Modelling Moisture Transport Processes in Cement Paste Systems

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Summary

Today, computer modeling technique's have been developed so far that almost the complete field of project design and engineering are computerized and interconnected to a far extend. The development of computational techniques for predicting material performances turned out to be a most promising way to achieve design information at a project's early stage. Models for predicting the evolution of cementitious material properties in general, and for calculating degradation processes in particular, are expected to be applicable to achieve knowledge about the material quality and to assist by setting-up a future maintenance plan as well. In line with this, the simulation model HYMOSTRUC is presented where the emphasis is on moisture transport processes in cement paste systems. The model promotes a multi-scale approach for predicting long and short-term performance of concrete.

Keywords: cement paste systems; multi scale modelling; moisture transport; computer simulations.

1. Introduction

Modelling engineering properties of cement-based materials may optionally start from different modelling levels. Today's way of approaching material modelling features is driven often by the so-called 'multi-scale' modelling approach. Physical material behaviour is modelled at the level at which it plays a dominant role. In this respect distinction is made between the micro- meso- and macro-level, where the output of these different modelling levels is encouraged to be complementary. This approach makes modelling more mature and bridges the gap between scientific research and engineering practice. Detailed research knowledge becomes available for designing processes and calculations of structural elements. The modern way of communicating this knowledge, on the other hand, is a challenge that requires knowledge of web-based services. At the TU Delft initiatives are currently worked out that pave the way for developments that will bring these kind of modern services to reality, starting with modelling material performances [1].

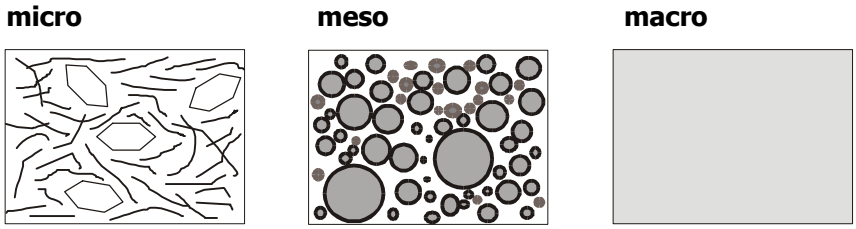


Fig 1. Definition of micro-, meso- and macro-level concrete [2].

2. Virtual Microstructure

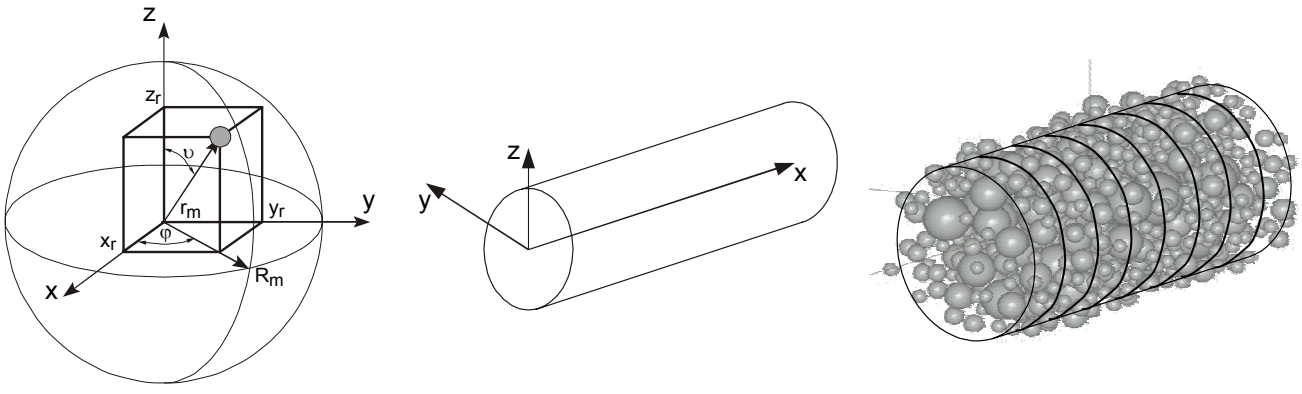
2.1. General

A possible way of simulating a virtual microstructure is by considering cement particles to be spherically shaped. From this on, a cement grain structure can be generated while considering a certain particle size distribution and where the positions of the spherical shaped grains are randomly chosen, in a closed predefined confined volume. The structure being build is assumed to be a representation of the initial stage of the mixed water-cement substance (cement particles in the aqueous phase). This initial particle structure represents the starting point for the calculation of the hydration process that evolves towards a virtual microstructure. The expansion of the hydrating cement grains represents the formation of hydration products. Simultaneously with this hydration process, the cement grain structure tends to form a load bearing structure. Modelling the development of a microstructure in accordance with the approach addressed provides the opportunity to generate a relatively large sample that can be adopted for the calculation of material properties, within acceptable limits of computation time. The simulations provide information about the micro-structural development in relation to evolving properties like porosity, permeability etc.

2.2. Structure generation

The formation of a virtual microstructure starts with the generation of a random particle structure. Within the HYMOSTRUC model this is based on random positions of the cement particles in a predefined confined space. The actual shape of this space is optional but is regularly chosen as tubular or spherically. Fig 2 provides an impression of the spherical volume and the (filled) tubular volume that represents the borders of a cement paste system and, hence, the size of the virtual microstructure to be simulated.

When it comes to the generation of a particle structure of a cement-based material, the question rises whether it concerns a plain Portland cement or a cements that contains special properties. The latter cement is most frequently used in the building and construction industry. So, there actually is a need to simulate the properties of special purpose cements or cements with tailored properties. In HYMOSTRUC, a feature is added that offers the opportunity to add filler particles to the random grain structure (see Fig 3). This creates the possibility to simulate the material properties of various types of cements adopted in a cement paste system. It can be considered as an added value that creates new challenges for modelling material properties of new innovative materials.



Spherical volume Tubular volume 'Filled' Tubular volume (Ribbon)

Fig 2. Schematic representation of the confined volumes for random particle structure

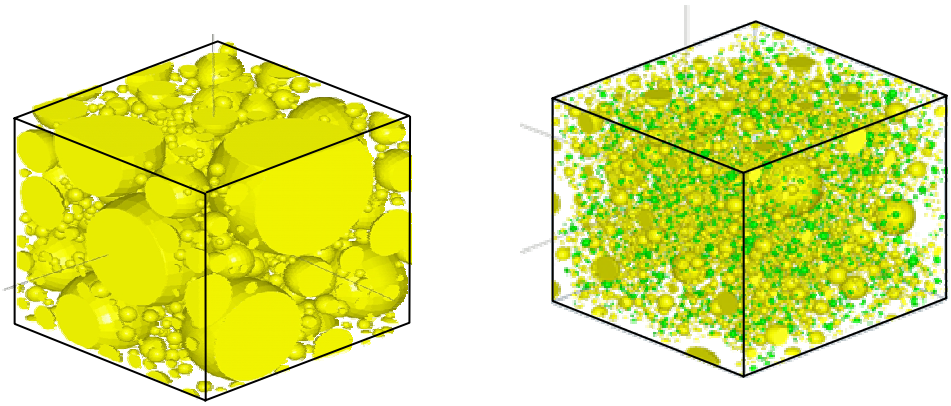


Fig 3. Generated particle structure, Left: cement, Right: cement with fillers.

The particles within a virtual microstructure may follow a certain distribution. The random particle structures generated in Fig 3 represents a paste that follow a particle size distribution (PSD) according to the Rosin-Rammler function G(x) (see eq. (1)).

$$G(x) = 1 - \exp(-bx^n) \qquad (1)$$

For enhanced particle structures, generated with this approach, fillers can be added with their own unique PSD. The predefined confined space (Fig 2) will than be filled randomly with cement as well as filler particles. It is a way to simulate a broad variety of cement types and its associating material properties.

2.3. Hydration

From the generated particle structure, the progress of the hydration process can be calculated. The growth of the particles is simulated by assuming the hydration products to growth in a uniform spherical direction while taking into account inner and outer growth. From the actual growth of the cement particles the degree of hydration can be calculated. With increasing degree of hydration, a microstructure is formed and the water volumes in the capillary pores decrease mainly at the expense of the larger pores. This process is associated with a reduction of the relative cross-section of the capillary pores, able to facilitate the movement of the capillary pore water through the cement paste system. This phenomenon is taken into account in the moisture transport model as presented next.

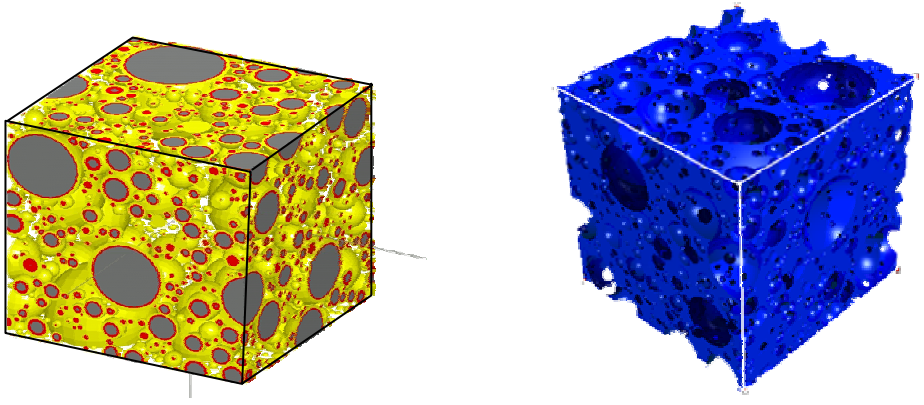


Fig 4. Generated particle structure Left: after hydration, Right: capillary water

3. Modelling moisture transport

Modelling moisture transport starts with equilibrating the pore-system thermodynamics and, with this, the associating changes of the capillary pressure p_w and the pressure in the gradually emptying capillary pores p_g. Existing pressure differences might move capillary water in the (partly) filled capillary pores, resulting in a rearrangement of the capillary pore water from the water-rich areas (Interfacial Transition Zone (ITZ)) to the water-lacking areas (inner parts of the cement matrix). Pores in the central matrix might be filled at the expense of the pores located at the porous ITZ's. These processes introduce drying of the emptied pores at the ITZ regions, resulting in large shrinkage deformations around the aggregates, potentially causing micro cracking. In addition to this, the rearrangement of water increases hydration of the cement matrix, resulting in a densification of the inner cementitious paste system.

3.2. Modelling transport of capillary water in porous systems

Consider an elementary volume V that is built up from a porous cementitious material, where the pores are filled partly with water and gas. The individual volumetric contributions of the constituents are assigned to be solid, water and gas [4,5]. Conservation of mass for the capillary water in an individual element leads to the following fluid-balance equation:

$$n\frac{\partial s}{\partial t} - \mathrm{div}\left(\frac{k_w}{\gamma_w}\,\mathrm{grad}\ p_w\right) = 0 \qquad (2)$$

This differential equation describes the movement of capillary water through the capillary pores in terms of variations of the degree of saturation s and assumes a constant porosity n between the incremental steps of the hydration progress calculation imposed by HYMOSTRUC [3].

While affecting the actual pressure in the empty pores, its volume will change proportionally. This relationship is described by Boyle's law. When it is assumed that either a change of the gas pressure or the gas volume takes place within a time increment dt, a relation can be elaborated:

$$\frac{\partial s}{\partial t} = \frac{(1-s)}{p_g}\frac{\partial p_g}{\partial t} \qquad (3)$$

The calculation of the moisture transport has been applied to a ribbon as presented in Fig 2 ('Filled' Tubular volume). It represents a volume of cement paste between two aggregates situated opposite to each other. With the model, the degree of saturation Fig 5 (left) and the shrinkage Fig 5 (right) as developed during hardening are calculated for three different water cement ratios (age = 100 hrs).

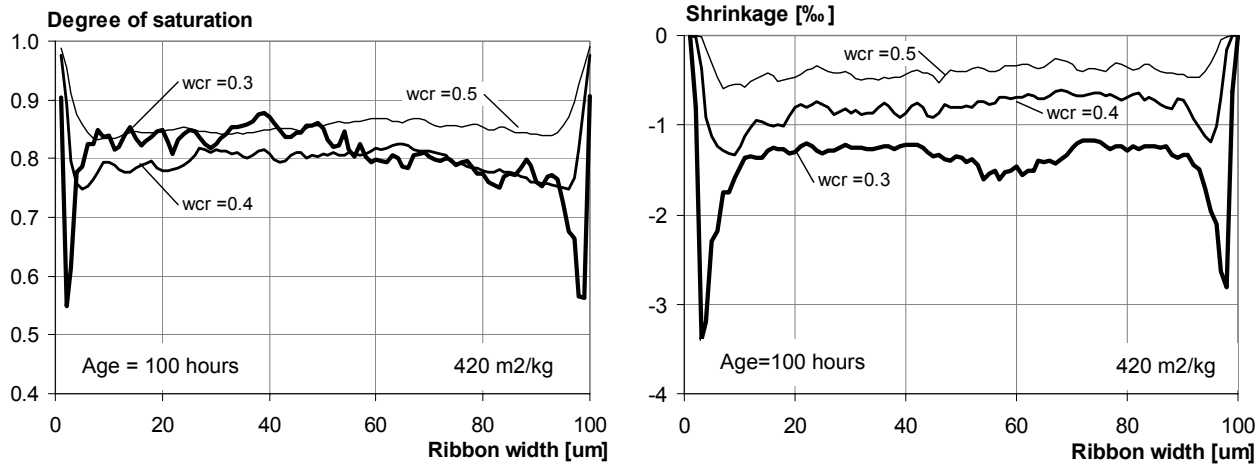


Fig 5. Left: Degree of saturation versus ribbon width, Right: Hardening shrinkage versus ribbon width.

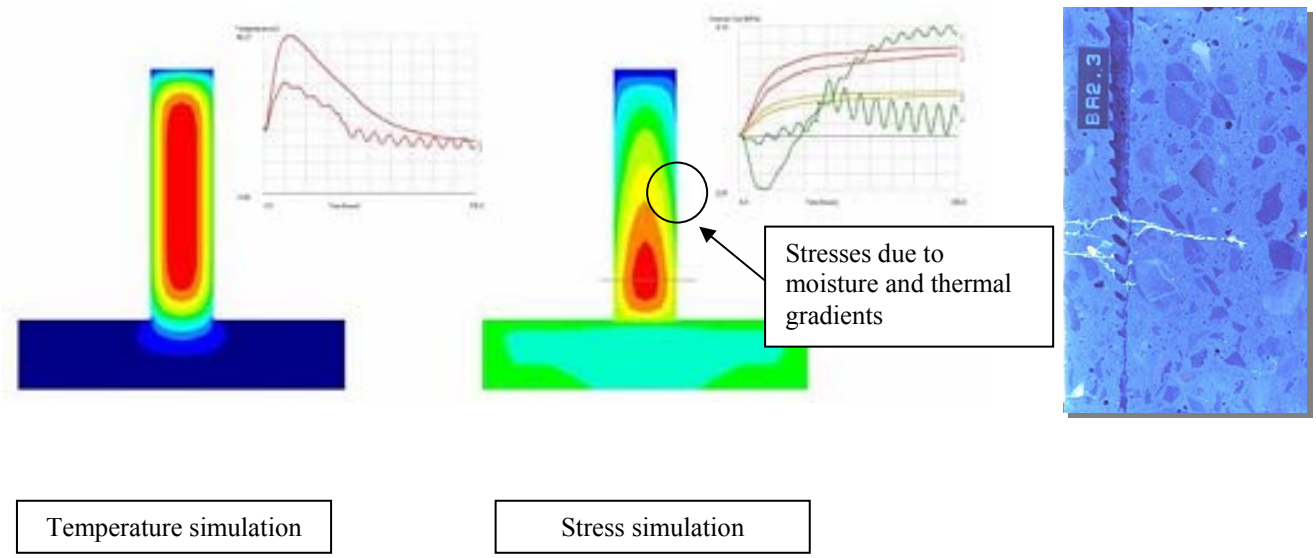


Fig 6. Example of macro-scale simulations [6], Left: Thermal analysis of hardening concrete wall, Right: Thermal crack in concrete, passing the rebar.

4. Application in Engineering Practice

When making the step from the 'modelling world' towards the engineering practice, the relationship between the simulated results and on-site observations becomes relevant. It is a matter of accuracy of the numerical simulation software and its potential to predict the probability of damage, being a measure for a concrete structure's lifetime.

When considering the multi-scale modelling approach, numerical simulations have to be performed at the different observation levels at which concrete (structures) can be analysed. Starting from a macro-scale observation level, full-scale structural elements can be simulated. In this respect the thermal stress analysis can be considered as a good example (see Fig 6). When downsizing the observation level, and with this, the modelling level, the focus is shifting towards the meso-level. In general, at this level, three phases are distinguished, viz. cement paste matrix, aggregates and ITZ. When applying the shrinkage results (wcr = 0.3), as calculated from the ribbon paste (Fig 5, left), to a meso-level model (Fig 7), the consequences of micro-structural volume changes can be reflected on a higher modelling level. The meso-level model as presented in Fig 7, shows a cracking pattern associated with a shrinkage profile where large shrinkage peaks occur around the aggregates (ITZ region) and more moderate shrinkage at the central cement paste matrix. It provides clear information about the applicability of numerical simulation models and its relevance for the engineering practice.

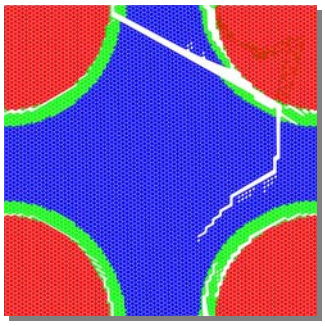


Fig 7. Crack formation calculated with a lattice model at meso-level [6].

5. Discussion and Conclusions

The present paper shows the potential of numerical simulation models to contribute to the demands that come up from the engineering practice and the building and construction industry. The multi-scale modeling approach, in this respect, offers the opportunity to go into more detail in order to get more accurate and reliable results or to get a more economical solution. All these options deal with the acceptance and applicability of multi-scale simulation models.

When it comes to the prediction of a structures life-time, the results as presented in this paper show that there is a serious option to get life-time information in advance, i.e. in the design stage of a project. Providing knowledge about the quality and crack sensitivity of the inner structures is welcome input that makes economical choices in the early design stage possible.

The paper shows how a particle structure can be generated and how, from this point further, a virtual microstructure can be calculated. The addition of fillers can be considered as a very promising feature as regards the development of new cement-based systems and with this, the development of new materials. It shows the potential of numerical models to simulate material and structural behaviour of concrete elements and the ability for the engineering practice to participate in these innovative developments.

6. References

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