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Finite Element Modeling of Chloride Ion Ingress and Reinforcement Bar Depassivation in UHPC

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Abstract. This study addresses the challenge of predicting chloride ingress in UHPC and depassivation of reinforcing steel, which is essential for durability assessment. A numerical model was calibrated using experimental data to estimate the time for chloride to reach the critical threshold (0.3%) at reinforcement depth. Simulations considered cover depths of 15, 20, and 25 mm under chloride concentrations of 0.5% and 1.95%. Results show that under low chloride exposure, the UHPC cover can protect steel for more than 100 years before depassivation, whereas under severe marine conditions, this duration drops to 16–25 years, depending on the cover. Matrix diffusivity and chloride concentration are the key parameters governing chloride ingress and the time to reach 0.3% at reinforcement depth, critically influencing service-life prediction. Numerical simulation proved efficient in overcoming the time limitations of experimental programs and supports service-life design.

Keywords: UHPC, Chloride ingress, service life predication.

1 Introduction

Concrete structures located in aggressive environments are exposed to ion ingress, for example, chloride ions, which can lead to the corrosion of reinforcing steel. This process may result in high maintenance costs and compromise the structural safety [1].

For this reason, utilizing advanced materials such as Ultra-High Performance Concrete (UHPC) is a prominent solution to increase the lifespan of structures in aggressive environments. UHPC has lower porosity than conventional concrete due to the dense particle packing, which can result in reduced chloride ion ingress [2,3]. Many studies, employing analytical, experimental, and numerical methods, have focused on determining the apparent chloride diffusivity of plain concrete and UHPC, as well as analyzing chloride ingress, calibrating numerical models, and examining the transition zone between the matrix and aggregates [4–11]. Wang and Kim [7] conducted a parametric study of a UHPC bridge deck with reinforcing bar covers of 50 mm and 75 mm to predict the time to initiation of depassivation (0.4%) under a surface chloride concentration of 3.5 kg/m³. However,

the French standard NF P 18-470 [12] specifies cover depths of 15, 20, and 25 mm for aggressive environments, depending on the exposure class. For such cases, few studies have explored this type of prediction.
Due to the very low porosity of UHPC, which lacks capillary pores [13], studies have shown that it is challenging to observe reinforcement depassivation at threshold chloride concentrations using standardized experimental methods, primarily due to the limited duration of typical testing programs. For UHPC, the threshold concentration to initiate the depassivation of embedded reinforcement is in the range of 0.3–0.5%[14]. Ahmad *et al.* [15] showed that after six months, the chloride concentration at a depth of 20 mm was approximately 0.1%. Soares *et al*. [5] reported a concentration of 0.18% at a depth of 10 mm after 311 days. Therefore, determining the time to reach the beginning of the depassivation experimentally requires significant time and effort, making numerical simulation a promising alternative for this purpose, not been deeply explored for UHPC.
Therefore, this study aims to calibrate a numerical model of chloride ion ingress in UHPC using the Abaqus software. Additionally, parametric studies are conducted to estimate the number of years required for chloride ingress to initiate the depassivation of embedded reinforcing bars with varying concrete covers.

2 Methodology

Three experimental programs on chloride ion ingress in UHPC were used to validate the numerical model. Table 1 presents the adopted experimental methods, average compressive strength, diffusion coefficient, specimen dimensions, chloride solution, exposure time in solution, and references, respectively.

Table 1. Chloride ion ingress experimental programs in UHPC

	Method	Compressive strength (MPa)	Diffusion Coef. (m²/s)	Dimensions (mm)	Chloride solution (%)	Time (Days)	Reference
Exp.A	Standard UNE-EN 12390-11:2019	150	3.0 E-13	Ø100 x 100	3,0	90	[4]
Exp.B	Nordtest method NT Build 443 (1995)	140 – 160	2.0 E-13	Ø90 x 100	16,5	90	[11]
Exp.C	Método de Volhard	167	-	Ø50 x 100	3,5	311	[5]
	NT BUILD 492		1.96E-13	Ø50 x 100	3,5	28	

2.1 Numerical modeling

The numerical chloride ion ingress simulation was made on Abaqus Standard. The diffusion analysis consists of transient mass diffusion. The chloride ion transport gradient, temperature effects, hydrostatic pressure, and non-uniform solubility of the material are accounted for. This model is particularly suitable for describing the spontaneous movement of particles in porous materials from regions of higher concentration to those of lower concentration. It is especially suitable for simulating the behavior of concrete under aggressive environmental conditions. The diffusion problem is formulated based on the mass conservation principle of the diffusive phase, as expressed in Eq. (1):

$$\int_V \frac{\partial c}{\partial x} dV + \int_V n \, \mathrm{J} \, dS = 0 \tag{1}$$

Where c is the mass concentration of the diffusing substance, and J is the concentration flux vector. V is the control volume, and S is the surface enclosing V. The vector n denotes the outward normal to S. In Abaqus, the primary solution variable is the normalized concentration ϕ, defined as $\phi = c/s$, where s is the solubility in the base material. The flux J indicates the direction of diffusion of chemical potential, for example, a concentration gradient of chloride ions. The constitutive flux equation, Eq. (2), is based on the generalized chemical potential and represents an extended form of Fick's law.

$$\mathrm{J} = -\mathrm{s}\,\mathrm{D}\,[\nabla \phi + K_s \nabla \ln(\theta - \theta^0) + K_p \nabla p_{eff} \tag{2}$$

Here, s is the solubility; D is diffusivity; K_s is the Soret effect factor, θ is the absolute temperature and θ^0 is the absolute zero reference temperature. K_p is the pressure stress factor, and $p_{eff} = -tr(\sigma)/3$ is the equivalent pressure, defined as the average of the principal stresses. This general formulation is particularly useful when modeling environments where multiple transport mechanisms act simultaneously, such as heat, moisture, and mechanical stresses. However, in situations where thermal and mechanical effects can be neglected, Eq. (2) can be simplified to the extended form of Fick's law, Eq. (3), retaining only the concentration and pressure gradients.

$$\mathrm{J} = -\mathrm{D}\left(\frac{\partial c}{\partial x} + K_p \frac{\partial p_{eff}}{\partial x}\right) \tag{3}$$

In this study, the classical form of Fick's law was adopted, assuming $K_p = 0$. As a result, the flux was expressed by Eq. (4).

$$\mathrm{J} = -\mathrm{D}\frac{\partial c}{\partial x} \tag{4}$$

The simplification is supported by the absence of significant thermal and mechanical effects, as well as the dominance of purely diffusive transport, as demonstrated by the experimental data used for model validation.
The transient mass diffusion formulation in Abaqus employs the implicit Euler method for solving the incremental problem (also known as the modified Crank-Nicholson operator). Although Fick's law is linear, the solution is computed in the time domain, with variations in normalized concentration over the model, necessitating incremental analysis. The solution technique is unconditionally stable for linear problems, allowing for large time increments. This enables the use of variable time steps throughout the simulation, adjusting to changes in normalized concentration.
When second-order elements are used, excessively small time increments may cause spurious oscillations in the solution. To prevent this, it is recommended that the time increment Δt satisfies the criterion in Equation 5, where D is the diffusivity and Δℓ is a representative element dimension.

$$\Delta \mathrm{t} > \frac{1}{6\mathrm{D}} (\Delta \ell)^2 \tag{5}$$

In transient analysis using first-order elements, the solubility terms are lumped, which eliminates such oscillations but can lead to locally inaccurate solutions for small time increments. If smaller time increments are required, a finer mesh should be used in regions where the normalized concentration changes occur.

2.2 Discretization and Sensitivity Analysis

The specimen was discretized using DCAX4 elements, which are 4-node linear axisymmetric quadrilateral elements for heat transfer. The specimen was considered axisymmetric to represent the geometry with radial symmetry about the vertical axis, which reduces computational cost. The sector geometry of each specimen was obtained from Tab. 1, which means half of the cross-section. Figure 1 illustrates the adopted hypothesis, boundary conditions, and mesh discretization. The material properties were taken from Tab.1. The diffusivity was expressed in square meters per hour (m²/h). The solubility was set to 1 in all simulations [16], implying that the concentration considered in the model is equivalent to that in the experiments, expressed in ppm. Three different diffusion coefficients were tested in the analysis. Diffusion coefficients were modeled based on the experimental results from Table 1. Sensitivity analyses were conducted to evaluate chloride ion ingress. Time increments of 12 hours, 1 day, and 14 days were tested to assess their influence on the chloride front, in accordance with Eq. (5).

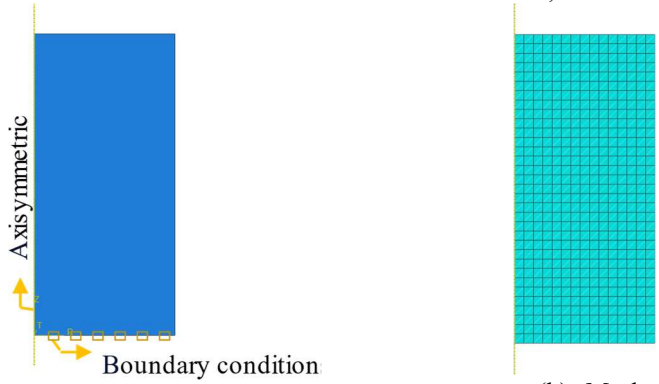


Figure 1. Numerical model

Mesh sizes of 3 mm, 1 mm, and 0.5 mm were tested to examine the impact of refinement on the stability and precision of the results. A transient Mass Diffusion step was used to simulate the continuous immersion period in hours, as shown in Tab. 1. The boundary conditions were applied at the same locations indicated in the experimental program presented in Tab. 1, as well as the chloride solution concentration.

3 Results and Discussion

3.1 Calibration

Sensitivity analyses were made to evaluate the importance of the chloride ion ingress profile. The increment size and mesh size were analyzed. Figure 2a shows the increment size analysis for Exp. A (Tab. 1). The results did not show significant differences for different increment sizes. This finding confirms that the implicit Euler method allows large increment sizes without affecting the results, as the solution process is unconditionally stable. Larger time increments reduce computational cost because fewer increments are needed to cover the total analysis time. Therefore, predicting long periods of chloride exposure can be efficiently model with the finite element method, as conducting long-term experimental programs may not be feasible. Figure 2b presents the mesh size analysis for Exp A (Tab. 1). Mesh sizes of 0,5 mm and 1,0 mm did not show significant differences. However, the 3.0 mm mesh showed a more pronounced diffusion up to 5 mm. No difference was observed in computational time cost for the mesh sizes. Even so, some experimental methods obtain chloride concentration in successive 1 mm layers. Therefore, mesh sizes of 0.5 mm and 1 mm enable discretization results of the same order of magnitude, providing a more accurate graphical representation of chloride ion ingress. After sensitivity analysis, a 0.5 mm mesh and a 30-day time increment were selected for the remaining simulations.

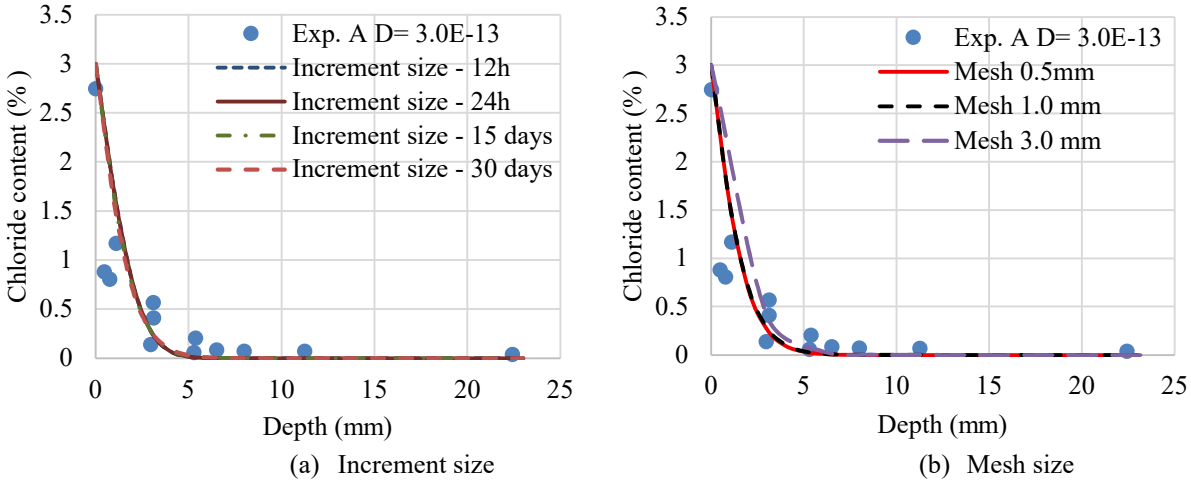


Figure 2. Sensitivity analyses for evaluating the chloride ion ingress profile.

Diffusivity is a material parameter that involves temporal and spatial uncertainties, as it depends on cement hydration, which introduces variability. Therefore, different diffusivity values were evaluated to understand their effect on the penetration front, using the experimental value from each reference (D = 3.0E-13 for A, D = 2.0E-13 for B, and D = 1.96E-13 for C) and two additional diffusivity coefficients, as shown in Figure 3. The experimental diffusion coefficient for Exp. C is 1.96E-13, but the best fit to the curve was with a diffusion coefficient of 3.0E-13 (Figure 3c). Similarly, the experimental diffusion coefficient for Exp. A is 3.0E-13, although some data aligned more closely with the curves for 1.96E-13 and 2.0E-13 (Figure 3a). Many variables can influence the prediction of experimental data, including the heterogeneity of the cementitious matrix, microstructural evolution during hydration, porosity, and microcracking. While the numerical model assumes a homogeneous material, the real matrix shows internal variations, particularly in pore size and distribution, which directly affect chloride transport. Figure 4 illustrates the UHPC microstructure.

Thus, if another point of the same sample were analyzed, the amount of absorbed chloride could vary due to the material heterogeneity. Moreover, the D value was kept constant throughout the simulation, although in the material's actual behavior, D changes over time, transitioning from a non-steady to a steady-state regime [5]. Finally, it can also be observed that the model behavior follows the expected trend: the lower the D value, the

lower the chloride flux and percolation in the UHPC [5]. Therefore, with D within this range, it is concluded that the model is adequately calibrated for UHPC.

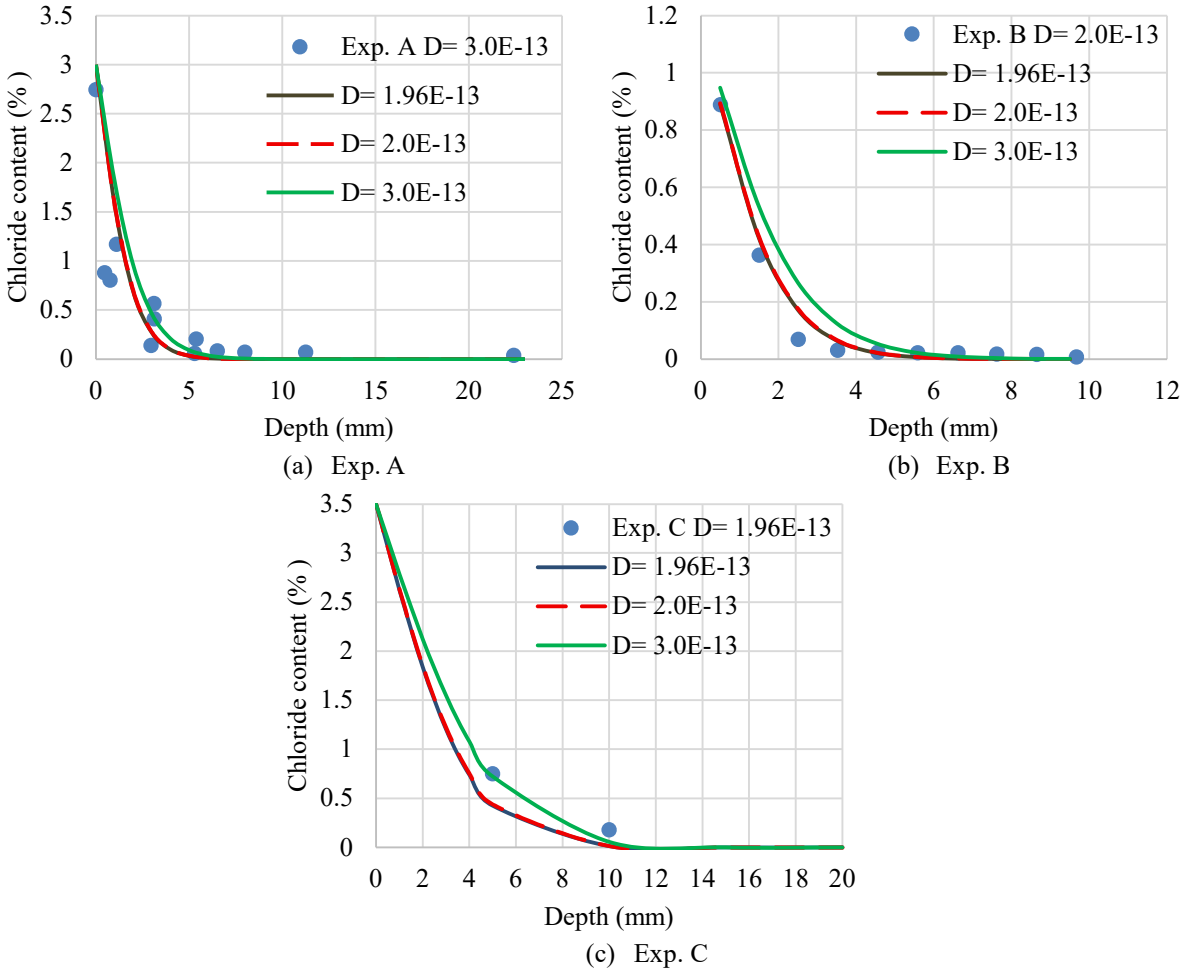


Figure 3. Avaliação da difusividade para calibração do modelo

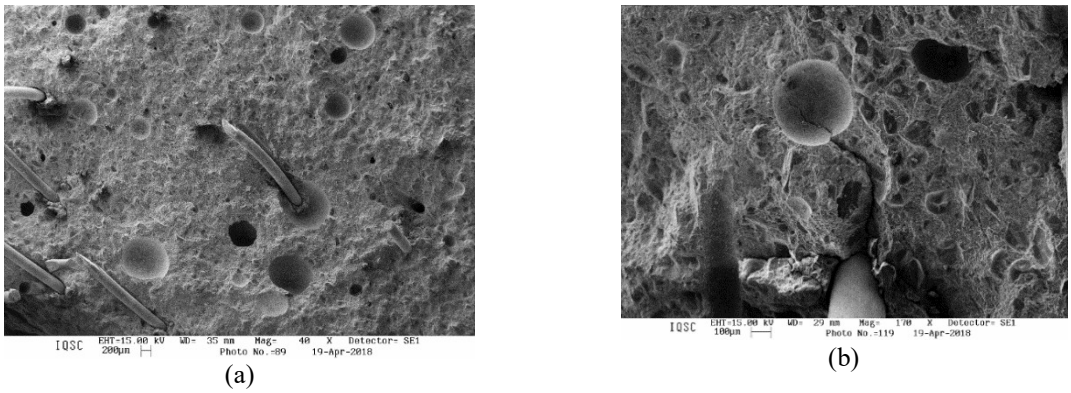
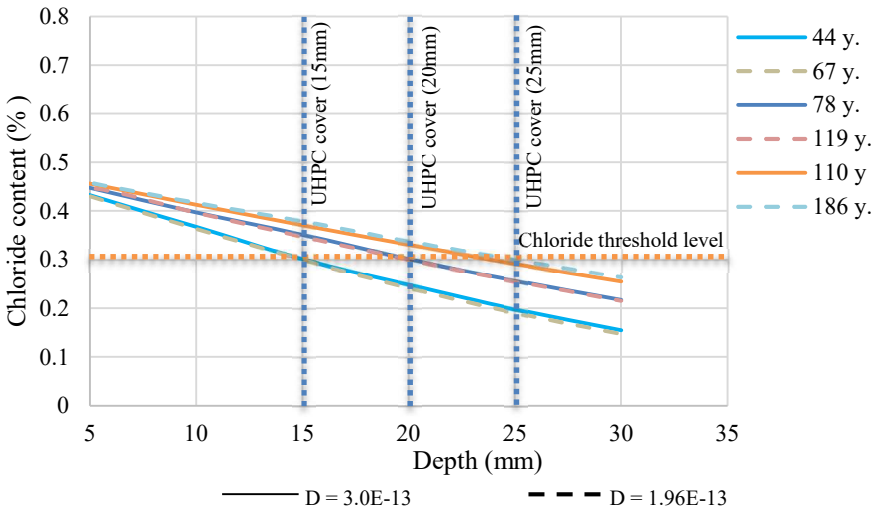


Figure 4 – Porosity and microcracking of UHPC matrix [17]

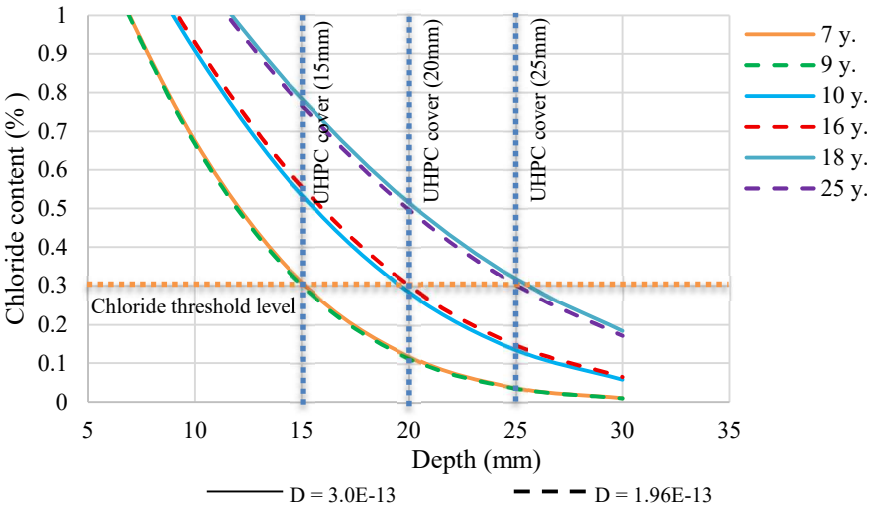
3.2 Time to steel despassivation

The validated model enables the analysis of the impact of the diffusion coefficient and chloride concentration on the initiation of reinforcement bar depassivation (0.3%) in UHPC. The study focuses on exposure class 4 (corrosion induced by chlorides from seawater) defined in NF P18-710 [12], which includes XS1 (airborne salt near the coast), XS2 (permanently submerged), and XS3 (tidal, splash, and spray zones). For these classes, concrete cover

depths of 15 mm, 20 mm, and 25 mm are recommended and will be considered, respectively. Two initial chloride concentrations were analyzed, 0.5% [18] and 1.95% [10], representing marine exposure conditions. For this purpose, a series of simulations were performed, iteratively adjusting the chloride ingress time until the threshold concentration was reached. Figure 5 presents the results of these simulations.



(a) Chloride concentration – 0.5%



(b) Chloride concentration – 1.95%

Figure 5. Time to reach the critical depassivation threshold

The results show that under low chloride concentrations (0.5%), the time to reach the critical depassivation threshold (0.3%) at 20–25 mm cover exceeds 100 years, suggesting low corrosion risk over a century. Under severe marine conditions (1.95%), the time drops to about 16–25 years, highlighting the need for protective strategies or maintenance in the short to medium term. This performance primarily stems from the UHPC dense matrix and significantly lower diffusivity compared to conventional concrete, which slows chloride ingress. While a 25 mm cover improves durability, it does not remove the need for maintenance, especially in aggressive environments where inspections and preventive actions should start after 10–15 years. This extended protection is a major advantage in marine settings, where constant chloride exposure poses a serious threat to reinforcement and service life.

4 Conclusions

This research presents a numerical model calibration of chloride diffusion in UHPC and conducts an analysis to estimate the time to depassivation of embedded reinforcement bars, which is fundamental for life cycle assessment.

The main conclusions are:

- A 2D numerical model for chloride diffusion in UHPC was successfully calibrated using experimental data from the literature.
- Sensitivity analyses showed that mesh size and time increment had minimal influence on numerical results applying Fick's Law for diffusion, allowing efficient cost-time performance by using large increments for long-term analyses.
- The results showed that matrix diffusivity and chloride concentration are key parameters controlling the time to reach the 0.3% threshold at reinforcement depth, directly influencing service life predictions.
- Numerical simulations proved to be an efficient tool to estimate long-term chloride ingress and reinforcement depassivation, overcoming the time limitations of experimental campaigns.

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