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ASPECTS OF PERMEABILITY IN MODELLING OF CONCRETE EXPOSED TO HIGH TEMPERATURES

C. T. Davie^{1*}, C. J. Pearce² and N. Bićanić²

¹ *School of Civil Engineering and Geosciences, Newcastle University, Newcastle upon Tyne, UK*

² *School of Engineering, University of Glasgow, Glasgow, U.K.*

*Correspondence to:

Colin T Davie

School of Civil Engineering and Geosciences,

Newcastle University

Newcastle upon Tyne,

NE1 7RU, United Kingdom

Email: colin.davie@ncl.ac.uk

Telephone: +44-(0)191 222 6458

Abstract

The development of heat and moisture transport in concrete is critical to the development of pore pressures, which are thought to be a primary driver of damage and thermal spalling in concrete exposed to elevated temperatures. In the light of uncertainty and variation in the value of certain material properties and constitutive or parametric descriptions found in the literature, various sets of numerical experiments were conducted to investigate the significance of the intrinsic permeability, the evolution of permeability related to temperature and the relative permeability of the fluid phases as functions of saturation in predicting and analysing the behaviour of concrete drying under normal, low temperature, isothermal conditions and under exposure to very high temperature conditions as might be encountered during a fire.

A fully coupled hygro-thermo-mechanical finite element model for concrete was employed with the permeability values and parametric functions altered in the model as required. Results of mass loss and the development of gas pressures with time were considered in relation to the potential for the occurrence of damage and thermal spalling, which is thought to be variously related to these processes.

The analyses showed that permeability, and its variation with temperature, are very important in controlling the predicted behaviour at both low and high temperatures. Most significant of all were the relationships chosen to define the relative permeabilities. These were shown to strongly control the results of analyses of both low and high temperature problems and to potentially imply apparently different permeability values for the same concrete.

Key words: permeability, concrete, high temperature, fire, spalling

1. Introduction

Problems concerning concrete exposed to elevated temperatures are significant and wide ranging. Some structures, such as nuclear reactor vessels, are designed to operate at elevated temperatures and others may be accidentally or deliberately exposed to fire. In all such cases safety, for example in terms of nuclear containment or structural collapse, is of primary concern while the economic consequences of thermally induced damage may also be very significant. These issues are particularly highlighted by incidents such as the Channel Tunnel fire in 1996, which resulted in significant damage to the tunnel liner, leaving it structurally unsound, and several months of closure with associated repair costs and loss of revenue of ~€1.5m/day (Ulm et al. 1999).

One of the key manifestations of damage under such circumstances is thermal spalling; i.e. the fracturing and loss of material (sometimes explosively) from heat exposed surfaces. In larger concrete structures such as pre-stressed concrete pressure vessels (PCPV), damage may develop inside the concrete, potentially affecting its structural integrity or that of internal steel liners that preserve nuclear containment (Pearce et al. 2005; Jason et al. 2007).

A primary driver of damage and spalling is thought to be the development of gas pressures in the concrete pore space (e.g. (Hertz 2003; Ichikawa, England 2004; Phan et al. 2001; Kalifa et al. 2000)) that result from the build up of vapour due to the movement and evaporation of water. If the stresses applied internally by these pressures exceed the tensile strength of the concrete, damage may be caused. It is therefore very important to understand the heat and moisture transport in concrete exposed to elevated temperatures and, to ensure safety in the design of structures, to be able to accurately predict the development of pressure in the pore space. Clearly this behaviour is dependent on the concrete material properties and particularly on the aspects of permeability that are explored here.

To predict this behaviour, over the last 30+ years, a number of authors have developed progressively more detailed (continuum based) numerical models for concrete exposed to elevated temperatures (e.g. (Bažant, Thonguthai 1978; Gawin et al. 1999; Baroghel-Bouny et al. 1999; Tenchev et al. 2001; Chung et al. 2006; Davie et al. 2006; Dwaikat, Kodur 2009)). The behaviour of concrete under such conditions is highly complex and ideally models must take into account numerous interdependent and coupled physical processes and material parameters.

In considering the state-of-the-art in this field the most sophisticated models consider the coupled multi-phase behaviour of concrete based on physical laws and are generally able to capture the observed heat and mass transport behaviour including the development of pore pressures. Of these, the least complex consider only the coupled hygro-thermal behaviour (e.g. (Baroghel-Bouny et al. 1999; Tenchev et al. 2001)). While they are capable of predicting the interaction of heat, liquid and gas flow in the pore space, without consideration of mechanical behaviour the role of pore pressure in the development of damage cannot be fully assessed. To address this some hygro-thermal models have been extended to include simplified assumptions to determine whether, as a result of the pore pressures, damage and spalling would occur (e.g. (Dwaikat, Kodur 2009)). Of course, the accuracy of the model predictions depends on the accuracy of the assumptions and it must be noted that without considering the mechanical behaviour directly they cannot account for the reverse effect of damage on heat and moisture transport, although this will arguably lead to conservative results.

A group of more complex models considers the coupled hygro-thermo-(chemo)-mechanical behaviour of concrete taking into account the development of stresses due to both mechanical and pore pressure behaviour (e.g. (Chung et al. 2006)). Furthermore, some of these models are extended either to include the development of damage as a result of stress (often employing an elastic-damage model) or to make assumptions based on the stress state in order to determine if spalling will occur (Tenchev, Purnell 2005; Gawin et al. 2006b).

However, the most comprehensive models also consider the fully coupled effects of the mechanical and transport behaviours and this has been shown to be critical in the prediction of pore pressures in concrete (e.g. (Gawin et al. 1999)). One such model is used in the work presented here (Davie et al. 2010).

Beyond the distinct formulations that have been discussed above the key differences between these state-of-the-art models lie in the form of the constitutive relationships employed. It is particular those functions relating to aspects of permeability and their implications for the prediction of damage and spalling that are investigated in this work. One reason for the variation found in these functions is the uncertainty surrounding concrete material properties and their evolution with temperature. Such properties are often not measured in experimental studies and even less so for real structures.

Where they are reported, investigation shows a very wide variation in values for permeability ranging over six orders of magnitude (Fig. 1). Similarly, there is considerable variation in the way that the evolution of permeability with temperature and saturation is described and numerous functions have been derived. Thus, without detailed understanding, it is extremely difficult to identify appropriate values or functions for numerical analysis of specific concretes.

Fig. 1 Reported values for Intrinsic Permeability for Ordinary (OC) and High Performance Concretes (HPC) ((Davie et al. 2010; Baroghel-Bouny et al. 1999; Tenchev,Purnell 2005; Schrefler et al. 2000; Zeiml et al. 2008; Ichikawa,England 2004; Gawin et al. 2002, 2004, 2006a))

Through the use of numerical experiment based on experimental case studies, this work sets out to investigate the influence of permeability and the relationships used to describe its evolution, the significance that they may have for the numerical prediction of the mass transport behaviours in concrete exposed to elevated temperatures and the implications that these findings have for concrete structures in terms of safety in the context of predicting spalling and damage. In doing so the work acts to review the literature and the qualitative suitability of the relationships presented there, identify the most representative and appropriate relationships for permeability development under elevated temperatures and further identify key areas where specific data is necessary for accurate analyses.

2. Numerical Model

A fully coupled hygro-thermo-mechanical model was employed in which concrete is treated as a multiphase porous continuum consisting of solid, liquid and gas phases. The solid skeleton is considered to behave elastically, and nonlinear responses to mechanical and thermal loadings are accounted for through an isotropic damage formulation. The ‘liquid’ phase considers free liquid water in pores, water liberated from the solid skeleton through dehydration and adsorbed water physically bound to solid skeleton. The gas phase is considered to be a

mixture of dry air and water vapour, which are assumed to behave as ideal gases. Many of the material properties are variable often, either directly or indirectly, as functions of temperature. A complete description of model formulation and implementation as well as auxiliary functions may be found in (Davie et al. 2010) and (Davie et al. 2006). Due to space constraints only a brief description of the governing and transport equations can be given here.

2.1. Governing Equations

The fully 3-dimensional model formulation is developed from four governing equations defining the conservations of mass of dry air (1), mass of moisture (2), energy (3) and linear momentum (4).

$$\frac{\partial(\varepsilon_G \tilde{\rho}_A)}{\partial t} = -\nabla \cdot \mathbf{J}_A \quad (1)$$

$$\frac{\partial(\varepsilon_G \tilde{\rho}_V)}{\partial t} + \frac{\partial(\varepsilon_L \rho_L)}{\partial t} - \frac{\partial(\varepsilon_D \rho_L)}{\partial t} = -\nabla \cdot (\mathbf{J}_V + \mathbf{J}_L) \quad (2)$$

$$(\underline{\rho C}) \frac{\partial T}{\partial t} - \lambda_E \frac{\partial(\varepsilon_L \rho_L)}{\partial t} + (\lambda_D + \lambda_E) \frac{\partial(\varepsilon_D \rho_L)}{\partial t} = \nabla \cdot (k \nabla T) + \lambda_E \nabla \cdot \mathbf{J}_L \quad (3)$$

$$\nabla \cdot (\boldsymbol{\sigma}' - \eta P_{Pore} \mathbf{I}) + \mathbf{b} = 0 \quad (4)$$

where, ε_θ is the volume fraction of a phase θ ($\theta = L, V, A, G, D$ refer to liquid water, water vapour, dry air, gas mixture and dehydrated water phases, respectively), ρ_θ is the density of a phase θ , $\tilde{\rho}_\theta$ the mass of a phase θ per unit volume of gaseous material, $\mathbf{J}_\theta$ the mass flux of a phase θ , $\underline{\rho C}$ the heat capacity of concrete, k the effective thermal conductivity of concrete, λ_E and λ_D are the specific enthalpies of evaporation and dehydration, T is the temperature, $\boldsymbol{\sigma}'$ is the Bishop's stress, $\mathbf{I}$ is the identity matrix, η is the Biot coefficient, P_{Pore} is the pore pressure, $\mathbf{b}$ is the body force and t is time.

2.2. Fluid Transport Equations

Within the pore space, fluids are assumed to flow under pressure according to Darcy's law, with the gas phase also diffusing according to Fick's law. The mass fluxes of dry air, water vapour and liquid water are then given by (5) - (7).

$$\mathbf{J}_A = \varepsilon_G \tilde{\rho}_A \left(-\frac{k_g K K_G}{\mu_G} \right) \nabla P_G - \varepsilon_G \tilde{\rho}_G D_{AV} \nabla \left(\frac{\tilde{\rho}_A}{\tilde{\rho}_G} \right) \quad (5)$$

$$\mathbf{J}_V = \varepsilon_G \tilde{\rho}_V \left(-\frac{k_g K K_G}{\mu_G} \right) \nabla P_G - \varepsilon_G \tilde{\rho}_G D_{AV} \nabla \left(\frac{\tilde{\rho}_V}{\tilde{\rho}_G} \right) \quad (6)$$

$$\mathbf{J}_L = \varepsilon_L \rho_L \left(-\frac{KK_L}{\mu_L} \right) \nabla P_L \quad (7)$$

where, K is the intrinsic permeability of the concrete, K_θ , μ_θ and P_θ are the relative permeability, dynamic viscosity and pressure of the phase θ , k_g is the gas-slip factor and D_{AV} is the coefficient of diffusion for the dry air/water vapour mixture.

Capillary suctions are considered via the Kelvin Equation (8).

$$P_L = P_G - P_C, \text{ with } P_C = \begin{cases} -R_V T \rho_L \ln \left(\frac{P_V}{P_{Sat}} \right) & \text{for } S > S_{SSP} \\ 0 & \text{for } S \leq S_{SSP} \end{cases} \quad (8)$$

where, R_V is the ideal gas constant for water vapour, P_V is the vapour partial pressure and P_{Sat} is the saturation vapour pressure. S_{SSP} is the solid saturation point, which is the degree of saturation below which all water exists as adsorbed water, physically bound to the concrete skeleton (Gawin et al. 1999).

The liquid water content in the concrete is calculated from the sorption isotherms (9) (Bažant, Thonguthai 1978; Tenchev et al. 2001).

$$\varepsilon_L = \frac{\varepsilon_{Cem} \rho_{Cem}}{\rho_L} \cdot f \left(\frac{P_V}{P_{Sat}}, T, \phi \right) \quad (9)$$

where, $\varepsilon_{Cem} \rho_{Cem}$ is the cement content, (P_V / P_{Sat}) is the relative humidity and ϕ is the porosity. Detail of the formulation can be found in (Davie et al. 2010).

2.3. Mechanical Constitutive Equations

Although coupling of the fluid transport and mechanical behaviours of the material is paramount, in the analysis of the problems considered here the formulation of the mechanical component of the model is not of primary importance and so is not given in detail. Briefly, it may be noted that a total strain formulation is developed ($\boldsymbol{\varepsilon}$) in which elastic strains ($\boldsymbol{\varepsilon}^e$), free thermal strains ($\boldsymbol{\varepsilon}^{ft}$) and load induced thermal strains ($\boldsymbol{\varepsilon}^{lits}$) are considered according to (10).

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^{ft} + \boldsymbol{\varepsilon}^{lits} \quad (10)$$

It may be further noted that the degradation of the concrete due to thermal and mechanical loading and the associated reduction of stiffness are accounted for by an isotropic scalar damage model where the Bishop's stress is given by (11).

$$\boldsymbol{\sigma}' = (1 - \omega)(1 - \chi) \mathbf{D}_0 : \boldsymbol{\varepsilon}^e \quad (11)$$

where, $\mathbf{D}_0$ is the initial elasticity tensor, ω is the mechanical damage parameter and χ is the thermal damage parameter.

2.4. Numerical Solution

The governing equations are discretised using the standard finite element approximation, with primary variables of displacements, $\mathbf{u}$, temperature, T , gas pressure, P_G , and vapour content, $\tilde{\rho}_v$. Discretisation in time is achieved by a generalised mid-point finite difference scheme. Boundary conditions for the temperature and vapour content are considered to be of the Neumann (flux) type, while the gas pressure is considered to be fixed at atmospheric pressure.

3. Numerical Analyses

To assess the influence and significance of permeability and its evolution on the fluid transport behaviour and particularly the development of pore pressures in concrete exposed to elevated temperatures with implications for spalling, various numerical experiments were conducted using the model described above.

To provide points of reference for the results two numerical models were developed that were representative of experimental problems from literature for which there are comprehensive results and for which the capability of the model in reproducing those results has been demonstrated (Davie et al. 2010).

The first problem (the ‘BB’ problem), reported in (Baroghel-Bouny et al. 1999), considers a cylinder of concrete allowed to dry under ambient isothermal conditions. This provides a control study through which temperature effects can be isolated. The second problem (the ‘K’ problem), reported in (Kalifa et al. 2000), considers a slab exposed to 600°C on one face. Through comparison with the BB problem, this allows the effects of temperature to be explored in detail. The set up and initial properties of both models are given in Fig. 2 and Table 1.

Fig. 2 Model Set Up for a) BB Problem and b) K Problem

For convenience the models were set up as 2-dimensional meshes (although it is noted that the problems are effectively 1-d) and preliminary studies showed that

discretisations of 100×1 (BB problem) and 120×1 (K problem), 8-noded, quadrilateral elements were suitable for the problems in question. Similarly, time-steps of 3600s and 1s were respectively found to be appropriate for the long running, isothermal, BB problem and the high temperature, K problem. In both cases the experimental results for ordinary concrete (OC) (mass loss with time - BB; gas pressure with time 20mm from the hot face - K) were used for parametric analysis and the models were initially tuned to those results.

Table 1 Parameter Values for BB and K Problems (Davie et al. 2010; Baroghel-Bouny et al. 1999)

Model	Parameter	Value
BB	Initial internal temperature, T	20°C
	Initial internal gas pressure, P_G	101325Pa
	Initial internal vapour content, $\tilde{\rho}_v$	0.016077kg/m ³ $\equiv$ ~93%RH
	External temperature, T	20°C
	External gas pressure, P_G	101325Pa
	External vapour content, $\tilde{\rho}_v$	50%RH
K	Initial internal temperature	25°C
	Initial internal gas pressure	101325Pa
	Initial internal vapour content	0.014525kg/m ³ $\equiv$ ~63%RH
	External hot face temperature	600°C
	Initial internal gas pressure	101325Pa
	Initial internal vapour content	0.05%RH
	External cold face temperature	25°C
	Initial internal gas pressure	101325Pa
	Initial internal vapour content	65%RH

Parametric effects related to the intrinsic permeability, the evolution of permeability related to temperature and the relative permeability of the fluid phases as functions of saturation were then investigated in detail. In considering the results particular attention was paid to moisture content and pore pressures in the concrete. As discussed above, these are thought to contribute to the development of thermal spalling and damage in concrete structures, which can have significant structural safety and economic consequences.

4. Numerical Investigations

4.1. Experimental Case Studies

In order to demonstrate the validity of the numerical model and to subsequently understand the comparative behaviours caused by varying parameters and formulae a calibrated benchmark set of results was required. To achieve this the two models were run several times while tuning by trial and error various parameters, such as the intrinsic permeability, thermal conductivity etc., that were

unspecified in the experimental procedures reported in the literature, until the best possible match was found between the results predicted by the model and the experimental results (Baroghel-Bouny et al. 1999; Kalifa et al. 2000). The parameters and functions found to give the best calibration are shown in Table 2.

Table 2 Material Parameters and Relationships for Analyses

Analyses	Intrinsic Perm. (m ²)	Perm. Func.	Rel. Perm. Func.
BB Model Calibration	4.0×10^{-21}	N/A	Baroghel-Bouny
K Model Calibration	9.0×10^{-20}	Bary	Chung & Consolazio
Intrinsic Perm. (BB)	Various	N/A	Baroghel-Bouny
Intrinsic Perm. (K)	Various	Bary	Chung & Consolazio
Perm. Function (K)	9.0×10^{-20}	Various	Chung & Consolazio
Rel. Perm. (BB)	4.0×10^{-21}	N/A	Various
Rel. Perm. (K)	9.0×10^{-20}	Bary	Various

A selection of results from the tuned BB and K problems are presented respectively in Fig. 3 & 4 to demonstrate the capabilities and performance of the model in predicting the fully coupled hygro-thermal behaviour that develops in concrete under ambient or hot conditions. Relevant example results are presented with time and distance across the sample at different times. Where possible the numerical results have been compared with the reported experimental results.

Fig. 3 BB Case Study results showing a) normalised mass loss with time, b) moisture contents across the sample, and partial pressures of c) dry air and d) vapour across the sample

Fig. 4 K Problem Case Study results showing a) temperature (10mm depth) with time, b) gas pressure (20mm depth) with time, c) temperatures across the sample, d) partial pressure of dry air across the sample, e) partial pressure of vapour across the sample, f) saturation across the sample, g) porosity across the sample, h) permeability across the sample

These results demonstrate the typical heat and moisture transport behaviours that occur under isothermal drying and high temperature conditions. As can be seen, in both the BB and K problems the model performance is good and the experimentally observed behaviours related to temperatures, moisture movements and gas pressures are well captured (Fig. 3a-b & Fig. 4a-b).

Particularly the variation of temperature across the heated sample and its effect on the movement of moisture in concrete is clearly observed where the gentle, slow drying process observed in profiles of moisture content shown in Fig. 3b is in sharp contrast to the steep drying front that can be identified in the saturation profiles shown in Fig. 4e. Associated with this is also a distinct difference in the gas flow behaviour. Where the isothermal BB problem produces very little vapour and gas pressures remain roughly constant (Fig. 3c), the high temperature K problem is characterised by large volumes of vapour and a sharp peak in gas pressure that moves through the concrete in time, driven by temperature and pressure gradients (Fig. 4b & d).

Further associated with the vapour it may be noted that the saturation in the high temperature problem increases ahead of the drying front (Fig. 4e). This is the result of evaporated water (vapour) being driven away from the hot face into cooler regions of the concrete where it re-condenses in a process originally described by Harmathy ((Harmathy 1965) as cited in (Tenchev et al. 2001)) as the ‘moisture clog effect’.

The typical effect of the temperature profile on the variation of the porosity and permeability may also be noted where significant increases in both are seen in time near the hot face (Fig. 4a, c, f & g). Clearly these changes influence the moisture and heat transport and so the development of these properties is critical to the prediction of gas pressure development in the concrete.

In the following parametric studies, the normalised mass loss with time (BB) and gas pressure with time 20mm from the heated face (K)¹ are used as key results by which to compare the relative behaviours controlled by the various permeability parameters (c.f. Fig. 3a & Fig. 4b).

4.2. Intrinsic Permeability

As discussed above a very wide range of values for intrinsic permeability are quoted in the literature ranging across six orders of magnitude from 10^{-16}m^2 to 10^{-21}m^2 for OC and from 10^{-18}m^2 to 10^{-22}m^2 for HPC (Fig. 1). There is little identifiable pattern to the quoted values other than, as would be expected for

¹ While gas pressures were recorded by (Kalifa et al. 2000) at various depths and consideration of any of these would have led to the same conclusions in this work, the results from 20mm were chosen for simple practical purposes in that they gave the clearest and most convenient plots.

denser material, HPC tends to have lower values. Consequently, for modelling and analysis, it is difficult to identify appropriate values for particular concretes.

To determine the significance of the intrinsic permeability for fluid transport behaviour two sets of numerical experiments were conducted. In the first investigation the model was applied to three analyses of the BB problem with intrinsic permeabilities of $1.0 \times 10^{-16} \text{m}^2$ (Ichikawa, England 2004), $1.0 \times 10^{-19} \text{m}^2$ (Gawin et al. 2006a) and $4.0 \times 10^{-21} \text{m}^2$ (Baroghel-Bouny et al. 1999). All other parameters were kept the same (Table 2).

The predicted normalised mass losses are shown in Fig. 5a.

Fig. 5 a) Normalised Mass Loss with Time (BB), with Various Intrinsic Permeabilities, b) Gas Pressures Developed in Time (K), with Various Intrinsic Permeabilities

As can be seen, distinctly different results are predicted in the three analyses. With the highest permeability, mass is initially lost very rapidly, over ~ 3 days, before slowing considerably as the concrete closest to the edge dries and the remaining moisture must travel further to the boundary, and with lower potential for flow as the internal moisture content approaches that of the atmosphere.

A similar profile is seen with the middle permeability although the mass loss takes significantly longer (>200 days) to level off. The low permeability analysis is notably different again, losing around half the total mass of the other two analyses and showing no tendency to level off even after 354 days.

Clearly the intrinsic permeability is extremely significant in controlling the drying behaviour of concrete. Without a good knowledge of the permeability it would therefore be very difficult to predict how much moisture might be present in a particular concrete at a given time. This could then have implications for determining the potential for spalling in concretes subsequently exposed fire.

In the second investigation three separate analyses of the K problem were conducted with intrinsic permeabilities of $4.0 \times 10^{-18} \text{m}^2$ (Ichikawa, England 2004),

$9.0 \times 10^{-20} \text{m}^2$ and $1.5 \times 10^{-21} \text{m}^2$ (Davie et al. 2010). All other parameters remained the same (Table 2). Gas pressure results developed in time, are shown in Fig. 5b.

As can be seen, the results show a very large increase in the predicted peak gas pressures over the three orders of magnitude decrease in intrinsic permeability, with a maximum pressure of $\sim 0.55 \text{MPa}$ at a permeability of $4.0 \times 10^{-18} \text{m}^2$, increasing to $\sim 3.7 \text{MPa}$ at a permeability of $1.5 \times 10^{-21} \text{m}^2$. While pressures of $< 1 \text{MPa}$, which are lower than the typical tensile strength of OC, would not suggest a potential for spalling, pressures of $\sim 3.7 \text{MPa}$ could present a spalling risk, especially when combined with thermally or mechanically induced stresses. This could be exacerbated for concretes with higher water contents. Pressures of that order would also have implications for the integrity of nuclear containment vessels, through damage of the concrete or associated steel liners and pipe work. The intrinsic permeability of the concrete is therefore critical in determining the fluid transport behaviour and ultimately the safety of concrete structures.

4.3. Variation of Permeability (with temperature)

The permeability of concrete is known to increase with temperature (e.g. (Bažant, Thonguthai 1978; Schneider, Herbst 1989; England, Khoylou 1995; Galle, Sercombe 2001; Kalifa et al. 2001; Jooss, Reinhardt 2002; Choinska et al. 2007; Kanema et al. 2007; Zeiml et al. 2008; Noumowe et al. 2009)). It may be noted that this is contrary to observed behaviour in some other porous materials (e.g. (Civan 2008)) where thermal expansion of the material grains leads to closing of the pore space (especially under confinement) and a reduction in permeability. However, the increase seen in concrete is a function of its material specific behaviour and results from degradation of the concrete microstructure due to processes such as dehydration of the cement gel and the development of micro-fractures caused by the differential thermal expansion of the cement and aggregate phases present in the material. Furthermore, while large concrete structures may experience relatively high uniaxial loads they do not typically experience the level of triaxial confinement experienced by materials such as rocks at depth in the ground and so any similar effect due to grain expansion may be mitigated by free thermal expansion of the concrete members as a whole.

There are various functions of differing forms suggested in the literature to describe the observed increase, any of which may be implemented in numerical

models, and it is not immediately clear which is most appropriate. Some are given as functions of temperature and gas pressure but recently descriptions in terms of an elastic-damage formulation have been favoured. To investigate the significance of the chosen function in influencing the predicted behaviour of concrete at elevated temperatures a series of numerical experiments were conducted based on the K problem.

Seven different functions for permeability, $K(f)$, were considered (12-18) and implemented in the model. For each analysis an intrinsic permeability, K_0 , of $9.0 \times 10^{-20} \text{m}^2$ was used. All other parameters remained the same (Table 2).

$$\text{Constant function} \quad K(T) = K_0 \quad (12)$$

$$\text{'Bary' function} \quad K(T) = K_0 (10^{4D}) \quad (13)$$

$$\text{'Tenchev' function} \quad K(T) = K_0 \left(\frac{\phi}{\phi_0} \right)^{\frac{2}{3}} \quad (14)$$

$$\text{'Gawin' 1} \quad K(T) = K_0 \left(10^{A_T(T-T_0)} \right) \left(\frac{P_G}{P_{Atm}} \right)^{A_P} \quad (15)$$

$$\text{'Gawin' 2} \quad K(T) = K_0 \left(10^{A_T(T-T_0)} \right) \left(\frac{P_G}{P_{Atm}} \right)^{A_P} 10^{A_D D} \quad (16)$$

$$\text{'Picandet' Function} \quad K = K_0 \exp \left((\alpha D)^\gamma \right) \quad (17)$$

$$\begin{aligned} \text{'Souley' Function} \quad K &= K_0 10^{C(D-D_0)} \quad \text{for } D > D_0 \\ K &= K_0 \quad \text{for } D \leq D_0 \end{aligned} \quad (18)$$

where, D is the damage parameter (between 0 and 1)(Davie et al. 2010), T_0 is the reference temperature (273.15K), P_{Atm} is the atmospheric gas pressure (101325Pa) and A_T , A_P , A_D , α , γ , C and D_0 are material coefficients, which have no physical meaning but are used to fit experimental data or observed behaviour. The values employed in this work (Table 3) are those given in the original references or mid-point values where a range is suggested.

The constant function (12) simply holds permeability steady with temperature. The 'Bary' function (13) was originally proposed by Bary et al. (cited in (Gawin et al. 2002)) to fit experimental data and describes permeability as a function of damage. However, since elevated temperatures lead to degradation of the concrete and the development of (thermal) damage, the permeability is also indirectly a function of temperature (Davie et al. 2010). The

‘Tenchev’ function (14) was proposed by (Tenchev et al. 2001) and describes permeability purely as a function of porosity, which is itself a function of temperature (Equation (A7) in that paper) and so the permeability is again indirectly a function of temperature. The first ‘Gawin’ function (15) was proposed by (Gawin et al. 1999) and describes permeability as a function of temperature and gas pressure. This function was subsequently modified in (Gawin et al. 2002) (16) to directly include the effects of damage according to the principles of Bary et al. The ‘Picandet’ function (17) (Picandet et al. 2001), which is exponential with damage, was similarly developed from experimental results. The ‘Souley’ function (18) was developed for the modelling of granite (Souley et al. 2001) and was adapted for concrete by (Jason et al. 2007).

Table 3 Material Parameters for Variation of Permeability Analyses

Equation	Parameter	Value	Source
(15)	A_T	0.005	(Gawin et al. 1999; Gawin et al. 2002)
	A_P	0.368	
(16)	A_T	0.0025	(Gawin et al. 2002)
	A_P	0.368	
	A_D	2	
(17)	α	11.3	(Jason et al. 2007)
	γ	1.64	
(18)	C	8.67	(Jason et al. 2007)
	D_0	0.035	

Due to the number of different variables involved it is difficult to show graphically the relative characteristics of these functions. However, it is notable that all, except (12), contain a power or exponential term and that these result in considerable increases in permeability over the 6 hour duration of the K problem. The maximum ratios of permeability to initial permeability that occurred during each analysis are shown in Table 4 and clearly there are significant differences. The results of the gas pressures predicted during the analyses are shown in Fig. 6.

As can be seen, there are also significant differences in these. Both the constant and ‘Tenchev’ functions result in peak gas pressures well in excess of 10MPa. These are considered inappropriate since, firstly, such pressures would be in excess of the typical tensile strength of OC (resulting in spalling before these pressures were reached) and secondly, they are much higher than the experimentally measured pressures (Kalifa et al. 2000). It is recognised that the gas pressures predicted are directly related to the chosen value of intrinsic permeability, and that by changing it, their magnitude could be tuned to match the

experimental results². However, to fit the results well the value of permeability would be outside the ‘realistic’ range (Fig. 1). It may thus be concluded that a constant permeability is unrealistic and that the magnitude of increase described by the ‘Tenchev’ function, solely as a function of porosity, is insufficient.

Table 4 Permeabilities at Hot Face (K) after 6 Hours

Perm. Function	Highest Permeability (m ²)	Ratio of Maximum to Initial Perm. (K_{max}/K_0)
Constant	9.00×10^{-20}	1
Tenchev	1.41×10^{-19}	1.57
Gawin 1	1.08×10^{-17}	120
Bary	3.79×10^{-17}	421
Gawin 2	2.10×10^{-16}	2333
Souley/Jason	2.02×10^{-14}	224444
Picandet/Jason	2.94×10^{-8}	3.27×10^{11}

Fig. 6 Gas Pressures Developed in Time (K), with Various Permeability Functions

By contrast, the other functions all result in peak pressures comparatively much closer to the expected range, although there are differences between them. ‘Gawin’ 1 (15), which considers temperature and gas pressure, produces a similar result to the ‘Bary’ function (13), which considers damage, but slightly over predicts the pressure. ‘Gawin’ 2 (16), which accounts for temperature, gas pressure and damage, predicts lower pressures, approximately half those predicted by ‘Gawin’ 1 and somewhat lower than both the experimental results and those predicted by the ‘Bary’ function. The ‘Souley’ function (18), which is similar to the ‘Bary’ function, produces even lower pressures and the ‘Picandet’ function (17), which is exponential with damage, produces the lowest pressures of all.

However, the shape of these five curves is very similar and they are indeed similar also to the shape of the experimental results. With tuning of the intrinsic permeability it is likely that they could all be made to fit reasonably well with the experimental results. However, the ‘Souley’ and ‘Picandet’ functions would seem

² Additional tuning may also be achieved by altering the various coefficients present in the functions. However, the values used in this study have been tuned already by the various authors and without a physical analogue for the coefficients it would be a complex trial and error process.

to require very low intrinsic permeabilities in comparison to the ‘realistic’ range. This leaves the two ‘Gawin’ functions and the ‘Bary’ function appearing to be most appropriate. But, ‘Gawin’ 1 slightly over predicts the pressure and ‘Gawin’ 2 somewhat under predicts it, and from the results of this work it is not clear that it is necessary to consider separately temperature, gas pressure and damage.

It is therefore recommended that the ‘Bary’ function is the most representative and appropriate formulation since it produces very good results and has the further advantage of including only one coefficient (which is simply representative of the observed increase in permeability and was universally set to 4 by Bary et al.) whereas the ‘Gawin’ functions require the specification of up to three coefficients, none of which have clear physical interpretations and for which a method of determination for a specific concrete is unclear.

It is accepted that this suggestion is in contrast to the findings of Jason et al. (Jason et al. 2007) who reported that the ‘Souley’ function best fit the permeabilities measured by Bary et al. However, they did not compare the associated heat and moisture transport behaviour and the suggestion is alternatively strongly supported by Dal Pont et al. (Dal Pont et al. 2005), who worked with a version of ‘Gawin’ 2 (16), and by Dwaikat and Kodur (Dwaikat,Kodur 2009) who similarly to this work showed ‘Gawin’ 1 to over predict the gas pressures. Dal Pont et al. showed the effects of temperature and gas pressure to be negligible in comparison to those of damage, ultimately reducing their formulation to that of the ‘Bary’ function, although they concluded that a value of $A_D=1$ was sufficient, despite the recommendation of $A_D=4$ from Bary et al. and $A_D=2$ from Gawin et al. This variation could be an effect of the different concretes being considered or the various damage models employed in these works³. The findings of this work imply that concrete permeability increases exponentially by up to 3 orders of magnitude over a 400°C increase in temperature (or with associated thermal damage).

4.4. Relative Permeability

The relative permeability of a fluid in a multi-phase environment describes the permeability of a given phase with respect to the intrinsic permeability. It is

³ It is recognised that the predicted behaviour is dependent on the damage model employed. This highlights the complex, coupled nature of the problem but is beyond the scope of the current study.

typically described as a weighting factor (between 1 and 0) that is a function of the relative saturation of the pore space (5-7).

There are numerous functions defined in the literature to describe the relative permeabilities of liquid water and gas phases in concrete. Again, it is not immediately clear which is most appropriate. To determine the significance of the chosen functions two sets of numerical experiments were conducted, respectively based on the BB and K problems. In both sets, five analyses were conducted implementing in the model five pairs of functions for K_L and K_G as described below (19-27). All other parameters remained the same (Table 2).

Baroghel-Bouny functions

$$K_G = \sqrt{1-S} \left(1 - S^{1/m}\right)^{2m} \quad (19)$$

$$K_L = \sqrt{S} \left(1 - \left(1 - S^{1/m}\right)^m\right)^2 \quad (20)$$

Chung and Consolazio functions

$$K_G = 10^{S(0.05-22.5\phi)} - 10^{(0.05-22.5\phi)} S \quad (21)$$

$$K_L = 10^{(1-S)(0.05-22.5\phi)} - 10^{(0.05-22.5\phi)} (1-S) \quad (22)$$

Monlouis-Bonnaire functions

$$K_G = (1-S)^p \left(1 - S^{1/m}\right)^{2m} \quad (23)$$

$$K_L = S^p \left(1 - \left(1 - S^{1/m}\right)^m\right)^2 \quad (24)$$

Gawin K_G function

$$K_G = 1 - \left(\frac{S}{S_{cr}}\right)^{A_G} \quad (25)$$

Gawin K_L function 1

$$K_L = \left(\frac{S - S_{ir}}{1 - S_{ir}}\right)^{A_L} \quad (26)$$

Gawin K_L function 2

$$K_L = \left[1 + \left(\frac{1 - RH}{0.25}\right)^{B_L}\right]^{-1} S^{A_L} \quad (27)$$

where, S is the saturation with liquid water, S_{cr} is critical saturation above which there is no gas flow in the medium, S_{ir} is the irreducible saturation, m , p , A_G , A_L and B_L are material parameters (with no physical meaning but used to fit experimental data or observed behaviour) and RH is the relative humidity.

It may be noted that the ‘Baroghel-Bouny’ and ‘Monlouis-Bonnaire’ functions are effectively the same and both take the form of the well known and well established van Genuchten functions (van Genuchten 1980). The difference lies in the values specified for the material parameters. As before, for all functions, where parameter values have been specified in the literature these have been used in this work (Table 5). Where, for the ‘Gawin’ functions a range is suggested, mid-point values have been chosen. This was found to maintain the character of the curves, while making them distinct from the other functions.

Table 5 Material Parameters for Relative Permeability Analyses

Equations	Parameter	Value	Source
(19), (20)	m	1/2.2748	(Baroghel-Bouny et al. 1999)
(23), (24)	p	5.5	(Monlouis-Bonnaire et al. 2004)
	m	0.56	
(25)	A_G	2	(Gawin et al. 1999)
	S_{cr}	1	(Gawin et al. 1999; Dal Pont et al. 2005)
(26)	A_L	2	(Gawin et al. 1999)
	S_{ir}	0	(Gawin et al. 1999; Dal Pont et al. 2005)
(27)	A_L	2	(Gawin et al. 1999)
	B_L	6

Fig. 7 Relative Permeability Functions for a) Gas b) Liquid

Fig. 8 a) Normalised Mass Loss with Time (BB), with Various Relative Permeability Functions, b) Gas Pressures Developed in Time (K), with Various Relative Permeability Functions

The relative characteristics of the functions can be seen in Figs 7a) & b). Two curves are shown for the ‘Chung and Consolazio’ functions as they are related to porosity, which differs between the two sets of analyses. It may also be noted that

for the two sets of ‘Gawin’ functions the K_G function is the same and that the curve shown for the second ‘Gawin’ K_L function is an approximation. This function is dependent on relative humidity and saturation, which is itself a function of relative humidity via the sorption isotherms and so the precise shape of the curve will be dependent on the characteristics of those functions. It may be further noted that, although unsaid, it has been inherently assumed by many of the original authors that these curves remain consistently applicable with increasing temperatures, irrespective of associated changes to the microstructure of the concrete. This assumption has been maintained for this work.

Normalised mass loss results for the first set of analyses are shown in Fig. 8a and gas pressure results for the second set of analyses are shown in Fig. 8b. As can be seen the results predicted using the different functions vary considerably.

Examining firstly the gas pressures it can be seen that the results follow a similar pattern to those seen in Section 4.2. (Fig. 5b), i.e. lower permeabilities produce higher gas pressures. The ‘Chung & Consolazio’ and ‘Monlouis-Bonnaire’ functions result in the highest predicted gas pressures and, in comparison to the other functions, both suggest low gas permeability at the high values of saturation initially present in the K problem (Figs. 4f & 7a). This trend is continued in the three lower gas pressure peaks with the ‘Baroghel-Bouny’ functions predicting a slightly higher peak pressure than the ‘Gawin’ functions.

This behaviour seems to be independent of the K_L functions, which do not have the same relative relationships as the K_G curves (Fig. 7). This suggests that the behaviour in the high temperature K problem is dominated by gas flow and that liquid flow plays only a small part. This is as may be expected given that the high temperatures will lead to large volumes of water vapour through evaporation.

Considering now the normalised mass loss results (Fig. 8a) it can be seen that they do not follow the same pattern. The first set of ‘Gawin’ functions has consistently the highest gas and liquid permeabilities and, as might therefore be expected, predicts the highest mass loss. The second set of ‘Gawin’ functions has the same K_G curve as the first but generally lower values of K_L . The fact that they predict a lower mass loss than the first set of ‘Gawin’ functions demonstrates that, in the case of drying at ambient temperature, both gas and liquid flow are significant. This is further confirmed in that the lowest mass loss is predicted

with the ‘Monlouis-Bonnaire’ functions, which indeed describe the lowest values of K_G and K_L of all the sets of functions.

What is most noteworthy is that the predicted mass loss can be varied by around 100% and the predicted peak gas pressures can be varied by around 60% by changing the relative permeability functions. This could have very significant consequences for the prediction of thermal spalling and so it is essential that appropriate functions are employed.

Considering the K_G curves (Fig. 7a)) they can be classified in two forms, concave and convex with saturation. Looking again at the predicted gas pressures, the ‘Chung & Consolazio’ and ‘Monlouis-Bonnaire’ functions seem to produce similar results and fit best with experimental results, not just with the magnitude, but also with the shape of the curves in time. Both of these K_G functions are concave with saturation suggesting that this is the most appropriate form, in agreement with the findings of (Jason et al. 2007) who showed concave functions of the ‘Monlouis-Bonnaire’ type fit best with measured values.

In contrast, these two sets of functions produce quite different predictions for the mass loss under drying conditions. Again, this is likely due to the form of the K_L curves. It is not completely clear from this work which is the most appropriate but it may be noted that where ‘Chung & Consolazio’ use a simple mirrored form of their K_G curve to define K_L , those of ‘Monlouis-Bonnaire’ are distinct and based on the van Genuchten formulation. Since (with modified parameters) this has been shown to be a good description for K_G in concrete it may be reasonable to assume that it is also appropriate for K_L . However, it may also be noted that, through the inclusion of the porosity term, the ‘Chung & Consolazio’ functions are the only ones that take any account of changes to the microstructure that develop with increasing temperature. While this may not be important for problems where gas flow is dominant more work is clearly required.

Certainly, the shapes of the mass loss curves suggest that both analyses could be tuned, via the intrinsic permeability, to match well with the experimental results and it is interesting to note that if this were done apparently different intrinsic permeabilities would be implied for the same concrete. Given the results of Section 4.1., this is in of itself significant.

5. Conclusions

In the light of uncertainty and variation in the value of certain material properties and parametric descriptions found in the literature, various numerical experiments were conducted to investigate the significance of the intrinsic permeability, the evolution of permeability related to temperature and the relative permeability of the fluid phases as functions of saturation in predicting the fluid transport behaviour in concrete drying under both ambient and high temperature conditions. This behaviour is critical for the prediction of pore pressures that are thought to contribute to the development of thermal spalling and damage in concrete, which in turn can have significant structural safety and economic consequences for structures exposed to fire and nuclear containment structures.

Results of mass loss and the development of gas pressures were considered in relation to the potential for the occurrence of thermal spalling and damage.

On the basis of the continuum description considered here, it was found that:

- Intrinsic permeability is extremely significant in controlling the fluid transport behaviour in concrete under ambient temperature and consequently pore pressures under high temperature conditions. The wide range in results seen in this work indicates that the identification of the concrete permeability may be critical in relation to prediction of the potential development of spalling, and this has implications for both the analysis of existing structures and the design of new structures. However, given the very large range in permeabilities reported in the literature it is difficult to identify even the appropriate order of magnitude without, for example, laboratory testing of specific materials.
- A formulation describing the increase in permeability caused by increasing temperature is essential in order to accurately predict gas pressures in concrete exposed to high temperatures⁴. Relationships expressing permeability as a function of damage appear most appropriate but the inclusion of dependency on gas pressure and temperature seem unnecessarily complicated and does not improve results. The exponential formulation developed by Bary et al. (cited in (Gawin et al. 2002)) was found to be most representative and appropriate.

⁴ Although as discussed previously a decrease in permeability with an increase in temperature has been observed in other porous materials (e.g. (Civan 2008)), particularly under confinement, the physical processes underlying such a decrease are different to those found in concrete exposed to elevated temperatures.

- The choice of relative permeability functions is critical in determining the fluid transport behaviour, in concrete under both ambient and high temperature conditions and the use of different formulations can have a very great effect on the development of pore pressures.

Relative gas permeability functions that suggest particularly low gas permeabilities at higher saturations, give the best comparisons with experimental data. The choice of relative liquid permeability curve has little control over the results of high temperature problems, where gas flow is dominant, but can affect the results of ambient temperature problems. It is suggested that the ‘Monlouis-Bonnaire’ curves, which are based on the well established van Genuchten formulations may be most appropriate although the ‘Chung & Consolazio’ functions are the only ones that can take any account of thermally induced changes to the microstructure. (While continuum descriptions are considered here, microstructural formulations may provide an appropriate alternative).

It is further noted that different formulations could result in the prediction of apparently different intrinsic permeabilities for the same concrete. This has implications not only for concrete but for all problems concerning multi-phase flow in porous media and more work may be required in this area.

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