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B.10 Analysis of Pore Pressure, Thermal Stress and Fracture in Rapidly Heated Concrete

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Abstract. A brief review of the problem of calculating the evolution of the distributions of pore pressure and thermal stresses in rapidly heated concrete is presented. The difficulties caused by order-of-magnitude jumps in permeability as a function of temperature and in water content as a function of pore pressure are discussed in some detail and the conditions for the movement of the interface between the saturated concrete and unsaturated concrete are established. Some aspects of the numerical difficulties caused by the jumps are elucidated. A weak point in explaining the explosive spalling of rapidly heated high-strength concrete by pore pressures is pointed out and clarified. It is argued that the main driving force of the explosive thermal spalling must be the release of the stored energy due to the thermal stresses, which requires fracture mechanics. Finally, a simplified analysis of the pore pressure distribution, based on the calculation of the movement of the fronts of drying and wetting, is outlined and some other relevant literature is briefly reviewed.

1 Introduction

The problem of brittle failure of rapidly heated concrete, which has recently surfaced in experimental studies of high strength concrete columns and other structural members, was investigated during the 1970's and early 1980's in relation to the safety of nuclear reactor containments and pressure vessels, especially those for liquid metal cooled breeder reactors [1-4]. The results of that research have direct relevance to the present problem, including that of explosive brittle failure and the build-up of pore pressure in concrete exposed to high temperature. The purpose of this brief paper summarizing the workshop presentation is to review some pertinent results of the studies of this problem at Northwestern University and Argonne National Laboratory during 1975-1982.

2 Finite element analysis of pore pressure

One important factor in brittle failure of concrete at high temperature, including the high strength concrete, is obviously the pressure p of water vapor in the capillary pores of concrete. The evolution of pore pressure distributions $p(\mathbf{x}, t)$ as a function of spatial coordinate \mathbf{x} and time t is governed by the following three equations that must be satisfied in every point of the body:

$$\frac{\partial w}{\partial t} = -\text{div} \mathbf{J} + \frac{dw_d}{dt} \quad (1)$$

$$\mathbf{J} = -a \text{ grad } p \quad (2)$$

$$dp = k dw \quad (3)$$

Here \mathbf{J} = mass flux of water (dimension kg/s m^3), w = specific water content (kg of evaporable water per m^3 of concrete), T = temperature, a = permeability, measured in seconds ($a = \bar{a}/g$ where g = gravity acceleration and \bar{a} = permeability with the dimension of velocity, m/s); $k = dp/dw$ = inverse slope of the desorption isotherm $w = w(p)$, and w_d = evaporable water released by the dehydration of hydrated cement caused by heating. Eq. 1 expresses the local mass balance at each point of the continuum; \dot{w}_d (where the superior dot denotes the time rate) is a distributed source term, an important term which has a great influence on the calculation of pore pressures.

In writing Eq. 1 governing the mass transfer of water, all the four phases of water, that is, water vapor, liquid capillary water, free adsorbed water, and hindered adsorbed water, are treated as one. This means that a thermodynamic equilibrium between these four phases is assumed to exist within each capillary pore and the adjacent micropores at all the times, i.e., thermodynamic disequilibrium exists only macroscopically, on the scale of the continuum approximating concrete as a whole.

There are other models in which the vapor phase and liquid phase are treated separately, but a more complicated approach appears unnecessary, for two reasons: (1) If the vapor phase and liquid phase are treated separately, then the adsorbed water ought to be treated separately, too. (2) Separation of the phases implies that water molecules in the vaporized phase and in the liquid phase can travel freely and independently of each other over finite distances macroscopically through concrete. But the latter implication is unreasonable because there is nothing to prevent the water molecules in the vaporized and liquid states as well as the adsorbed state to readily exchange their Gibbs' free energy (chemical potential), and, even more importantly, because the water molecules in the vaporized state cannot pass through pores of subcapillary dimensions, which are known to block the passages through concrete. The reason is that the mean free path of a water molecule in the vaporized state is about $80\text{m} \times 10^{-9}\text{m}$ at room temperature, and much more at high temperature, while the width of the necks on the passages through concrete is about 10^{-9}m or less. When the mean free path of water molecules is larger than the opening, the passage of a molecule through such opening is virtually impossible.

Some authors (e.g., Luikov) express the flux as a separate function of the gradient of pressure and the gradient of temperature, or use the gradient of water concentration w (distinguishing Fick's flux, Dufour flux and Soret flux in the coupled heat and mass transfer equations). However, fitting of extensive test data during the 1970's has shown that little can be gained by considering the temperature gradient as a separate driving force of diffusion.. It only complicates the formulation. The pore pressure p depends on both w and T and thus Eq. 1 implies the dependence of J on both $\text{grad } w$ and $\text{grad } T$. Eq. 1 is of course nothing but the classical Darcy law for the permeation of a fluid through a porous medium.

An interesting phenomenon apparent in Fig. 1 (top left), which was deduced by indirect reasoning rather than direct measurements, is that the slope of the desorption isotherm in the saturation region $p > p_s(T)$ (the saturation vapor pressure) is apparently far higher than what one would calculate for liquid water fully filling a perfectly rigid container (as determined, e.g., from the ASTM Steam Tables) [9]. The explanation is that the micropores (gel pores of molecule dimensions) that are inaccessible to evaporable water at less than the saturation pressure become accessible to evaporable water at higher pressures, which is not an illogical hypothesis to make. If the isotherm in the over saturation region were assumed to have the same slope as calculated for liquid water completely filling a perfectly rigid container, the pressures calculated would be orders of magnitude higher than those observed in experiments, and all the concrete would have to explode when heated to high temperature.

The typical diagrams of permeability as a function of temperature and of the sorption and desorption isotherms at room temperature and high temperatures are shown in Fig. 1 (top right). From these diagrams, two difficulties become immediately apparent:

1) The permeability of concrete to evaporable water as a function of temperature exhibits an almost sudden upward jump of more than 2 orders of magnitude (about 200 times), a phenomenon that was discovered at Northwestern University in 1979 [5] and became in a milder, less conspicuous form also apparent from the experiments of England and coworkers [6]. The microscopic physical reason for this phenomenon has not been clarified experimentally, but a plausible hypothesis, advanced in [5] (see also [1]) is that, at high temperature, the surfaces of the pores become more smooth (less rough), and in particular the necks of gel-pore dimensions (only a few water molecules in thickness, containing hindered adsorbed water) become widened, without any significant change of porosity overall, thus opening continuous passages of capillary dimensions for the flow of water; see the illustration in Fig. 1 (inserted box on top right)).

2) The desorption isotherms in Fig. 1 (top left) at high temperature exhibit a sharp jump, by a factor of at least $50 \times$, as the point of saturation of vapor, that is the pressure $p_s(T)$, is crossed.

The foregoing two phenomena, that is, the jump of permeability and the jump of water content on desorption isotherm, create considerable difficulties in numerical modeling.

During the years of collaborative research between Northwestern University and Argonne National

Laboratory in nuclear safety reactor problems, many typical problems of pore pressure evolution were analyzed by finite elements on the basis of Eqs. (1)-(3). Some typical results obtained are shown in Fig. 1 (bottom). Many further results and a comparison with some test data, calculation procedure, input parameters, etc., are given in [1, 5, 7, 8] and in further extensive literature quoted in [1]. In these studies, the heating was generally not as rapid as in fire because nuclear reactor structures were considered to be always protected by thick thermal insulation.

An interesting point is that the calculated pressures were considerably smaller than initially expected, and never exceeded about 10 bars (1 MPa, or 144 Psi). Likewise, experimental measurements of pore pressure in heated concrete never indicated pressures in excess of the aforementioned value. The reason is no doubt twofold: (1) the enormous increase in permeability upon exceeding 100°C, and (2) the aforementioned phenomenon of the inflation of pore space when the pressure exceeds the saturation vapor pressure, $p_s(T)$.

3 Explosive thermal spalling

The explosive thermal spalling, which was first observed by Harmathy in normal concrete exposed to fire, has recently been identified as a major problem for high strength concrete. The explosive thermal spalling is a brittle failure which can conceivably be caused by the following two phenomena:

1. Development of a high pore pressure caused by oversaturation of the region of concrete at the front of heating (called the "moisture clog" by Harmathy); and
2. brittle fracture, particularly the sudden unstable release of the potential energy of thermal stresses stored in the structure.

The relative importance of these two phenomena, however, is debatable. On careful scrutiny it appears that the second mechanism, that is, the fracture mechanics aspect, is the major one. The first mechanism, that is, the development of high pore pressure due to moisture clog can play only the triggering role. However, it is also clear that the first mechanism, the pore pressure, must have at least some effect because recent experiments have confirmed that the explosive thermal spalling occurs only in wet concrete in which over saturation by water can develop.

The problem is schematically illustrated in Fig. 2 (top left). Assume that a high pressure develops at a certain distance below the heated surface and creates a crack, as shown. However, as soon as the crack starts opening, the volume available to the water vapor and liquid in the crack is suddenly increased by several orders of magnitude. This means that the water is suddenly forced to expand enormously. Because additional water cannot flow into the crack from the surrounding concrete suddenly, the pore pressure must immediately drop to nearly zero, as soon as the crack starts opening up. Only after the passage of some time, which is certainly far longer than the fraction of a second during which an explosive spalling occurs, additional water can flow from the pores of the surrounding concrete into the crack.

From this consideration, it appears that the pore pressure can only serve to trigger a crack but cannot drive the explosion, cannot force the crack to open widely. That must be caused by another supply of energy, which is of course available in the form of the potential energy of the thermal stresses.

In this context, it is not surprising at all that the high strength concrete appears to be much more prone to explosive spalling than the normal strength concrete. The high strength concrete is known to be far more brittle. The size effect method of the measurement of fracture energy revealed [11] that an increase of the strength of concrete from 5,000 to 14,000 psi was accompanied by no increase in the fracture energy, G_f , and a decrease of the fracture process zone size, c_f .

Thus it appears imperative to analyze the explosive thermal failure of high strength concrete on the basis of fracture mechanics. This of course further implies that the explosive thermal spalling should exhibit a pronounced size effect, which is observed in all brittle failures of concrete. Experiments checking the size effect in the explosive thermal spalling ought to be conducted.

4 Propagation of saturation interface

The jumps in permeability as a function of temperature and in the desorption isotherm (apparent in Fig. 1 top right) can cause major 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 overcome the problem:

1. To spread the jump of the curves in Fig. 1 (top right) over a sufficient width, replacing the jump of w with a gradual transition (e.g., introducing a linear change of w as a function of relative humidity $h = p/p_s$ in the range from 0.8 to 1.05), and, for the permeability, a linear transition from temperature 70° C to 120° C.
2. To model the movement of a sharp interface between the regions of saturated and unsaturated pores, or the regions of high and low permeability.

Consider the interface curve $f(x, y, t) = 0$, in two spatial coordinates x, y . During time dt , the interface moves as shown in Fig. 2 (top right), and a small element ds of the interface curve moves through the cross hatched rectangular region shown. The flux into this element is J_{n1} , and the water flux out of the element is J_{n2} . The area swept by the element is $ds v_n dt$ where v_n = velocity of the interface in the direction of the normal. Mass balance during time dt requires that the mass increase of the element

$$(J_{n1} - J_{n2})ds dt = (w_2 - w_1)ds(v_n dt) \quad (4)$$

in which $J_{n1} - J_{n2} = [J]$ = jump in flux across the interface, and $w_2 - w_1 = [w]$ = jump in specific water content across the interface. It follows that the velocity of the interface in the direction normal to the interface curve is

$$v_n = -\frac{[J_n]}{[w]} = \frac{[a \text{ grad } p]}{[w]} \quad (5)$$

For an accurate solution, the interface and its velocity according to Eq. (2) should be directly simulated in a computer program.

Due to the self-desiccation of concrete prior to rapid heating, 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, and 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 [12]. In that numerical example, it was found that, if there were no self-desiccation, i.e., $p = p_s$ as an initial condition, the hydraulic pressure from the reservoir would spread through the whole thickness of a concrete dam (about 80 m) in 56 days. However, taking into account the self-desiccation of concrete, it is found that the hydraulic pressure $p > p_s$ will spread from the reservoir across the dam thickness in 156 years. This difference is enormous.

So the problem is entirely dominated by the filling of the pores at the moving interface between hydraulic over pressure and the unsaturated concrete. The diffusivity of concrete has negligible influence. The rate of movement of the interface depends only on the permeability of concrete, a . The distribution of pressure between the interface and the boundaries is governed essentially by the Laplace differential equation, which does not contain time, that is, by the equation

$$\text{div } (a \text{ grad } p) = 0 \quad (6)$$

where $p = p(x, y, t)$ and permeability a depends on $T(x, y, t)$, and also possibly on p . Within a region in which the permeability is uniform, this differential equation is $\nabla^2 p = 0$.

Differentiating the equation of the interface curve, $f(x, y, t) = 0$, 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

$$\frac{\partial f}{\partial t} = -\frac{\partial f}{\partial x} \frac{1}{[w]} \left[a \frac{\partial p}{\partial x} \right] - \frac{\partial f}{\partial y} \frac{1}{[w]} \left[a \frac{\partial p}{\partial y} \right] \quad (7)$$

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, as shown in Fig. (top right), and the fluxes can be taken separately in the directions shown by the arrows across the element boundaries. This offers one possibility for numerical simulation of the movement of the saturation interface.

5 Simple one-dimensional analysis of pressure with moving saturation interface

Consider a wall uniformly heated on its surface, such that the surface temperature T is equal to a prescribed environmental temperature $T_e(t)$. Rapid heating will desiccate a layer up to depth $x = x_d(t)$. Below it, there will be a layer of saturated concrete up to depth $x = x_w(t)$. Further below it, there will be unsaturated concrete, either self-desiccated mass concrete or concrete that has lost water due to previous drying. Consider that the heating front reaches up to depth $x_h(t)$, which is also the front of pressure increase (Fig. 2 bottom).

For approximate analysis, one may assume the profiles of temperature, pore pressure and water content to be as shown in Fig. 2 (bottom). 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 is piece-wise constant, as shown. With the notations defined by the figures, the equations for the fluxes are

$$\begin{aligned} J_d &= -a_1 p_d(t), & a_1 &= a/x_d \\ J_w &= -a_2 [p_w(t) - p_d(t)], & a_2 &= a/(x_w - x_d) \end{aligned} \quad (8)$$

and the jump conditions for the interface velocities are

$$\begin{aligned} \dot{x}_d &= -\frac{J_w - J_d}{w_s - w_1} \approx \frac{J_d - J_w}{w_s} \\ \dot{x}_w &= -\frac{J_0 - J_w}{w_0 - w_s} \approx \frac{J_w}{w_0 - w_s} \end{aligned} \quad (9)$$

At the front of drying and at the front of saturation, the pore pressures must be equal to the saturation vapor pressures corresponding to the local temperatures, i.e.,

$$\begin{aligned} p_d &= f[T_d(t)] \\ p_w &= f[T_w(t)] \end{aligned} \quad (10)$$

where $p_s = f(T) =$ function defining the saturation vapor pressure corresponding to temperature T (according to ASTM Steam Tables [9]). Furthermore, the specific water content at saturation, w_s , must be specified as a function of temperature T i.e.,

$$w_s = g(T) \quad (11)$$

The flux of water in the third layer of unsaturated concrete may be assumed $J_0 \cong 0$. The differential equation governing heat transport may be written as [1]:

$$\rho C \dot{T} = C_w J \cdot \text{grad} T + C_a \dot{w} - \text{div } q \quad (12)$$

in which the first term on the right hand side represents the heat convection, the second term represents a distributed source of heat due to the latent heat of the phase transition of water, and the last term represents the heat conduction; $C, C_w =$ specific heats of dry concrete and of pore water (per unit mass and per degree C); $\rho_0, \rho =$ specific mass of concrete without or with water; $C_a =$ latent heat of adsorption or condensation of water; and $C_e =$ latent of heat of evaporation of water; and $q =$ heat flux, determined by heat conductivity b ,

$$\mathbf{q} = -b \text{ grad } T \quad (13)$$

Neglecting the effect of the latent heat of evaporation, the conditions of the heat balance in the wet layer (second layer) and the dry layer (the first layer) may be written as

$$\begin{aligned} & (\rho C + w_s C_w) \left[\frac{\dot{T}_d + \dot{T}_w}{2} (x_w - x_d) + (T_w - T_d) \frac{\dot{x}_d + \dot{x}_w}{2} \right] \\ = & C_w J_w \frac{(T_w - T_d)}{(x_w - x_d)} (x_w - x_d) + \left(-b \frac{T_d - T_b}{x_d} \right) - \left(-b \frac{T_w - T_d}{x_w - x_d} \right) \end{aligned} \quad (14)$$

$$\begin{aligned} & \rho C \left[\frac{\dot{T}_b + \dot{T}_w}{2} x_d + (T_d - T_b) \frac{\dot{x}_d}{2} \right] \\ = & C_w J_d (T_d - T_b) + q_b - \left(-b \frac{T_d - T_b}{x_d} \right) - C_e J_d \end{aligned} \quad (15)$$

in which the temperatures at the boundaries of the layer are averaged to obtain the mean temperature in the layer, the coordinates of the boundary are averaged to obtain the mean velocity of the layer, and the first terms represent heat supply due to convection. The surface temperature T_b may be assumed approximately equal to the prescribed environmental temperature $T_e(t)$.

The jump conditions at the moving interface yield the interface velocities:

$$\dot{x}_d = \frac{1}{g[(T_d + T_w)/2]} \{a_2 [f(T_w) - f(T_d)] - a_1 f(T_d)\} \quad (16)$$

$$\dot{x}_w = \frac{a_2}{w_o - g[(T_d + T_w)/2]} [f(T_d) - f(T_w)] \quad (17)$$

Eqs. (14) and (15), provide the conditions:

$$\begin{aligned} & \left[\rho C + C_w g \left(\frac{T_d + T_w}{2} \right) \right] \left[\frac{\dot{T}_d + \dot{T}_w}{2} (x_w - x_d) - (T_d - T_w) \frac{\dot{x}_d + \dot{x}_w}{2} \right] \\ = & -C_w (T_d - T_w) a_2 \{f(T_d) - f(T_w)\} + \frac{b}{x_d} (T_b - T_d) + \frac{b}{x_w - x_d} (T_w - T_d). \end{aligned} \quad (18)$$

$$\rho C \left[\frac{\dot{T}_b + \dot{T}_d}{2} x_d + (T_d - T_b) \frac{\dot{x}_d}{2} \right] = -C_w a_1 f(T_d) (T_d - T_b) + b \frac{T_d - T_b}{x_d} \quad (19)$$

Eqs. (16) - (19) represent a system of four nonlinear ordinary differential equations for four unknowns $x_d(t)$, $x_w(t)$, $T_d(t)$, and $T_w(t)$. These equations may be integrated in time by a standard library computer program for a system of nonlinear ordinary differential equations. In this manner, the maximum pore pressure that can develop in the wall, occurring at interface x_d , can be approximately calculated.

Fracture analysis of the brittle explosive failure requires knowledge of the fracture energy dependence on temperature. Some information in this regard has been reported in [13]. Furthermore, calculation of the energy stored by thermal stresses necessitates a good model for creep and thermal shrinkage of concrete at high temperature. Many studies have been devoted to this effect; see e.g., [15, 16, 17, 18, 20, 27, 28]. Further relevant information on the calculation of pore pressure and other aspects can be found in [21, 22, 23, 29, 24, 25, 26].

6 Conclusions

1. Calculations of pore pressure in rapidly heated concrete must take into account the jumps in permeability as a function of temperature and in water content as a function of pore pressure. The most realistic numerical simulation of these jumps requires following the movement of the interface curve over which the jumps occur.
2. The pore pressure may be realistically expected to serve only as a trigger of the explosive thermal spalling of high strength concrete. Whether the explosive failure actually occurs depends mainly on the amount of energy stored due to thermal stresses, whose release needs to be analyzed according to fracture mechanics.
3. A simplified analysis of the pore pressures may be based on the calculation of the movement of the interfaces between the dried hot zone, the wet heated zone, and the heated not yet saturated frontal zone.

7 References

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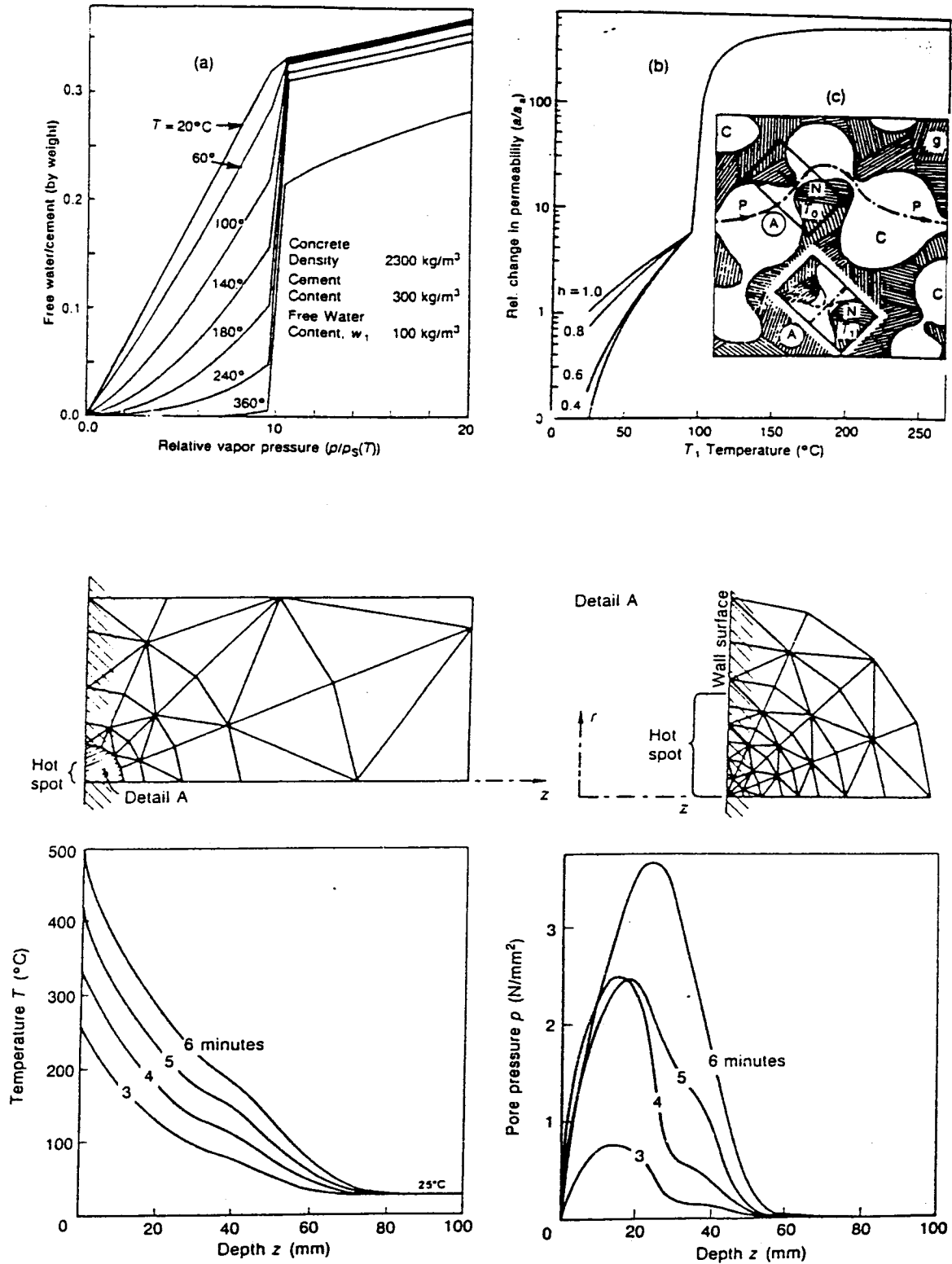


Figure 1: Top: Desorption isotherms at various temperatures (left) and permeability dependence on temperature (right), as established in [5]. Bottom: Two-dimensional finite element analysis of the temperature distributions and pore pressure caused by a rapid heating of a hot spot on a concrete wall, at various times [7, 21].

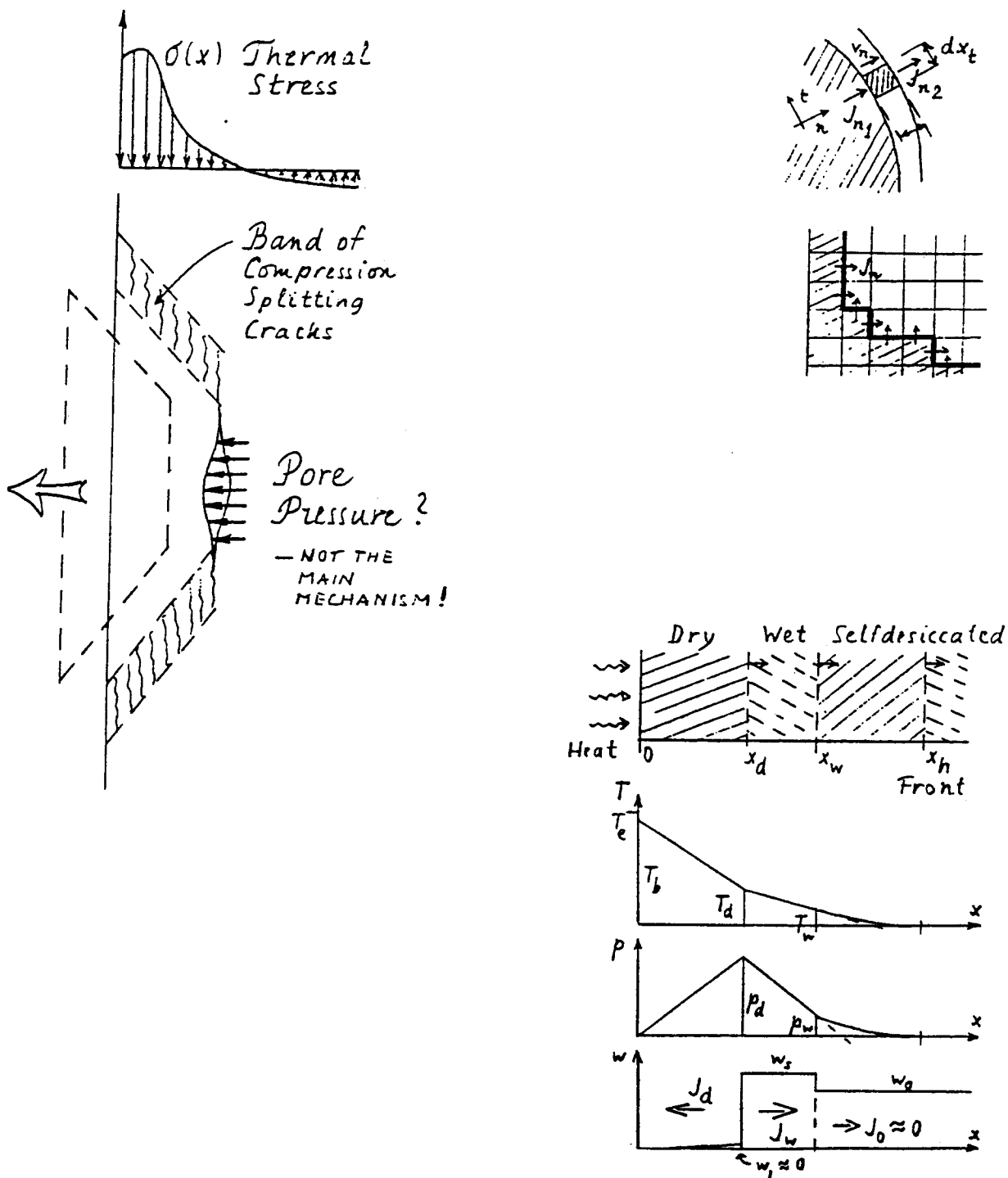


Figure 2: Top Left: Possible mechanism of explosive thermal spalling. Top Right: Moving interface between saturated and nonsaturated concrete, and its representation by a zig-zag interelement boundary. Bottom: Profiles of temperature T , pressure p and specific water content w in a rapidly heated wall, with moving interfaces and fronts.