Lattice model as a tool for modelling transport phenomena in cement based composites

Numerical Modeling
Strategies for Sustainable Concrete Structures

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1. Introduction

Reinforced concrete structures are not durable enough. That is the conclusion in both the research and engineering communities. In the past, design of concrete structures has mainly been focused on strength considerations. A clear relationship between concrete strength and durability was implied. In recent years, however, there is an increasing level of understanding that strength alone cannot be considered as a reliable durability parameter. Other factors clearly need to be taken into account.

Reinforced concrete is, yet still, a construction material of choice for aggressive environmental conditions. An increasing number of structures are built in very cold and very hot climates, as well as in the marine environment. And yet, the structures are expected to have a long service life in these harsh conditions.

Service life demands for concrete infrastructure have become more stringent in recent years. Structures are expected to serve their purpose for 100 or even 200 years without major repairs. In order to achieve that, reliable empirical or numerical models are needed. Major deterioration mechanisms affecting reinforced concrete structures include sulphate attack, alkali-silica reaction, freeze-thaw damage, and corrosion of reinforcing steel due to chloride ingress or carbonation. All of these mechanisms include transport of aggressive species through concrete, whether moisture, ions, electrical current, and so on. In general, water is involved in every type of deterioration [6]. On top of that, in most cases it is necessary to consider coupling of two or more mechanisms. For coupled physico-chemical phenomena, numerical models are clearly a way to go.

Lattice models have long been successfully used in modelling fracture processes in cement based materials [8, 11]. This concept can be considered as a discrete approach, as opposed to the continuum approach of most finite element models. In this approach, a continuum is discretized as a set of beam or truss elements. This approach makes it possible to obtain realistic crack patterns and fracture properties of composite quasi-brittle materials. The model has recently been fully extended to three dimensions [7]. Also, by assigning different material (mechanical) properties to different beam elements in accordance with the material microstructure, the composite nature of concrete can be taken into account. This enables modelling concrete on the meso-scale: as a composite material consisting of aggregates, the mortar matrix, and the ITZ (interface transition zone).

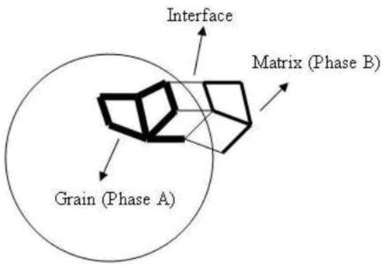

Figure 1: Determining the lattice element material properties [7]

Recently, several studies have dealt with the possibility of extending the lattice model concept to modelling transport phenomena in cement based materials. Using this approach, a continuum is discretized as a set of “pipes”, through which the transport takes place. Bolander [1] developed a lattice-type model to simulate shrinkage induced cracking in cement overlays. Grassl [2] used a similar (although two dimensional) approach to model flow in cracked concrete. These models consider concrete as a quasi-homogeneous medium, with respect to mechanical and transport properties of the material. Also, coupling with fracture models and effects of cracking on transport properties are taken into account. Very recently, Wang [12] proposed a two-dimensional lattice-based model for simulating chloride penetration in the concrete cover. In this work, similarly to the mechanical model described in [7], concrete is considered as a three phase composite, comprising of the mortar matrix, aggregate, and the ITZ. Since transport of species in the domain takes place through a set of one-dimensional “pipe” elements, computational effort needed to solve the governing set of equations can be chiefly reduced, when compared to continuum-based models.

In this paper, a three dimensional lattice modelling approach for simulating transport phenomena in cement based composites is presented. An irregular (random) lattice is used for the analyses. The spatial discretization procedure based on Voronoi tessellation is laid out in the paper. A set of governing equations for the diffusion-type transport (e.g. of moisture, chloride ions, etc.) is presented. As is the case with the fracture lattice model, it is possible to model the material on both the macro (homogeneous) and meso scale (heterogeneous). Several analysis cases are therefore presented and discussed.

2. Method

2.1. Spatial discretization

For the spatial discretization of the specimen in three dimensions, the basis is the prismatic domain. If the specimen has a shape different than prismatic (irregular), a prismatic domain enclosing the specimen is specified. Discretization of the domain is then performed according to the following procedure:

- The rectangular domain is first divided in a number of cubic cells. As an input value, number of cells in x, y and z direction is specified (figure 2).

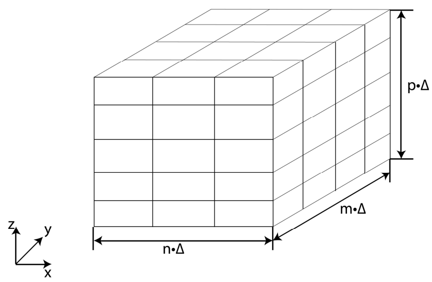

Figure 2: Subdivision of the prismatic domain

– A node is randomly placed in every cell using a (pseudo) random number generator. The degree of randomness can be set so that either a regular (tetrahedric for a 3D case) or an irregular lattice is obtained in the end.

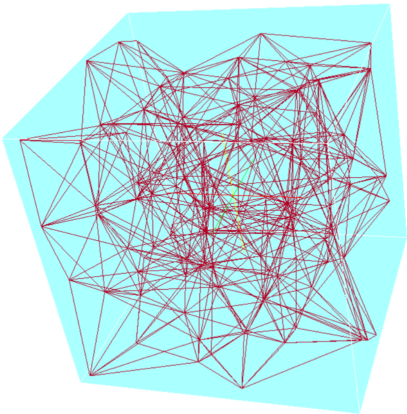

Figure 3: A random 5x5x5 lattice within a cubic domain

– Voronoi tessellation of the prismatic domain with respect to the specified set of nodes is preformed using the Multi-Parametric toolbox (MPT) for MATLAB [3].

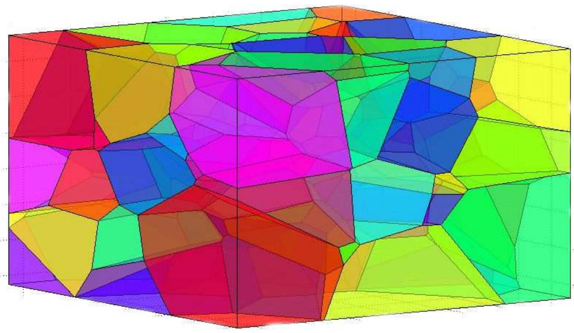

Figure 4: Voronoi tessellation of a prismatic domain, using MPT

– Nodes with adjacent Voronoi cells are connected by lattice elements. Since Voronoi diagrams are dual with Delaunay tessellation, this approach is equivalent to performing a Delaunay tessellation of the set of nodes, as outlined in [13].

If the domain in question is not prismatic, the lattice is "extracted" from the prismatic one which was created according to the outlined procedure. Also, since the cells are cubic for a three-dimensional case, it is possible to use a voxel-based image (e.g. a generated microstructure or a micro-CT scan image- see, for example, [10] for "mapping" individual elements in the domain. Then, different properties (e.g. conductivity, permeability, diffusivity) can be assigned to elements belonging to different material phases. Heterogeneous nature of the material with respect to transport properties can therefore be simulated.

It is important to note that, in general, nodes are not placed on the boundary of the analyzed domain. The implications of this fact on the boundary-condition application, and therefore the result, are discussed later.

2.2. Governing equations

An assembly of lattice elements as presented here can be considered as a set of one-dimensional linear finite elements. If transport of one agent (e.g. moisture, heat, chloride, sulphate, etc.) is considered, an element has two degrees of freedom- one for every node. A generic governing partial differential equation for diffusion-type transport phenomena has the following form:

$$\frac{\partial C}{\partial t} = D \cdot \frac{\partial^2 C}{\partial x^2} + Q \tag{0.1}$$

Here, C is the unknown concentration (e.g. chloride content or temperature), D is the material property (e.g. diffusion coefficient for chloride transport or thermal conductivity for heat transport), and Q is a term accounting for any sinks or sources that might be present in the system (e.g. for heat transport than can be heat of hydration). If this equation is discretized using the standard Galerkin method [5], the following set of linear equations arises (in matrix form):

$$M\dot{C} + KC = f \tag{0.2}$$

Here, M is the element mass matrix, K is the element diffusion matrix, and f is the forcing vector. Vector C is the vector of unknown quantities (e.g. temperatures or chloride concentrations), and the dot over C indicates the time derivative. Elemental matrices have the following generic forms:

$$M = \frac{Al}{6\omega}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}, K = \frac{DA}{l}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, f = \begin{bmatrix} -q_i \cdot D \cdot A \\ -q_j \cdot D \cdot A \end{bmatrix} \tag{0.3}$$

In the matrices, *l* is the length of the element, *A* is its cross sectional area, and *D* its conductivity. Cross sectional areas of individual elements are assigned using the so-called Voronoi scaling method [1] - cross section of an element is equal to the area of a facet of a Voronoi cell which is common to two nodes (see chapter 2.1). Depending on the analysis, ω takes value of 1, 2 or 3 for one, two, and three-dimensional cases respectively [1]. In the discretization, any sources and/or sinks have been neglected. Forcing vector *f* consists of the fluxes which can be applied on the domain boundaries.

If a time-independent (i.e. steady-state) problem is analyzed, equation (1.2.) takes the form:

$$KC = f \tag{0.4}$$

When elemental matrices of all the elements are calculated, the usual finite element assembling procedure is performed [5]. The resulting set of linear equations is then solved for unknown nodal values of C.

3. Results

3.1. Steady-state diffusion through a homogeneous medium

When observed on a macro (structural) level, concrete can be modelled as a homogeneous medium. If that is the case, transport properties of the whole domain can be approximated as the same. For most analyses and models available in the literature, this approach is taken. It can be considered that, if the problem at hand is of a significant size (e.g. hydration induced heat transport in large dams or tunnels), it is appropriate to do so.

In order to assess the ability of the 3D random lattice to simulate transport processes in cement based materials, the following benchmark case was selected. A concrete element subjected to steady-state transport of species is simulated. Without loss of generality, it is subjected to the following (Dirichlet) boundary conditions: one side of the prism has a prescribed value of C equal to 1, while the opposite side has a prescribed concentration of C equal to 0. It has to be borne in mind here, again, that the surface nodes are somewhat offset from the domain boundary, and that the boundary conditions are applied directly to those nodes. Although this may affect the result to a certain (mainly insignificant) extent, the effect can be reduced through suitable mesh refinement of areas close to the boundary. It can be considered that all the other sides of the prism are completely sealed (no flux boundary condition). Also without loss of generality, the value of the conductivity parameter (D in the K matrix, see equation 1.3) is taken as 1. Other input analysis parameters can be found in table 1.

For this case, it is possible to obtain the analytical solution:

$$C(x) = \frac{C_2 - C_1}{l} x + C_1 \tag{0.5}$$

Here, C1 and C2 are the prescribed values of C at the inlet and outlet side, respectively, x is spatial coordinate in the "loading" direction, and l is the specimen dimension in the same direction. For the observed example, C1 and C2 are equal to 1 and 0, respectively, so the following solution is obtained:

$$C(x) = 1 - \frac{x}{l} \tag{0.6}$$

Length (mm)	Width (mm)	Thickness (mm)	Total number of nodes	**Number of lattice elements**
50	**10**	**10**	**5000**	**34532**

Table 1: Analysis input parameters

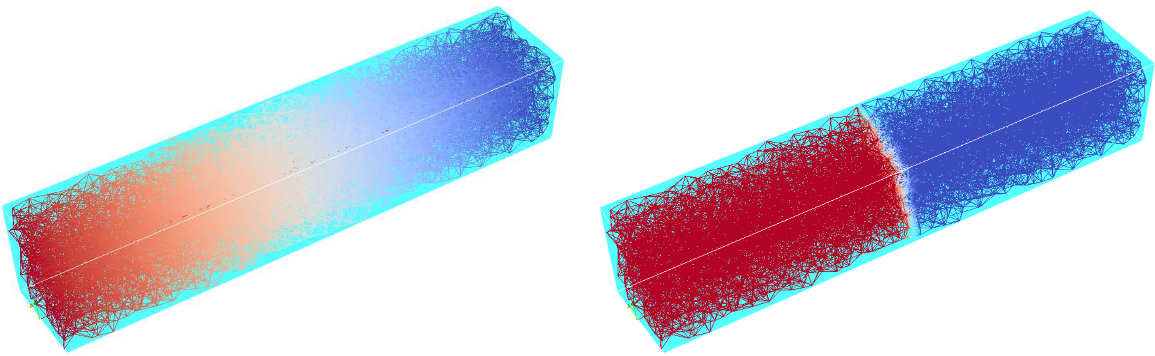

Figure 5: Gradient of C (left) and a front of C (right) in the homogeneous 3D lattice

3.2. Steady-state diffusion through a heterogeneous medium

On the material level, concrete is a heterogeneous medium. When it comes to transport of aggressive species trough the material, different phases of the material have different transport properties (D in equation 1.3). These properties depend on the porosity of the certain phase, pore connectivity, existence of microcracking, etc. It is therefore advisable to model concrete on the meso-scale, in order to get more insight on the role of different phases on transport processes that occur.

When observed on the meso (mm to cm) scale, concrete can be considered as a composite consisting of coarse aggregate, ITZ (interfacial transition zone), and the mortar matrix. In order to get the three-dimensional meso-structure of concrete as an input for the analysis, several approaches are possible. Firstly, it is possible to use micro-CT scanning. This approach must be combined with some "tricks"(see e.g. [9, 10,4]). Namely, since it is difficult to distinguish between the aggregate and the matrix in the scan, either less dense particles are used to simulate the aggregate, or the matrix is simulated by a material which is less dense than the aggregate. This enables the analyst to easily distinguish between the matrix and the aggregates.

In this research, another approach is taken. The concrete meso-structure is computer generated, using realistic aggregate shapes [14]. A 150x150x150 mm cube was generated, out of which a 50x10x10 mm slice was taken for the analysis, in accordance with the previous analysis. A lattice was projected on top of that image. The generated heterogeneous lattice is depicted in figure 6. The brown parts are the aggregates, and the blue parts the matrix. For simplicity, existence of the permeable ITZ is neglected in the analysis.

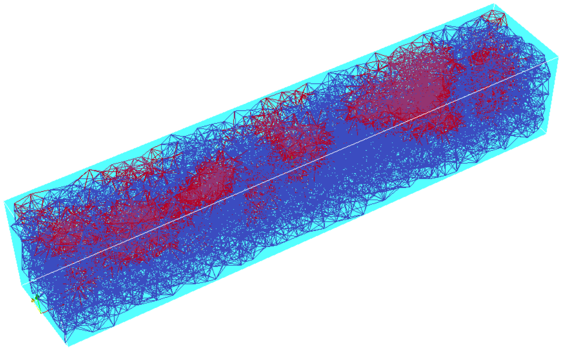

Figure 6: Computer generated meso-structure

The same analysis as for the homogeneous case was repeated with different input values. The D value was set to 1 and 10^{-15} for the matrix and the aggregate elements, respectively. This means that the aggregate particles present an obstacle for the transport.

In the following figure, results of the analysis are depicted.

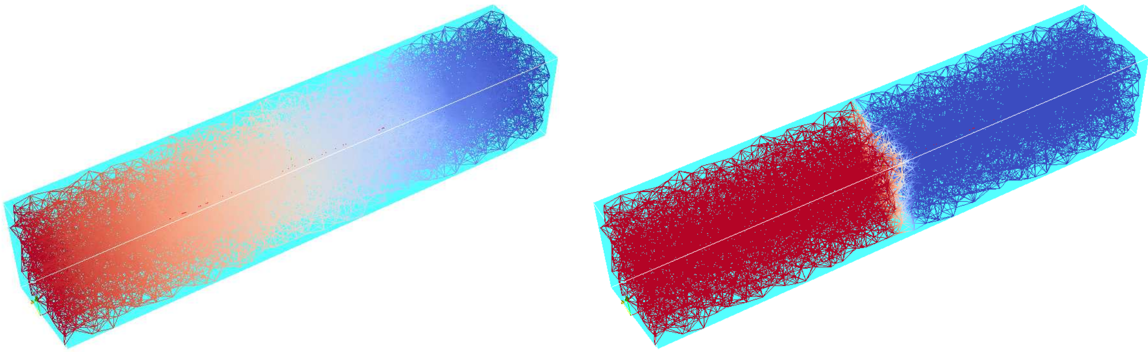

Figure 7: Gradient of C (left) and a front of C (right) in the heterogeneous 3D lattice

4. Discussion

4.1. Homogeneous lattice analysis

Comparison of the lattice-based simulation with the numerical solution is given in the figure:

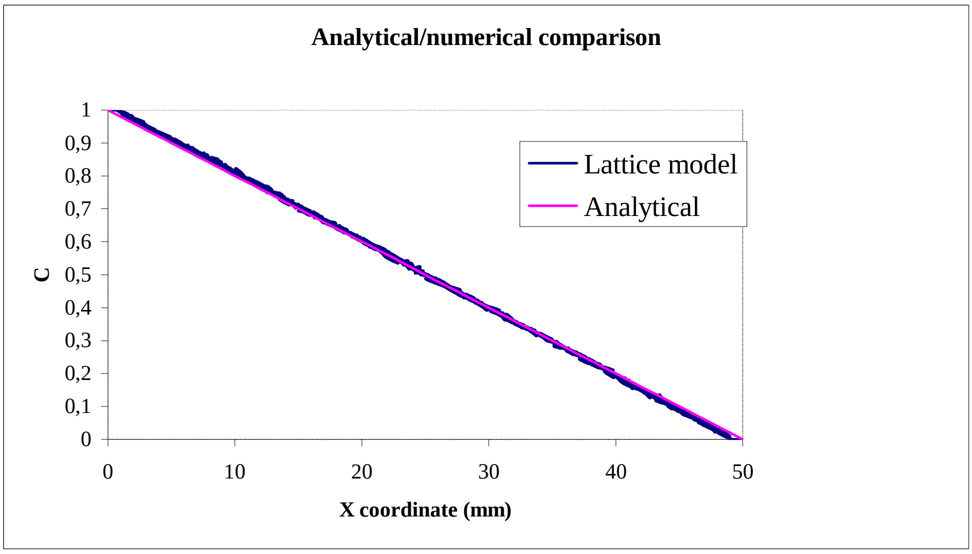

Figure 8: Comparison of the analytical and lattice model solution

Figure 8 shows that the deviations between the analytical and the numerical solution are minimal when a three-dimensional homogeneous random lattice is used. This signifies that no numerical artifacts occur due to the random configuration of the lattice. The small differences that do occur can be attributed entirely to the fact that boundary nodes are not placed exactly at the domain boundaries. This error can be, if necessary, reduced with mesh refinement, as already mentioned. However, in practice, this is mostly not needed.

Figure 5 shows, on the left-hand side, the gradual change of quantity C along the lattice, as expected. On the right-had side a front of equal concentrations close to the middle of the lattice is depicted. It can be concluded that a uniform concentration front occurs when using the random lattice, again without any numerical errors caused by the randomness.

4.2. Heterogeneous lattice analysis

For the steady-state diffusion, it is possible only to qualitatively assess the influence of aggregate inclusions on the transport simulation. Figure 7 shows, on the left hand side, that the change of C along the lattice is gradual, although somewhat different than that of the homogeneous lattice. On the right-hand side, again, a front of equal concentrations close to the middle of the lattice for this case is shown. A concentration front is not uniform in this case- the deviations are caused by presence of aggregate particles in the matrix. Since this is not observed in the homogeneous case, it is clearly not a numerical error. Also, preliminary simulations of the non-steady state diffusion process show an even more significant role of material heterogeneity on the transport process.

5. Conclusions

In the paper, basics of the three-dimensional random lattice based model for transport processes in cement based composites are outlined. A discretization procedure based on the Voronoi tessellation of the prismatic domain and Voronoi scaling method is presented. A generic diffusion type transport partial differential equation is discretized using the Galerkin method. A discrete form of the equation, along with the element matrices, is presented. The efficiency of the approach is tested using two steady-state diffusion examples: one for homogeneous and the other for heterogeneous material microstructure. These examples have yielded the following:

- When compared to the analytical solution for the homogeneous case, the deviations are minimal.
- The sole cause of the error is the fact that the boundary nodes are not placed exactly on the domain boundary. This can be further reduced by mesh refinement in the boundary regions.
- The penetration is uniform in the random lattice for the homogeneous material properties, meaning that no numerical error is introduced by the lattice randomness.
- It is possible to model concrete on the meso-scale, i.e. as a heterogeneous material. Computer-based or concrete structure obtained by micro-CT scanning can be used as a basis for the analysis.
- The addition of aggregates in the matrix makes the penetration profile non-uniform. This is not observed in the case of a homogeneous medium, and can be attributed to the material inhomogenity.

It can be concluded that lattice-based models are suitable for modelling transport phenomena in cement based composites. Further work will include non-steady state diffusion analysis, with emphasis on chloride transport. Also, it is envisioned that the transport model will be coupled to the fracture lattice model, which would enable taking into account effect of cracking on penetration of aggressive substances into concrete.

6. Acknowledgements

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