Propagation of Concentration Jump Interfaces as a Rate-Controlling Mechanism of Diffusion in Concrete

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pp. 1150-1153
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Abstract
Attention is focused on the role of jump interfaces, such as jump in water content or in the concentration of chloride ions, in the diffusion problems affecting concrete cracking, heat resistance and durability. It is shown that the process of mass transfer at the propagating interface may often totally dominate the rate of the diffusion process (e.g. its characteristic half-time), and the flow outside of the interface may be almost steady-state.

Introduction
Solution of various diffusion problems of concrete is a problem of considerable interest for its durability or resistance to thermal spalling. The problem is normally formulated in the form of a diffusion equation, whose coefficients often depend of the dependent variable such as pore humidity or concentration of various chemical species. Consequently, a numerical solution is required. However, the variation of the diffusion equation coefficients often exhibits nearly sudden jumps. This causes sharp interfaces which are hard to resolve in a numerical approach. At the same time, the propagation of the interface may become the rate-controlling mechanism, such that the distribution of the dependent variable outside the interface obeys a differential equation in which time has almost no effect, for example the Laplace differential equation.

The conference paper discusses various examples of such behavior, for example the propagation of a front of chloride ions into a concrete pavement slab, the propagation of saturation front into a self-desiccated concrete dam, and the propagation of a drying front into a concrete rapidly heated in fire. Here we mention only the principles of analysis and discuss the basic type of response.

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Analysis

The water permeability as a function of temperature exhibits a sudden upward jump at temperature 100°C. The desorption isotherm of hot concrete, i.e., the curve of pore water content versus pore water pressure at constant temperature, exhibits a sudden downward jump just below the saturation pressure. The sorption isotherm of concrete exhibits a sudden upward jump as the saturation is approached (e.g., Bažant and Kaplan 1996).

Such jumps can cause difficulties in finite element modeling. The time step required for numerical stability on each side of the interface is of a different order of magnitude. Furthermore, the roughness of the interface in finite element modeling does not make it possible to accurately capture the transfer of water. There are two ways to deal with the problem: (1) To spread the jump of these curves over a sufficient width, i.e. replace the jump of the diffusion equation coefficient with a gradual transition. 2) To directly model the movement of the sharp interface.

Consider the interface curve \( f(x, y, t) = 0 \), in two spatial coordinates \( x, y \). By mass balance considerations, it is easy to show that the velocity of the interface in the direction normal to the interface curve is

\[
\mathbf{v}_n = -\frac{\mathbf{J}_n}{\mathbf{w}} = \frac{[a \, \nabla \mathbf{p}]}{[w]}
\]

(e.g., Bažant 1997) in which \([..]\) denotes the jump across the interface, \( J_n \) = mass flux across the interface in the direction normal to it, \( w \) = mass concentration of the diffusing substance, for example water, \( p \) = pressure of that substance in the pores, and \( a \) = permeability.

For an accurate solution, the interface and its velocity according should be directly simulated in a computer program. One may consider the evolution of the interface curve \( f(x, y, t) = 0 \) in two-dimensional diffusion \( (x, y = \text{spatial coordinates}, \, t = \text{time}) \). Differentiating this equation, we have \( f_x \dot{x} + f_y \dot{y} + f_t = 0 \), where \( \dot{x} = v_x, \dot{y} = v_y \) with \( v_x \) and \( v_y \) being the components of the velocity vector of the interface points. It follows that \( f_t = -f_x v_x - f_y v_y \) or (Bažant 1997)

\[
\frac{\partial f}{\partial t} = -\frac{\partial f}{\partial x} \left[ a \frac{\partial p}{\partial x} \right] - \frac{\partial f}{\partial y} \left[ a \frac{\partial p}{\partial y} \right]
\]

Now we see that the right-hand side represents the jump conditions based on the velocities in the \( x \) and \( y \) directions, considered separately. This means that instead of a smooth interface curve, one may consider a zig-zag interface curve following the inter element boundaries, with the flux vector components considered separately in the \( x \) and \( y \) directions across the element boundaries. This offers one possibility for numerical simulation of the movement of the interface.

It turns out that the rate of the process at the interface, e.g., the filling of the pores of concrete that must precede development of hydraulic overpressure, is often the rate-controlling mechanism of the whole diffusion process. In other words, the diffusion equation outside of the interface reduces to the time-independent Laplace equation, for example,

\[
\nabla \cdot (a \, \nabla p) = 0
\]
where \( p = p(x, y, t) \) = pore pressure, and \( a = \) permeability which depends on pressure and temperature. Within a region in which the permeability is uniform, this differential equation simplifies as \( \nabla^2 p = 0 \).

Due to the self-desiccation of concrete prior to rapid heating in fire the arrival of hydraulic water pressure front in a dam, the pores of concrete are never saturated even if there is no drying. The amount of water that needs to be added to the pores in order to achieve full saturation \( (p = p_s) \) is significant. A long time is required for the diffusion through concrete to supply that water.

An example has been given in the calculation of the spread of pore pressure \( p > p_s \) into a dam from a reservoir (Bažant 1975). In that numerical example, it was calculated by solving the one-dimensional diffusion equation that, if there were no self-desiccation, i.e., \( p = p_s \) as an initial condition, the hydraulic overpressure from the reservoir would spread through the whole thickness of a concrete dam (about 80 m) within the time of

\[
t_1 = 56 \text{ days}
\]  

(4)

However, taking into account the self-desiccation of concrete, the solution shows that the pressure profile between the upstream face of dam subjected to water pressure and the propagating saturation front is almost linear (Fig. 1 left). So the flux of water into the saturation front can be calculated from permeability as if the flow were a steady-state flow. Thus it is found that the hydraulic pressure \( p > p_s \) will spread from the reservoir across the dam thickness in the time of

\[
t_1 = 156 \text{ years.}
\]  

(5)

(Bažant 1975). The difference is enormous, and highlight the importance of the interface propagation as the dominant mechanism. This behavior is confirmed by the experiment of Carlson at University of California, Berkeley, in which the a long pipe was filled with concrete and was exposed to hydraulic overpressure at one end; the measurements could not register any hydraulic pressure in the pores of concrete even after many years and showed the propagation of the pressure front to be orders of magnitude slower than expected from the diffusivity of concrete (see Bažant 1975).

Another example discussed in the conference presentation deals with a concrete wall uniformly heated on its surface by fire, with the surface (environmental) temperature \( T_s(t) \) given. Rapid heating will desiccate a layer up to a certain depth \( x = x_d(t) \) increasing with time \( t \) (Fig. 1 right) (Harmathy, 1965, 1970; Bažant and Kaplan 1996). Deeper than that, there will be a layer of saturated concrete up to depth \( x = x_w(t) \). Still deeper, there will be unsaturated concrete, either previously self-desiccated mass concrete or concrete that has lost water to the environment due to previous drying. Approximately it may be assumed that the heating front depth \( x_h(t) \) is the same as the front of pressure increase (Fig. 1 right).

For approximate analysis, one may assume the profiles of temperature, pore pressure and water content to be as shown in Fig. 1 right. The profiles of \( T_p \) in the first two layers are assumed to be linear, with the interfaces moving, and in the third layer parabolic, with a horizontal tangent at the front. The slope of the temperature profile in the third layer is continuous with the slope of the
temperature profile in the second layer, as sketched. The profile of the water content may be assumed as piece-wise constant, as shown.

Based on the foregoing assumptions, the problem may be reduced to a set of four nonlinear first-order differential equations for the depths of the two sharp interfaces and the temperatures at these interfaces as functions of time (Bazant 1975). This solution (which is being prepared for publication by Beltoise, Ulm and Bazant) appears simpler, more instructive and more transparent than finite element analysis of the problem.

Concluding Comment

The analysis makes it clear that more attention should be paid to the rate of mass-exchange process at the diffusion fronts in concrete, and that simplification may often result from such approach.

References


