Towards realistic microscale simulation of reactive transport in cement pore space using advanced LBM

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Introduction

The vast majority of the concrete structures and infrastructure were built in the 20th century. Degradation problems started to appear after half a century later.
The potential to understand degradation mechanisms is trending for optimizing the functionality of concrete structures, and for increasing the life time of the material.

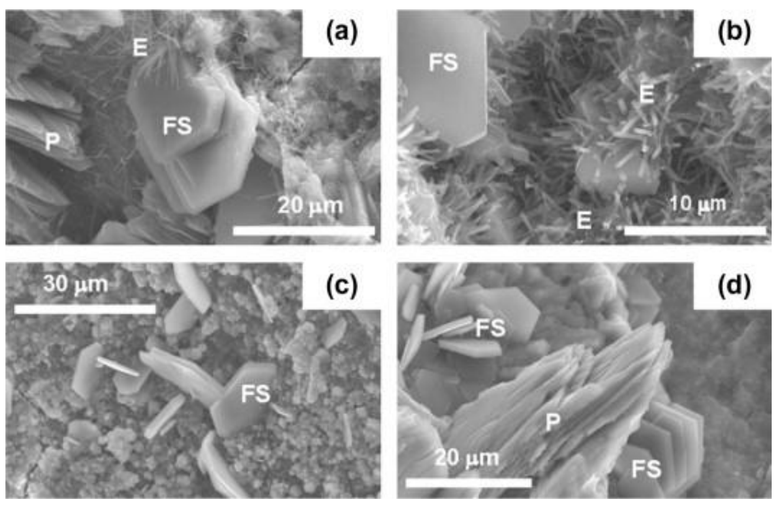


Fig.1 The dissolution of the calcium hydroxide (P), and the forming of Friedel's salt (FS) [3]

Deterioration mechanisms are determined on the microscopic level, especially the chemical and physical phenomena that occur in the pores (Fig.1) i.e. the dissolution of the material structure when attacked by the advected and diffused aggressive ions such as (sulphate, nitrate, carbonate, etc.).
With the development of computational power in the few past decades, modelling of transport phenomena in cementitious materials received a greater attention.
The scope of our research is to introduce a state of the art model for multicomponent reactive flow in cementitious materials to assist in estimating service-life of concrete structures.
Historically, fundamental processes like ion transport occurring in complex geometry i.e. porous media were studied in isolation, until the emergence of reactive transport modelling.

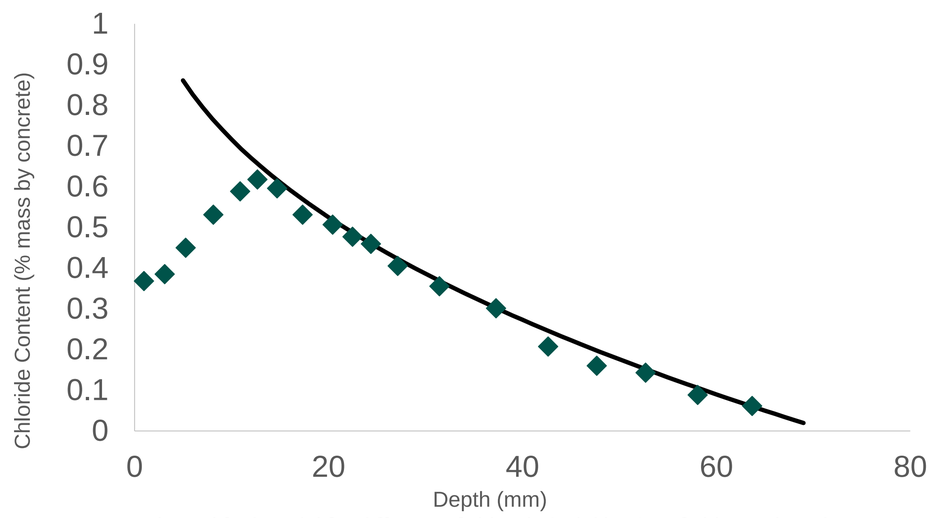


Fig.2: Typical simplified model for diffusion of chloride (solid line) vs. field samples , deviation is due drying/wetting cycles (max. concentration is not on the surface)[1]

Marchand et. al. [1] raised the awareness of the lack of reliability of simplified models, as seen in (Fig.2), to predict the behaviour of concrete exposed to chemically aggressive environments.
The proposed research is trying to give a thorough look at these processes, developing an approach to simulate dissolution/ precipitation of minerals using Lattice Boltzmann Method [2].
The chemical reactions will be simulated with a coupled geochemical solver, taking into account the development of the pore volume due to the chemical reaction in 3-D geometry.
The challenge for simulating reactive flows is that sub-grid distances, have to be recomputed at each time step.

Theory and numerical model

1. The physicochemical model

The physicochemical model incorporates the governing equations for fluid flow, mass transport namely, Navier-Stokes equations, the advection-diffusion equation, and dissolution/ precipitation heterogeneous reaction.

$$\nabla . \boldsymbol{u} = 0$$

$$\partial_t \boldsymbol{u} + \nabla . (\boldsymbol{u}\boldsymbol{u}) = -\nabla p + \frac{1}{Re}\nabla^2 \boldsymbol{u} + \frac{1}{Fr}\boldsymbol{g}$$

$$\partial_t c^j + \boldsymbol{u} . \nabla c^j = \frac{1}{Pe}\nabla^2 c^j + R$$

$$\boldsymbol{n} . (\nabla c^j)_0 = Da . c^j \quad at\ the\ interface$$

2. Lattice Boltzmann Method

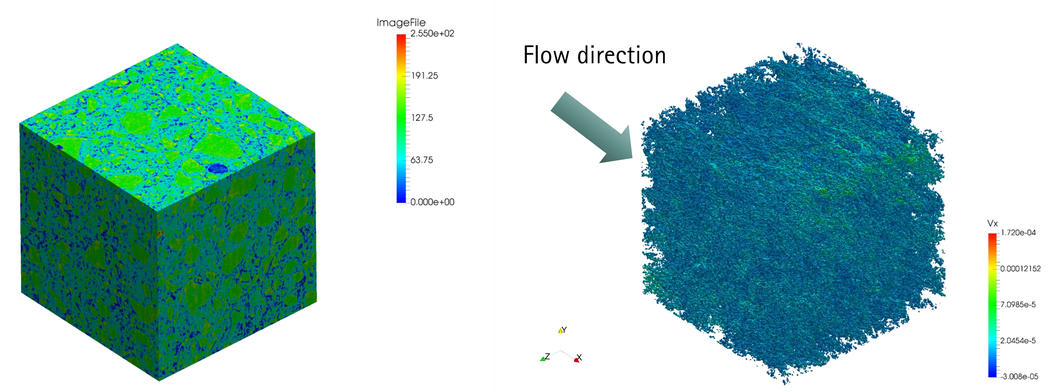
$$f_i(\boldsymbol{r} + \boldsymbol{e}_i \Delta t , t + \Delta t) = f_i(\boldsymbol{r}, t) + \Omega_i^{\mathrm{BGK/MRT/CUM}}(\boldsymbol{r}, t)$$

Results

Permeability test

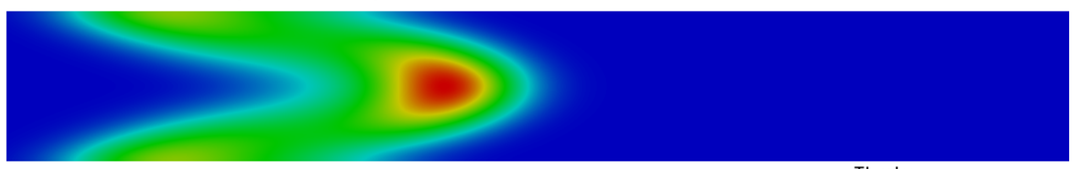
First result of flow simulation obtained from VirtualFluids in terms of permeability using µ-CT geometry is quite satisfying (about 10^{-16} m^2) the result lies within the range of values obtained from previous numerical and experimental results.

Permeability simulation of CCRL133 sample (w/c=0.45 by mass)



Taylor Aris dispersion

The dispersion of a concentration profile ø is considered under a background flow with a parabolic profile velocity between two parallel plates.

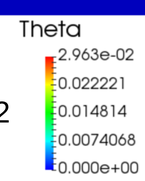


$$D_n^{\mathrm{L}} := \frac{1}{2}\frac{d(\sigma^2)}{dt}$$

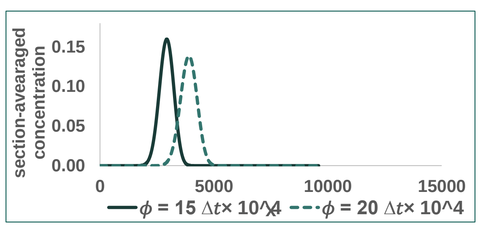
$$D_a^{\mathrm{L}} = D(1 + \mathrm{Pe}^2/210)$$

$$Pe := \frac{\bar{u}L}{D}$$

Evolution of concentration profile
Pe=50, t= 5000 ts, N=64 points, D=0.02

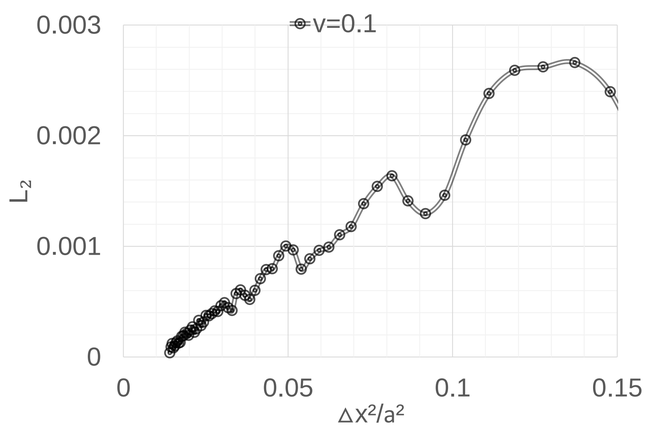


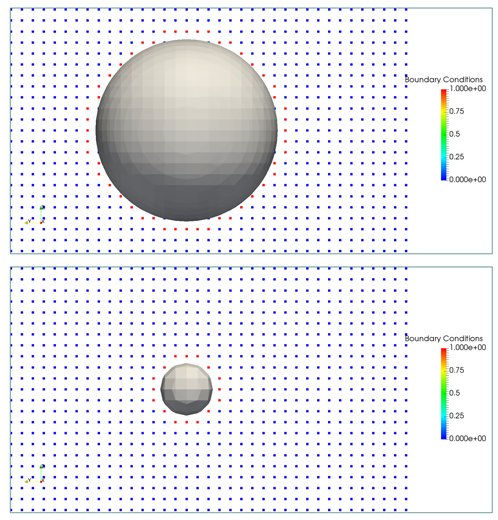
Pe	D_n^{L}/D	D_a^{L}/D	Error (%)
25	4.018	3.976	1.053
50	13.154	12.905	1.929



Sharp interface reconstruction

$$L_2 = \frac{1}{N}\sqrt{\frac{\Sigma_m (a - r_m)^2}{a^2}}$$





References

1. Marchand J, Samson E. Predicting the service-life of concrete structures – Limitations of simplified models. Cem. Concr. Compos. 2009;31(8):515-521.
2. Geier M, Schönherr M, Pasquali A, Krafczyk M. The cumulant lattice Boltzmann equation in three dimensions: Theory and validation. Comput. Math with Appl. 2015;70(4):507-547.
3. Goñi S., Frias M., Vegas I., García R., Sodium sulphate effect on the mineralogy of ternary blended cements elaborated with activated paper sludge and fly ash, In Construction and Building Materials, 2014 ;54:313-319.