MRI validation of FEM models to describe moisture induced spalling of concrete

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ABSTRACT: Fire safety of buildings and structures is an important issue, and has a great impact on human life and economy. One of the processes negatively affecting the strength of a concrete building or structure during fire is spalling. Many examples exist in which spalling of concrete during fire has caused severe damage to structures, such as during the fires in the Mont Blanc and Channel Tunnel. Especially newly developed types of concrete such as HPC and SCC, have shown to be sensitive to spalling, hampering the application of these new concrete types. To reduce risks and building costs, the processes behind spalling need to be understood. Increasing our knowledge allows us to predict and take effective and cost friendly preventive measures. One of the mechanisms that drives spalling of concrete, is the heating of the moisture present inside concrete. When concrete is heated water will evaporate, which results in a high gas pressure inside the pores of the concrete.

In recent years much research has been performed on the processes behind spalling. Using this knowledge, a Finite Element Model (FEM) describing the moisture transport processes in heated concrete has been developed. However, the validity of all current models (including our own) is unknown because of debatable input parameters and lack of experimental techniques to follow the transport process in situ. In cooperation with the Eindhoven University of Technology moisture transport in heated concrete can now be investigated using a home built dedicated 1D Magnetic Resonance Imaging (MRI) setup. Using the results of the MRI experiments the validity of our FEM model is being assessed.

1 INTRODUCTION

Over the past decades concrete has improved in strength, workability, and durability, and the research on improving concrete still continues (Aitcin 2000). In modern structures such as tunnels, bridges, and buildings so-called high performance concrete (HPC) is preferred more and more over ordinary concrete (OC). In order to achieve a higher strength and better durability the water cement ratio is reduced. As a result, the porosity, and hence permeability of the concrete is also greatly reduced. On one hand, this reduction in permeability has resulted in a higher durability of concrete. On the other hand, due to these modifications the risk of (violent) spalling has increased when the concrete is subjected to high temperatures as occur in a fire (Gabriel 2000; Kalifa et al. 2000).

Two mechanisms are assumed to contribute to the process of spalling. First, upon heating water inside the concrete will evaporate and boil at a certain temperature (depending on the pressure). The high gas pressure drives the transport of water vapour out of the concrete, but is hindered due to a low permeability, and as a result the pressure inside the pores further increases. Second, due to the difference in thermal strain between the cement, and aggregates thermal stresses occur in the material. This stresses can introduce internal cracking of the concrete. In most cases a combination of both mechanisms is needed for spalling to occur (Gabriel 2000).

Numerous techniques are developed for research on fire spalling of concrete, such as mathematical models, full scale experiments, chemical analysis, and strength measurements (Gawin et al. 1999). To our opinion the full complexity of the spalling process can only be modeled fully, when subsequent modeling steps are validated. To validate subsequent modeling steps a suitable technique is required. However, no direct measurements of the moisture content and moisture transport are available. As a result only measurements of temperature and pressure are generally used for validation. With Nuclear Magnetic Resonance (NMR) it is now possible to nondestructively measure the moisture content as a function of the position inside porous
building materials (Kopinga et al. 1994; Valckenborg et al. 2001). With a new home built MRI setup the moisture transport can now be measured while being heated at one side.

In this paper we describe a study in which results of a FEM model that describes moisture transport in heated concrete is compared to MRI measurements of the moisture content inside concrete during heating. First we will explain some basic MRI principles and describe the setup used. Additionally the basic assumption and ingredients for the FEM model will be described.

2 MRI THEORY AND TRANSPORT MODEL

2.1 MRI setup
Almost all nuclei have a magnetic dipole moment, resulting from their spin-angular momentum. (One can think of a nucleus as a charged sphere spinning around its axis, which corresponds to a current loop, generating a magnetic moment.) In an NMR experiment the magnetic moments of the nuclei are manipulated by suitably chosen electromagnetic radio frequency (RF) fields. The frequency of the resonance conditions is given by:

\[ f_i = \frac{\gamma}{2\pi} B_0 , \]

where \( f_i \) is so-called Larmor frequency [Hz], \( B_0 \) [T] the externally applied static magnetic field and \( \gamma \) is the gyromagnetic ratio which is dependent on the type of nucleus (for \(^1H\) \( \gamma/2\pi = 42.58 \text{ MHz T}^{-1} \)). Because of this condition the method can be made sensitive to only hydrogen and therefore to water. When a known magnetic field gradient is applied, the constant magnetic field \( B_0 \) in the resonance condition (Eq. 1) has to be replaced by the spatially varying magnetic field \( B \):

\[ B(x) = B_0 + Gx , \]

where \( G \) [T m\(^{-1}\)] (see Fig. 1) is the magnetic field gradient and \( x \) is the position of the precessing magnetic moment. The resonance condition is then spatially dependent. Therefore the moisture content at different positions \( x \) in the sample can be measured by varying the resonance frequency without moving the sample.

In a pulsed NMR experiment the orientation of the moments of the spins are manipulated by short RF pulses at the resonance frequency. The amplitude of the resulting signal emitted by the nuclear spins, the so-called ‘Hahn spin-echo’ (Hahn 1950) signal is proportional to the number of nuclei taking part in the experiment. The spin-echo signal also gives information about the rate at which this magnetic excitation of the spins decays. The system will return to its magnetic equilibrium by two mechanisms: interactions between the nuclei themselves, causing the so-called spin-spin relaxation, and interactions between the nuclei and their environment, causing the so-called spin-lattice relaxation.

For the experiments described in this study, a home built NMR scanner is used. This instrument was especially designed for quantitative measurements of moisture in porous materials with short transverse relaxation (T2) times (unlike standard Magnetic Resonance Imaging (MRI), which is generally used in a qualitative way). The machine makes use of the magnet of a whole body MRI scanner (Gyroscan, Philips) which operates at a main field of 1.5 T corresponding to a frequency of 63.9 MHz. The setup is placed within the scanner and a schematic diagram is given in Fig. 3. Two Helmholtz coils provide the magnetic field gradient \( G \) in the direction of \( B_0 \). The magnitude of the gradient is 100 mT m\(^{-1}\), providing a spatial resolution of the order of 2 mm.

A home built birdcage coil is used for applying the RF pulses, and receiving the NMR signal from the sample. The coil is 60 mm long and has a diameter of 60 mm.

A birdcage coil is used because it generates a homogeneous \( B_1^\text{-field} \) perpendicular to the sample. Therefore, the coil can be placed parallel to the main magnetic field providing optimal use of the available space inside the bore. The sample is heated with a halogen lamp. The reflector of the lamp was gold plated to ensure maximum reflection of the infra-red radiation. The sample is placed inside the birdcage coil and is thermally insulated using mineral wool in order to create a 1D experiment (van der Heijden et al. 2007).

2.2 FEM model
Concrete is a porous material, which contains voids that are filled with air, water vapour and liquid water. To describe transport of moisture and heat the three phases, concrete (s), water (l), water vapour (gw) and air (ga), present in concrete have to be taken
into account. By introducing the Representative Elementary Volume (REV) it is possible to describe the microscopic level by macroscopic variables. An important issue within the averaging theory is the size of the REV. The REV has to be small enough to be considered as infinitesimal, and at the same time must be large enough with respect to the heterogeneities of the material, to provide average quantities (Hassanzadeh et al. 1979). After having applied the averaging theory a continuum description using differential equations may be used.

2.3 Simplifying the model using suitable assumptions

To describe the process of spalling of concrete several assumptions have to be made to simplify the model and limited it to the major processes involved. The following list summarizes the assumptions made for the model in this report.

- No change in porosity (n) is assumed. The change of porosity will affect the pore volume and the permeability. Because the peak of the gas pressure will be located at temperatures much lower than 1000°C, the increase in volume will decrease the gas pressure only slightly. However, the induced change in permeability is of importance, but that effect is incorporated in the equations describing the permeability.
- Dehydration of concrete is an important source for water inside the pores, and is therefore included as a source term (Gawin et al. 1999; Li et al. 2002).
- At high temperature diffusion of water vapour is no longer an important process (Ichikawa et al. 2004). At high temperatures moisture and water vapour transport is gas-pressure.
- Liquid water and water vapour are always in local equilibrium, so that the change in Gibbs free energy of liquid water and water vapour is always equal: \( dG_w = dG_{gw} \). As a result the evaporation of water can be described by the Clausius-Clapeyron equation. Note that, assuming thermodynamic equilibrium also means that all materials in one representative volume have equal temperatures and pressures.
- Heat capacity of gas is omitted in the effective capacity, since the heat capacity (density times specific heat capacity) of gas is low compared to that of water and concrete. However, in case of convection the speed of the gas, and therefore the flux can be sufficiently high to be of relevance, so for convection of heat the heat capacity of the gas is included.
- Water is assumed to be incompressible, as a result the density of water is only a function of temperature.
- Influence of gravity is neglected.

2.4 Basic ingredients

To describe moisture and heat transport in concrete the three conservation equations are constructed, for dry air, for water (including water vapour), and one for energy. To construct these equations several general conservation equations are used. For a conserved variable ψ (e.g. like mass, momentum and energy) the general conservation equation may be written as

\[
\frac{\partial \psi}{\partial t} + \nabla \cdot (\psi \mathbf{v}) = H,
\]

with \( \psi \mathbf{v} \) the transport flux and \( H \) the source or sink of \( \psi \). In our model the conserved averaged variables are respectively: \( \psi \in (1-n)\rho_a, nS_w\rho_w, nS_g\rho_gw, nS_g\rho_gv, C_{eff} T \), where \( n \) the porosity (between 0 and 1), \( S \) the saturation of the respective phase (sum of water and gas phase is 1) and \( C_{eff} \) the effective heat capacity of concrete and \( T \) the temperature. The subscripts denote the phase, \( s \) for solid matrix, \( w \) for water, \( ga \) for air, and \( gw \) for water vapour.

Besides the conservation equations several state equations and material properties are required. For the state equations we use the Kelvin equation, the Clausius-Clapeyron equation, Darcy’s law (for both water and water vapour), and ideal gas law, and for the material properties we use an equation for the dehydration, the water density as a function of temperature, the permeability for different levels of saturation (for both water and water vapour), and the van Genugten equation (Hall et al. 2002) (for the hydrodynamic potential). Each of these equations has its own limitation, introducing deviations in the final calculations.

After some mathematical operations the model was implemented. Finally, the last step before simulations can actually be performed the boundary conditions need to be specified. At the right side the boundary is closed. At the left side of the sample is open for water vapour. To achieve the best correspondence with the experiments the surface temperature of the experiment is used as the boundary condition at the left side of the sample.

3 RESULTS OF SIMULATIONS AND MRI MEASUREMENTS

3.1 Yellow fired-clay brick

In figure 2 the saturation profiles measured with NMR for fired-clay brick are shown every 15 minutes for a total of 7.5 hours. Initially the sample is fully saturated, so the first profile corresponds to \( S = 1 \). After 1.5 hours a clear drying front develops. From 0 to 1.5 hours the moisture profiles are more homogeneous. In figure 3 the simulations are shown for the fired-clay brick.
A general correspondence is seen between the saturation profiles and the simulation profiles. The homogeneous drying, in the beginning of the drying experiment, is due to the capillary forces inside the fired-clay brick. In the experiment when the saturation equals approximately 0.4, the signal at the right side of the front starts to drop less fast. In the simulations this effect is not as pronounced.

The temperatures measured by the 8 thermocouples are shown in figure 4, with thermocouples positioned every 5 mm, and the first 5 mm from the surface. At 100°C a change in curvature can be seen, corresponding to the boiling of water inside the pores. The temperatures obtained from the simulation are shown in figure 5. It can be seen that the experiment and the simulations correspond rather well, except that the boiling temperature in the simulation is higher approximately 125°C due to the higher gas pressure. This can be attributed to the fact that the drilled holes, in which the thermocouples are inserted, allow the gas to escape.

As the sample is heated a 100°C front is formed and moves through the sample. The water at this front will start to boil and evaporate. In figure 6 the position of both the 100°C front and the drying front are shown. The evaporation front moves slower than the 100°C front, indicating an increased gas pressure inside the fired-clay brick (boiling is taking place at a higher temperature). This corresponds to the simulations, which showed that the boiling point was approximately 125°C. The gas pressure inside the samples, determined from the simulations, is boundary at the right side is closed in the simulations (figure 7).
3.2 Concrete containing poly-propylene fibers

In figure 8 moisture profiles measured by MRI are presented, which show a gradient in the moisture content. The measured saturation profiles measured are shown every 5 minutes. Initially the sample is fully saturated, so the first profile corresponds to $S = 1$ (in the measurements the data is normalized). In this concrete sample polypropylene fibers were added which melt at approximately 165°C. The profiles correspond rather well to the simulated profiles shown in figure 9.

In figure 10 the measured temperature is plotted at different positions: 5, 10, 15, 20, 30 mm from the surface. In figure 11 the temperature of the simulations is plotted at different positions. Note that in this figure 10 the temperature remains constant at 100°C for a short period, indicating that boiling is occurring at that position. In fact the boiling takes place at a higher temperature, as in case of the fired-clay brick, the high gas pressure can escape from the sample in the experiment via the drilled holes. Note that the same temperature is reached after 100 min for all thermocouples, which is not observed in the MRI experiment (figure 10). This difference can be explained by the fact that in the simulation the sample is ideally insulation, which is not the case in the NMR experiments.

4 CONCLUSIONS AND DISCUSSION

In first order the global features observed in the simulations correspond to those observed in the MRI experiments. However, several differences are observed. For instance the temperatures in the simulations with respect to the boiling of water do not correspond to the temperatures measured in the experiment. The boiling in the simulations takes place at 125°C and in the experiment at 100°C. This can be explained by the fact that gas can escape from the drilled holes,
Another difference between simulations and experiments is the final temperature that is reached. In the simulations the temperatures at different depths reach the same value. However, in the MRI experiment different final temperatures are reached, the difference is caused by heat loss to the environment from the walls of the sample, which is not the case for the 1D simulations.

In all simulations the input parameters describing the material properties were a best guess and were then optimized for the best correspondence between experiment and simulation. Further research should not only focus on optimizing the simulations, but also on determining the most relevant material properties, such as permeability, porosity, dehydration, permeability for water and water vapour as a function of temperature and saturation. Additionally in a next step interaction between moisture transport and mechanical behaviour should be investigated. All these future steps require subsequent validation, in which MRI as a validation tool has proven to be very valuable.

To validate the model at high temperatures the MRI setup has still to be improved to be able to measure at these high temperatures. Additionally the size of the sample is still rather small. At this moment the Eindhoven University of Technology is working on both these improvements.

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