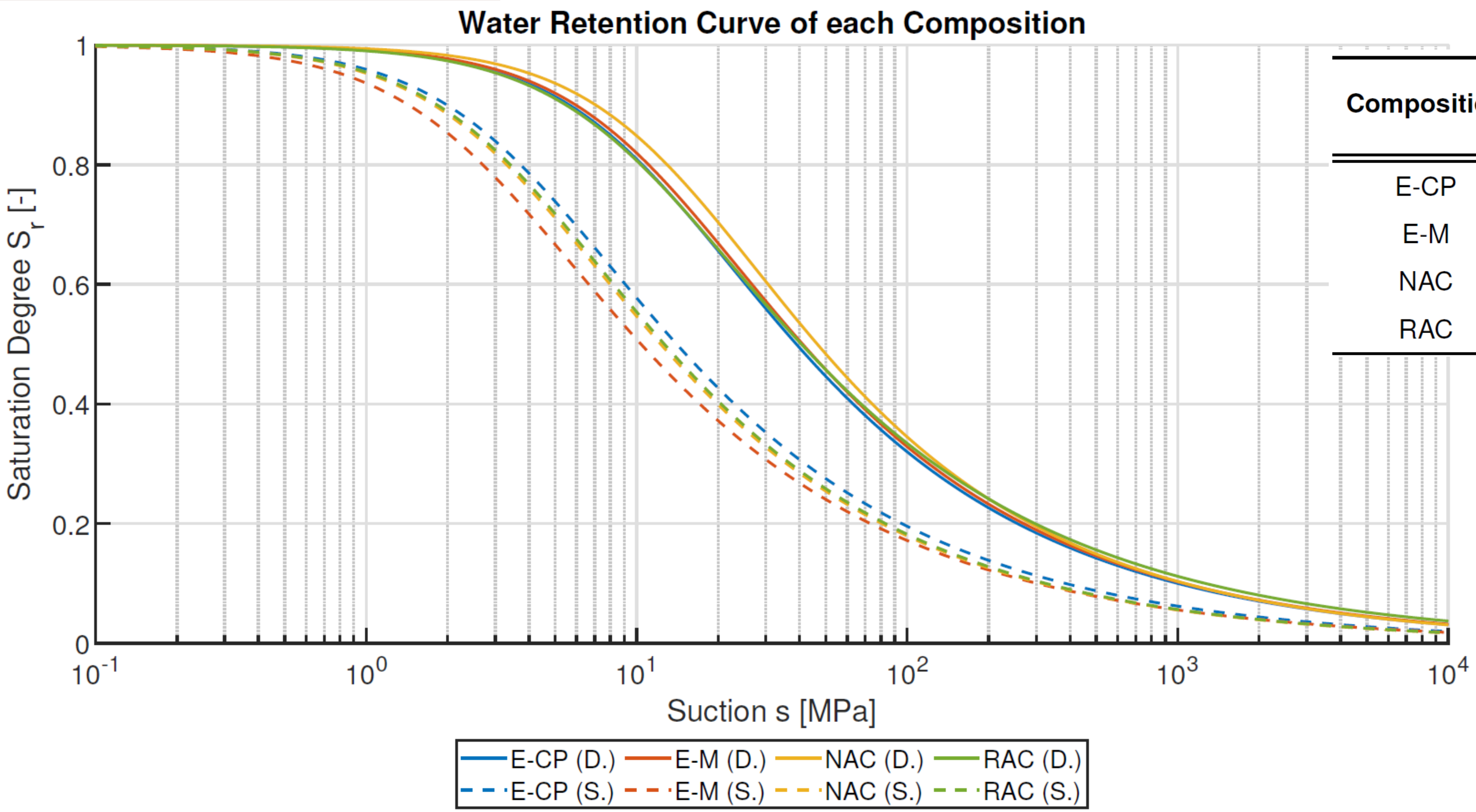
Static Sorption and Desorption



Static Sorption and Desorption



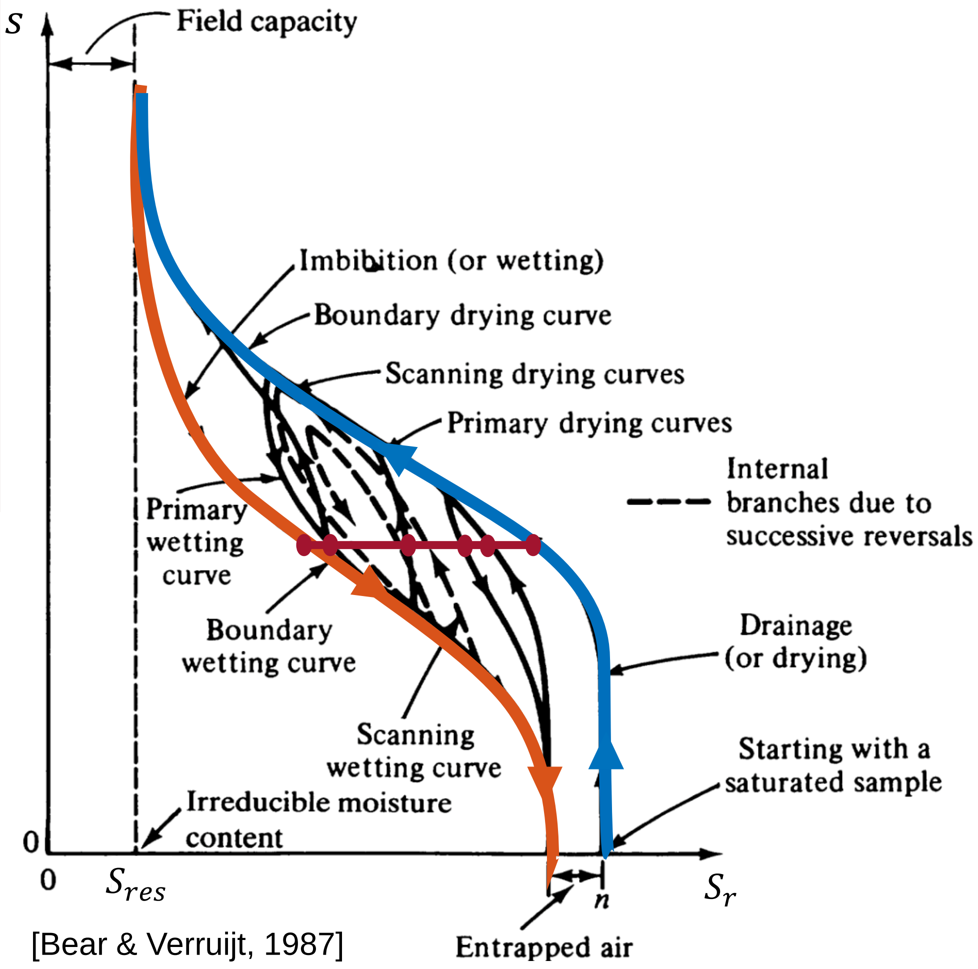
Static Sorption and Desorption



Composition	Desorption		Sorption	
	n_{vG} [-]	α_{vG} [MPa]	n_{vG} [-]	α_{vG} [MPa]
E-CP	1.51	10.95	1.50	3.84
E-M	1.51	11.55	1.49	2.75
NAC	1.53	13.83	1.51	3.45
RAC	1.48	10.43	1.51	3.56

- The greater (smaller) the air-entry pressure in drying, the smaller (bigger) the maximum pore size;
- The greater (smaller) the air-entry pressure in wetting, the smaller (bigger) the minimum pore size.

Static Sorption and Desorption



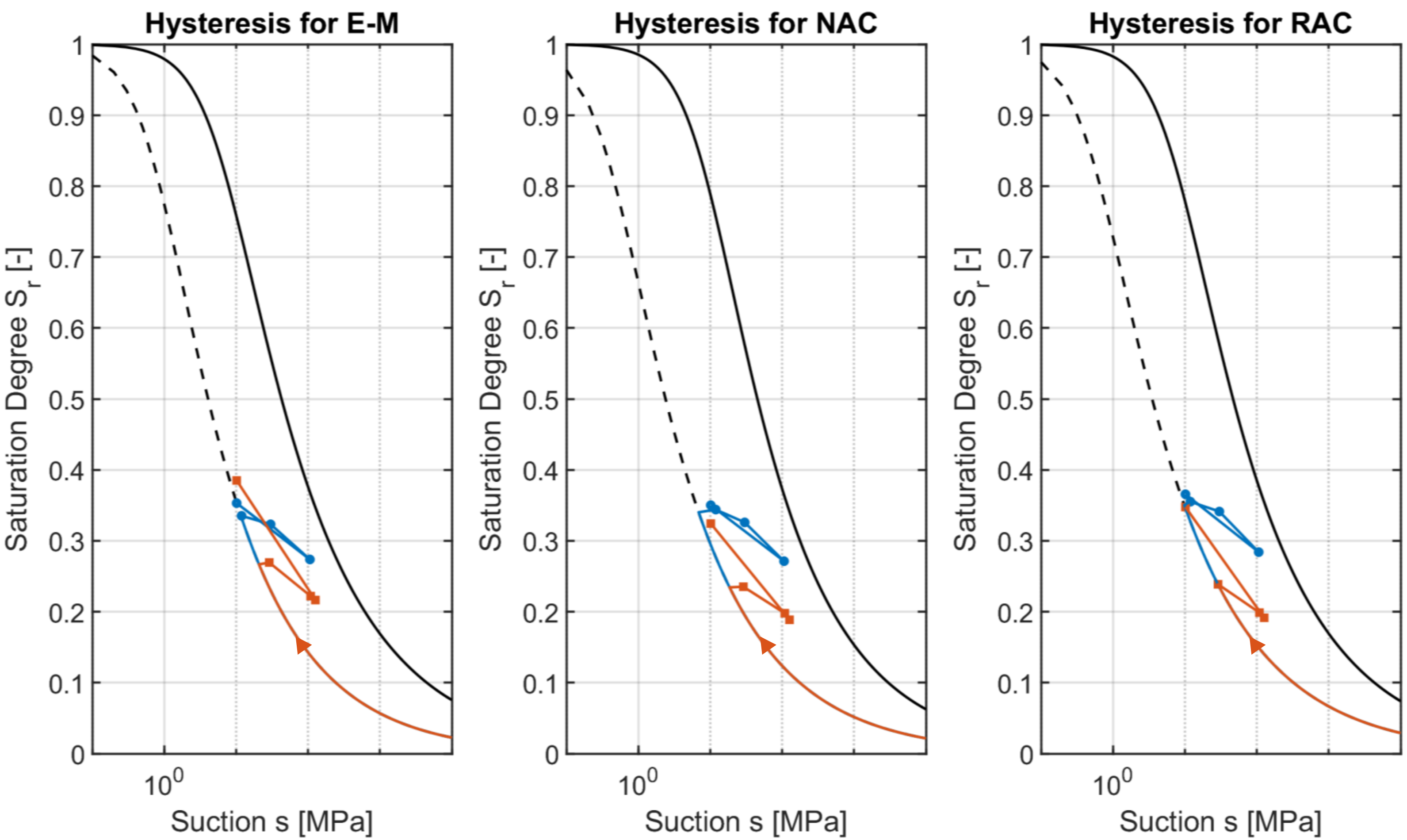
[Bear & Verruijt, 1987]

Causes of the hysteresis:

- Ink-bottle effect (water reentering narrow channels)
- Raindrop effect (different contact angles)
- Entrapped air

Starting RH	Chamber 1	Chamber 2	Chamber 3	Chamber 4
0%	91.60%	80.30%	45.74%	92.78%
0%	80.84%	45.31%	39.37%	92.78%

Static Sorption and Desorption



Starting RH	Chamber 1	Chamber 2	Chamber 3	Chamber 4
0%	91.60%	80.30%	45.74%	92.78%
0%	80.84%	45.31%	39.37%	92.78%

Experimental plan

- Chloride ions transfer properties
  - Chloride diffusion under steady-state
  - **Chloride diffusion under unsteady-state**
    - Apparent diffusion coefficient
    - NBN EN 12390-11
    - 80x50mm cylinders

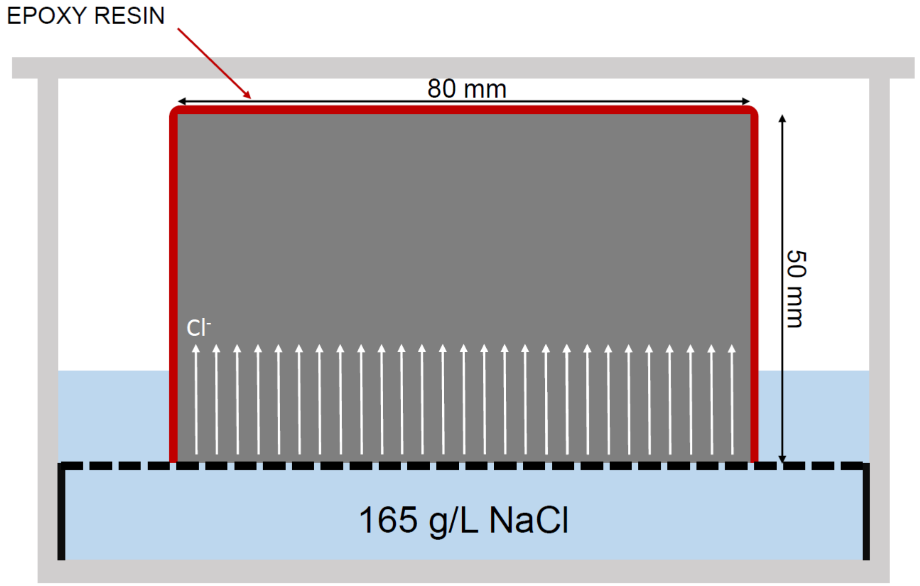
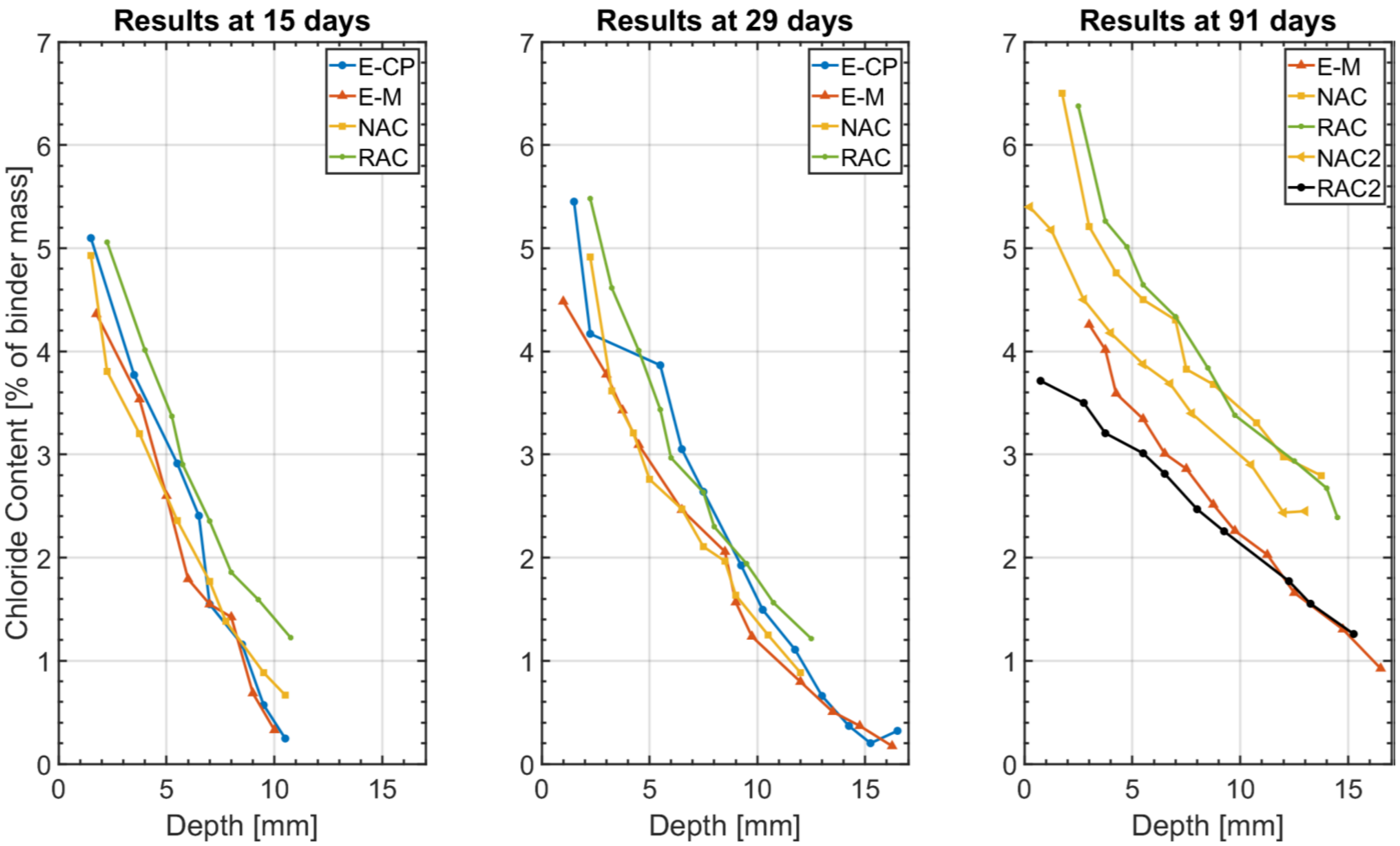


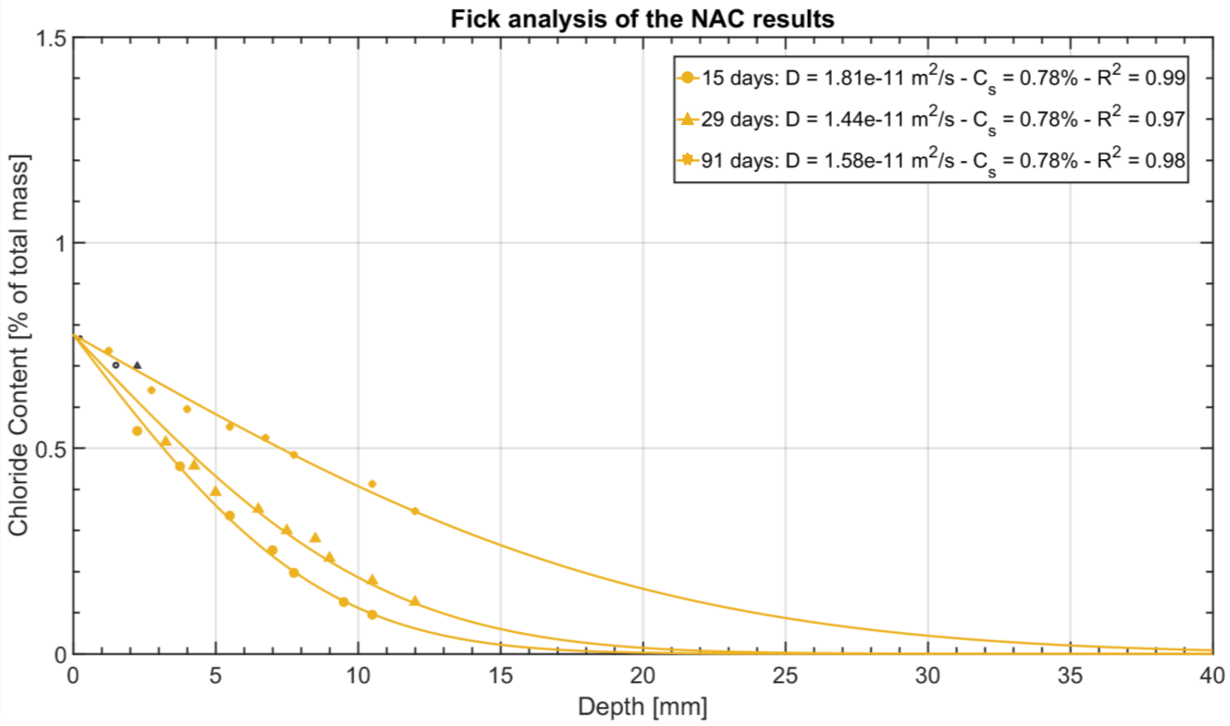
Figure 4.5: Experimental system for the diffusion under unsteady-state.

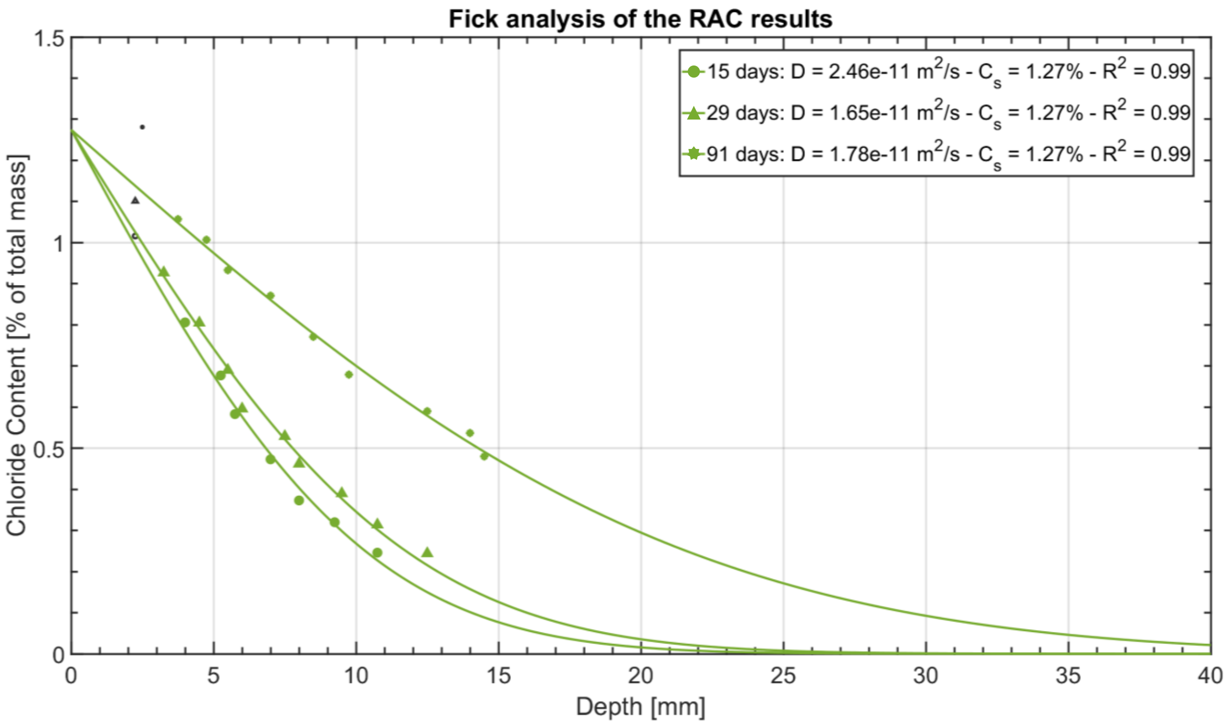
Diffusion under Unsteady-State



- E-CP has the greater chloride content;
- When expressed in term of binder mass, all compositions regroup in a spindle.

Diffusion under Unsteady-State





$$C(x,t) = C_s\left(1-\mathrm{erf}\left(\frac{x}{2\sqrt{D_{app}t}}\right)\right) \quad \text{with} \quad C_s[\%] = C_{sol}\ [\mathrm{g/L\ Cl^-}]\ \frac{n\ [\%\ \mathrm{volume}]}{\rho_d\ [\mathrm{kg/m^3}]}$$

- Fick's second law solution fits nicely the experimental results;
- At constant surface concentration, the diffusion coefficient remains relatively constant with time;
- RAC is more diffusive than NAC.

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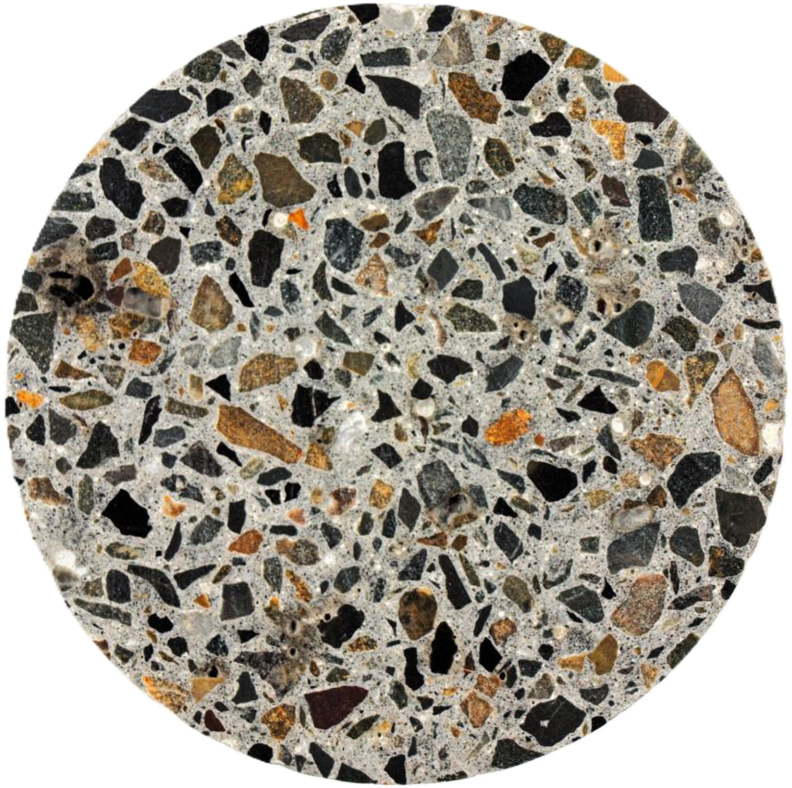
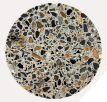


- Concrete is highly heterogeneous due to its components;
- RCA add heterogeneity.

Numerical Approach

- Multiscale modelling allows to account for (partial) heterogeneity while keeping the cost acceptable:

  - Macroscale: homogeneous material using the mixture theory [Bowen, 1980] to introduce multiple phases in the same porous medium.



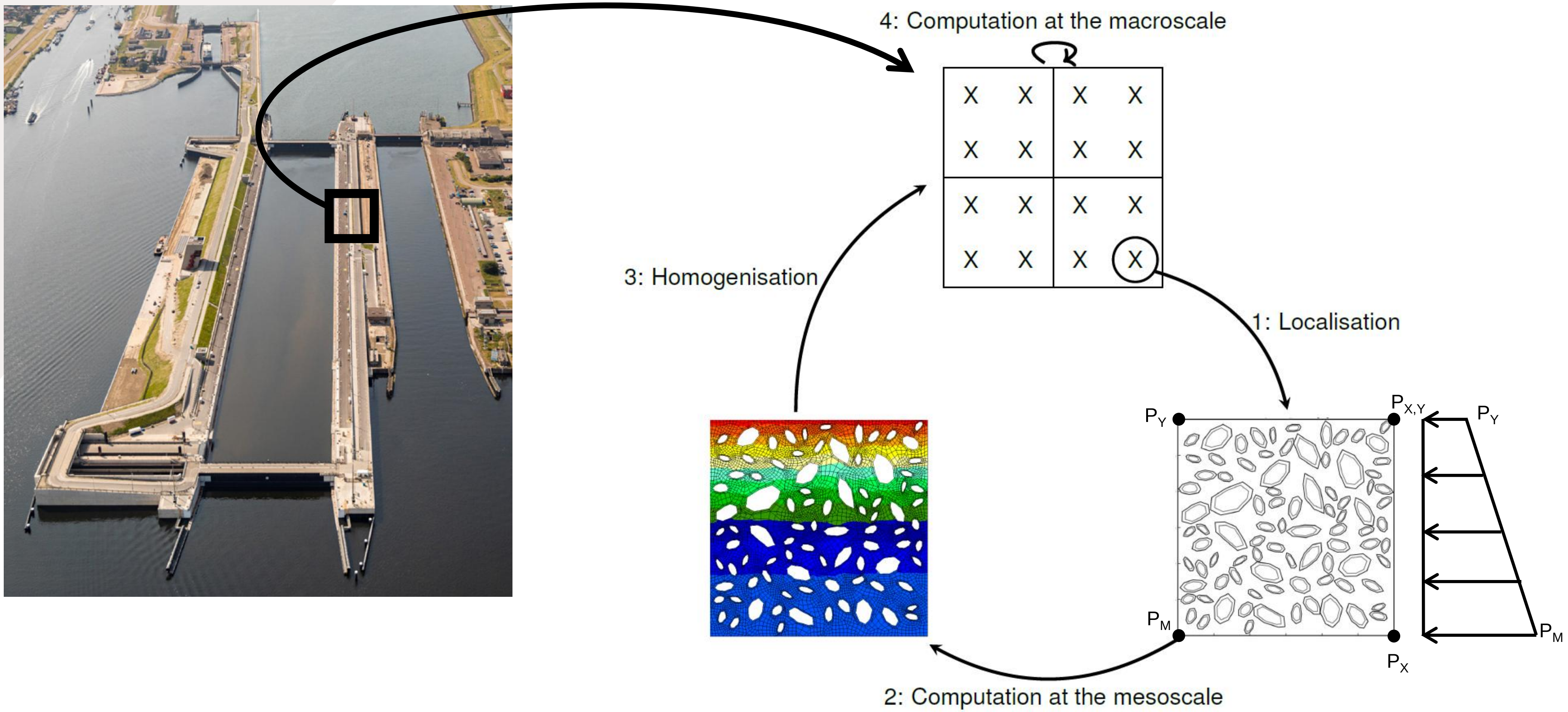
  - Mesoscale: heterogeneities are modelled, and each constituent has its own set of constitutive equations and intrinsic properties.

- Homogenisation is necessary to go from one scale to the other: numerical homogenisation (unit cell method) is implemented, based on the concept of Representative Volume Element (RVE) [Smit et al., 1998].

- FE² (= FEM-FEM) method for engineering structures and liquid/gas/chloride flows.

- Implemented in Lagamine, a FE software from the University of Liège.

Numerical Approach



Numerical Approach

- Introduction to Multiscale Modelling;
- **Model Constitutive Laws;**
- Modelling of the RVE;
- Application to a Lock Wall under Realistic Conditions.

Homogenised Macroscale Response

- Macroscale constitutive equations:

$$\frac{\partial}{\partial x_i}\left(\rho_w \times v^w_{i,\text{homogenised}}\right) + \frac{\partial S_w}{\partial t} = 0$$

$$\frac{\partial}{\partial x_i}\left(\rho_g \times v^g_{i,\text{homogenised}}\right) + \frac{\partial S_g}{\partial t} = 0$$

$$\frac{\partial}{\partial x_i}\left(C_M \times v^w_{i,\text{homogenised}} + v^c_{i,\text{homogenised}}\right) + \frac{\partial S_c}{\partial t} = 0$$

Mesoscale Constitutive Laws

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Water

$$\frac{\partial}{\partial x_i}(\rho_w v_i^w) + \cancel{\frac{\partial S_w}{\partial t}} = 0$$

$$\rho_w = \rho_{w0} \times \left(1 + \frac{P_{w,average} - P_{w0}}{\chi_w}\right)$$

$$v_i^w = -\frac{k_{int}\, k_{rel,w}}{\mu_w}\left(\frac{\partial P_w}{\partial x_i} + \rho_w\, g_i\right)$$

$$k_{rel,w} = \sqrt{S_{r,w}} \times \left(1 - \left(1 - S_{r,w}^{1/m}\right)^m\right)^2$$

Gas

$$\frac{\partial}{\partial x_i}(\rho_g v_i^g) + \cancel{\frac{\partial S_g}{\partial t}} = 0$$

$$\rho_g = \rho_{g0} \times \left(\frac{P_{g,average}}{P_{g0}}\right)$$

$$v_i^g = -\frac{k_{int}\, k_{rel,g}}{\mu_g}\left(\frac{\partial P_g}{\partial x_i} + \rho_g\, g_i\right)$$

$$k_{rel,g} = \sqrt{1 - S_{r,w}} \times \left(1 - S_{r,w}^{1/m}\right)^{2m}$$

$$S_{r,w} = S_{res} + (S_{sat} - S_{res})\left(1 + \left(\frac{s}{\alpha}\right)^n\right)^{-m}$$

$$s = P_g - P_w$$

Chlorides

$$\frac{\partial}{\partial x_i}(v_i^c) + \cancel{\frac{\partial S_c}{\partial t}} = 0$$

$$v_i^c = \cancel{v_i^{\text{advection}}} + v_i^{\text{diffusion+dispersion}} = -D\,\frac{\partial C_m}{\partial x_i}$$

Stiffness matrix

$$F_i = K_{i,j} \times P_j$$

- Mesoscale stiffness matrix obtained analytically:

$$K_{i,j} = \frac{\partial \mathrm{Flux}_i}{\partial P_j}$$

- Macroscale stiffness matrix obtained by perturbation:

$$K_{i,j} = \frac{\mathrm{Flux}_{i,\mathrm{perturbated}} - \mathrm{Flux}_{i,\mathrm{original}}}{\mathrm{Perturbation}_j}$$

Water Retention Curves' model

- Concrete is subjected to temperature and relative humidity variations;
- Water content inside concrete is always changing;
- Necessity to implement a hysteresis model for the water retention curve.

Water Retention Curves' model

- Van Genuchten model:

$$S_e = S_{res} + (S_{max} - S_{res}) \left(1 + \left(\frac{s}{\alpha}\right)^n\right)^{-m} \quad \text{with} \quad m = 1 - \frac{1}{n}$$

- Zhou et al. (2012) model:

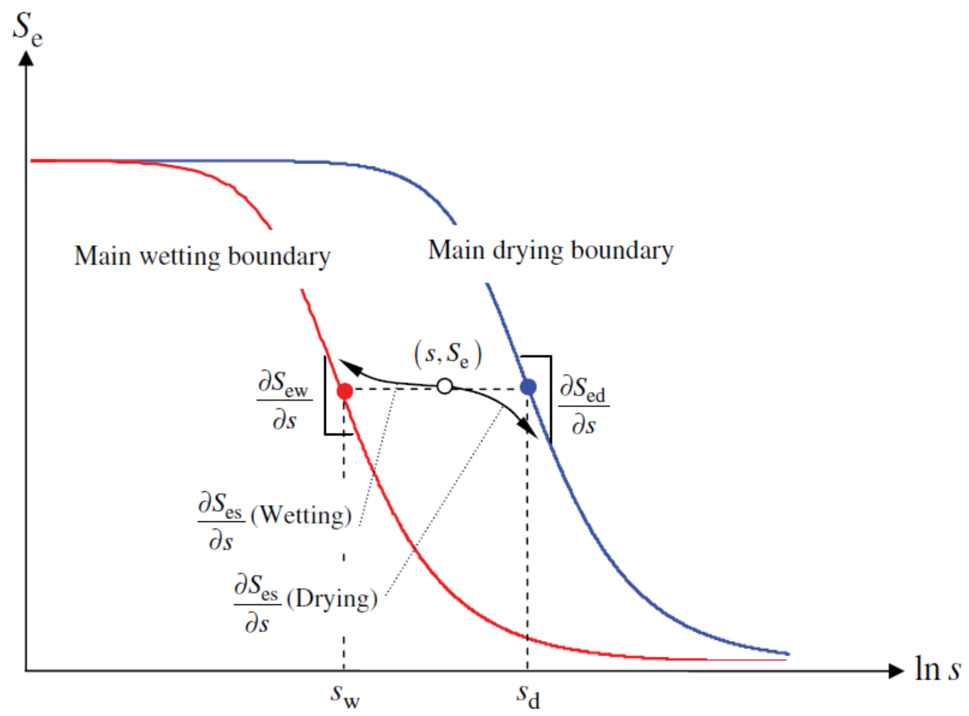
$$S_{ed} = S_{res} + (S_{max} - S_{res}) \left[1 + \left(\frac{s}{\alpha_d}\right)^{n_d}\right]^{-m_d}$$

$$S_{ew} = S_{res} + (S_{max} - S_{res}) \left[1 + \left(\frac{s}{\alpha_w}\right)^{n_w}\right]^{-m_w}$$

$$\frac{\partial S_{ed,s}}{\partial s} = \left(\frac{s_d}{s}\right)^{-b} \left(\frac{\partial S_{ed}}{\partial s}\right) \text{ with } s_d = \alpha_d \left(S_e^{-1/m_d}\right)^{1/n_d}$$

$$\frac{\partial S_{ew,s}}{\partial s} = \left(\frac{s_w}{s}\right)^{b} \left(\frac{\partial S_{ew}}{\partial s}\right) \text{ with } s_w = \alpha_w \left(S_e^{-1/m_w}\right)^{1/n_w}$$

$$S_e^t = S_e^{t-1} + \left(\frac{\partial S_{e,s}}{\partial s}\right) \times ds$$

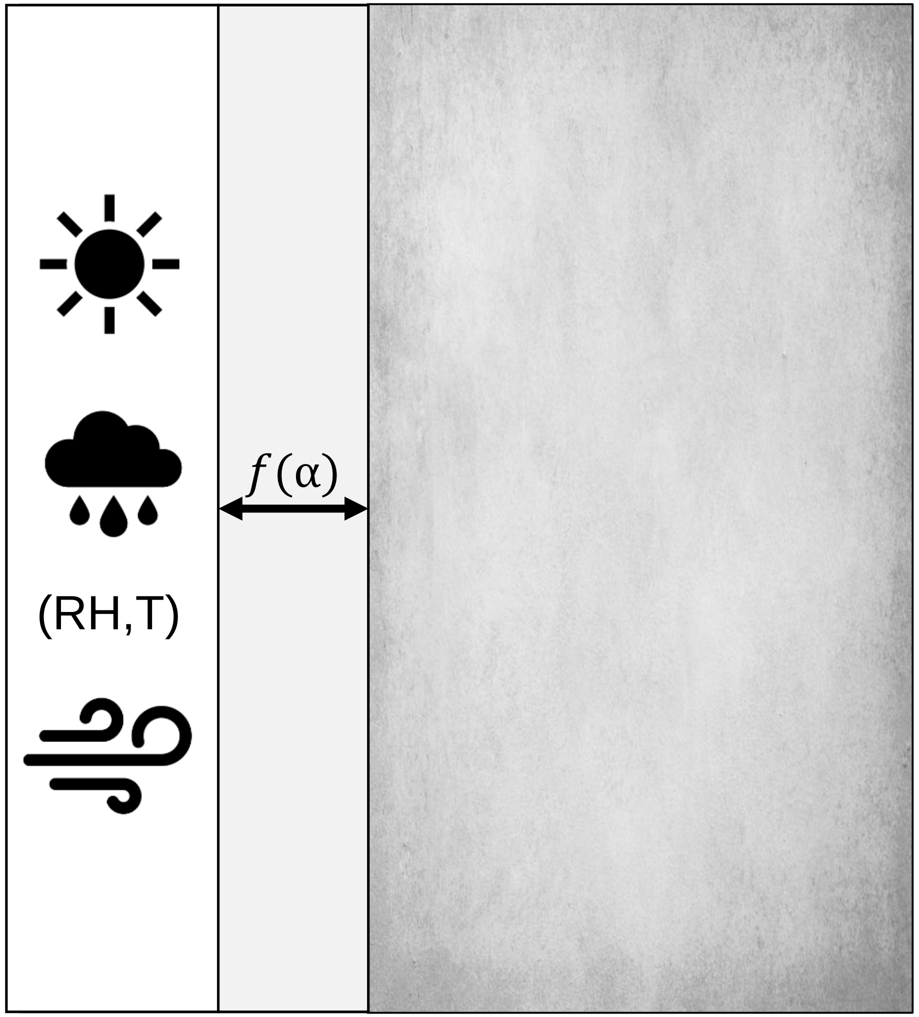


[Zhou et al., 2012]

Boundary Layer Model

- Not a direct equilibrium between concrete and its environment;
- Depends on many parameters such as wind speed, …;
- Exchanges between the concrete and its environment are penalised by a coefficient α.

$$\bar{q} = \alpha_{b.l.m.}(\rho_{v,surf} - \rho_{v,air})$$



Numerical Approach

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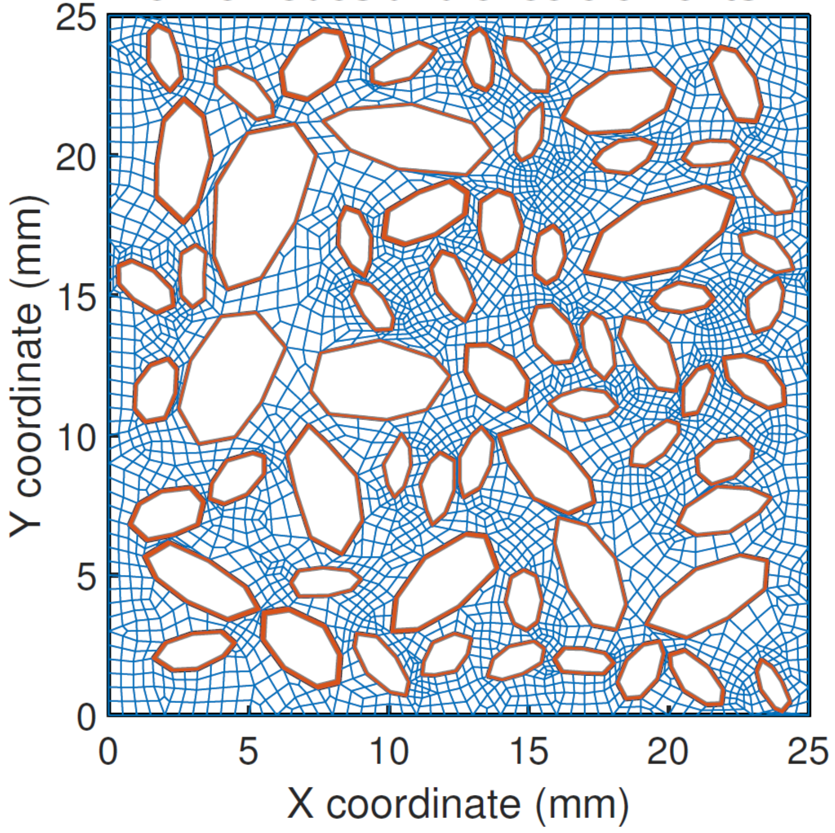
- Introduction to Multiscale Modelling;
- Model Constitutive Laws;
- **Modelling of the RVE;**
- Application to a Lock Wall under Realistic Conditions.

Representative Volume Element

- Maximum packing of octagonal inclusions algorithm:
  - No overlapping of aggregates
  - Random spatial distribution of aggregates
  - Maximised packing density
  - Periodic RVE boundaries

- It requires:
  - Particle Size Distribution of aggregates
  - Surface Fraction of aggregates
  - Aspect Ratio of aggregates
  - Cement content if RCA

Mesh generated by the GMSH software: 5723 nodes and 5188 elements.



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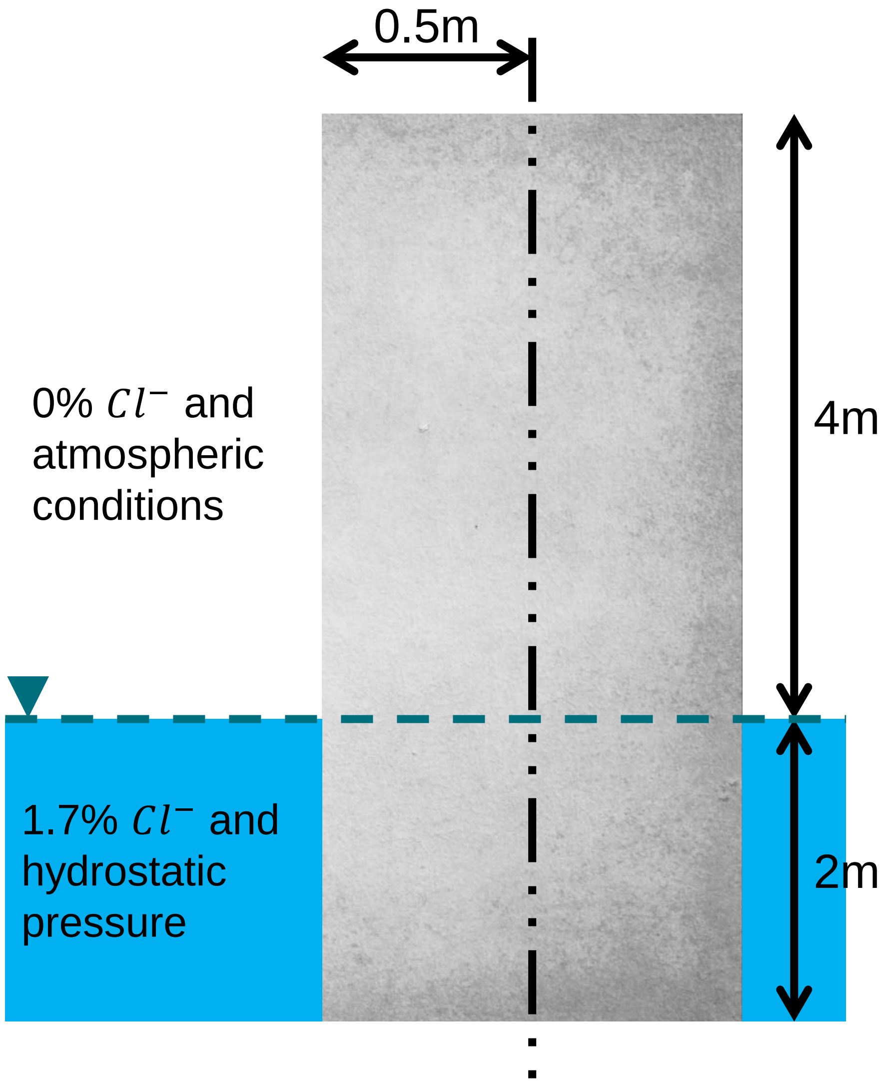
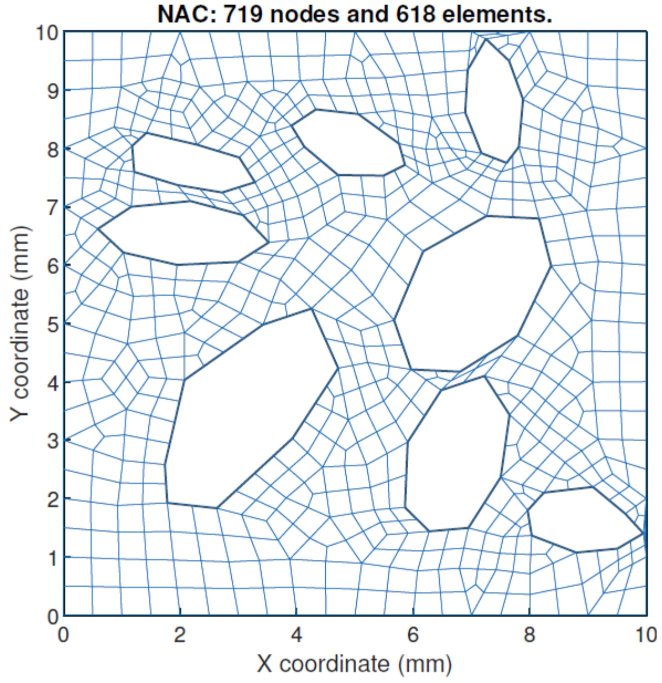
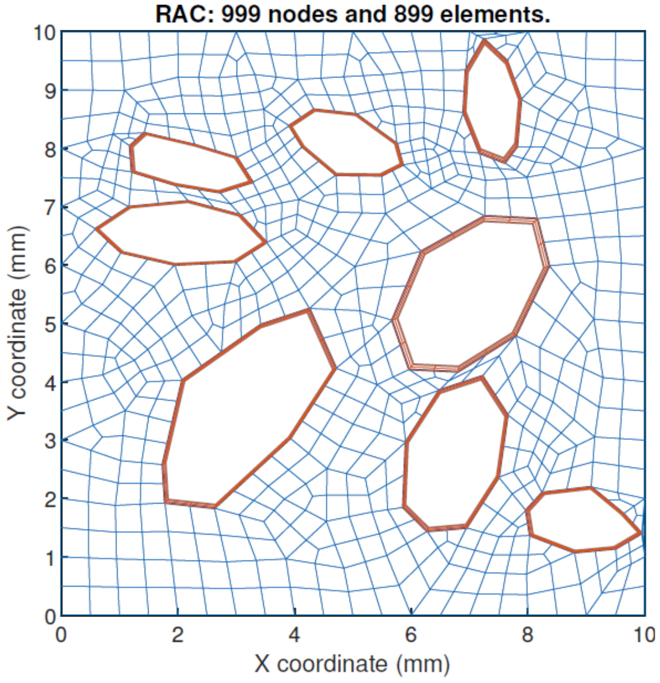
Application under Realistic Conditions

Maritime lock wall



Application under Realistic Conditions

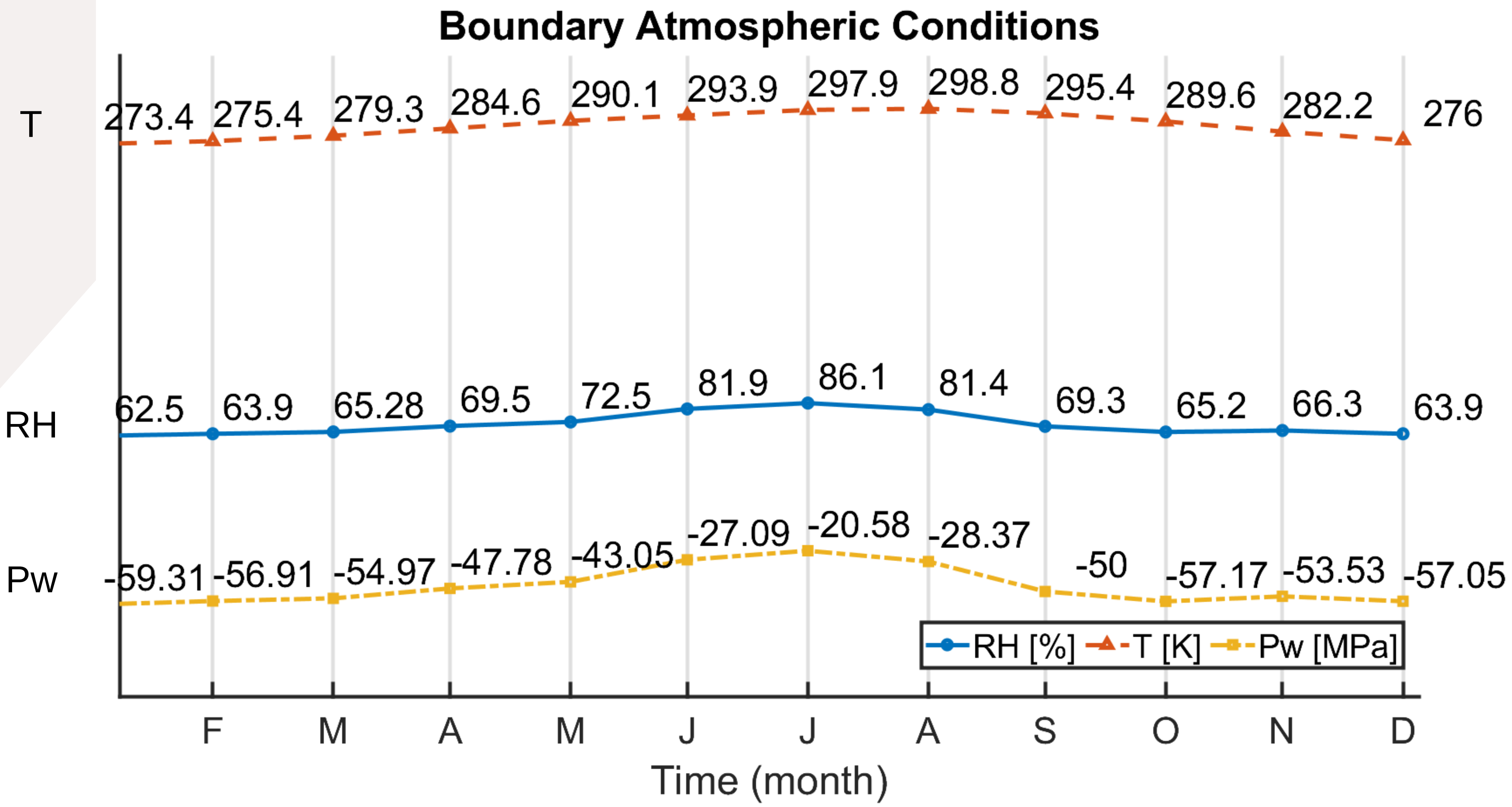




Property	NAC	RAC	Adherent mortar of RCA
Intrinsic Permeability [m^2]	5.02E-18	5.02E-18	5.02E-17
Porosity [% Volume]	29.68	29.68	59.36
Diffusion Coefficient [m^2/s]	1.86E-11	1.86E-11	1.86E-10
n_{VG} Sorption [-]	1.51	1.51	-
α_{VG} Sorption [MPa]	3.45	3.56	-
n_{VG} Desorption [-]	1.53	1.48	-
α_{VG} Desorption [MPa]	13.83	10.43	-
b [-]	1.20	1.20	-
$\alpha_{b.l.m.}$ [m/s]	1.99E-3	1.99E-3	-

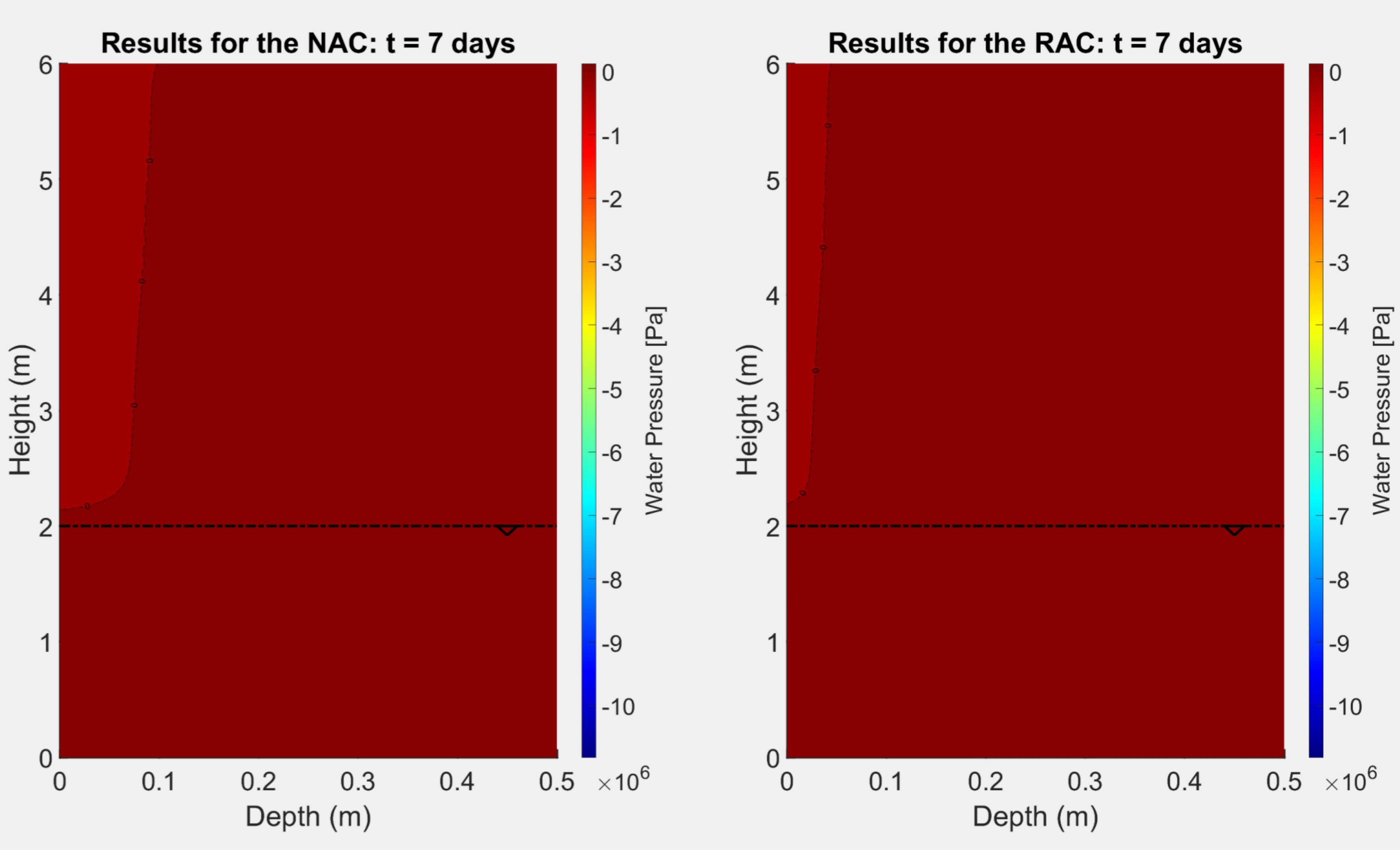
$$C_s[\%] = 17\ [\text{g/L Cl}^-]\ \frac{n\ [\%\ \text{volume}]}{\rho_d\ [\text{kg/m}^3]}$$

Application under Realistic Conditions



$$P_w = P_g - \frac{\rho_w RT}{M} \ln(RH)$$

Application under Realistic Conditions



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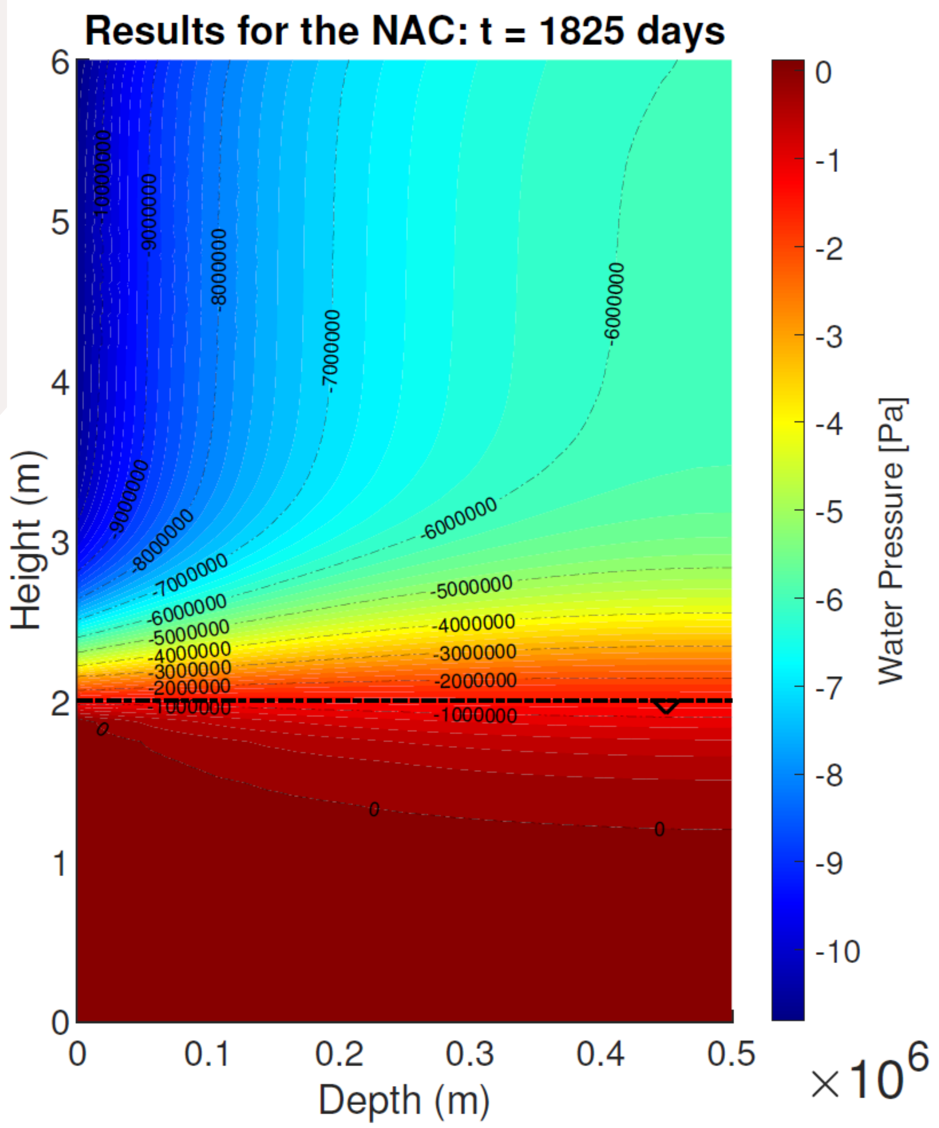

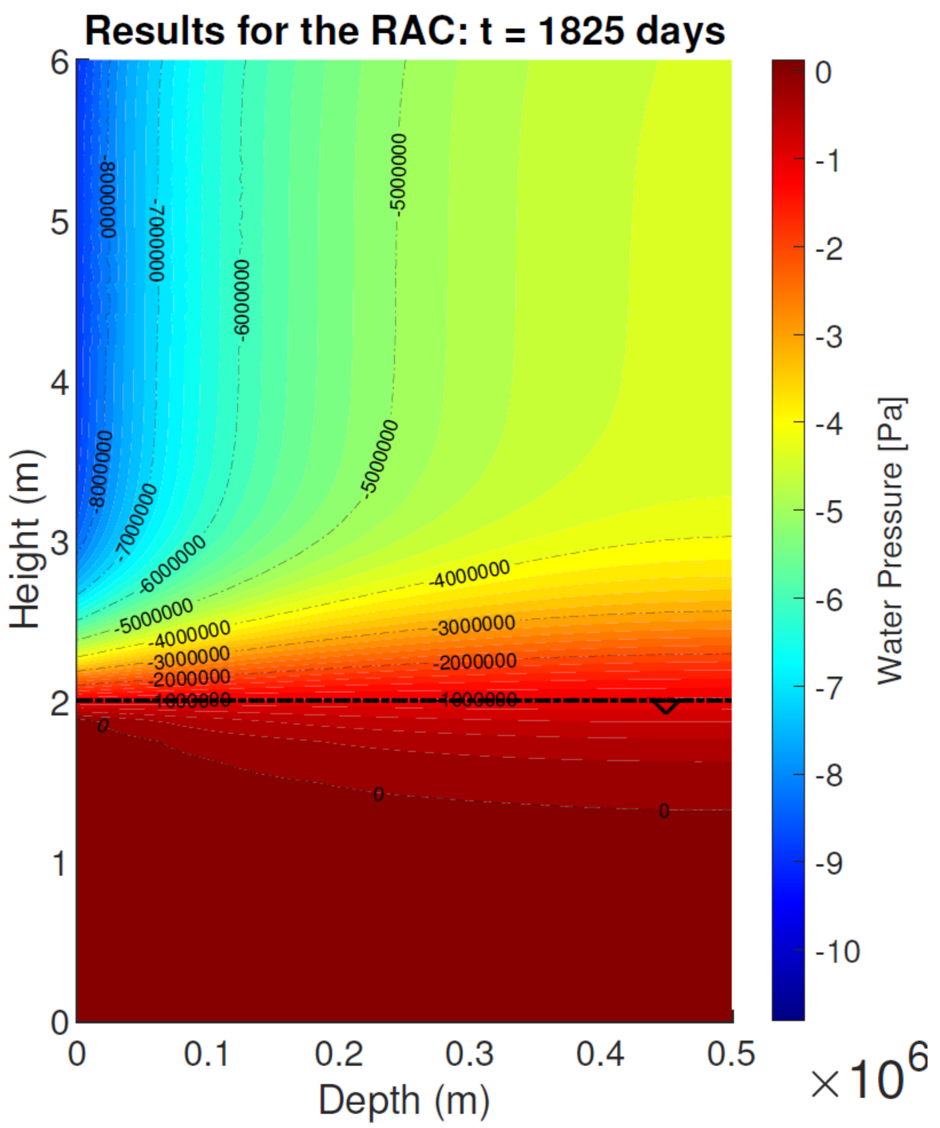

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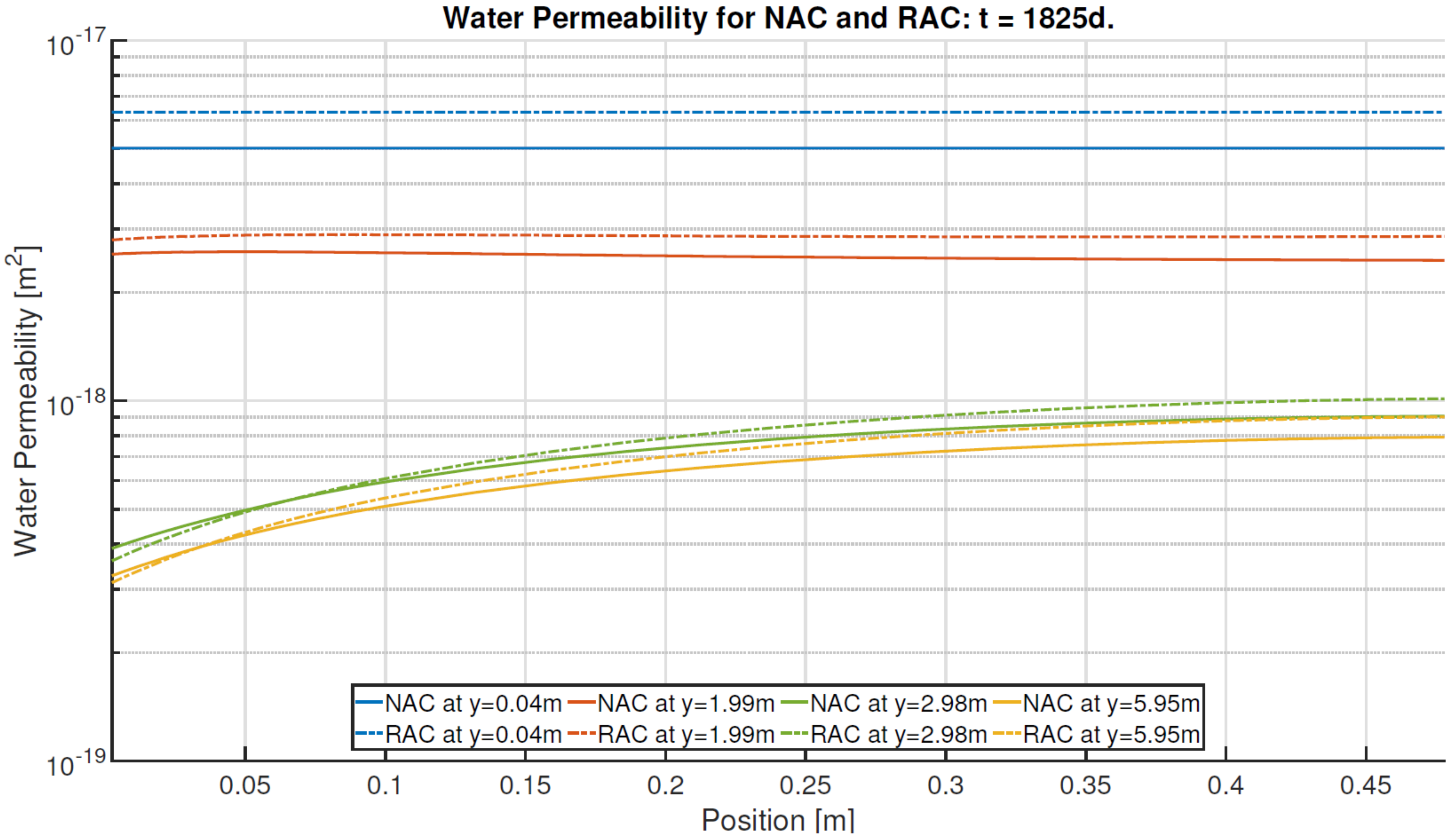

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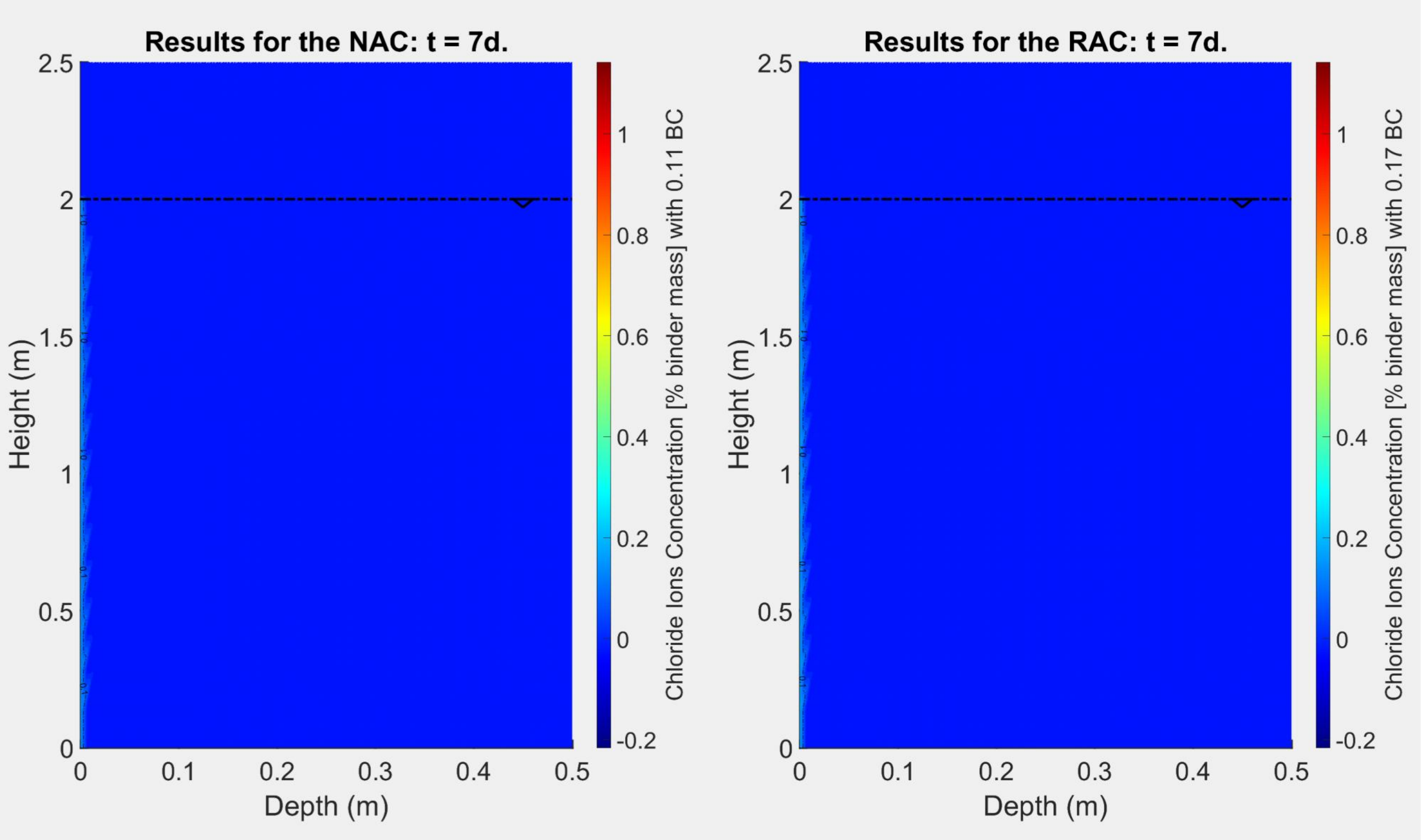

Application under Realistic Conditions

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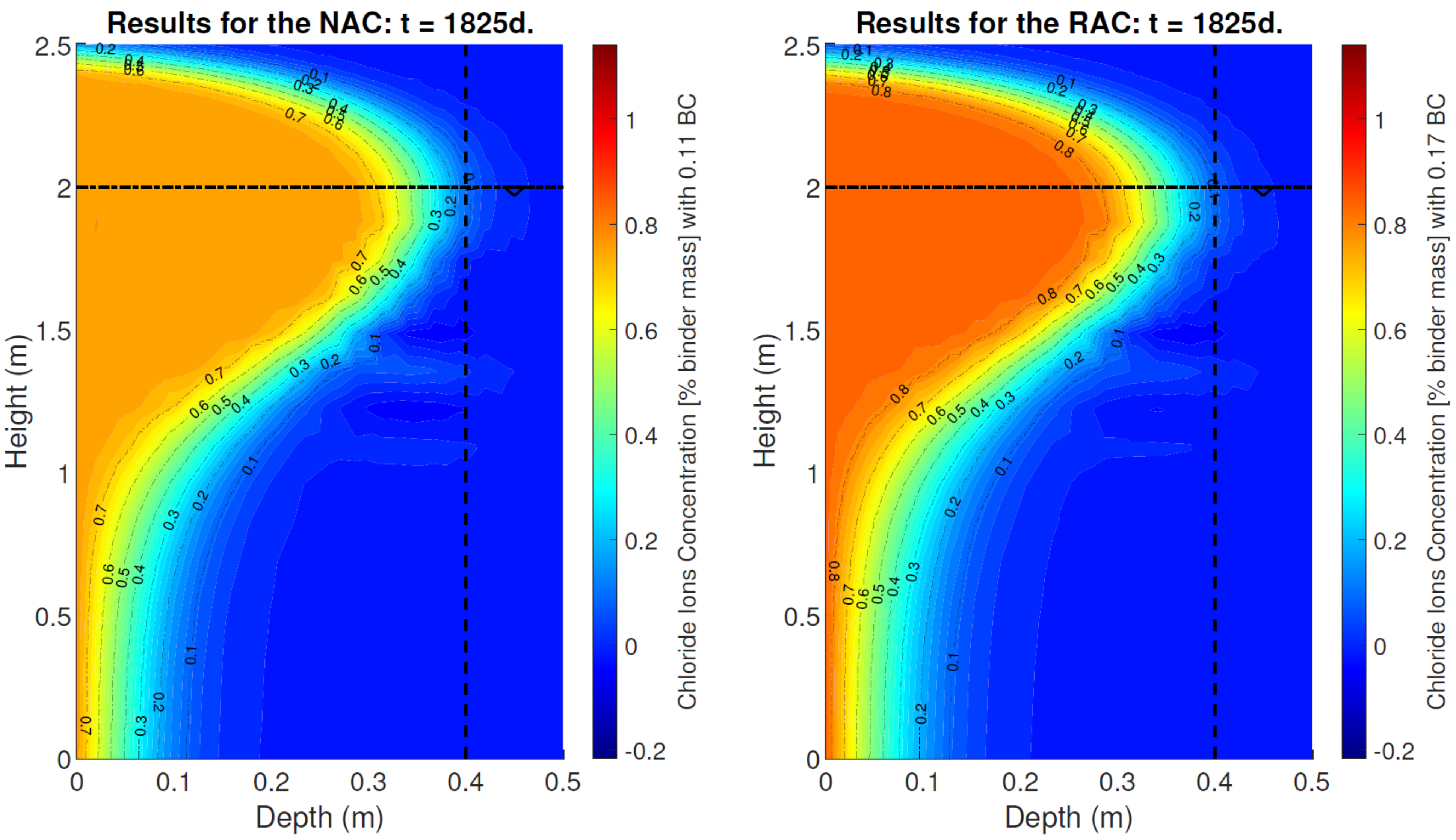

Application under Realistic Conditions

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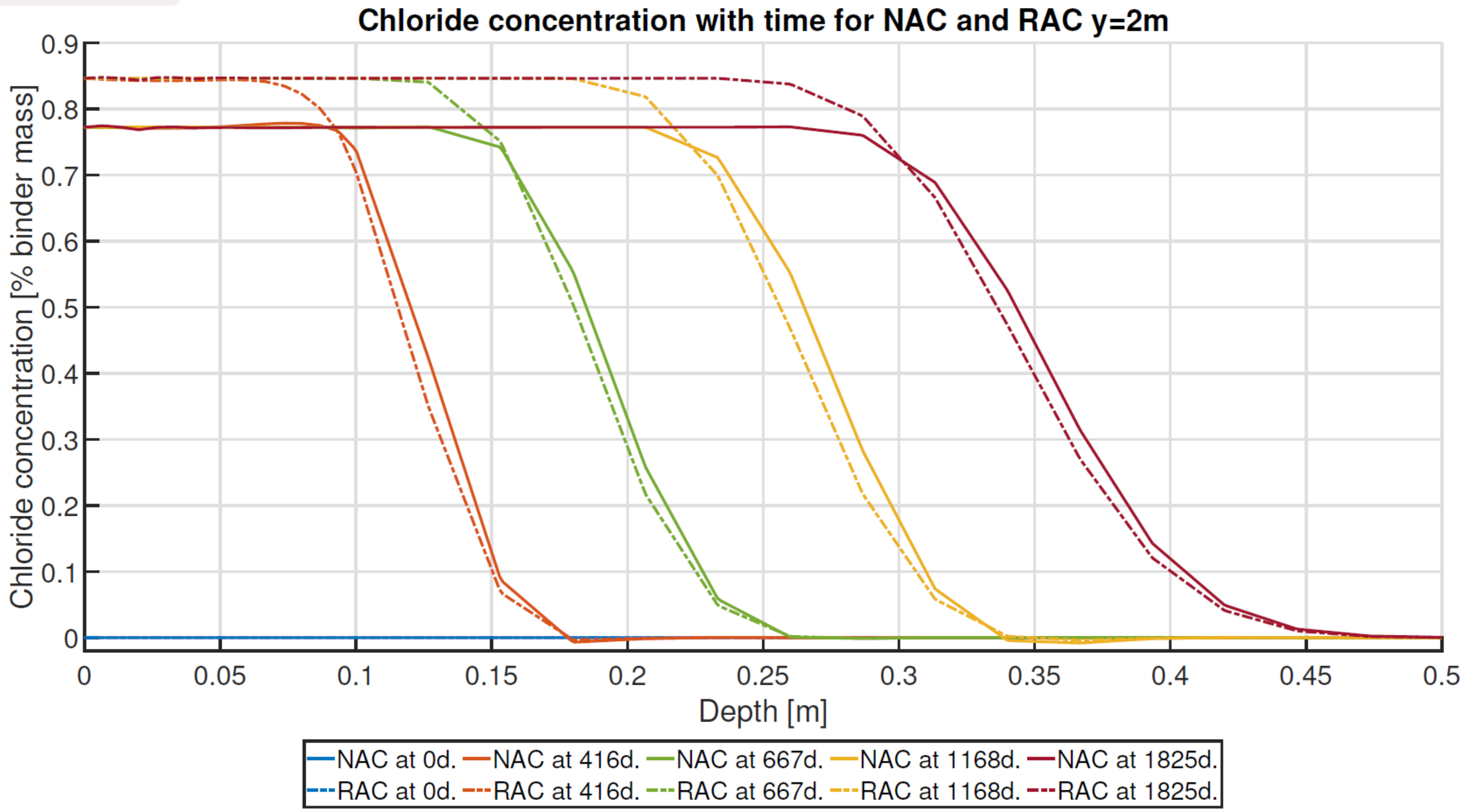

Application under Realistic Conditions

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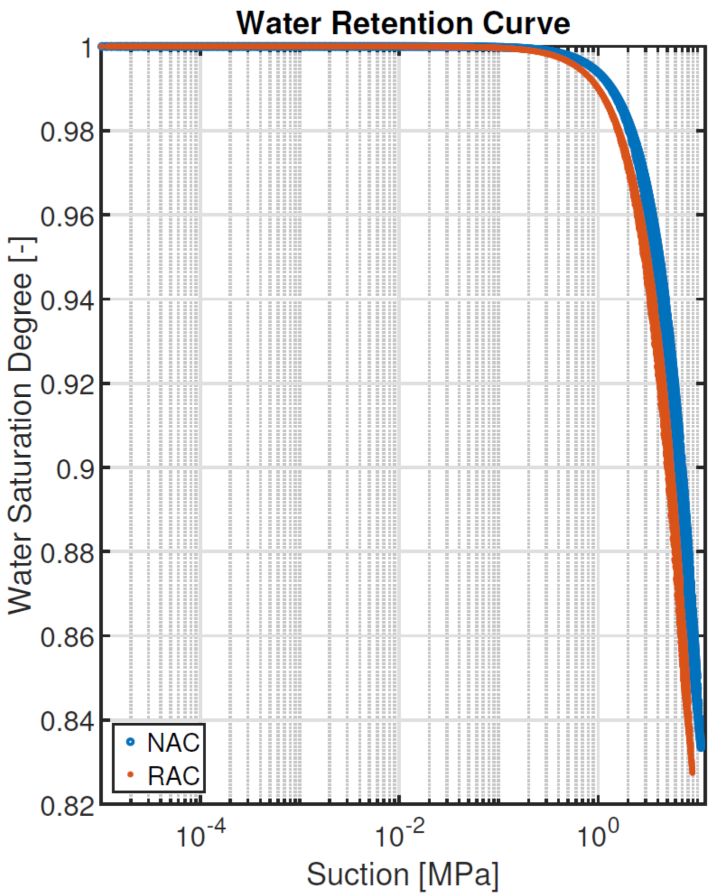

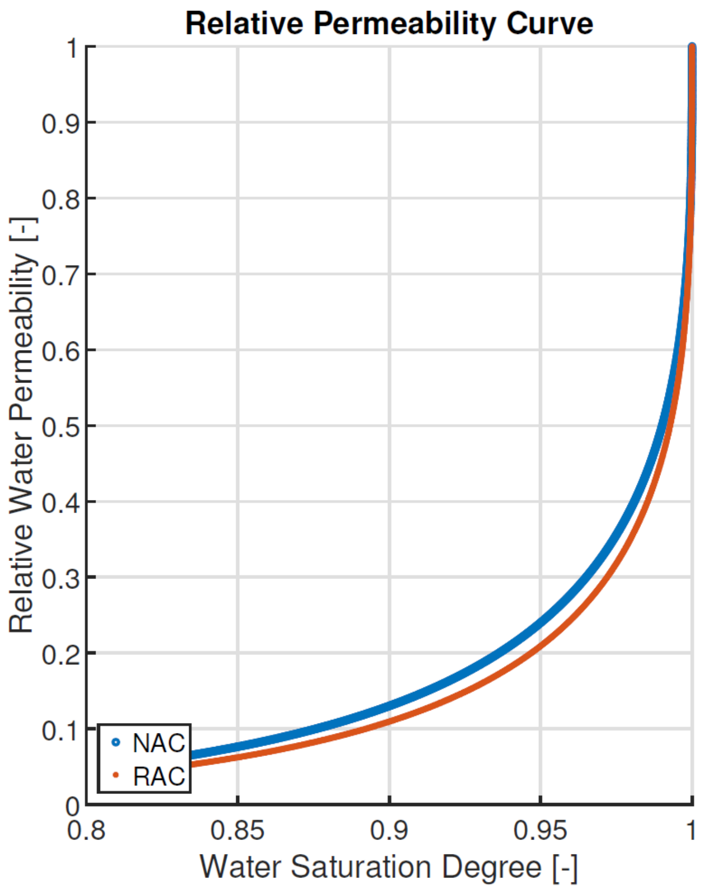

Table of Contents

Experimental Conclusions

Using recycled concrete aggregates in concrete:

- **Increases** the material's **overall porosity** due to their inherent porosity. Water absorption also increases by an amount equivalent to the absorption of the aggregates themselves;
- **Increases** the **intrinsic water permeability**, possibly because of a greater interconnectivity of the pores or due to the creation of a larger Interfacial Transition Zone;
- **Increases** the **chloride diffusion coefficient** for both steady and unsteady-state diffusions. This is expected as the substitution of NA by RCA worsens all water transfer properties, and chloride ion transport is directly related to theses;
- **Increases** the **larger maximum pore size**, as demonstrated by the water retention curves. However, it is important to note that this may not have a negative impact due to the relative permeability.

Numerical Conclusions

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- **Small errors in the cement content and diffusion properties of the RCA** would not significantly impact the accuracy of the model;
- In relation to the hysteresis model, the value of the **increment of suction** should be limited to the value to the **air-entry pressure**, and the value of the parameter ***b*** is not critical to the chloride ingress.
- The application showed that **the chloride content is marginally higher in the RAC than in the NAC**, which is a logical conclusion given its worse intrinsic properties and boundary conditions.

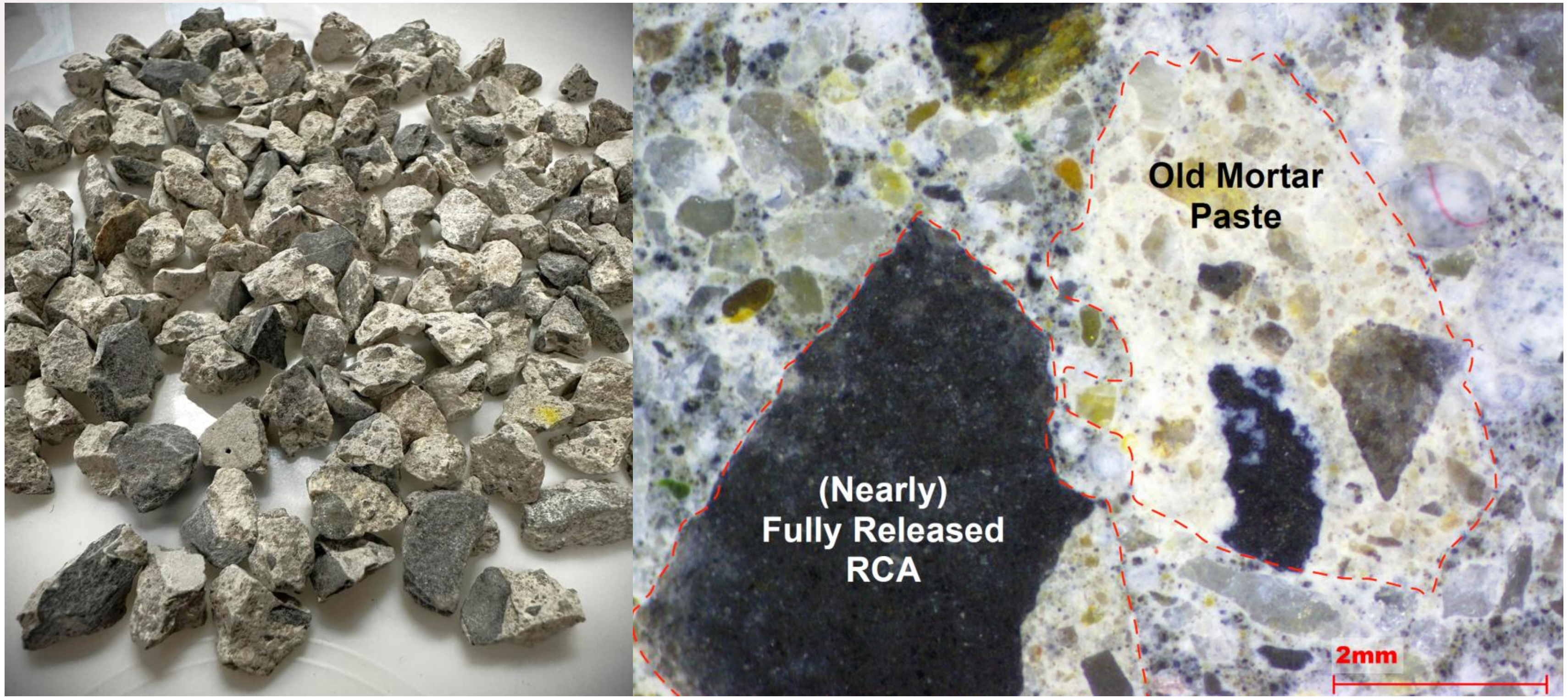
“ How does the incorporation of Recycled Concrete Aggregates affect the durability of concrete in terms of chloride attacks? ”

→ The **detrimental effects** of the substitution of aggregates are therefore **relatively limited**.

Thank you for your attention.

This work is co-funded by the FNRS and the Walloon Region as part of a FRIA grant (FC38499).

Context



- Increased heterogeneity; [Rao et al., 2007]
- Increased porosity, water absorption; [Rao et al., 2007]
- Reduced workability; [Guo et al., 2018]
- Chemical contamination; [Debieb et al., 2010]
- Depends on the substitution ratio; [Pacheco et al., 2023]
- Decreased durability properties?

Origin and Properties of RCA

RCA from the SeRaMCo project:

- OC1.2 (Sandstone) because of lower density and compressive strength;
- Jaw crusher because of higher water absorption.

Name	Reference OC1.0	Sandstone OC1.2	Low Cement OC2
Aggregate's Nature	Limestone	Sandstone	Limestone
Cement Type	CEM I 52.5	CEM I 52.5	CEM I 52.5
Cement Quantity $[\mathrm{kg/m^3}]$	400	400	320
Sand 0/4 $[\mathrm{kg/m^3}]$	604.9	604.9	664.4
Aggregates 2/7 $[\mathrm{kg/m^3}]$	368.8	368.8	405.1
Aggregates 7/14 $[\mathrm{kg/m^3}]$	345	345	379
Aggregates 14/20 $[\mathrm{kg/m^3}]$	433.5	433.5	476.2
Efficient Water $[\mathrm{kg/m^3}]$	224.2	224.2	180.6
W/C Ratio	0.56	0.56	0.56
Volume of Cement Paste $[\mathrm{dm^3/m^3}]$	351.2	351.2	282.2
Density $[\mathrm{g/cm^3}]$	2.35	2.31	2.36
Compressive Strength [MPa]	56.0 ± 2.4	52.7 ± 2.5	56 ± 6.4

Table 4.1: Original concrete compositions manufactured in the laboratory and their properties.

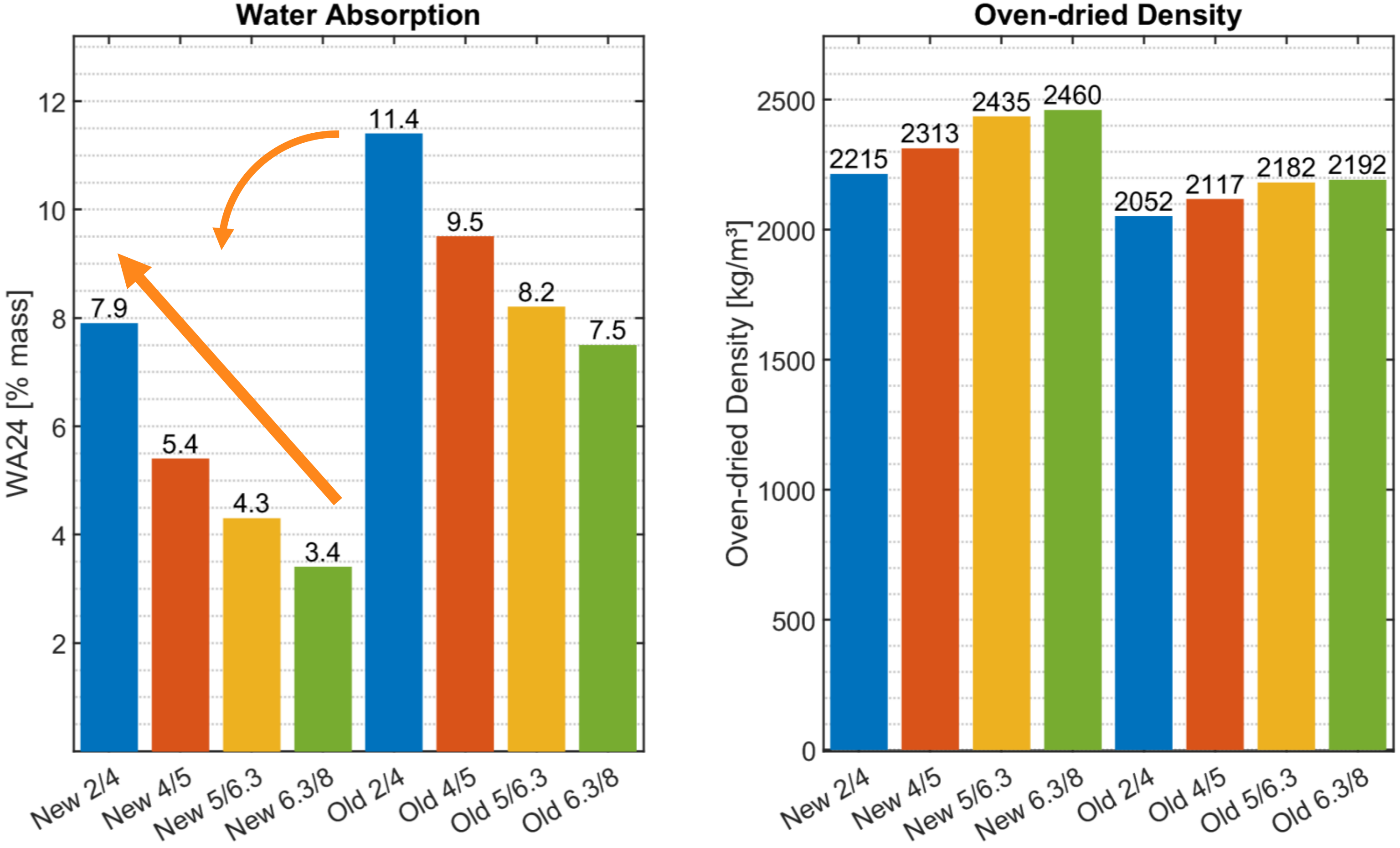
Name	OC1.0		OC1.2		OC2	
Crusher Type	Jaw	Impact	Jaw	Impact	Jaw	Impact
Global Flakiness Index [%]	14	8	13	6	11	7
Shape Ratio (L/E) 4/8	3.62	2.77	3.62	3.01	3.44	3.04
Water Absorption 0/4 [% mass]	11.75	10.96	12.47	11.58	8.9	7.92
Water Absorption 4/6.3 [% mass]	8.18	-	7.14	-	-	-
Water Absorption 6.3/8 [% mass]	7.72	7.15	8.58	8.12	7.02	6.27
Water Absorption 8/12.5 [% mass]	6.9	-	8.14	-	-	-
Water Absorption 12.5/20 [% mass]	7.09	6.92	7.95	6.7	6.39	6.03
Water Absorption 20/25 [% mass]	6.9	7.65	6.53	6.83	6.96	6.11

Table 4.2: Properties of the RCA obtained from the compositions OC1.0, OC1.2 and OC2.

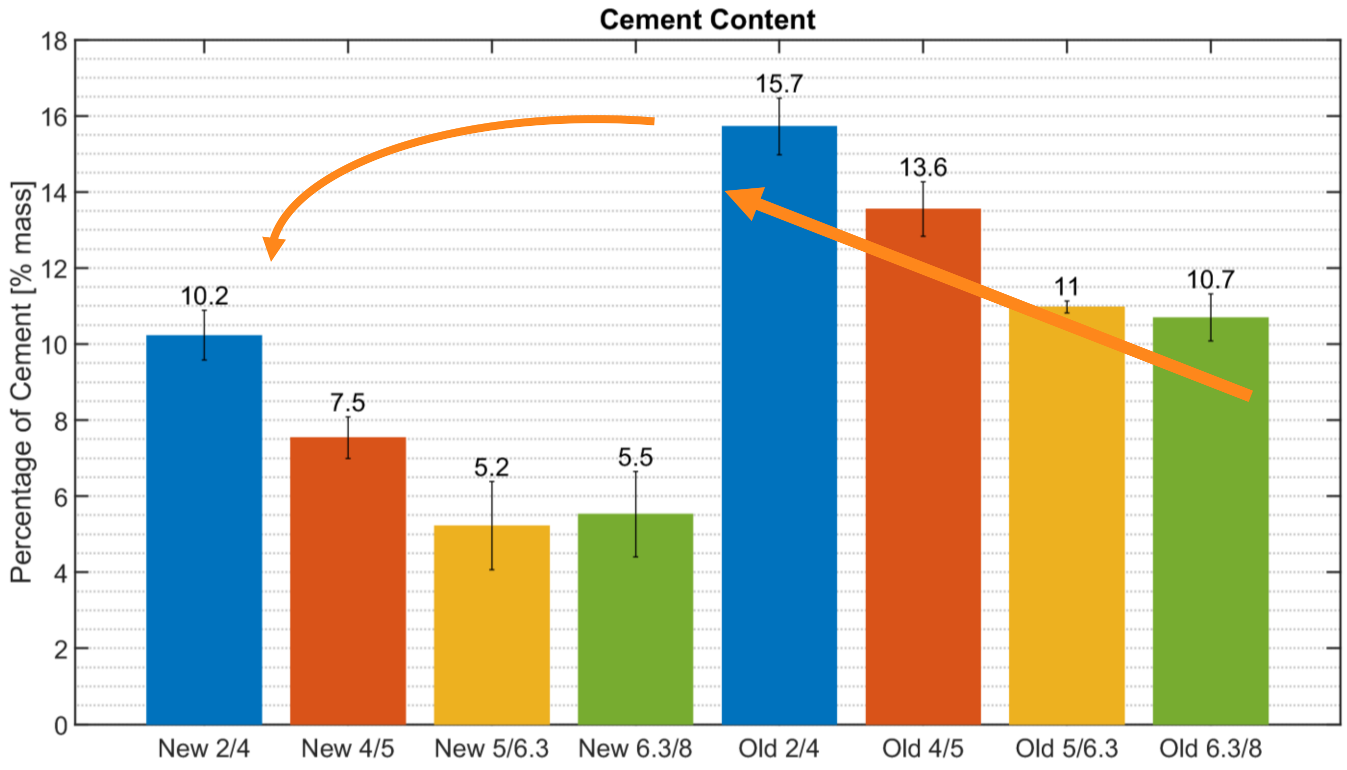
Origin and Properties of RCA

RCA from the SeRaMCo project [Hubert et al., 2023]:

- OC1.2 (Sandstone) because of lower density and compressive strength;
- Jaw crusher because of higher water absorption;
- Not enough materials → third crushing step (Old vs. New);
- The smaller the particles, the greater the water absorption;
- The more crushing steps, the smaller the water absorption and the greater the density.



Origin and Properties of RCA



- The smaller the particles, the greater the cement content;
- The more crushing steps, the smaller the cement content.

Water Absorption by Immersion

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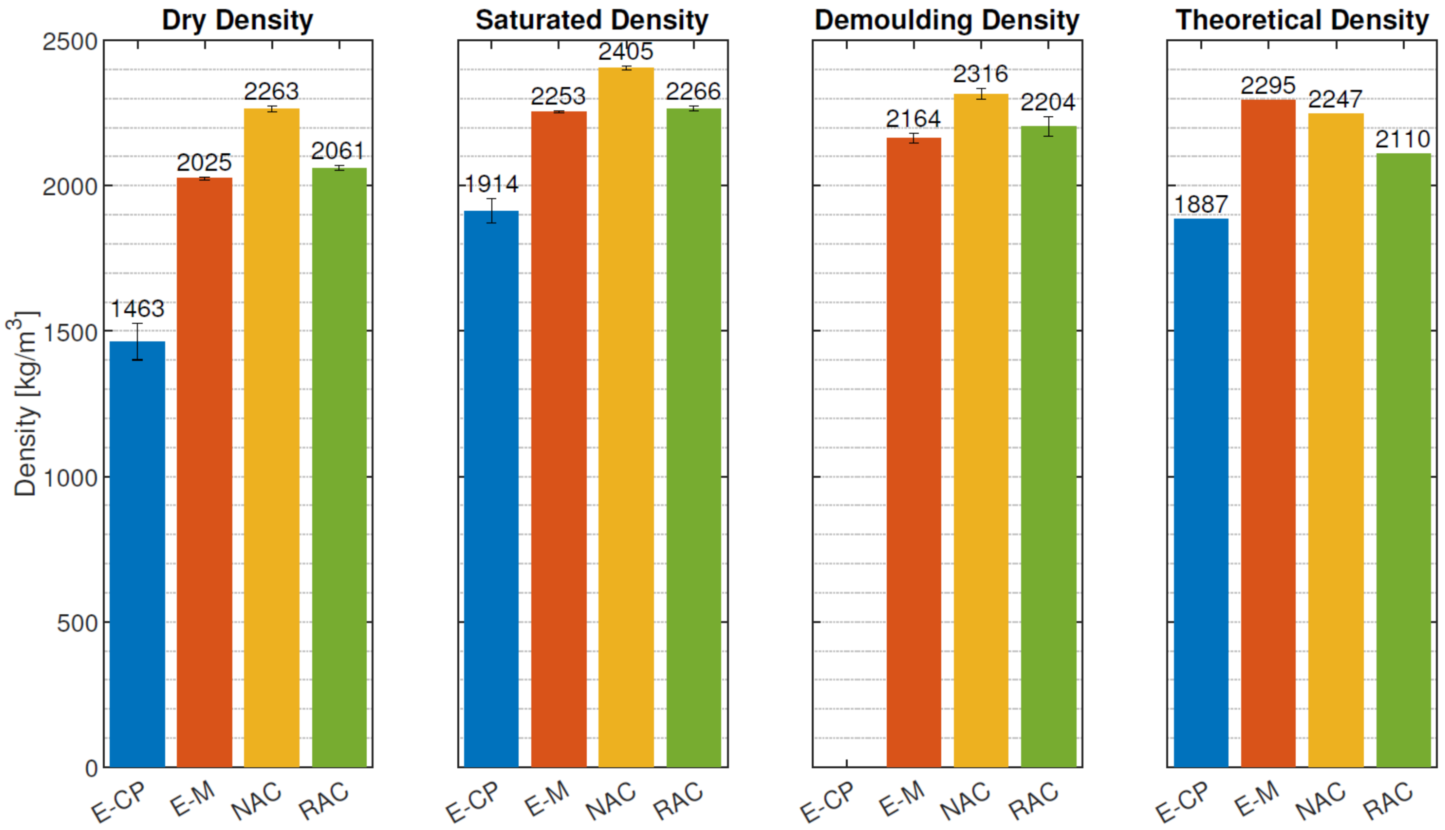
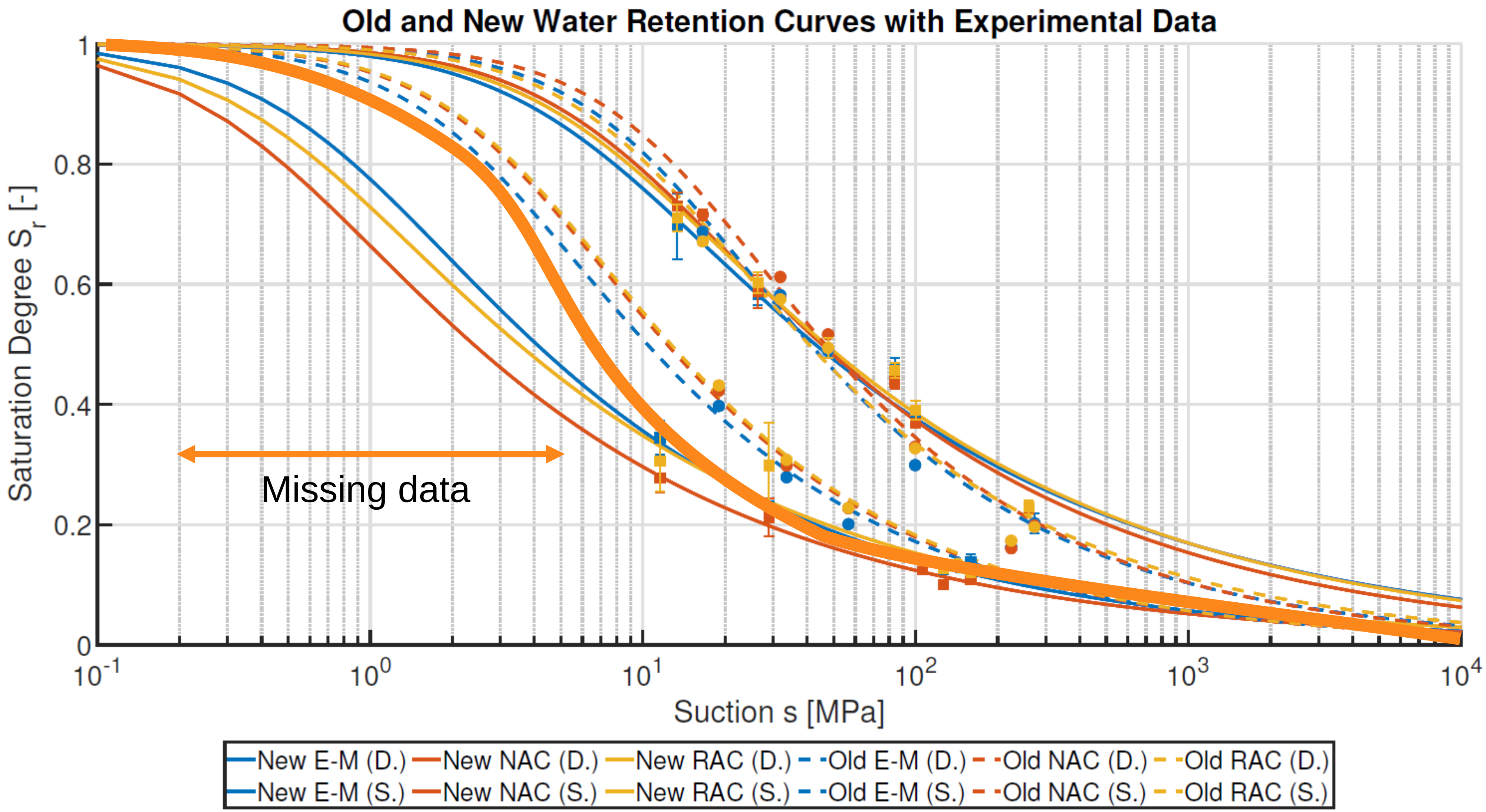


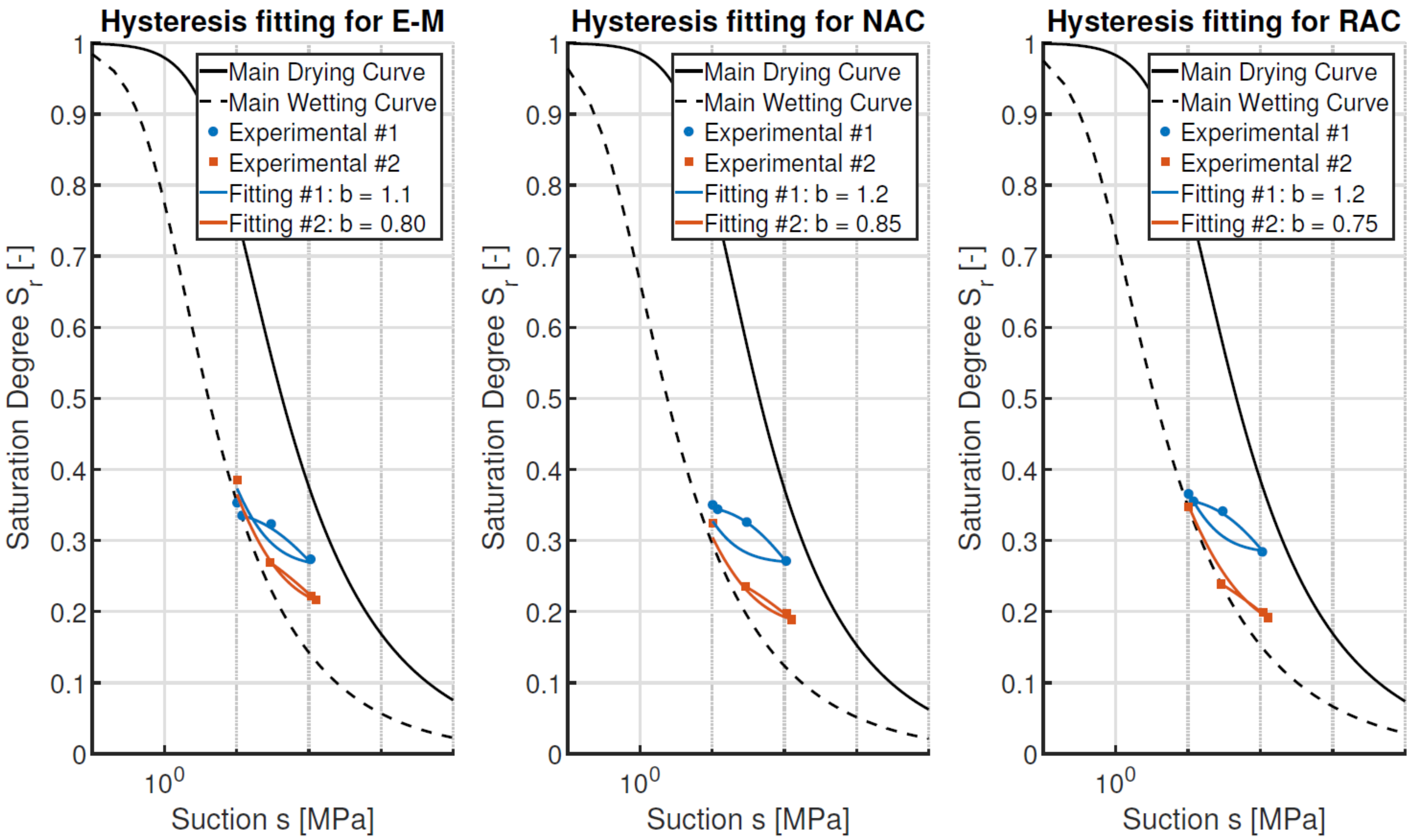
- Aggregates are denser than mortar → NAC is denser than RAC;
- E-CP has the greater density gain from dry to saturated → greater water absorption ?
- Demoulding density of E-M smaller than the theoretical one → greater porosity ?

Static Sorption and Desorption



Static Sorption and Desorption

- Fitting by the model by Zhou et al. (2012), introducing parameter b.



Diffusion under Unsteady-State

Composition	E-CP		E-M			NAC			RAC		
Time [day]	15	29	15	29	91	15	29	91	15	29	91
D_{app} [E-11 m^2/s]	1.63	1.51	1.71	1.43	0.92	1.81	1.44	2.93/1.58	2.46	1.65	1.78
C_s [% total mass]	4.15		1.45			0.78			1.27		
$X_{0.4\%t.m.}$ [mm]	12.1	16.2	11.9	15.1	21.5	12.3	15.2	38.4/28.2	14.8	16.9	31.1

Table 5.4: Apparent diffusion coefficient, surface concentration and threshold depth for each composition, obtained from the Fick analysis of the experimental results.

$$C_s[\%] = 106\ [\text{kg/m}^3\ \text{Cl}^-]\ \frac{n\ [\%\ \text{volume}]}{\rho_d\ [\text{kg/m}^3]}$$

Mixture	Theoretical		Experimental		Difference
	C_s [% total mass]	n [% volume]	C_s [% total mass]	n [% volume]	
E-CP	3.34	45.6	4.15	56.7	+24.3%
E-M	1.18	22.6	1.45	27.8	+22.8%
NAC	0.67	14.4	0.78	16.65	+16.7%
RAC	1.06	20.7	1.27	24.8	+19.8%

Table 5.5: Comparison of the theoretical and experimental (obtained by fitting) surface concentrations.

Diffusion under Unsteady-State

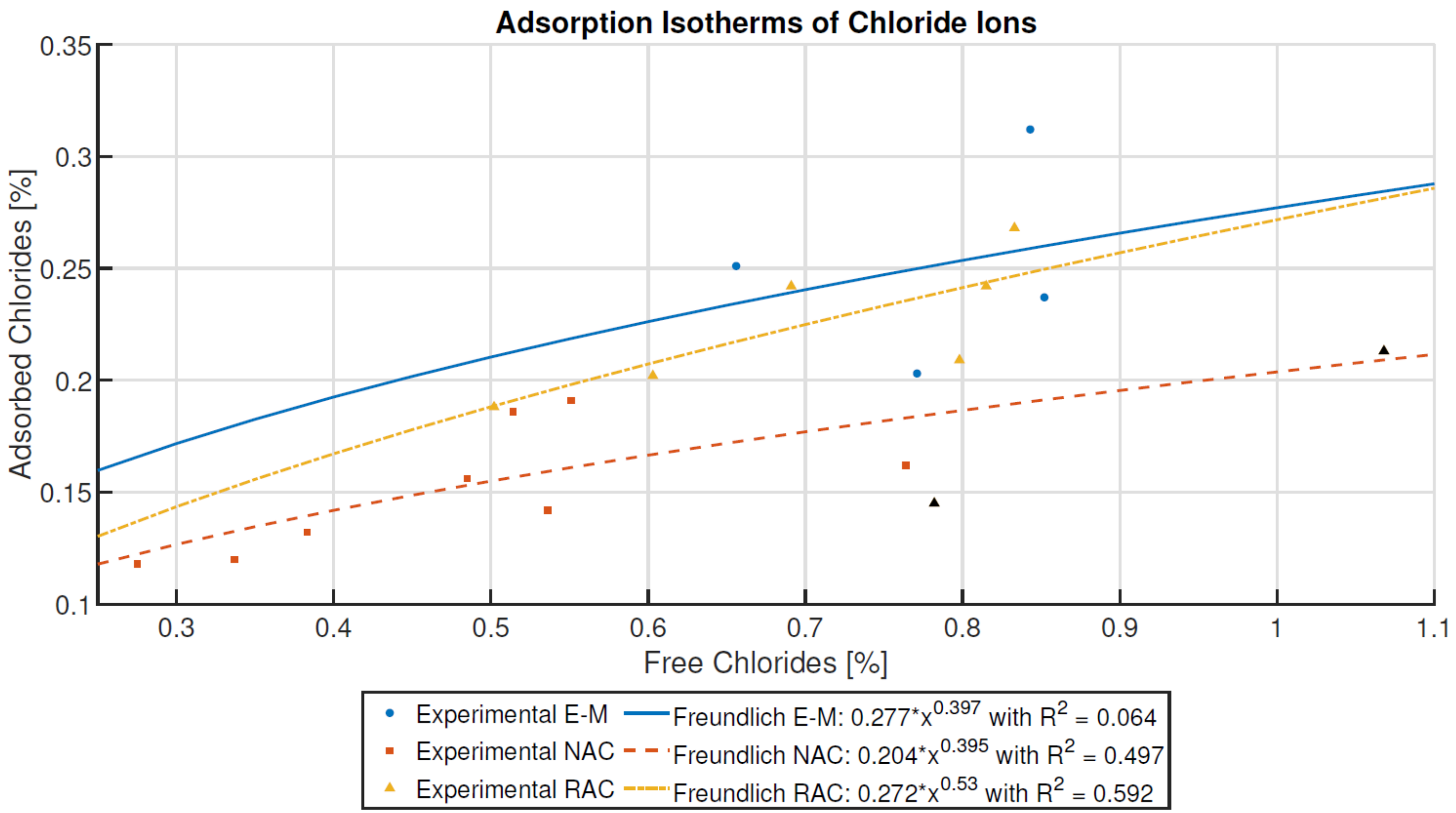
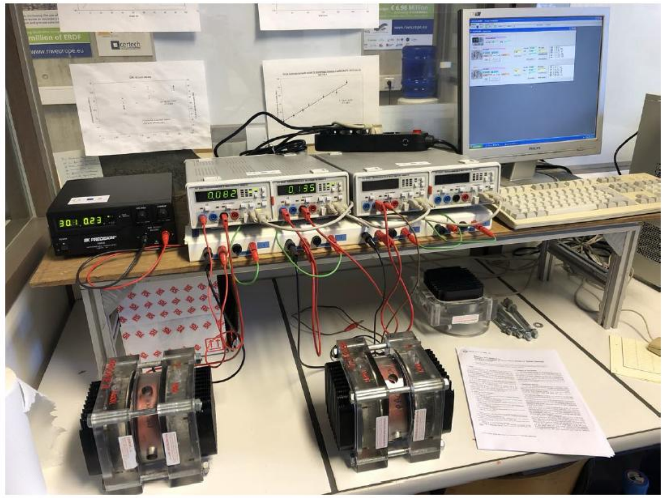


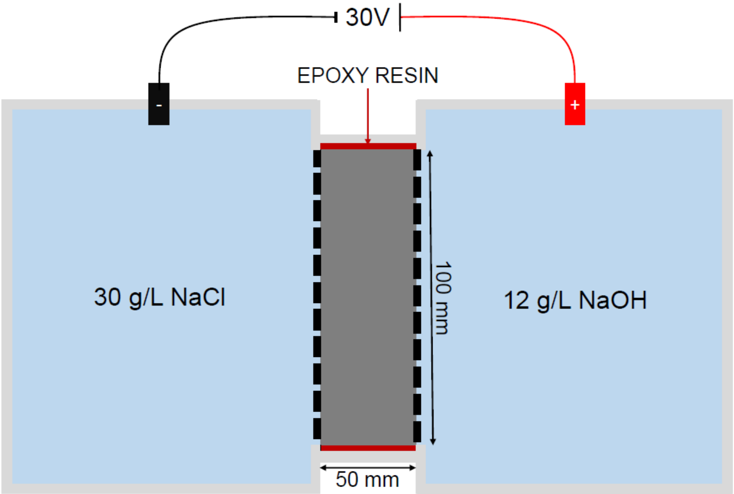
Figure 5.23: Chloride Adsorption Isotherms obtained with our chloride diffusion experiment under unsteady state.

- Results are inconclusive;
- RAC tends to adsorb chloride ions more rapidly than NAC, as depicted by the slope.

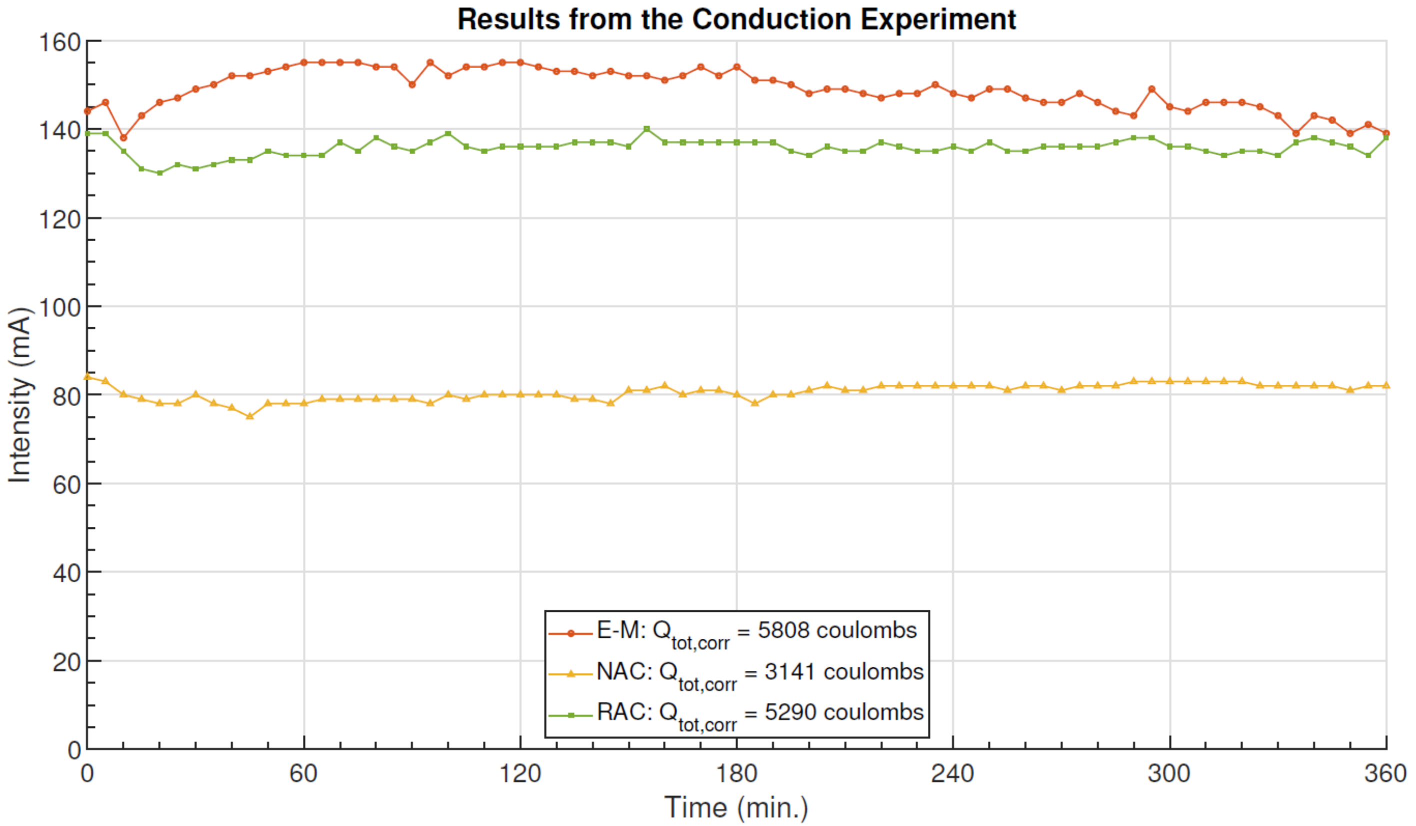
Experimental programme

- Water transfer properties
  - Water Absorption by Immersion (WAI)
  - Intrinsic Water Permeability experiment
  - Static Sorption and Desorption experiment
- Chloride ions transfer properties
  - Chloride diffusion under steady-state
  - Chloride diffusion under unsteady-state
  - **Conduction**
    - Chloride ion permeability
    - ASTM C 1202-05
    - 100x50mm cylinders.





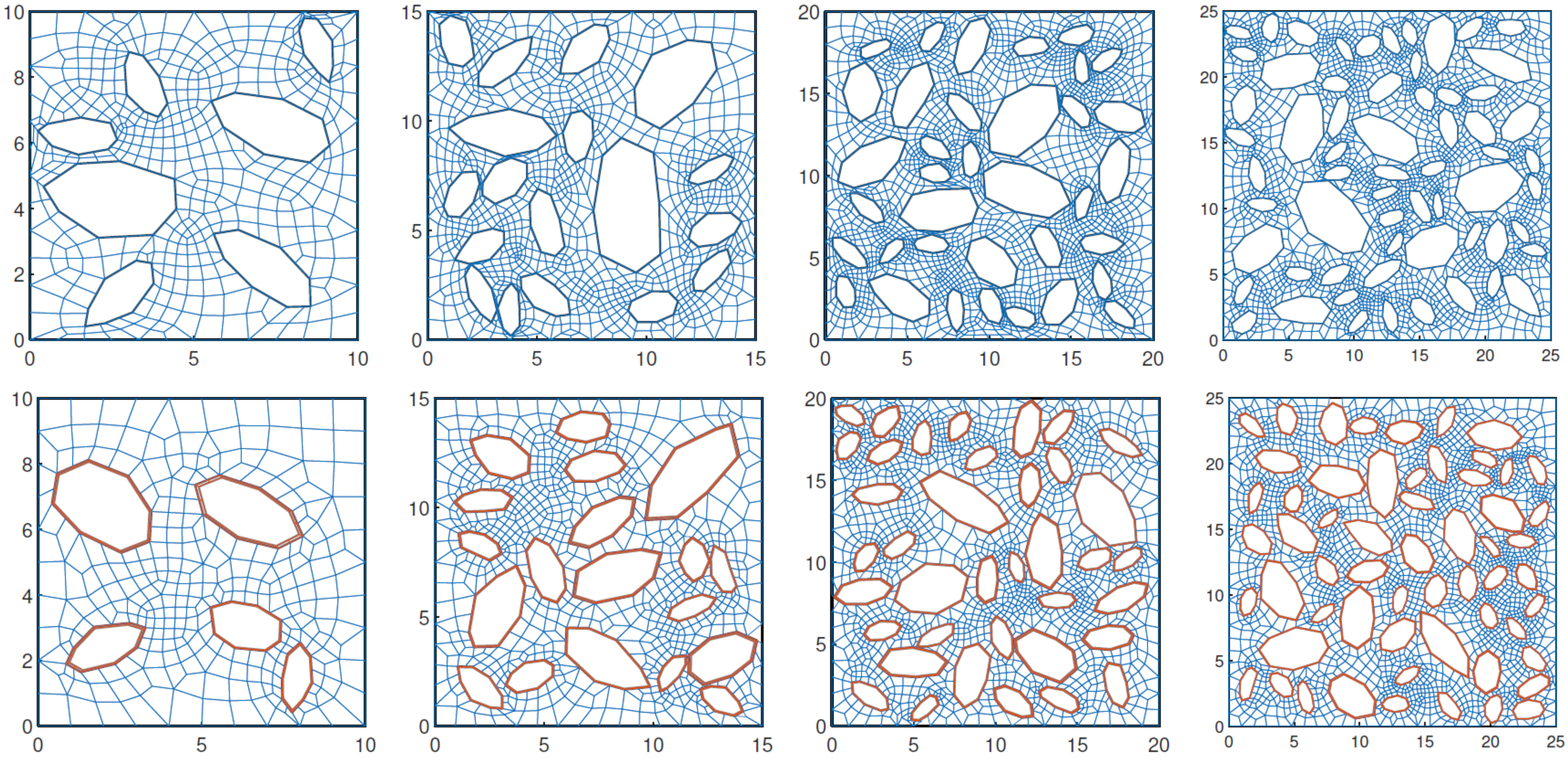
Conduction



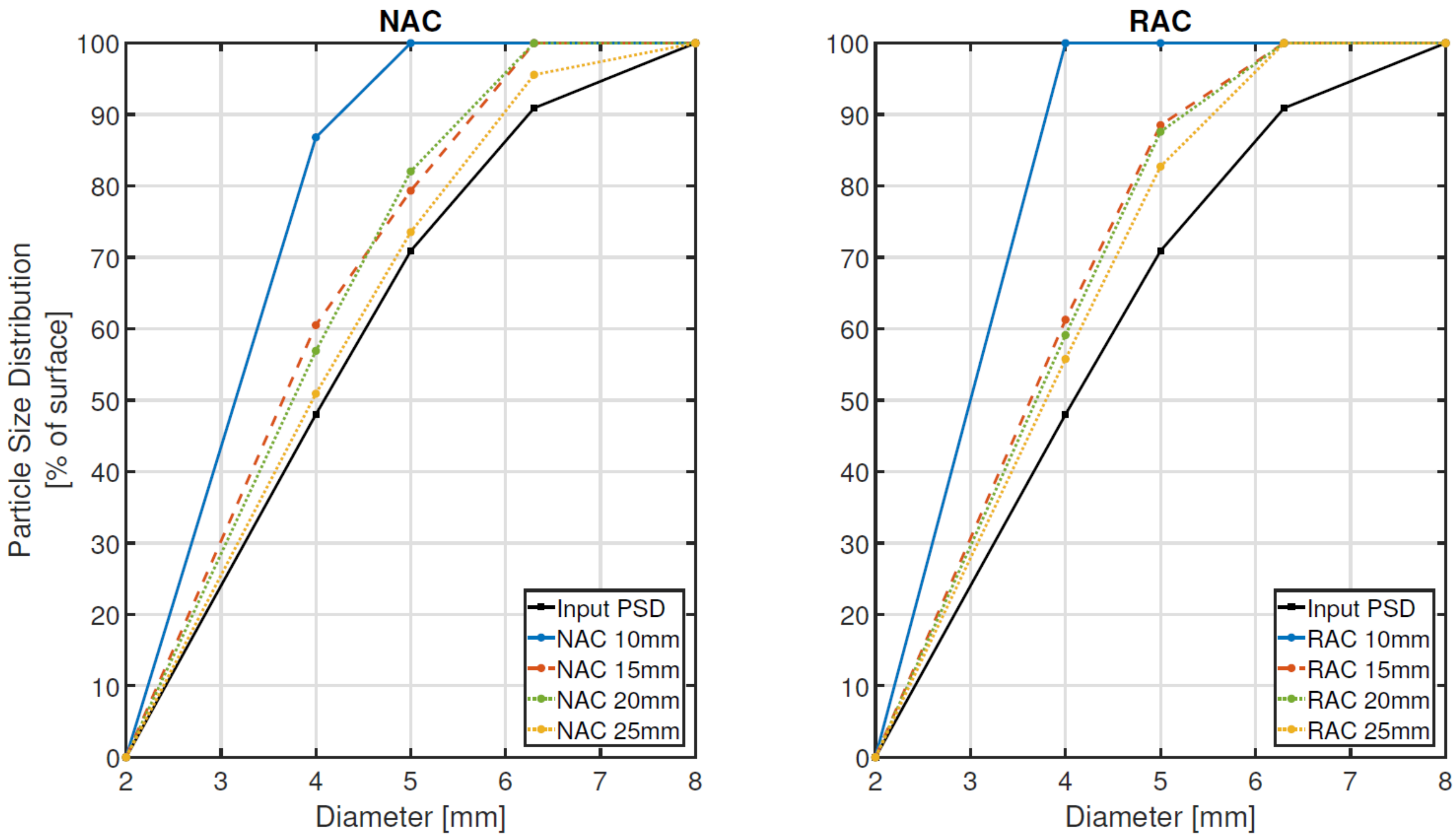
Sample	**Charge passed** [Coulombs]	Chloride Permeability Class
E-M	5808 (>4000)	High
NAC	3141 (2000-4000)	Moderate
RAC	5290 (>4000)	High

Table 5.6: Comparison of the results from the conductivity experiment with the chloride permeability class from [Whiting, 1981].

Influence of RVE' Size



Influence of RVE’ Size



Influence of RVE' Size

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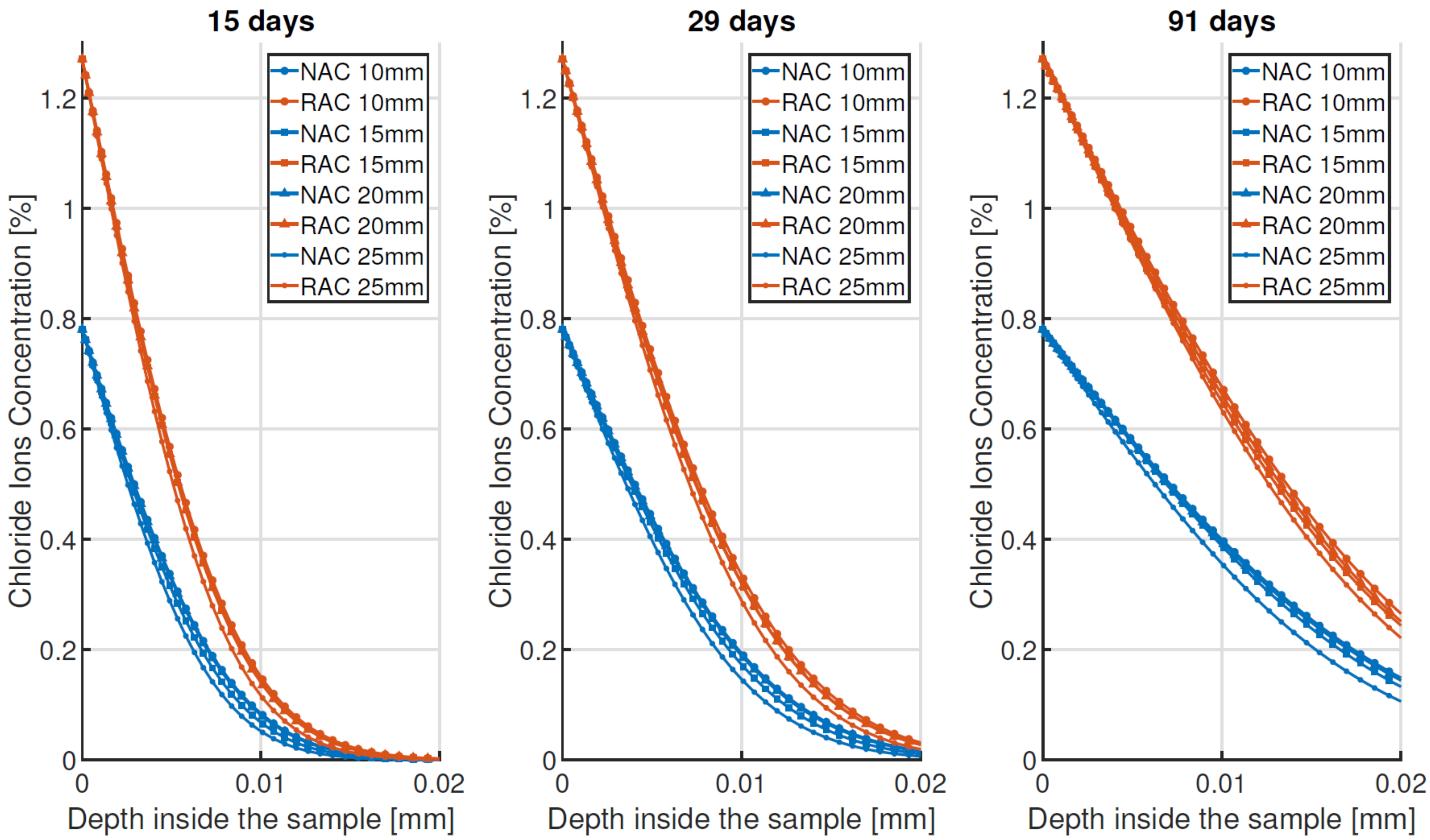
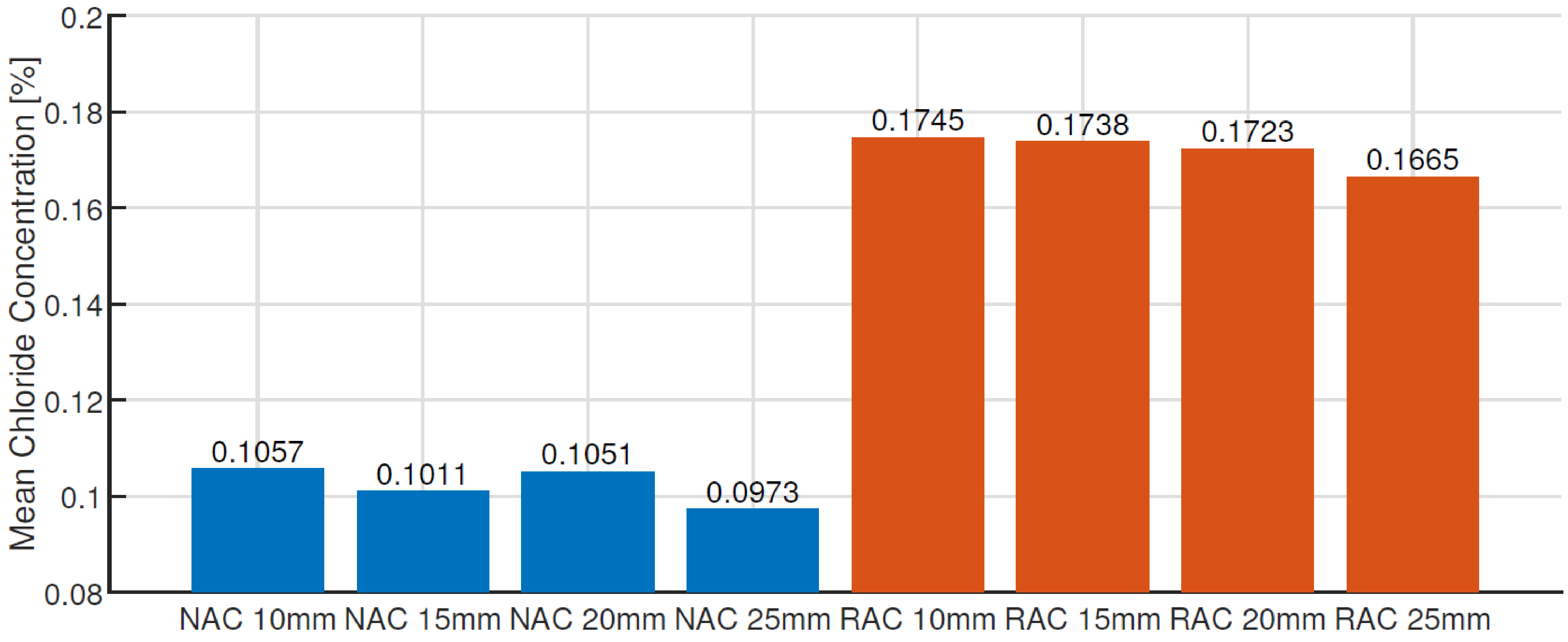
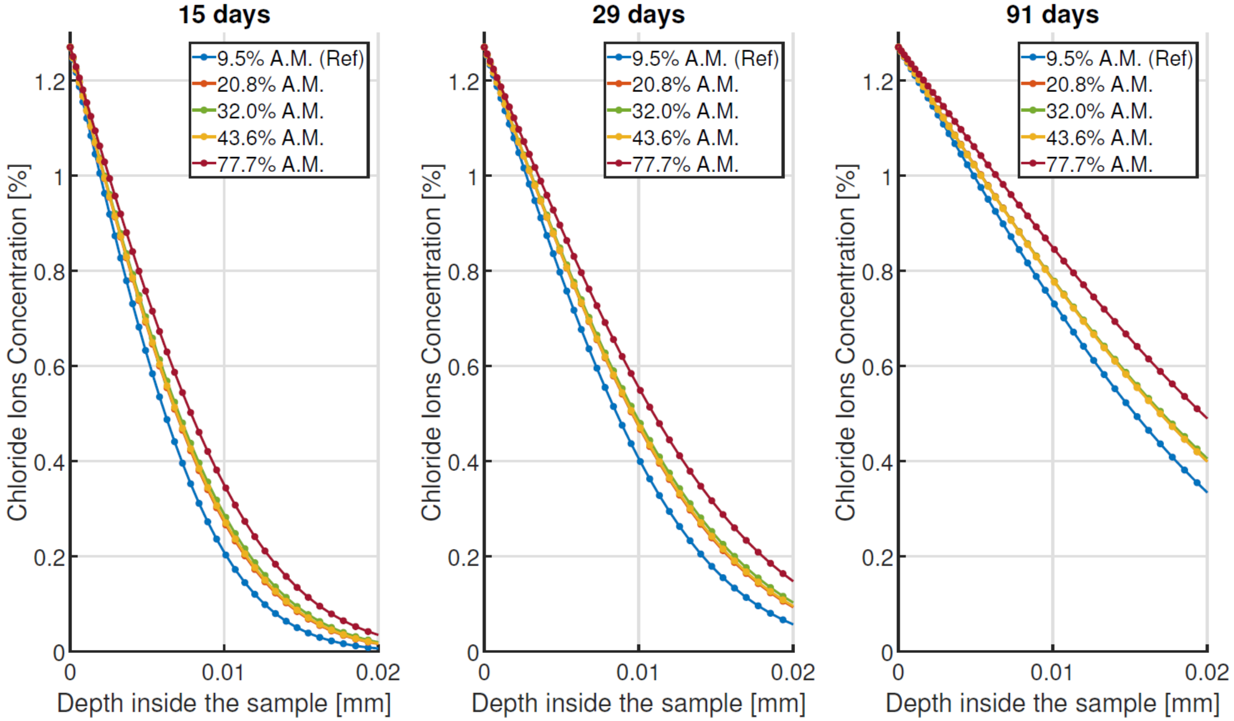


Influence of RVE' Size



Influence of RCA's cement content

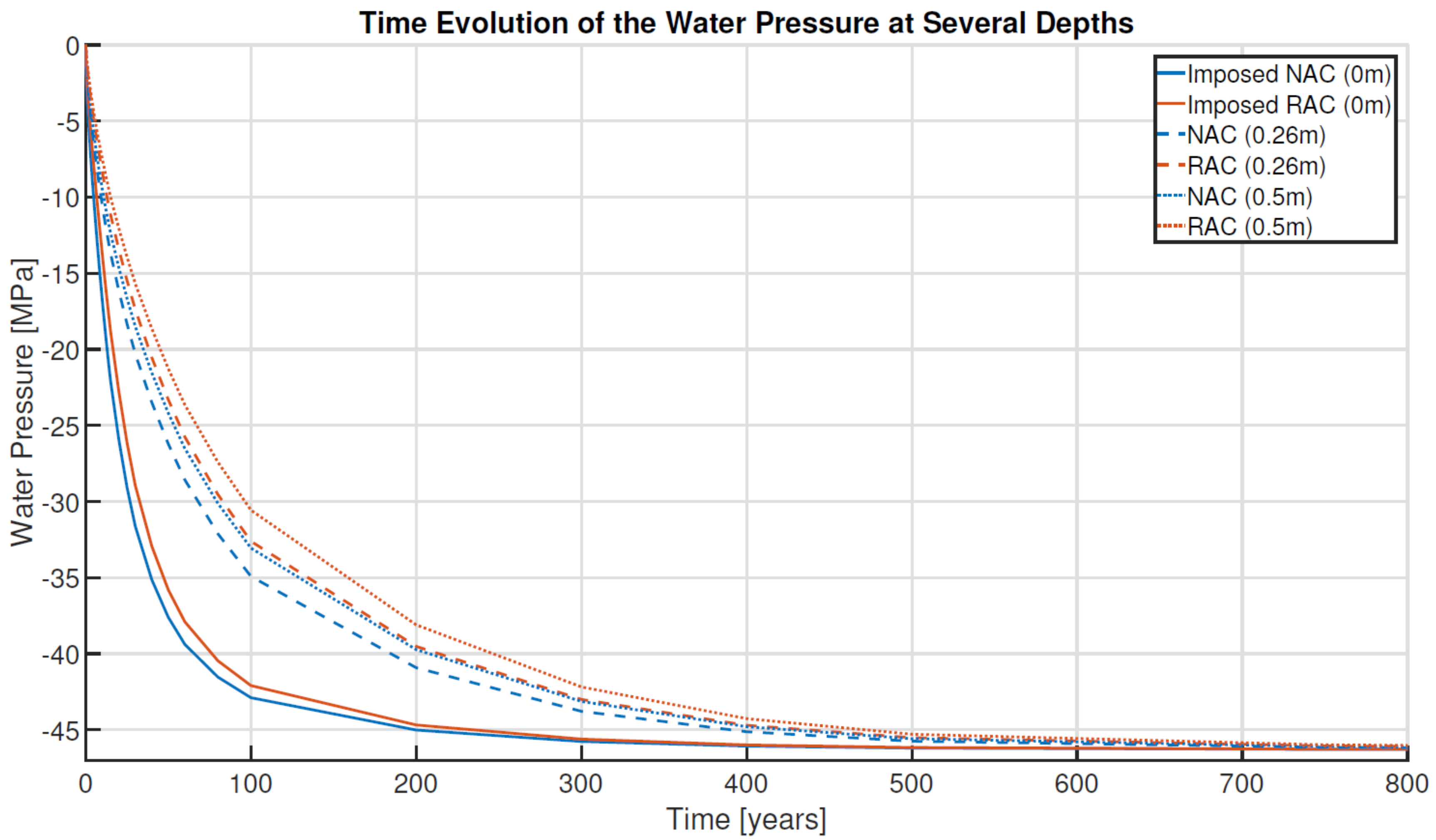


- Diffusion coeff. x10
- Intrinsic perm. x10
- Porosity x2

Simulation	Reference	Times 2	Times 3	Times 4	Times 7
Adherent Mortar (% Ref.)	100	218.7	337.5	459.4	818.7
Results at 15 days (% Ref.)	100	107.97	110.62	108.78	116.56
Results at 29 days (% Ref.)	100	107.73	110.29	108.51	116.05
Results at 91 days (% Ref.)	100	107.37	109.76	108.07	115.29

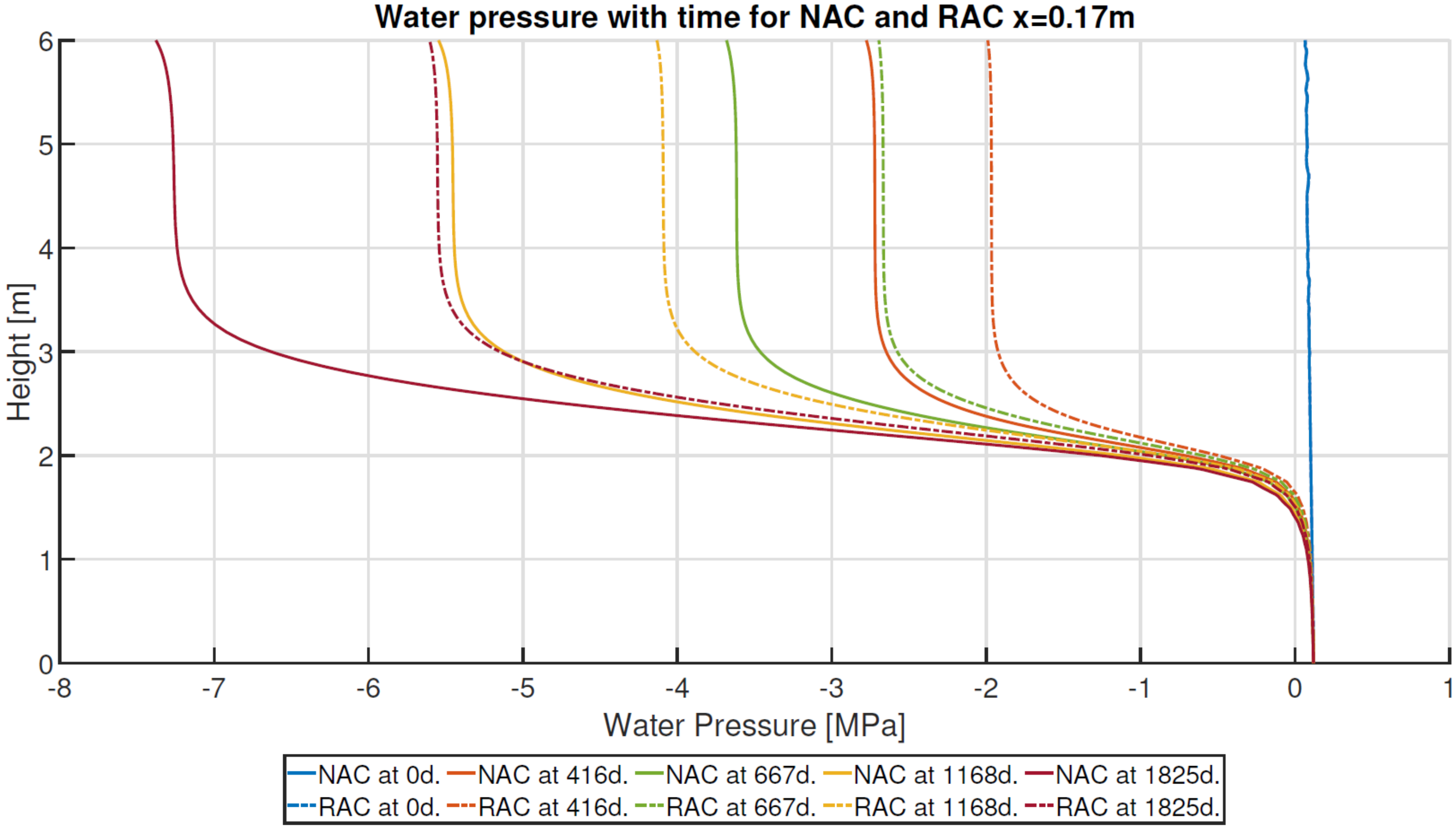
Table 7.9: Relative percentage of adherent mortar content and mean concentration at 15, 29 and 91 days compared to the reference simulation, after increasing the properties of the adherent mortar.

Application to a Real Life Scenario

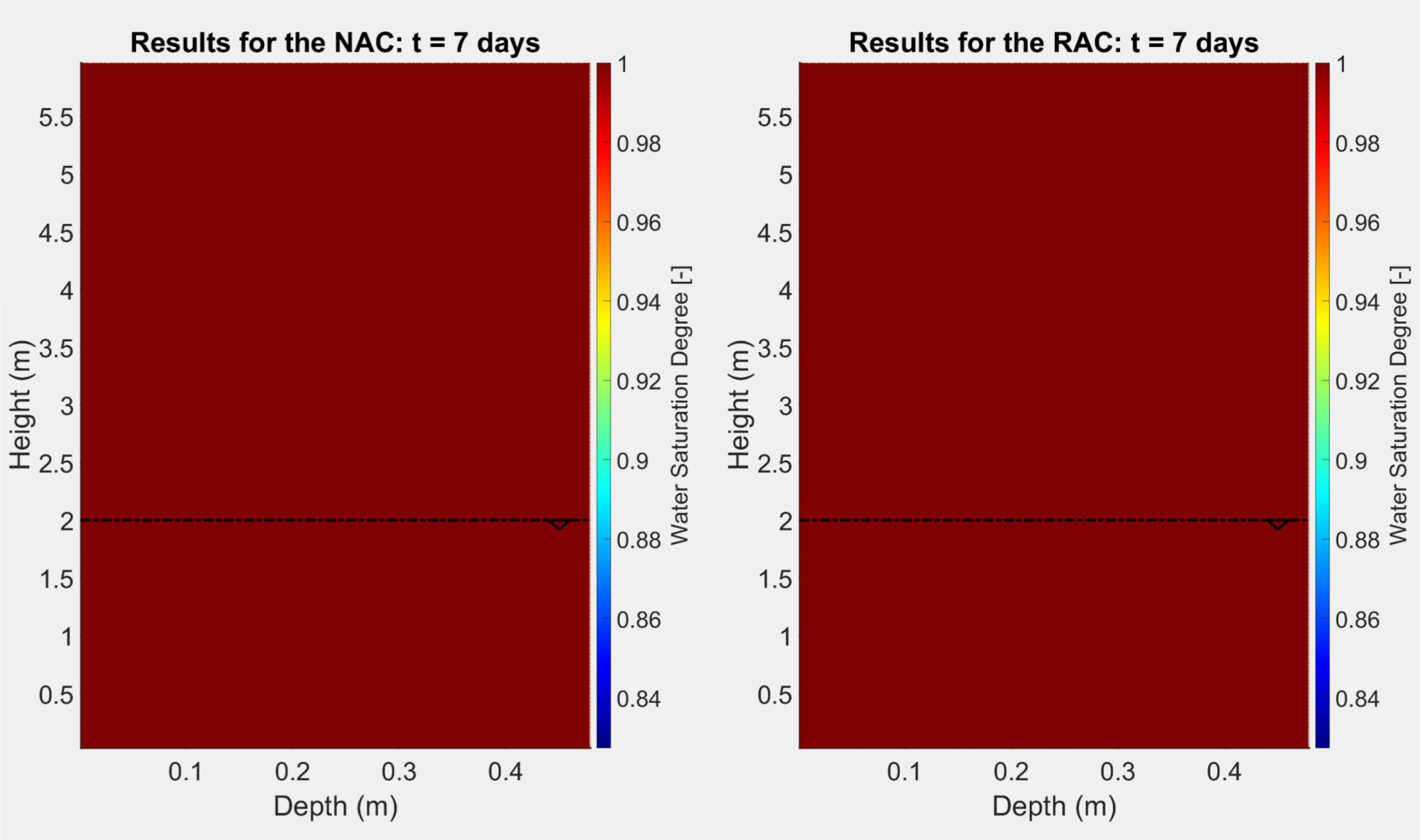


- Due to the Boundary Layer Model, the BC are fully applied after 400 years.

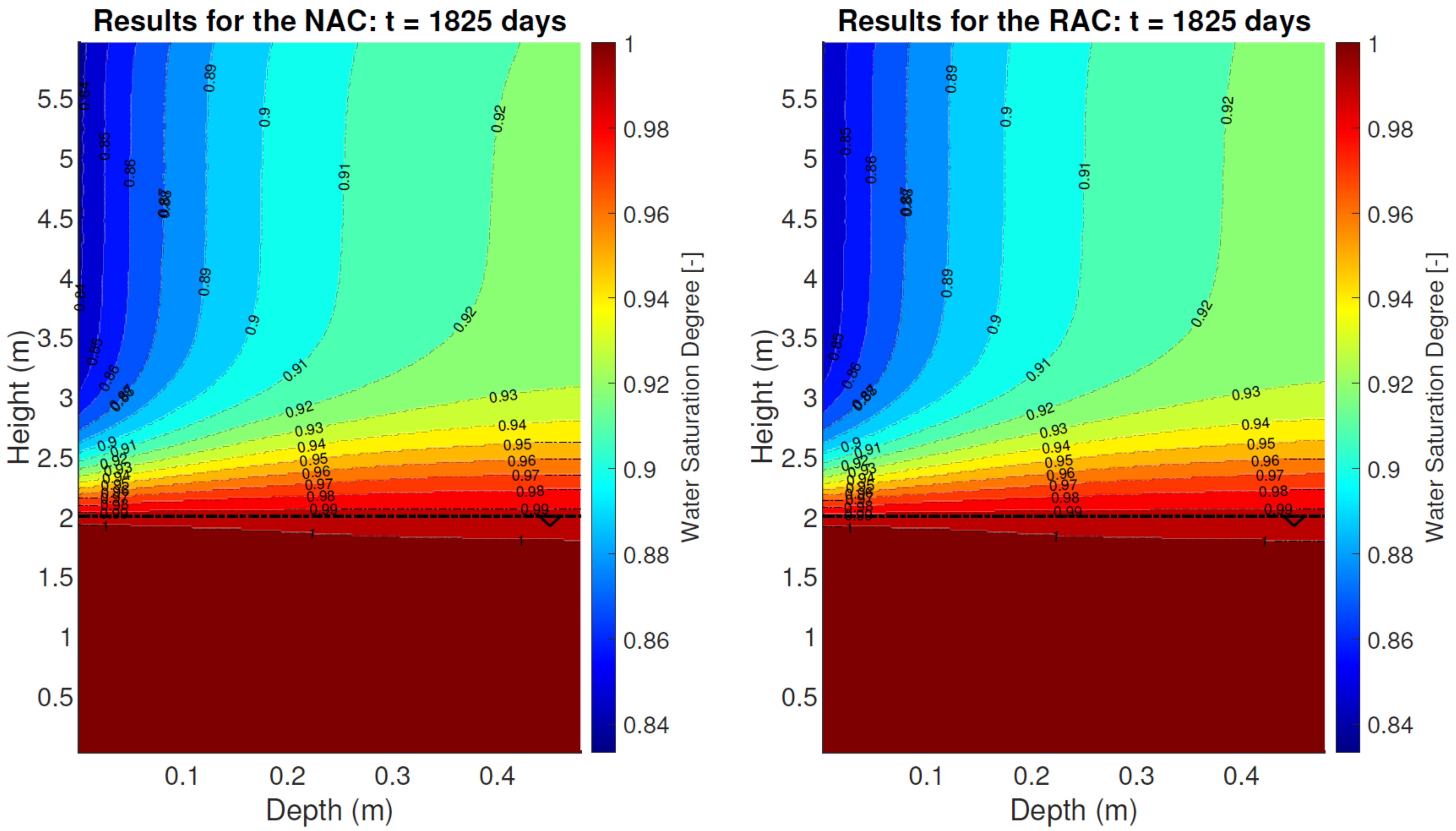
Application to a Real Life Scenario



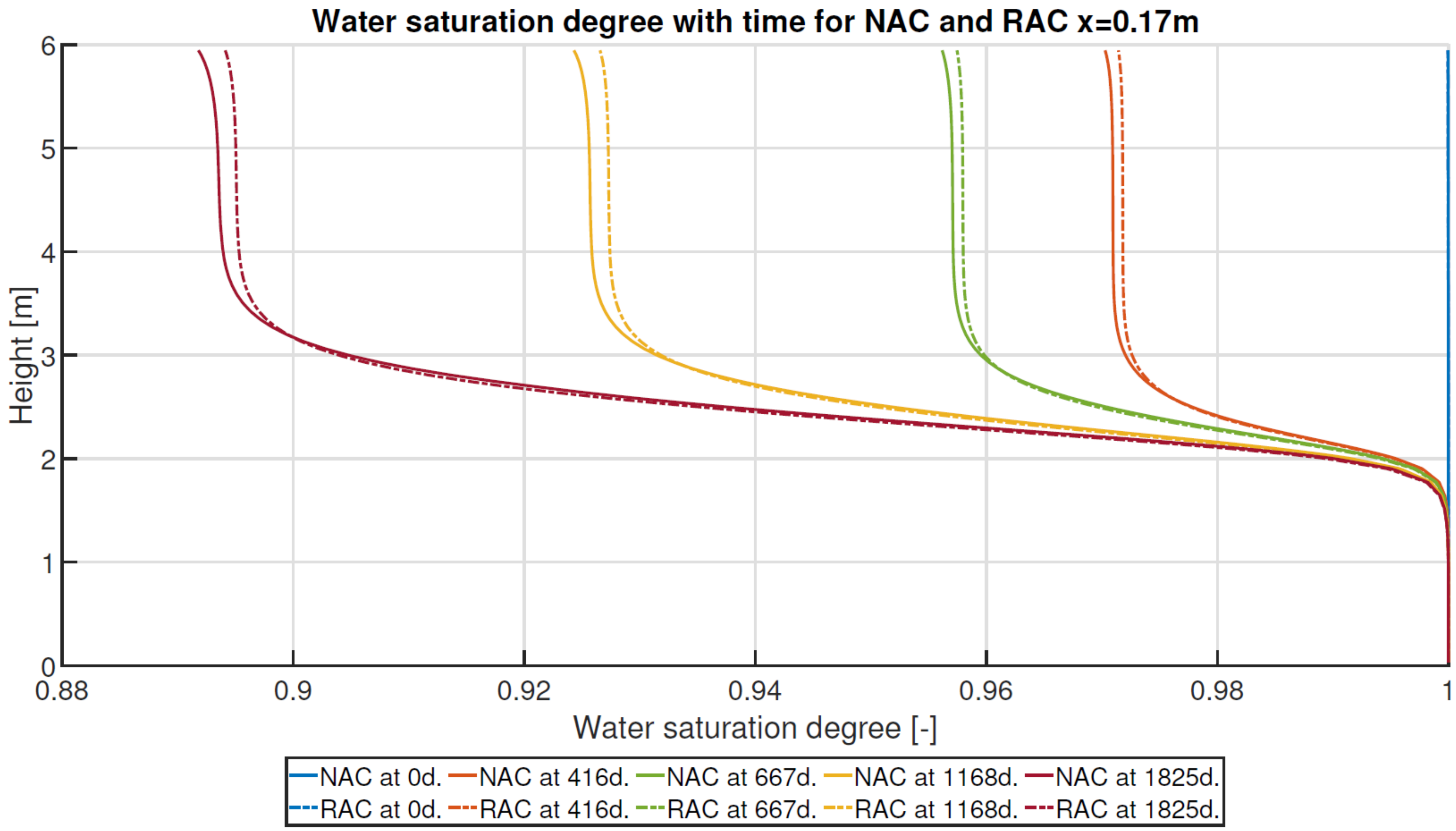
Application to a Real Life Scenario



Application to a Real Life Scenario



Application to a Real Life Scenario



Application to a Real Life Scenario

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Time of the day [hours]	7	12	19	24
Height of the tide [m.]	0	2	0	2

Table 8.3: Amplitude of the tides at a given time of a day.

Application to a Real Life Scenario

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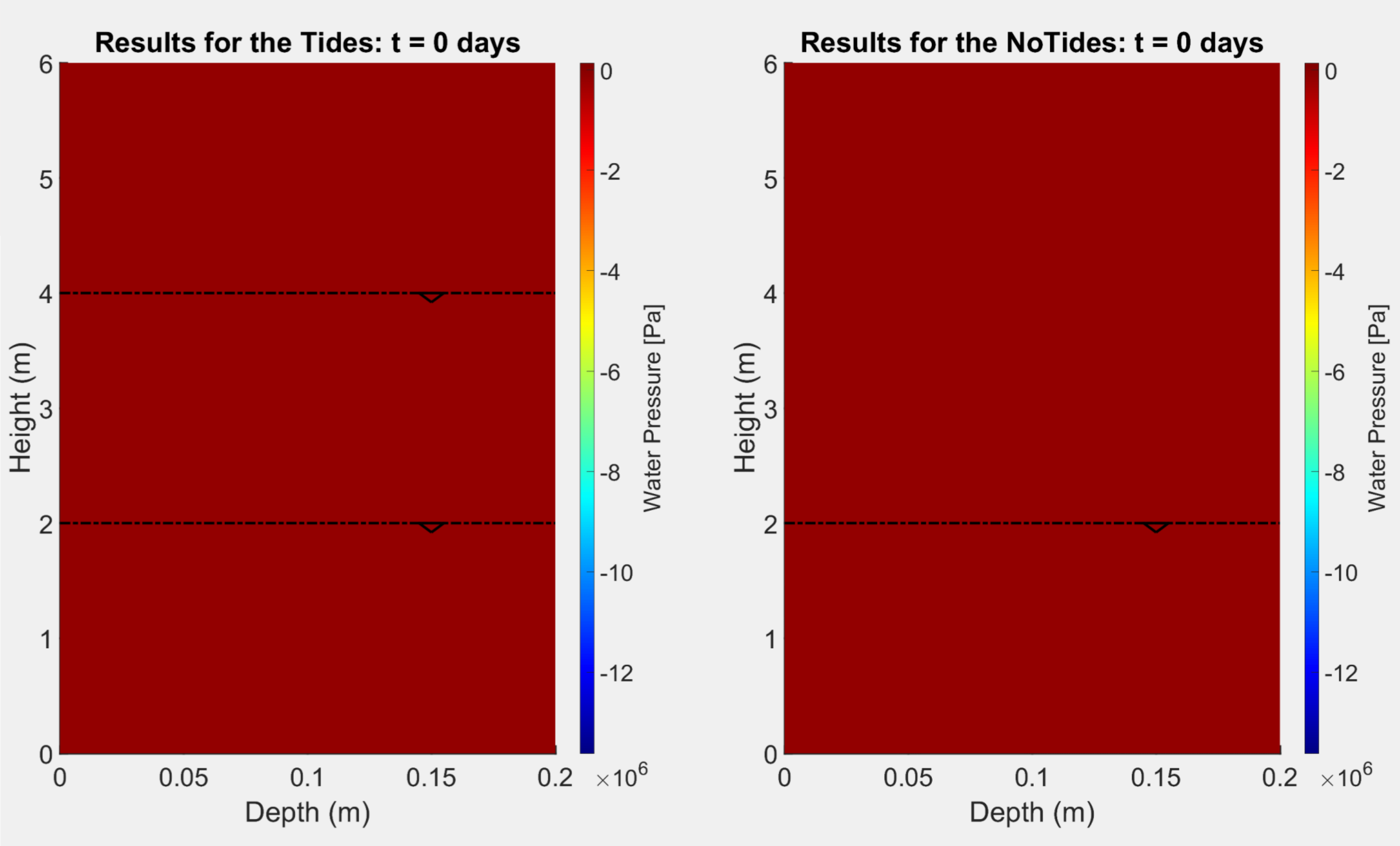
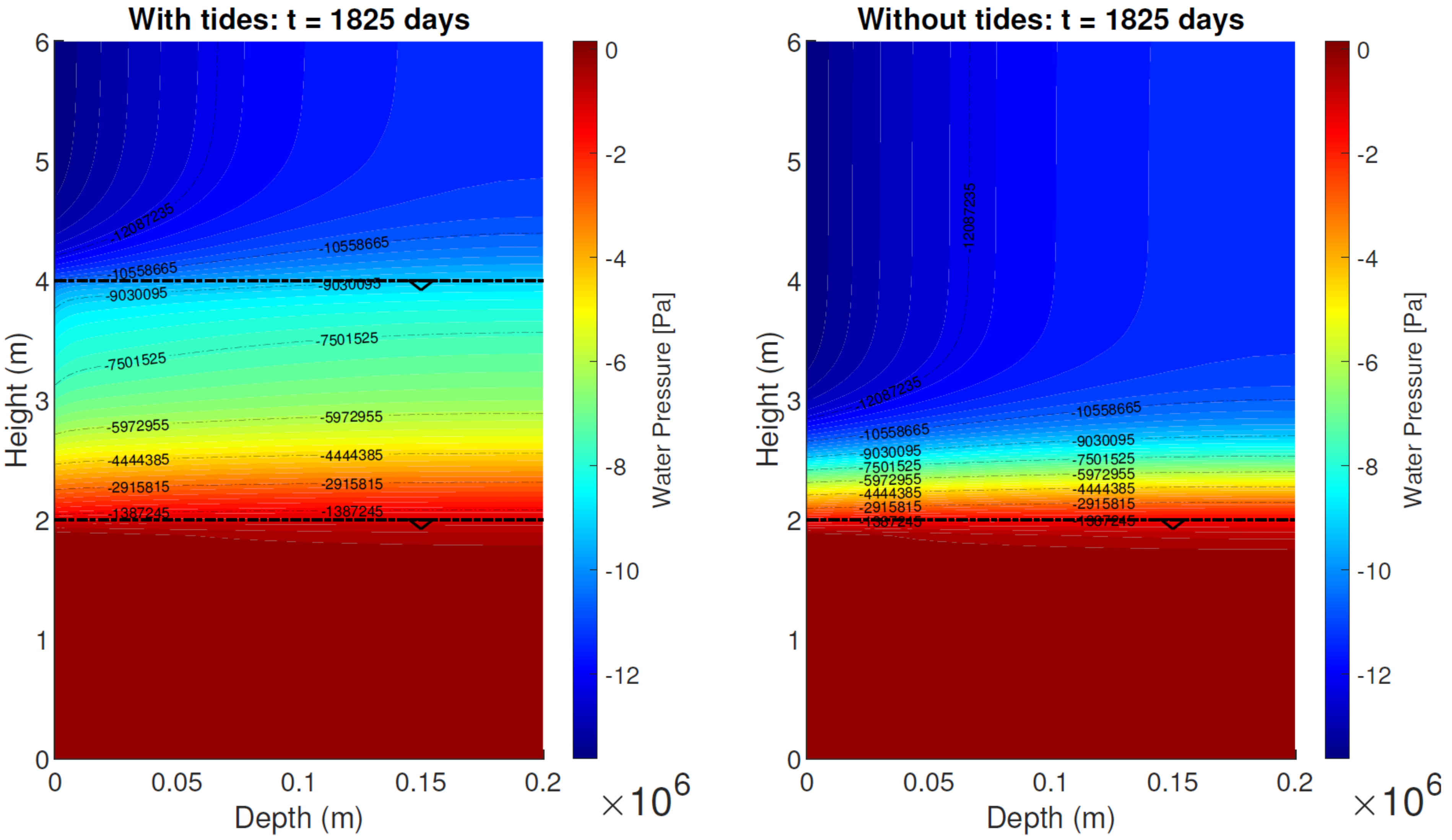
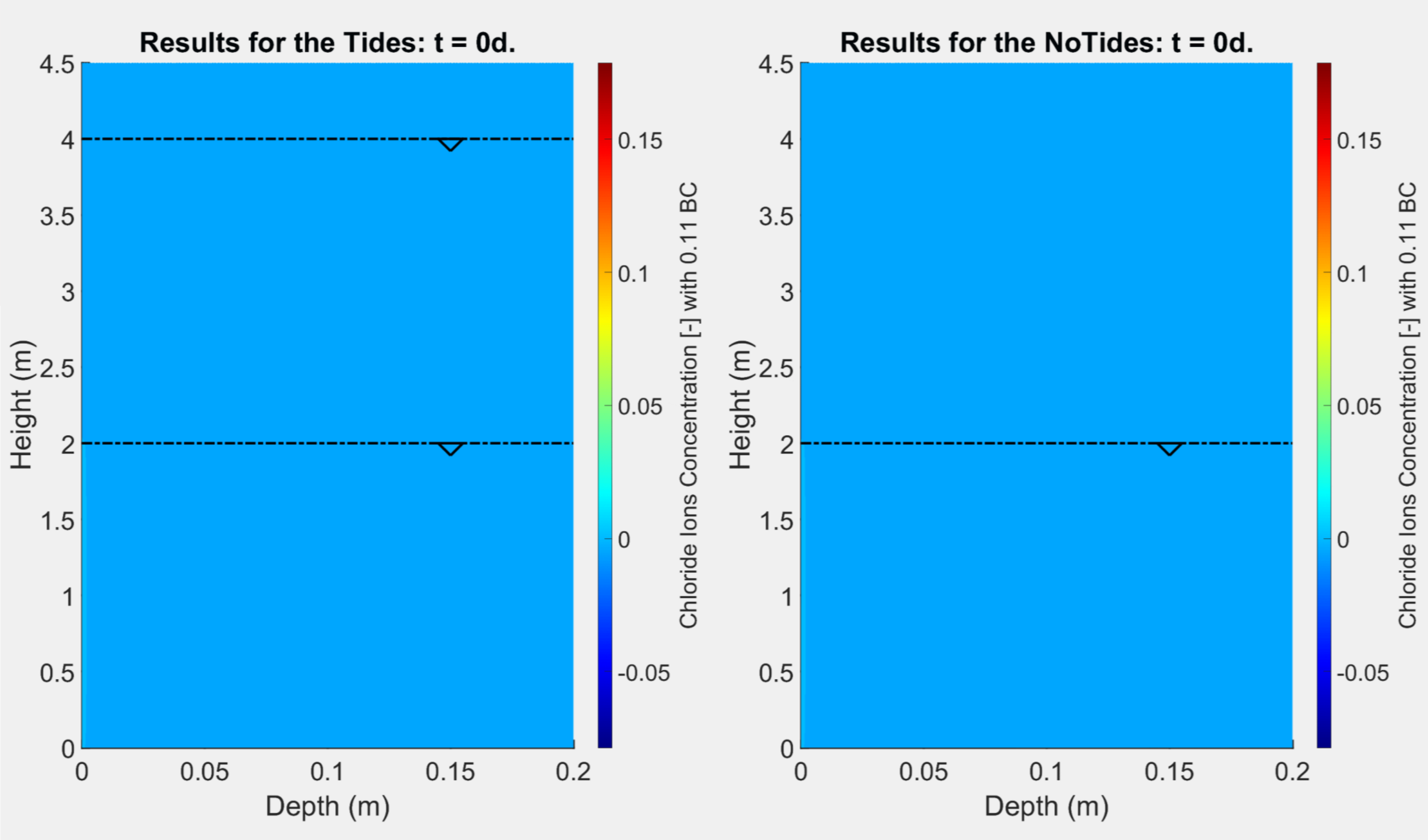


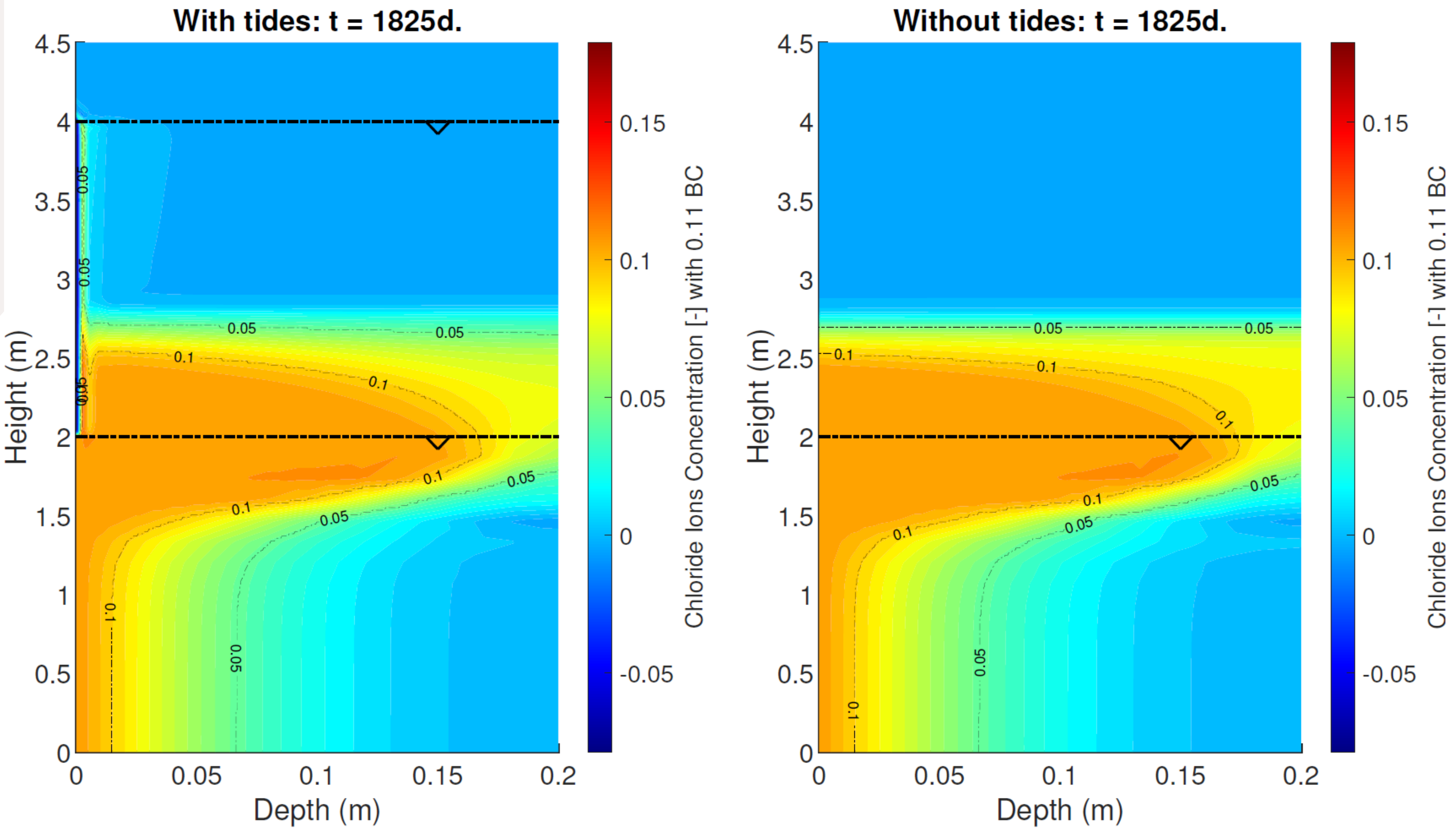
Application to a Real Life Scenario



Application to a Real Life Scenario



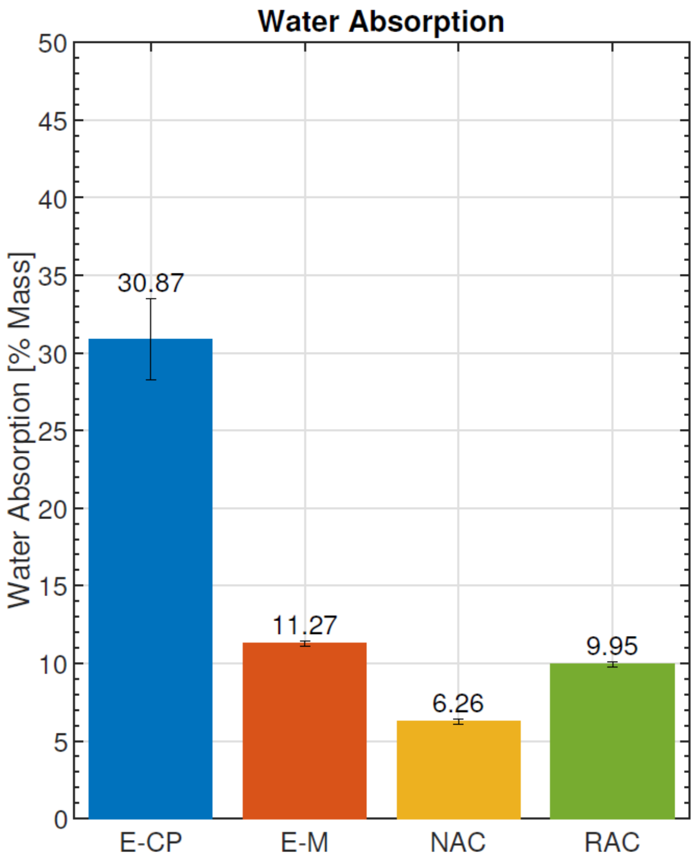
Application to a Real Life Scenario



Scientific Perspectives

- To increase the heterogeneity of concrete and make simulations more realistic, a **different RVE** could be used **for each integration point**.
- The creation of a database of RVE, with varying cement content, transport properties of the adherent mortar, and substitution rates of the aggregates, among other parameters.
- The **stiffness matrices** obtained by **perturbation** could only be calculated at the **initial iteration of each step** and then maintained at a constant value throughout the remainder of the current step.
- In terms of application of the model, it could be applied to **a road salt application** instead of obtaining chloride ions from seawater.
- It would be of interest to study concrete made from industrial recycled concrete aggregates with a **smaller substitution ratio**.

Water Absorption by Immersion



- Comparison of WA between the concrete and their aggregates:

$$\begin{cases} \Delta WA_{\text{NAC-RAC}} = WA_{\text{RAC}} - WA_{\text{NAC}} = 9.95 - 6.26 = 3.69\% \\ \Delta WA_{\text{NA-RCA}} = WA_{\text{RCA}} - WA_{\text{NA}} = 3.62 - 0.61 = 3.01\% \end{cases}$$

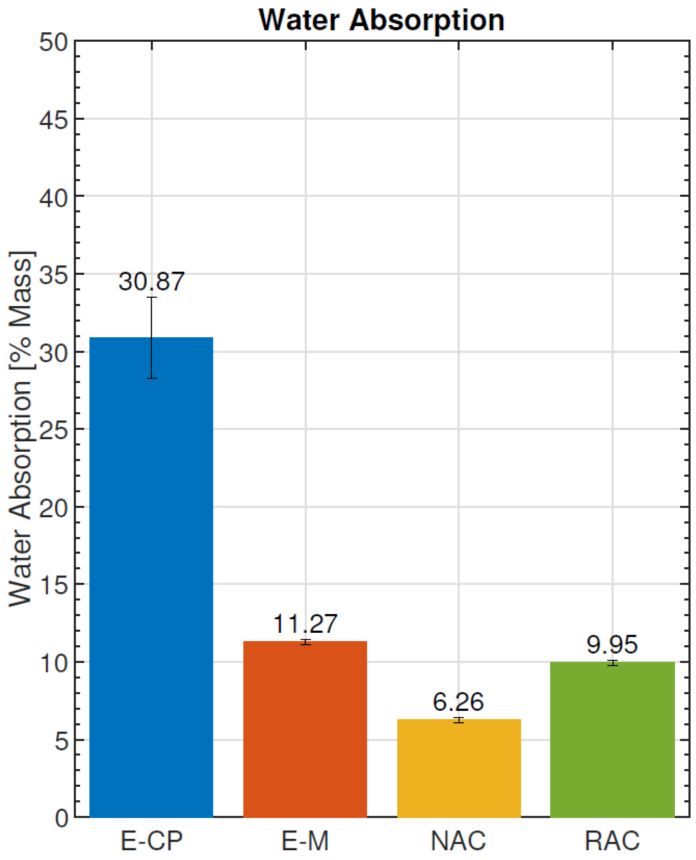
- Comparison of WA between the mortar of the concretes and the E-M:

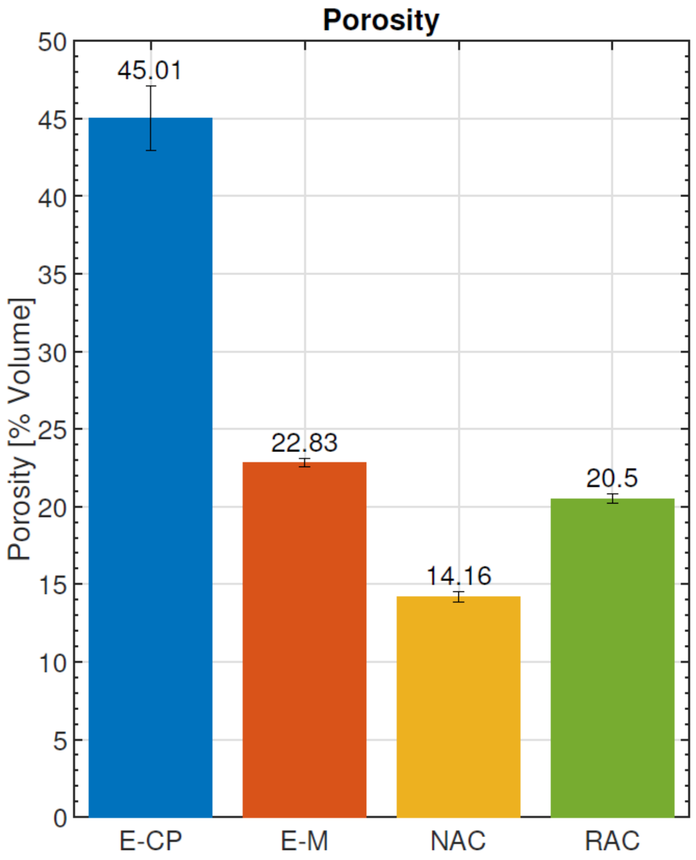
$$\begin{cases} WA_{\text{NAC}} = 5.95\% \text{ for } \frac{2247 - 1111}{2247} \times 100 = 50.55\% \longrightarrow WA = 11.77\% \text{ for } 100\% \text{ of mortar} \\ WA_{\text{RAC}} = 6.33\% \text{ for } \frac{2110 - 945}{2110} \times 100 = 55.21\% \longrightarrow WA = 11.46\% \text{ for } 100\% \text{ of mortar} \end{cases}$$

Experimental plan

- Water transfer properties
  - **Water Absorption by Immersion (WAI)**
    - Water absorption, porosity, and humid and dry densities
    - NBN B 15-215:2008, NBN EN 772-4, ASTM C 642-97
    - 100x100x10mm square plates.
  - Intrinsic Water Permeability experiment
  - Static Sorption and Desorption experiment

Water Absorption by Immersion





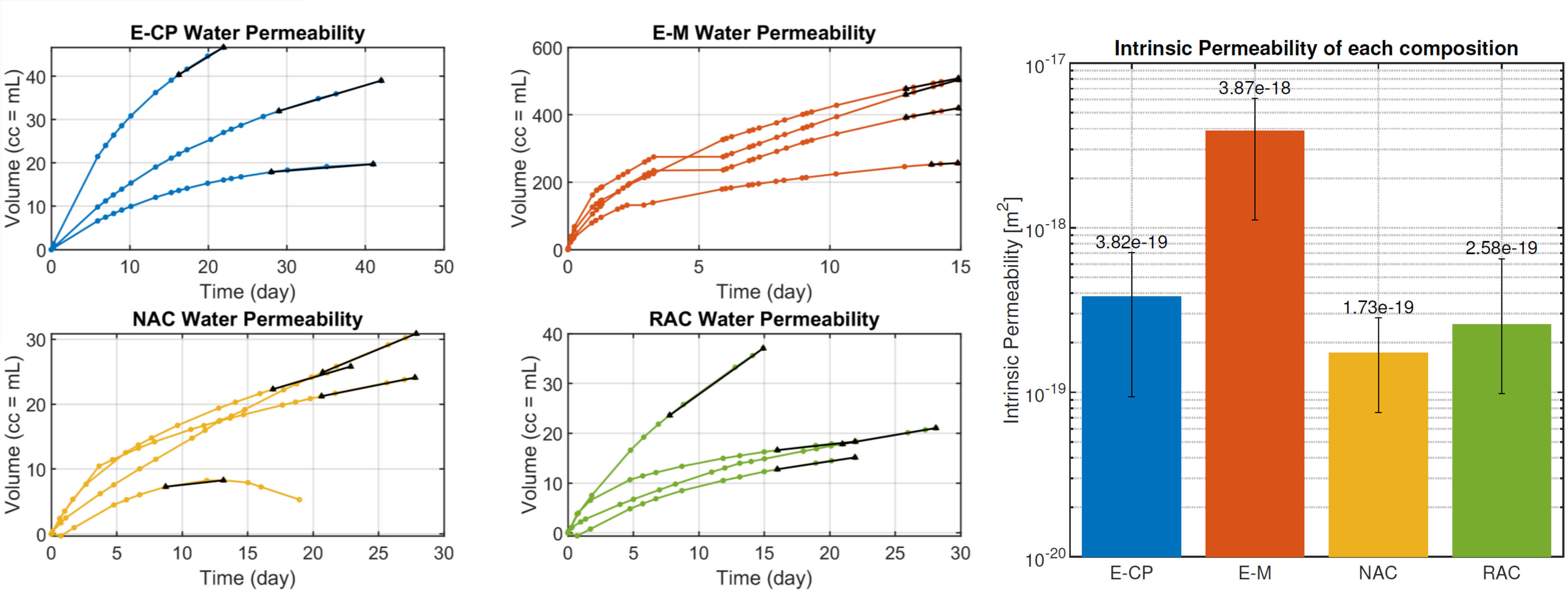
E-CP = Cement Paste
E-M = Mortar
NAC = Natural Aggregate Concrete
RAC = Recycled Aggregates Concrete

- Cement paste is more porous than the other materials;
- The greater the cement paste content, the greater the porosity.

Experimental plan

- Water transfer properties
  - Water Absorption by Immersion (WAI)
  - **Intrinsic Water Permeability experiment**
    - Water intrinsic permeability
    - NBN EN ISO 17892-11:2019.
    - 100x100mm cylinders.
  - Static Sorption and Desorption experiment

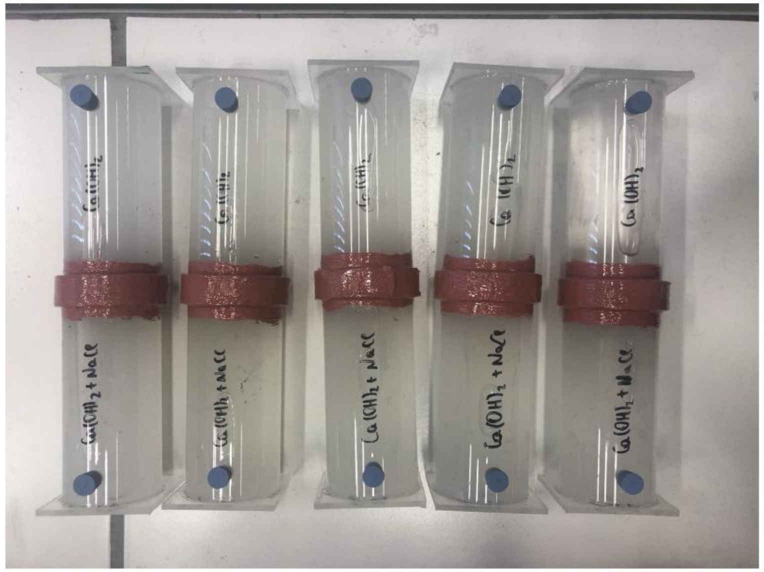
Water Permeability

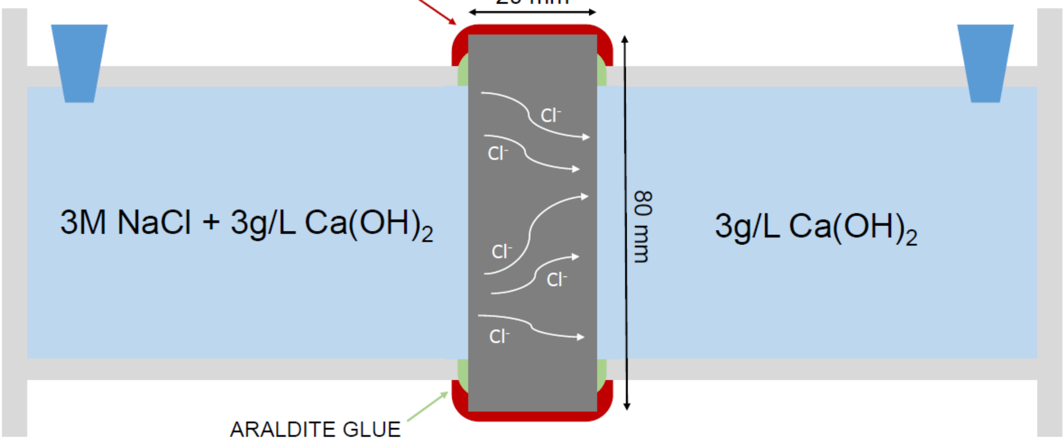


- Mortar’s porosity is coarser or more connected than the cement paste’s one;
- NAC and RAC have a similar intrinsic water permeability.

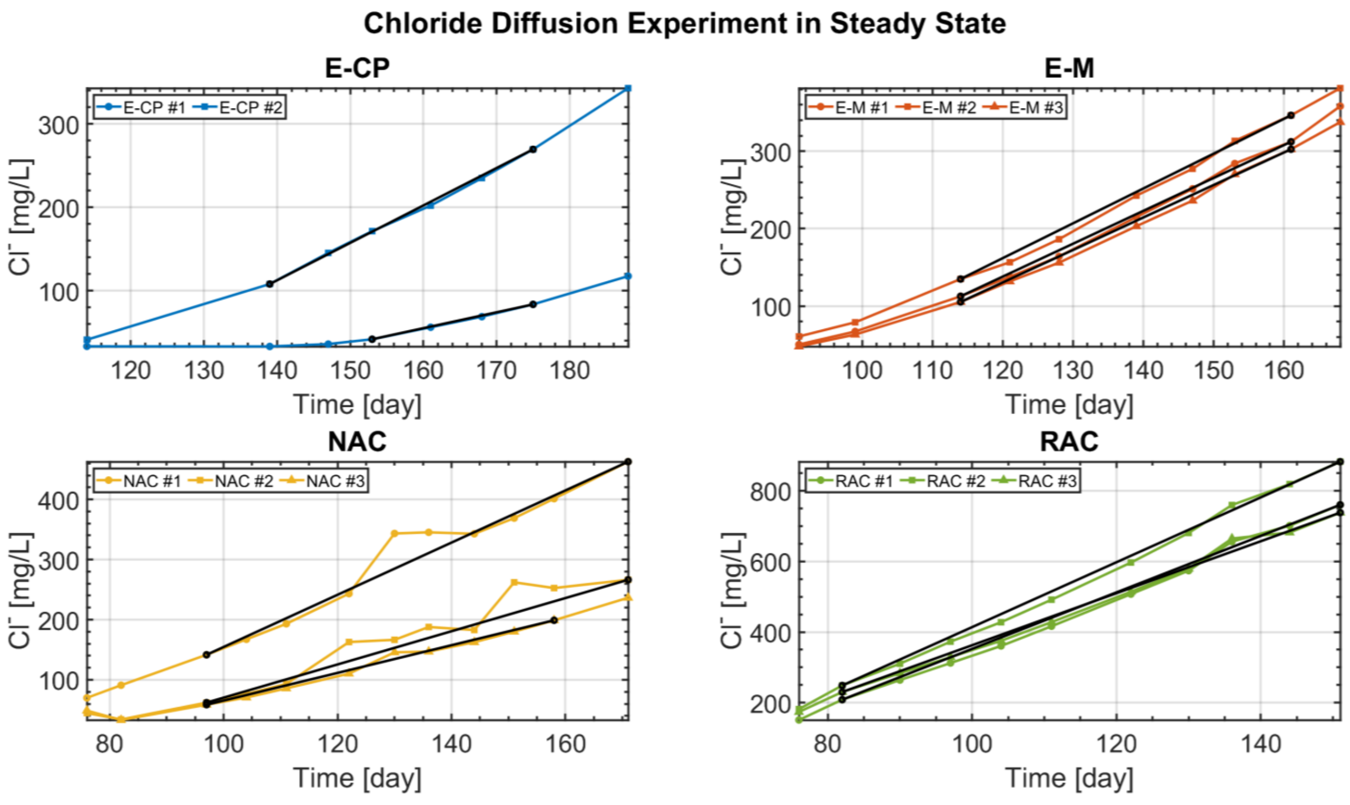
Experimental plan

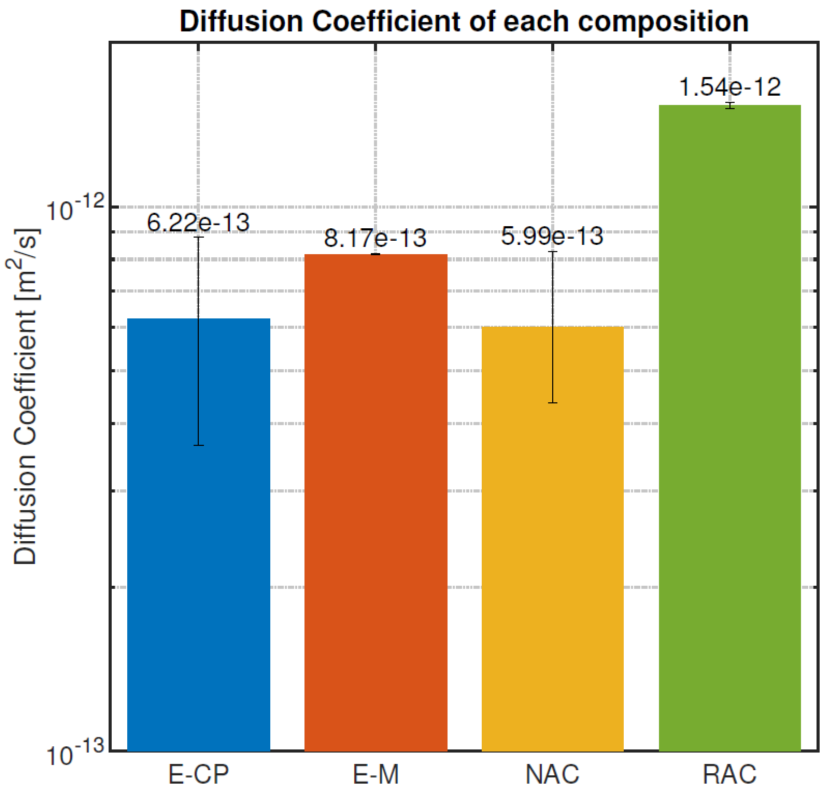
- Chloride ions transfer properties
  - **Chloride diffusion under steady-state**
    - Effective diffusion coefficient
    - 80x20mm cylinders.
  - Chloride diffusion under unsteady-state





Diffusion under Steady-State





- RAC is more diffusive than NAC;
- Not a significant difference in between the E-CP, E-M and NAC.

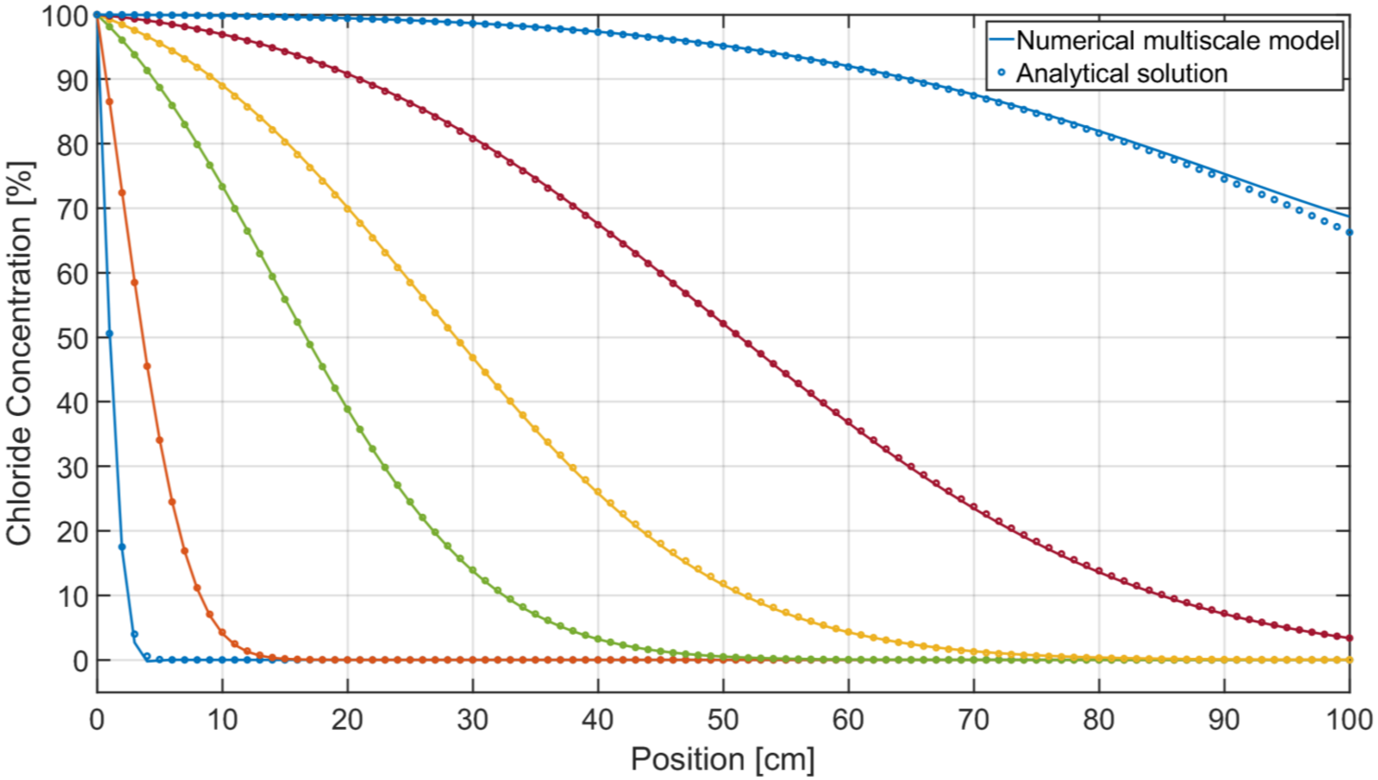
Numerical Approach

- Introduction to Multiscale Modelling;
- Model Constitutive Laws;
- Modelling of the RVE;
- **Validation of the Model;**
- Sensitivity Analysis;
- Application to a Lock Wall under Realistic Conditions.

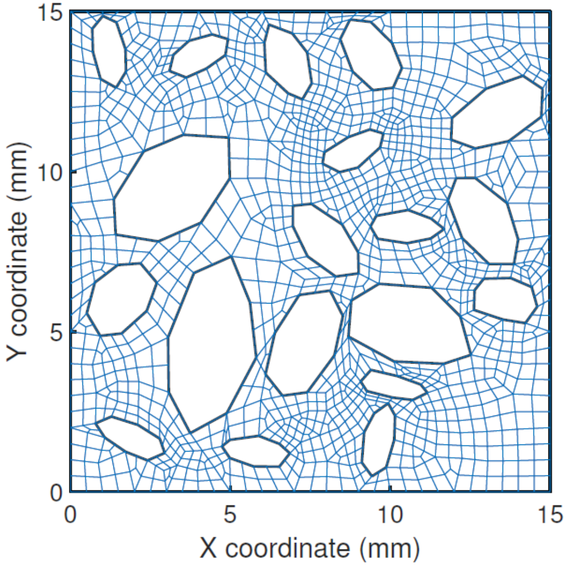
Validation: Saturated Conditions

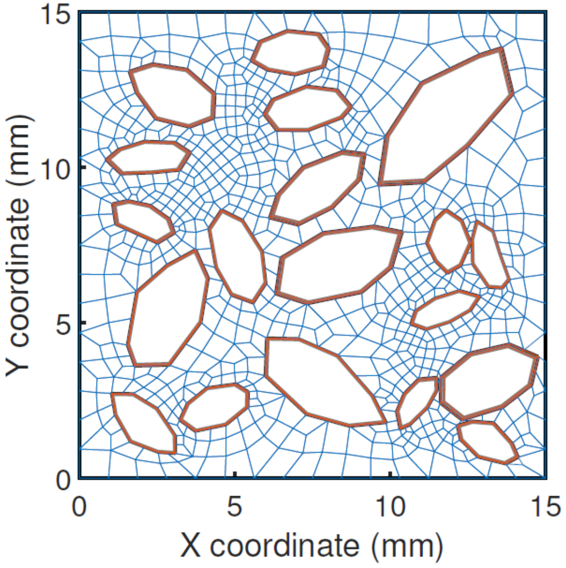
- Biver' solution (1993) for a 1D semi-infinite medium:

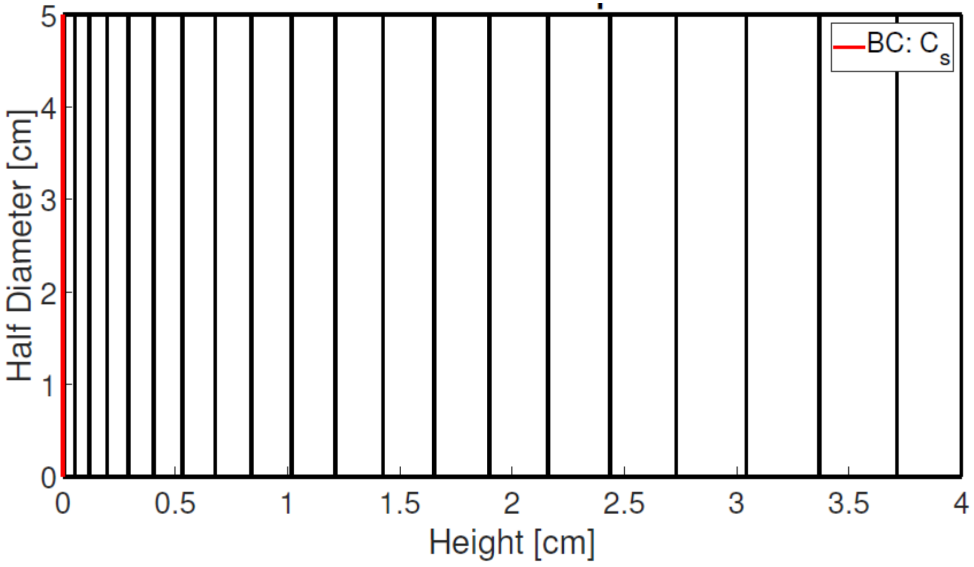
$$C(x,t) = \frac{C_0}{2}\exp\left(\frac{ux}{2D}\right)\left[\exp\left(-x\frac{u}{2D}\right)\operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}} - \sqrt{\frac{u^2t}{4D}}\right) + \exp\left(x\frac{u}{2D}\right)\operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}} + \sqrt{\frac{u^2t}{4D}}\right)\right] \text{ with } u = -\frac{k_{int}}{\mu_w}\times\frac{\partial P_w}{\partial x}$$



Validation: Experimental







Property	E-M	NAC	RAC	E-M +30%
Intrinsic Permeability [m^2]	3.87E-18	1.73E-19	2.58E-19	5.02E-18
Porosity [% Volume]	22.83	14.16	20.50	29.68
Diffusion Coefficient [m^2/s]	1.43E-11	1.41E-11	1.65E-11	1.86E-11
C_s [-]	1.45	0.78	1.27	

Validation: Experimental NAC

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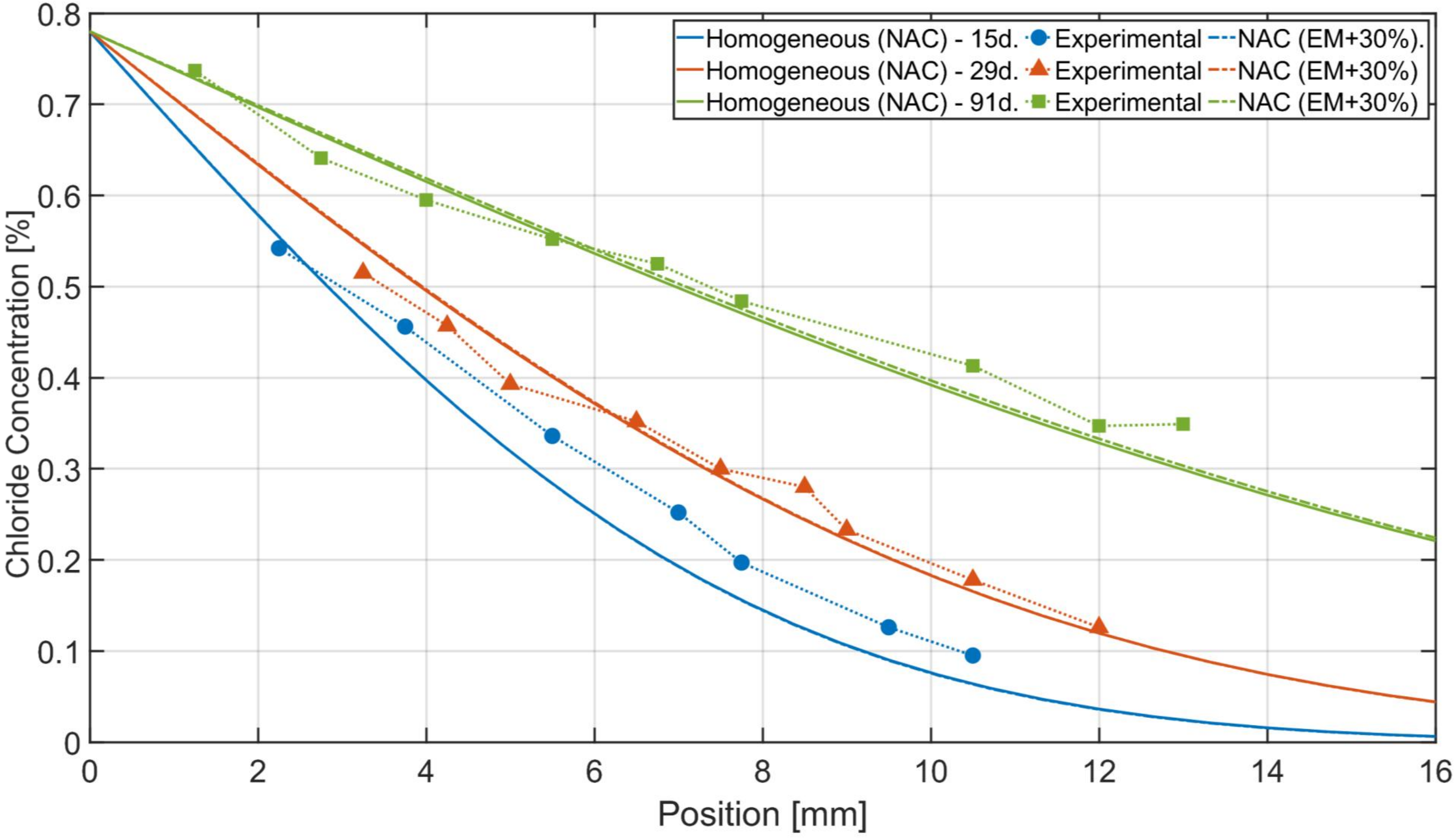
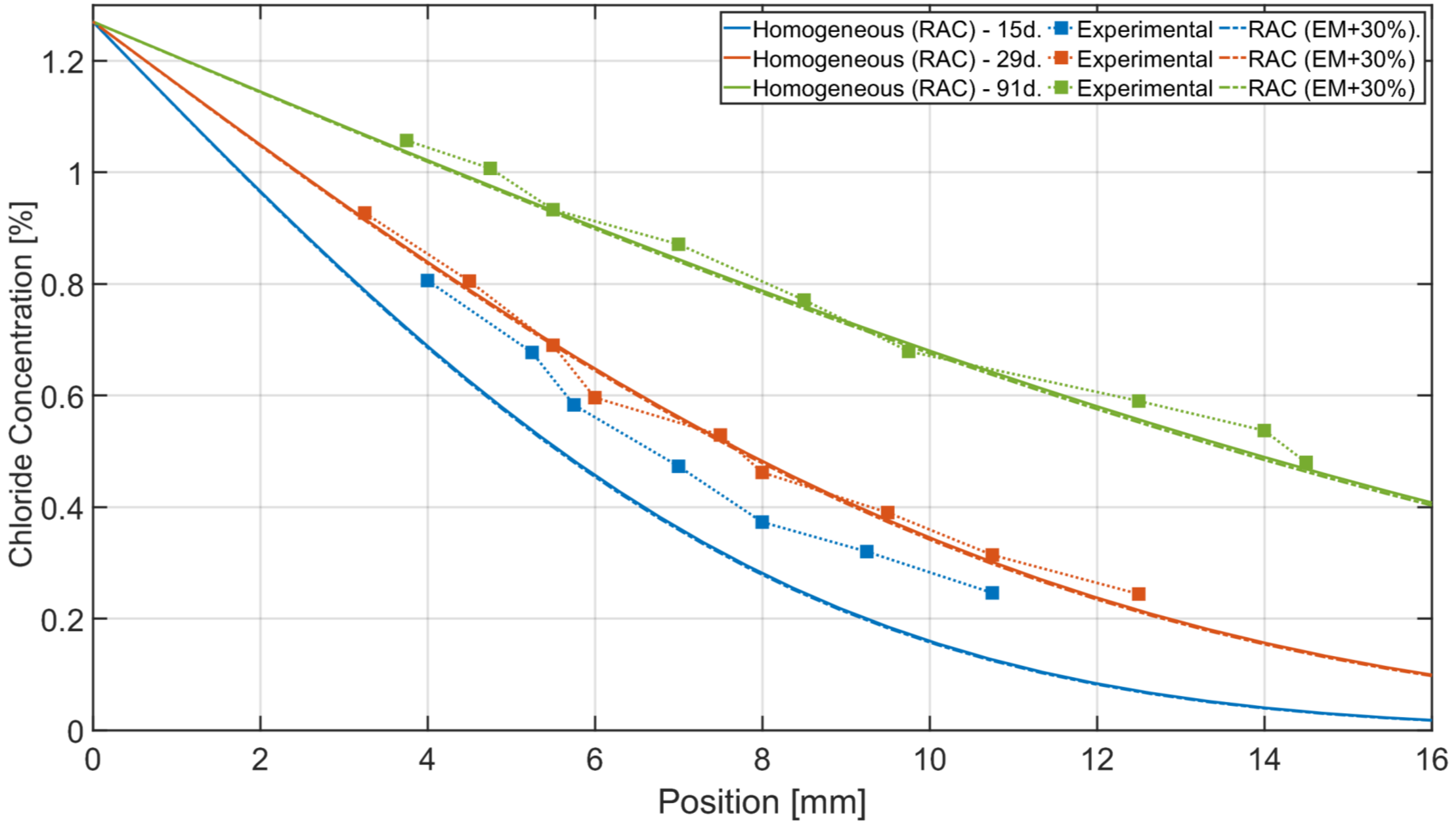
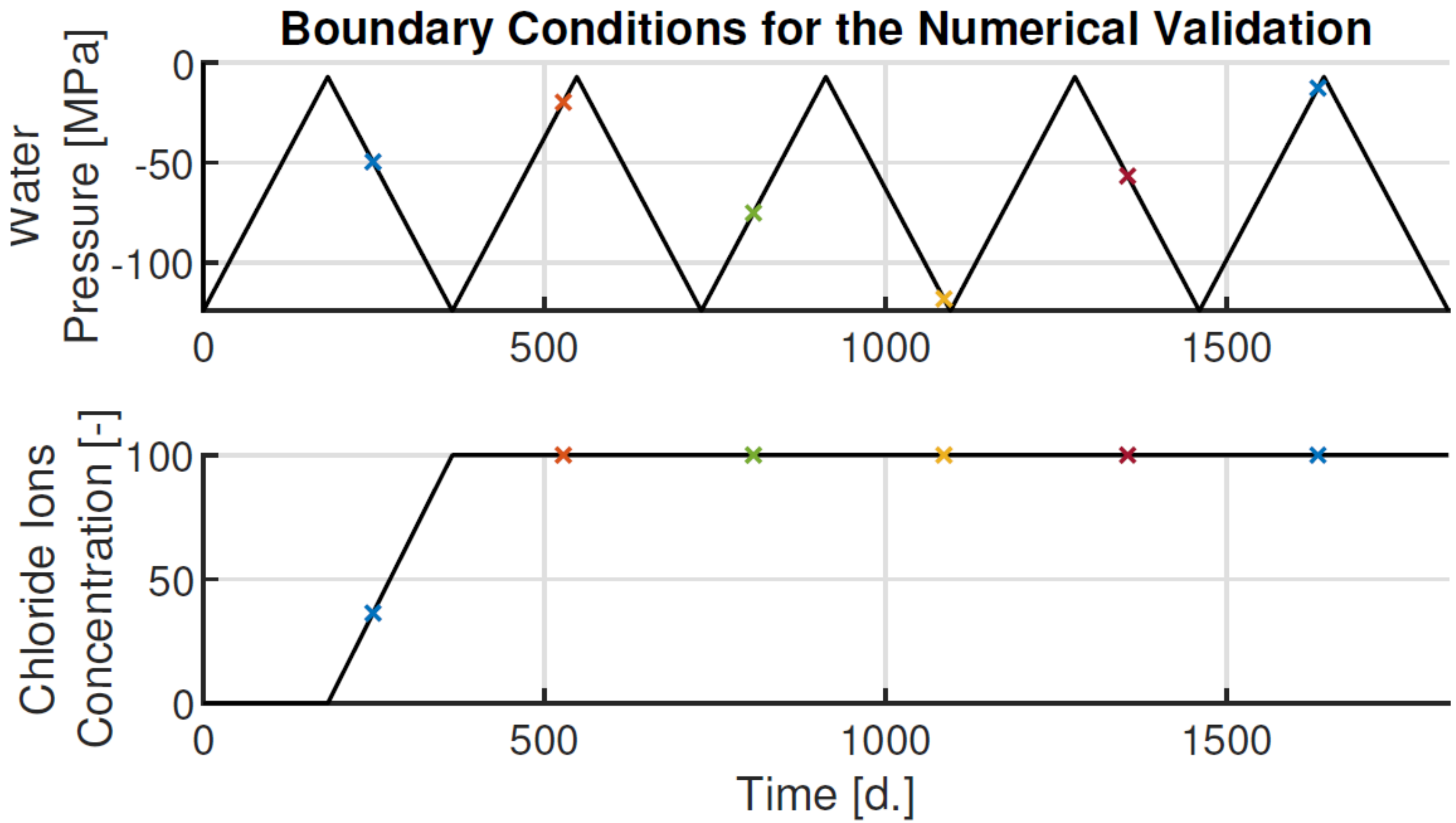


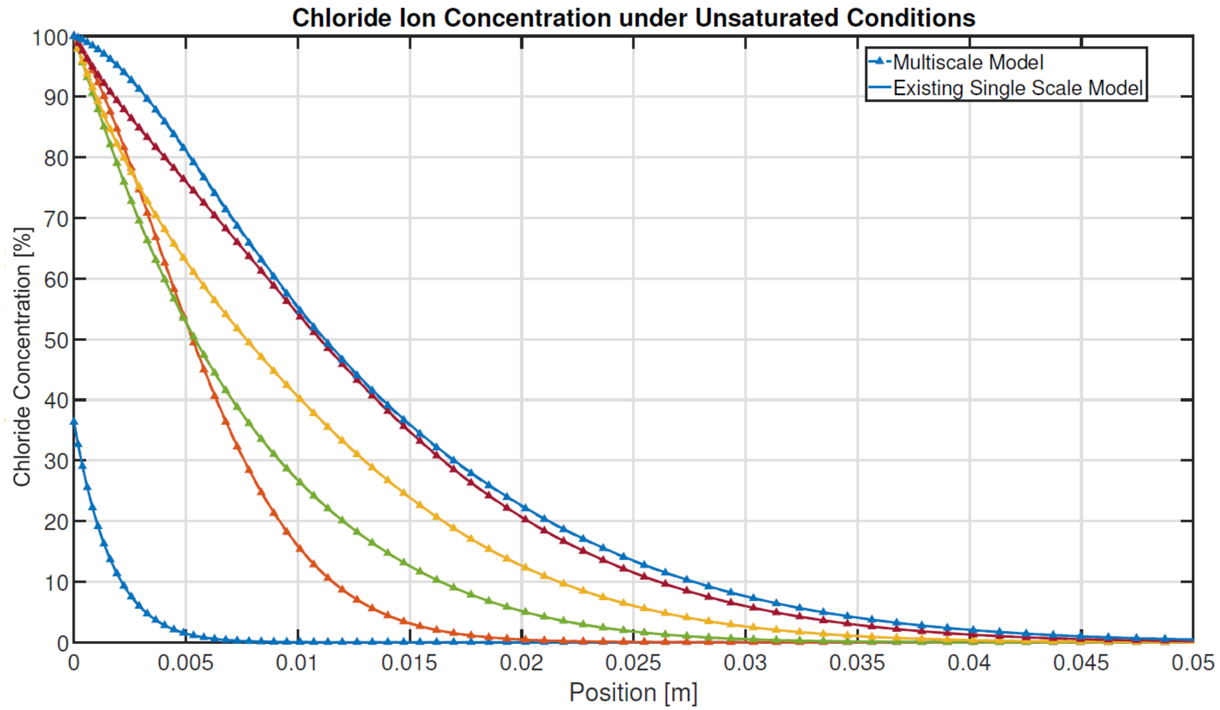
Validation: Experimental RAC

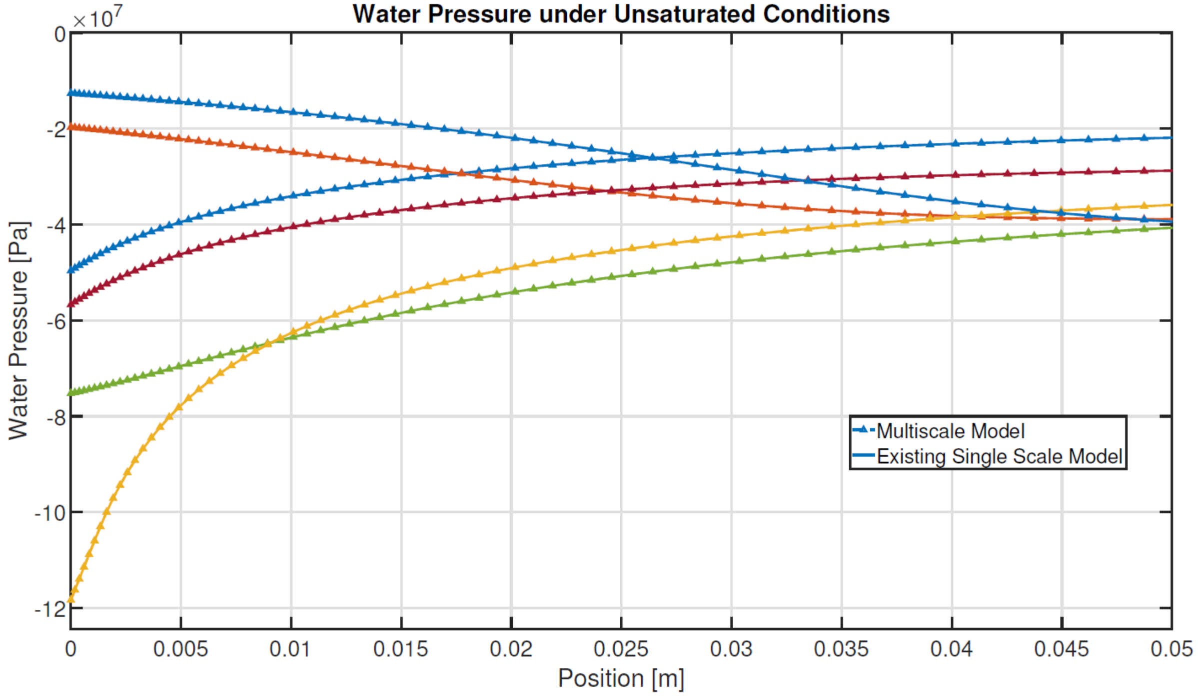


Validation: Unsaturated Conditions



Validation: Unsaturated Conditions





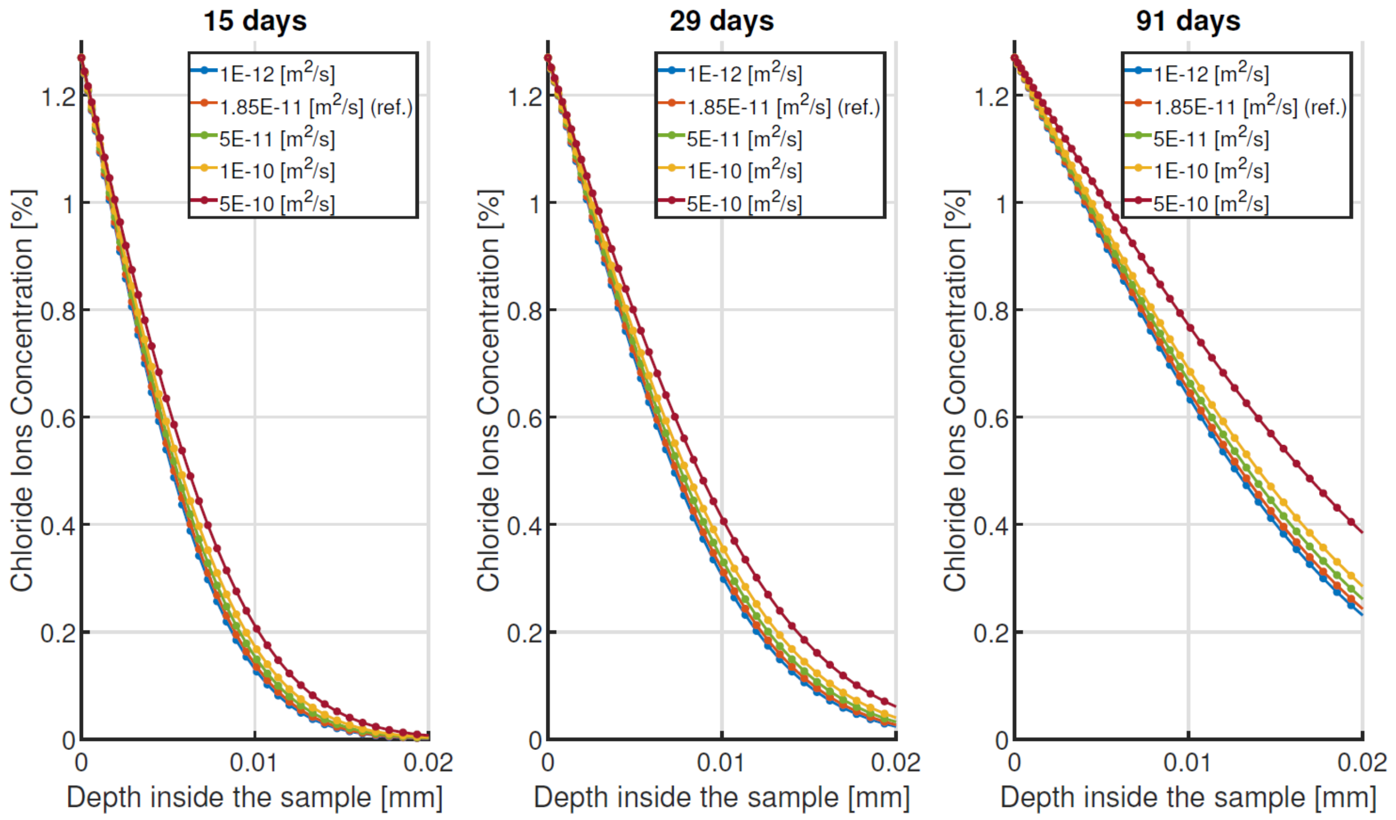
Numerical Approach

- Introduction to Multiscale Modelling;
- Model Constitutive Laws;
- Modelling of the RVE;
- Validation of the Model;
- **Sensitivity Analysis;**
- Application to a Lock Wall under Realistic Conditions.

Influence of RCA's diffusion coefficient

Mortar Matrix's Properties					
Intrinsic Permeability [m^2]			5.03E-18		
Porosity [% Volume]			29.68		
Diffusion Coefficient [m^2/s]			1.85E-11		
Adherent Mortar's Properties					
Intrinsic Permeability [m^2]			5.03E-18		
Porosity [% Volume]			29.68		
Diffusion Coefficient [m^2/s]	1E-10	5E-10	1.85E-11	5E-11	1E-12

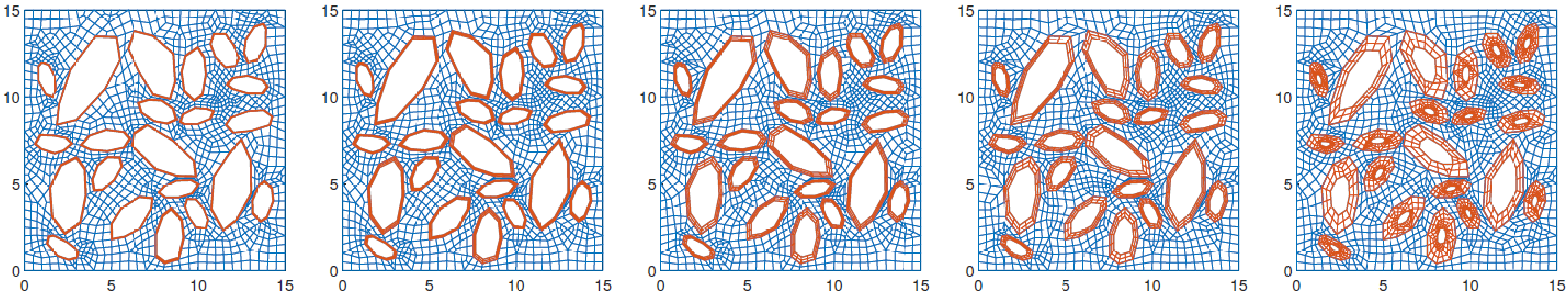
Influence of RCA’s diffusion coefficient



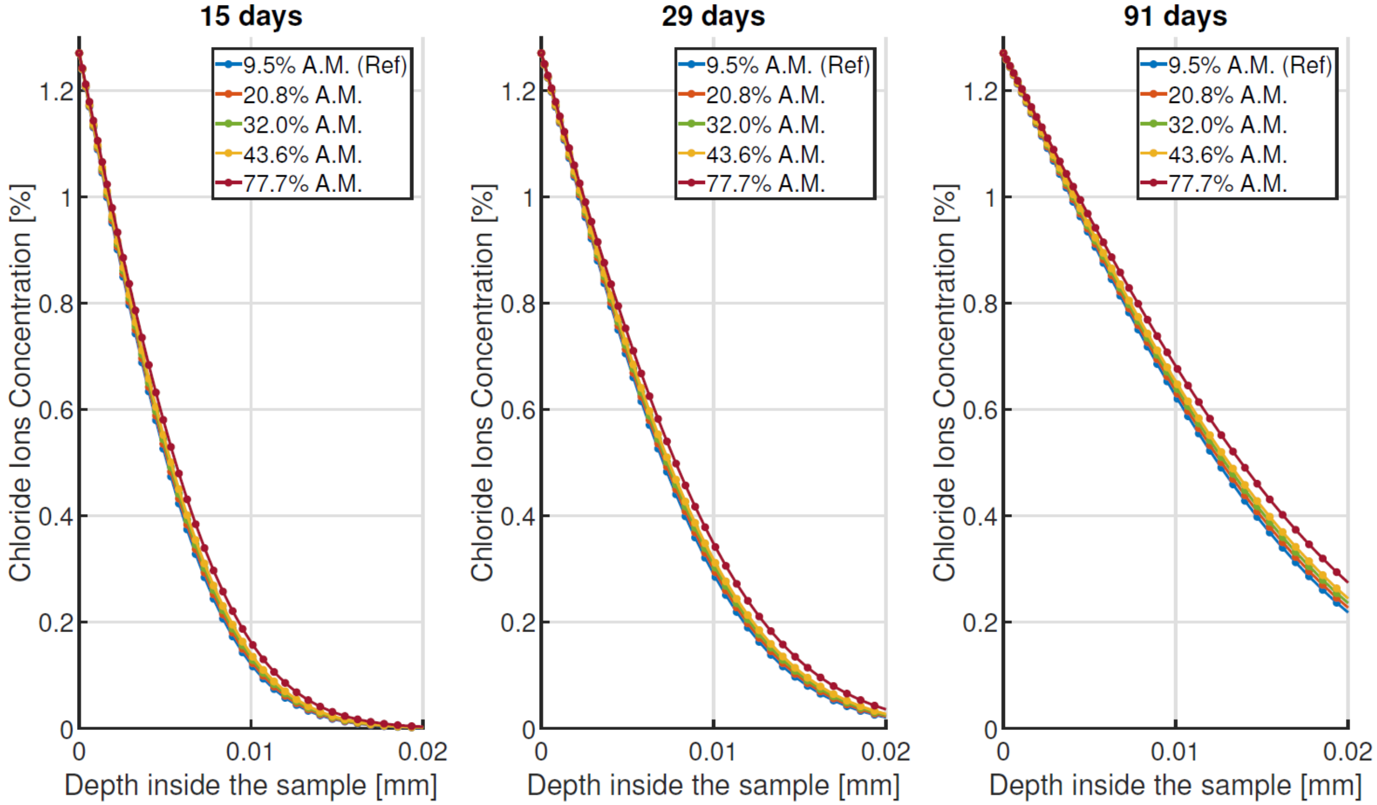
Diffusion Coefficient [m²/s]	1E-12	1.85E-11 (Ref.)	5E-11	1E-10	5E-10
Diffusion Coefficient [% Ref.]	5.40	100	270.27	540.54	2702.70
Results at 15 days [% Ref.]	98.72	100	101.94	104.54	115.77
Results at 29 days [% Ref.]	98.75	100	101.91	104.41	115.31
Results at 91 days [% Ref.]	98.81	100	101.82	104.21	114.63

Influence of RCA's cement content

Simulation	Reference	x 2	x 3	x 4	x 7
Mortar paste (% overall surface)			66.3		
Adherent Mortar (% overall surface)	3.2	7.0	10.8	14.7	26.2
Adherent Mortar (% RCA' surface)	9.49	20.77	32.05	43.62	77.74

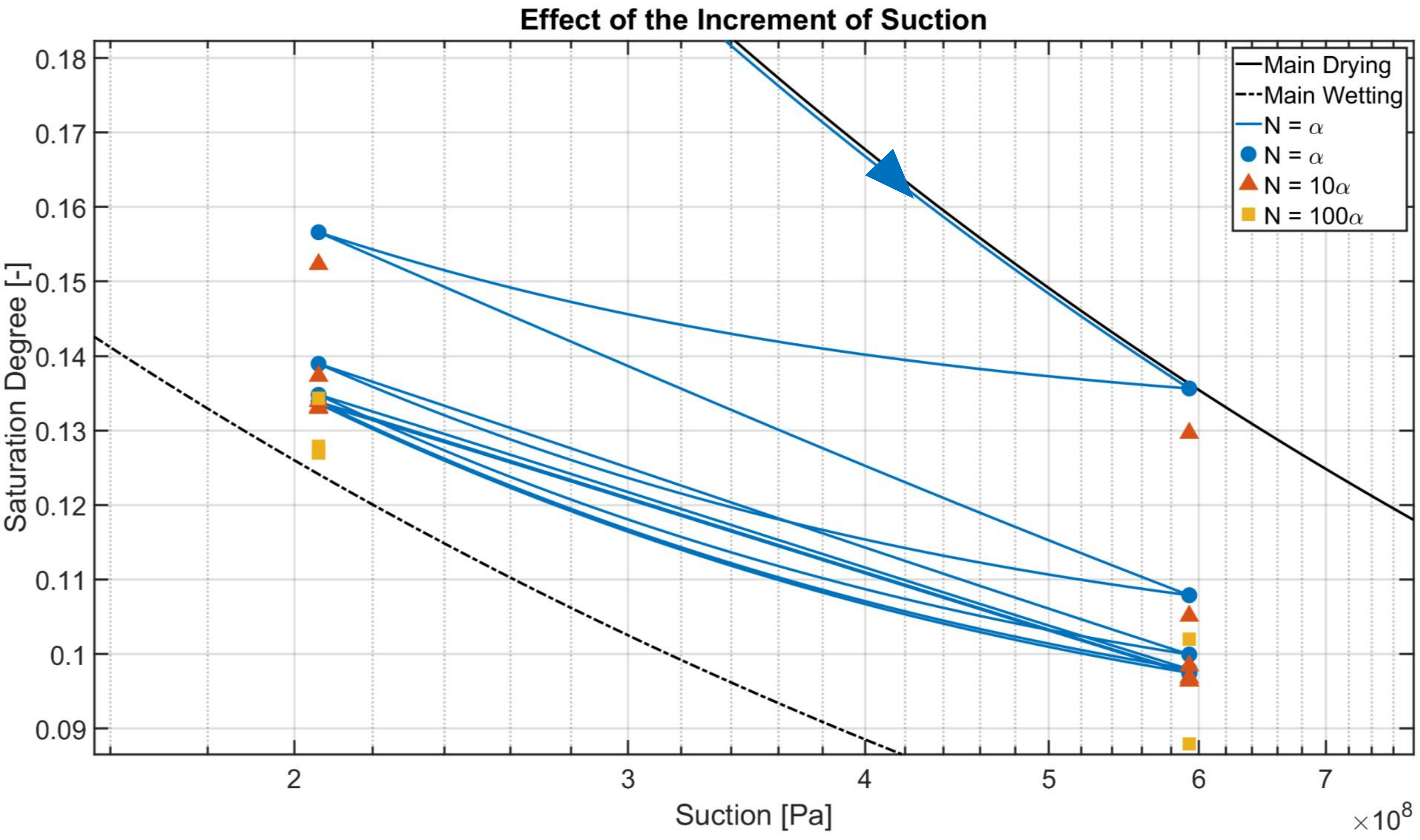


Influence of RCA's cement content

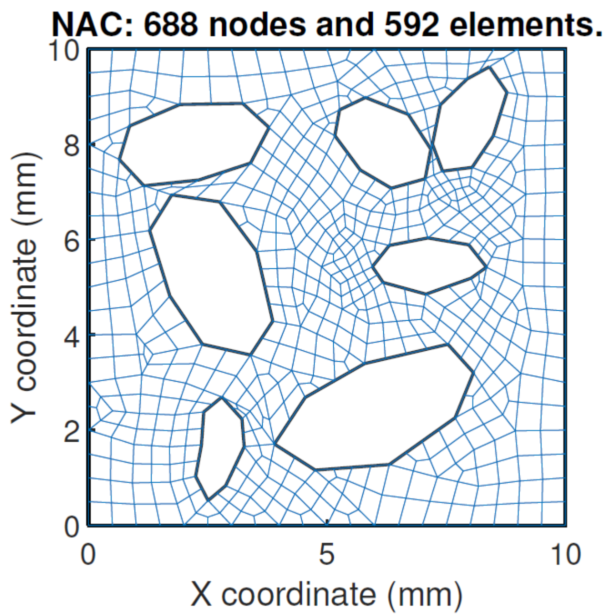


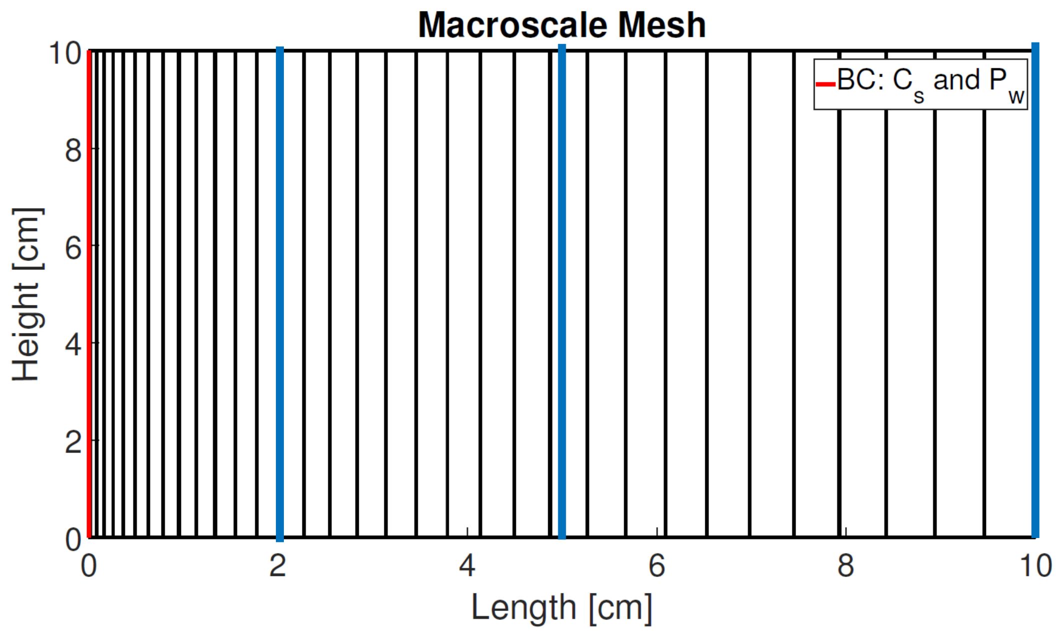
Simulation	Reference	x 2	x 3	x 4	x 7
Adherent Mortar (% Ref.)	100	218.7	337.5	459.4	818.7
Results at 15 days (% Ref.)	100	100.93	101.81	102.72	105.83
Results at 29 days (% Ref.)	100	100.91	101.76	102.65	105.66
Results at 91 days (% Ref.)	100	100.87	101.68	102.53	105.40

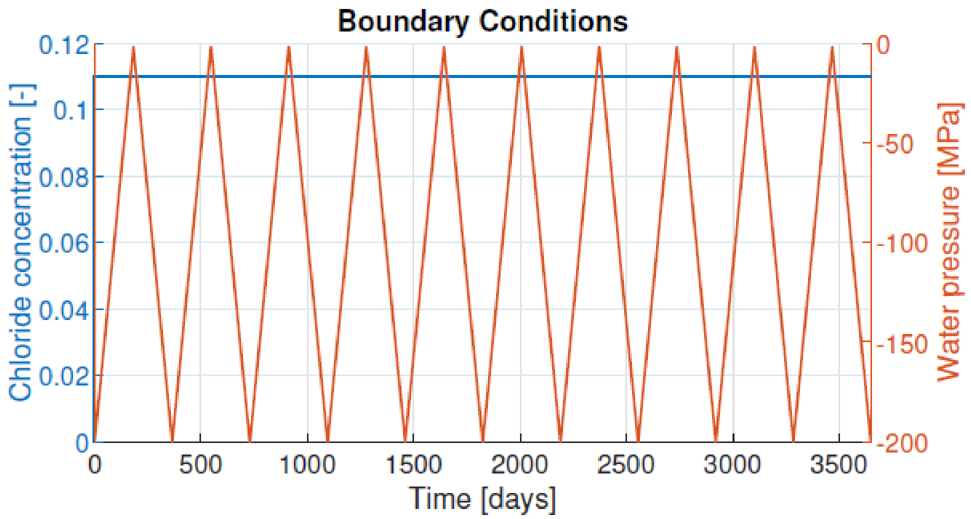
Influence of the hysteresis' parameters



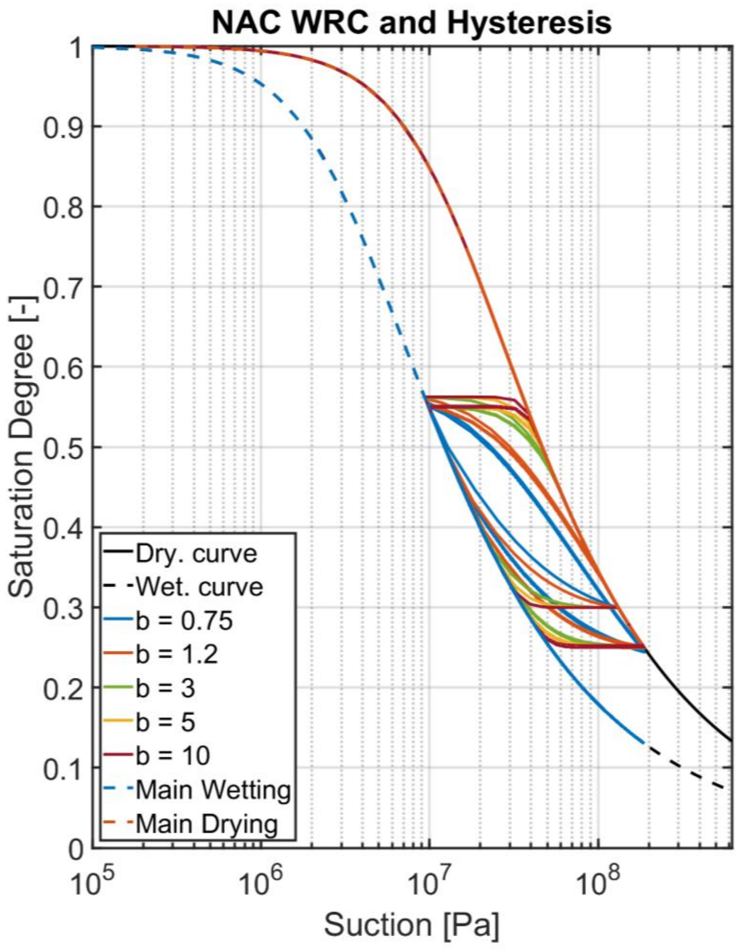
Influence of the hysteresis' parameters

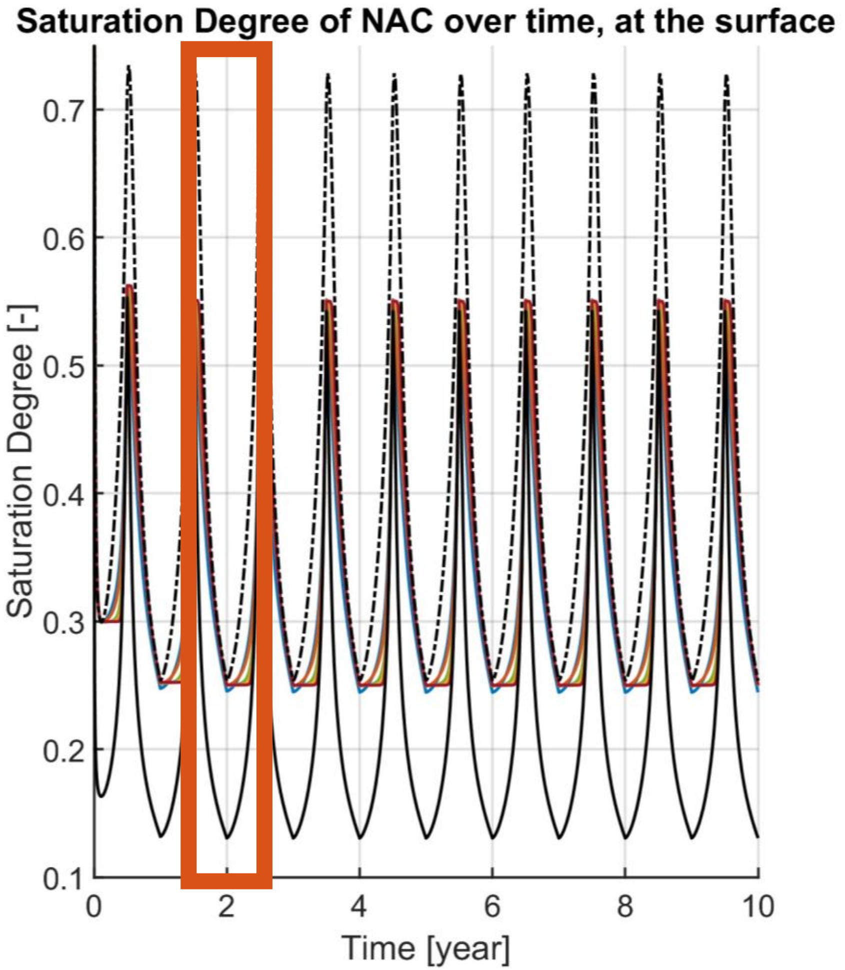


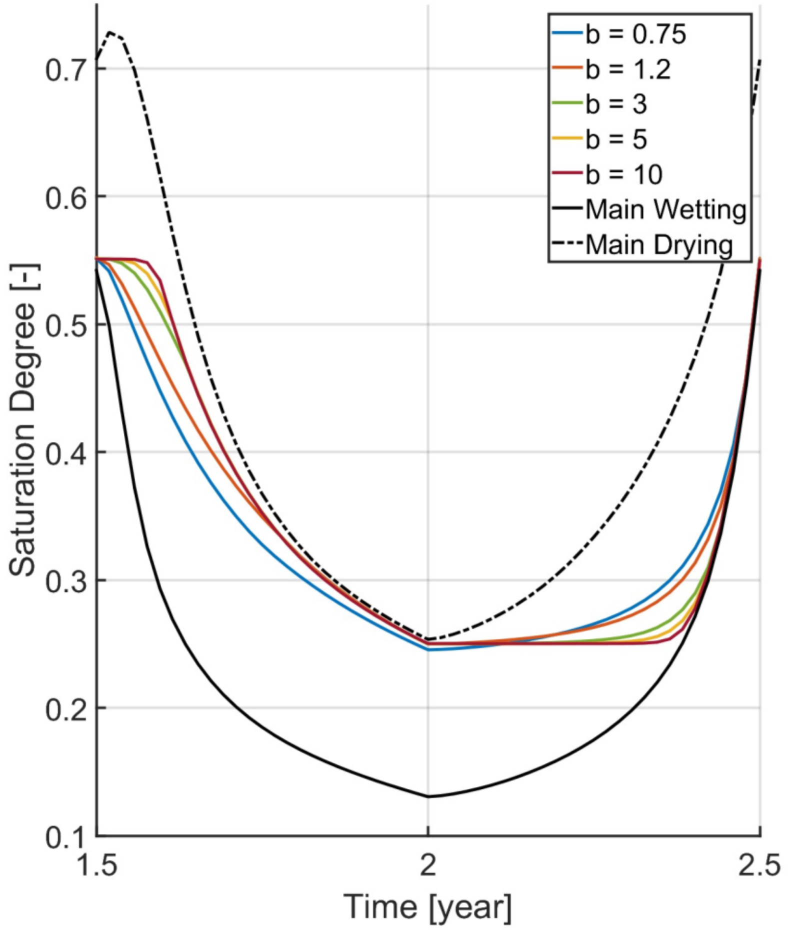




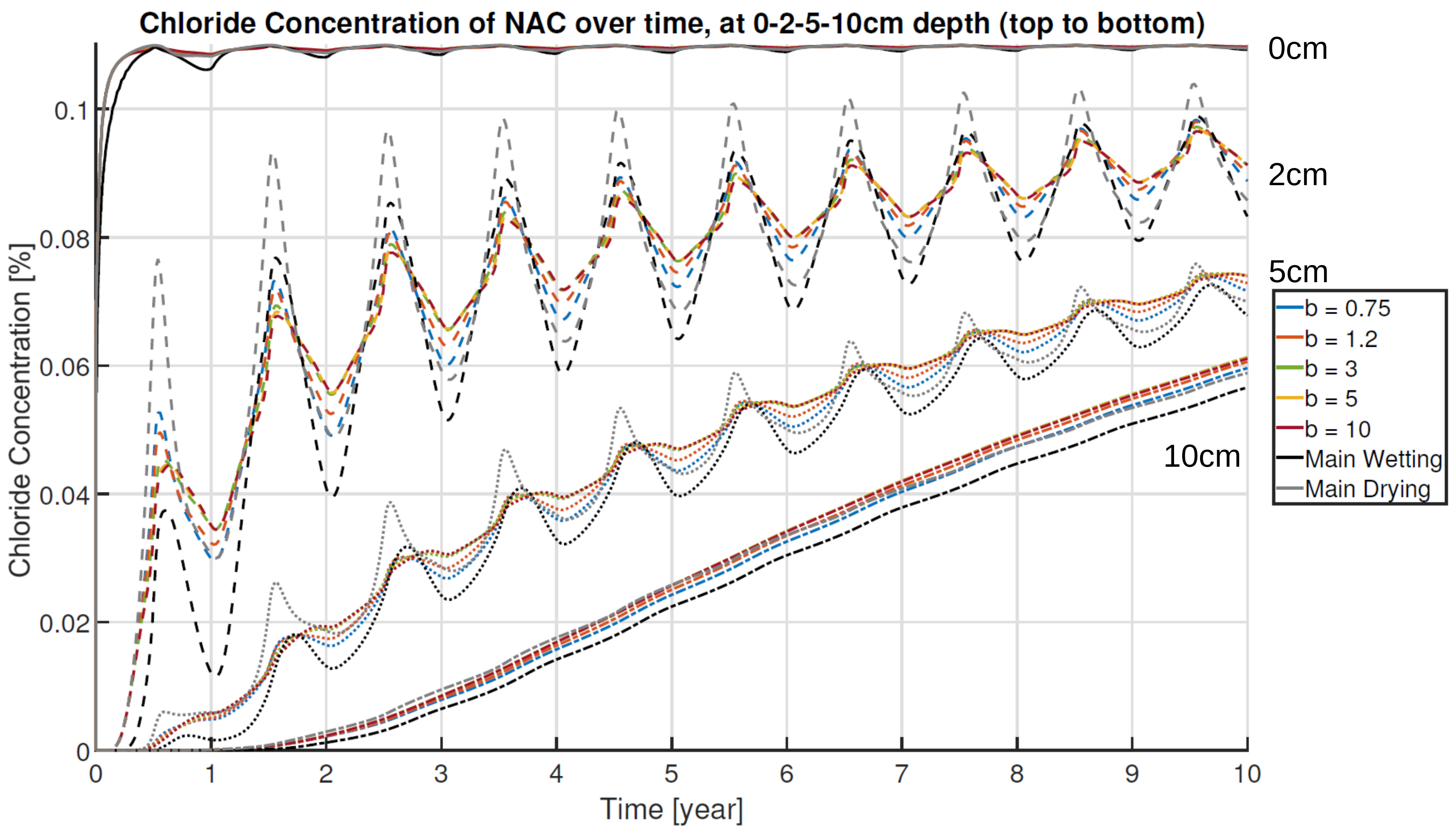
Influence of the hysteresis' parameters

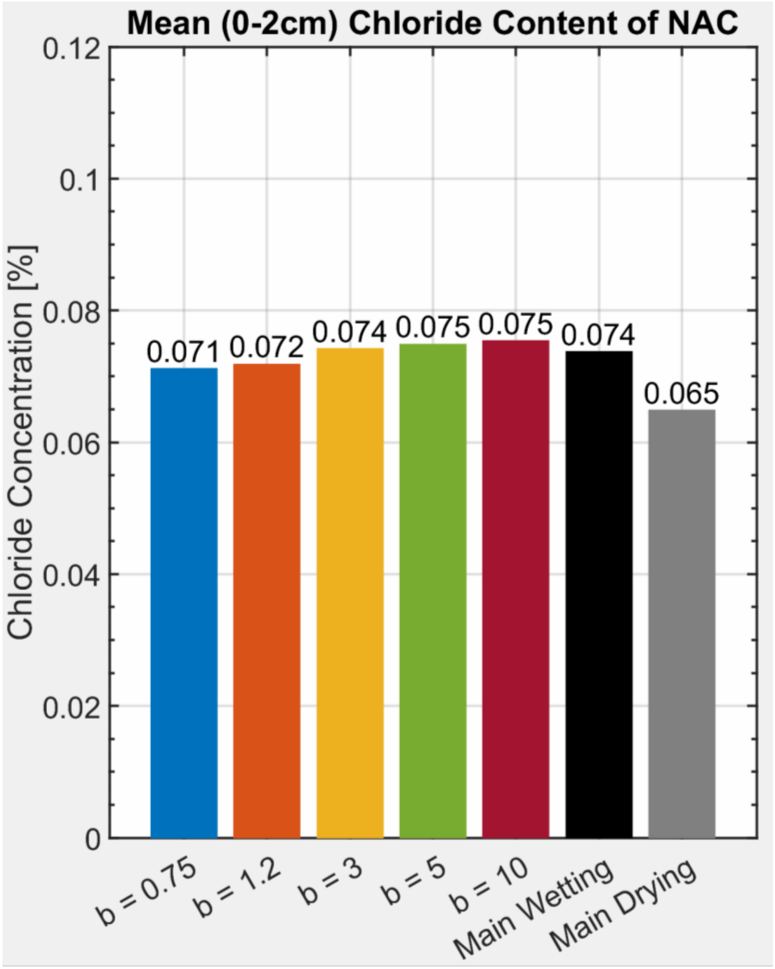






Influence of the hysteresis' parameters





Original Contributions

The principal **experimental** contributions of this work are as follows:

- The study of the **water retention curves** and their **hysteresis** in **concrete**.
- The study of **chloride ions diffusion**, in steady and unsteady state, in **recycled aggregates concrete**.

The main **numerical** contributions of this work include:

- The development of a **multiscale model** that couples the transport of **water** and **pollutants**, specifically chloride ions in this case.
- The **implementation of a hysteresis model** that follows the Van Genuchten model for Water Retention Curves.
- The creation of an **algorithm to generate a RVE** that emulates a concrete slice.

Scientific Perspectives

- Regarding the ingress of chloride ions, our model could be improved by introducing **adsorption isotherms of chloride ions**;
- Additional processes, such as **carbonation** or **alkali-aggregate reactions**, could be incorporated into the model. The **corrosion reactions** could be implemented.
- A new degree of freedom, **temperature**, could also be added to the model;
- In terms of modelling the mesoscale, a **3D model** could be developed to significantly increase accuracy and eliminate the need to increase the intrinsic properties of the mortar by 30%.