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FINITE ELEMENT PROGRAM FOR MOISTURE AND HEAT TRANSFER IN HEATED CONCRETE

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A new axisymmetric finite element program for the analysis of pore pressure, moisture content and temperature in heated concrete is described. The program is based on the diffusion equations for coupled heat and moisture transfer and uses a step-by-step time integration. The finite element scheme is based on Galerkin method. For time integration a step-by-step solution with iterations is used. The numerical analysis is complicated by the fact that the sorption isotherms exhibit a steep jump at saturation–nonsaturation transitions, and that the permeability dependence on temperature exhibits a jump of two orders of magnitude at 100°C. The mathematical model takes into account the release of chemically bound water due to dehydration and the associated changes in the pore space. The program may also be used at normal temperatures. Predictions of the program are compared with tests by HEDL as well as two other existing programs.

1. Introduction

Concrete is a material which contains extremely fine pores with a great amount of water. Therefore, heating of concrete produces significant pore pressure which causes migration of moisture through concrete and eventual drying. At the same time, the movement of moisture through concrete may appreciably contribute to the heat transfer and affect the temperatures. The pore pressures depend on the pore space available to water, which is known to change in response to heating and other factors. The material characteristics entering the diffusion problem of moisture and heat transfer are strongly variable. Therefore, analysis of pore pressures, moisture content and temperature in heated concrete necessitates a numerical approach, and the objective of this paper is to report on the development of a finite element program to accomplish this task.

The movement of moisture and the magnitude of pore pressure is of concern in predicting the behavior of nuclear reactor structures, particularly prestressed concrete reactor vessels, in response to certain hypothetical core disruptive accidents. In one scenario, for example, liquid sodium may come in contact with the steel liner of the concrete wall and cause its sudden heating to temperatures close to 600°C. Moreover, in case of some damage to the steel liner, the sodium might react with the water present in the pores of concrete below the liner. If the liner is not disrupted, the sudden heating would produce significant pressure build-up in the pore water under the liner. Predictions of water content are also of interest for radiation shielding capability of concrete. Aside from nuclear technology, the high temperature behavior of concrete is also of acute interest in fire resistance predictions.

One phenomenon for which the calculations of pore pressure are of great interest is the explosive spalling of concrete which is sometimes caused by a rapid heating during the fire. Although the major factor in this phenomenon is no doubt the thermal stress produced by rapid heating in a restrained concrete, a significant factor may also be the rise of the pore pressure caused by heating. This is suggested by the fact that explosive spalling is observed only in concrete of high moisture content.

2. Theoretical model

The computer program uses the finite element method to solve the following system of governing differential equations for the coupled heat and moisture

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transfer in concrete [1,2]:

$$\frac{\partial w}{\partial t} = -\operatorname{div} \boldsymbol{J} + \frac{\partial w_d}{\partial t}, \tag{1}$$

$$\boldsymbol{J} = -a \operatorname{grad} p, \tag{2}$$

$$\rho C \frac{\partial T}{\partial t} - C_a \frac{\partial w}{\partial t} = -\operatorname{div} \boldsymbol{q} + C_w \boldsymbol{J} \cdot \operatorname{grad} T, \tag{3}$$

$$\boldsymbol{q} = -b \operatorname{grad} T, \tag{4}$$

in which

- t = time,
- T = temperature in concrete,
- w = water content = mass of all free (not chemically bound) water per unit volume of concrete,
- $\boldsymbol{J}$ = moisture flux,
- $\boldsymbol{q}$ = heat flux,
- w_d = total mass of free (evaporable) water that has been released into the pores by dehydration of the hydrated cement paste,
- p = pore water pressure,
- a = water permeability,
- ρ = unit mass of concrete,
- C = isobaric heat capacity of concrete per unit volume of concrete,
- C_a = heat adsoprtion of free water,
- C_w = mass density and isobaric heat capacity of liquid water,
- b = heat conductivity.

Note that eq. (3) includes the effect of heat convection due to the movement of water, which is however significant only at very rapid heating. Another characteristic aspect of the foregoing equations is the effect of dehydration, given by w_d. Dehydration is the opposite of hydration and is produced by heating concrete to temperatures over about 125°C. At room temperatures this same term may be used to represent the water lost due to hydration.

The foregoing equations must be complemented by the equation of state, which relates w, p and T. One distinguishes the case of saturated and nonsaturated concrete. For saturated concrete, the equation of state is based on the thermodynamic properties of water, as given by the ASTM tables. The specific volume must be determined from the changes in porosity of concrete. These are caused by dehydration and are related to w_d. In the nonsaturated region, the capillary and adsorption phenomena in the pores govern the equation of state, and a semi-empirical equation of state has been developed for this region. The temperature is a very significant factor in the sorption relation. The equation of

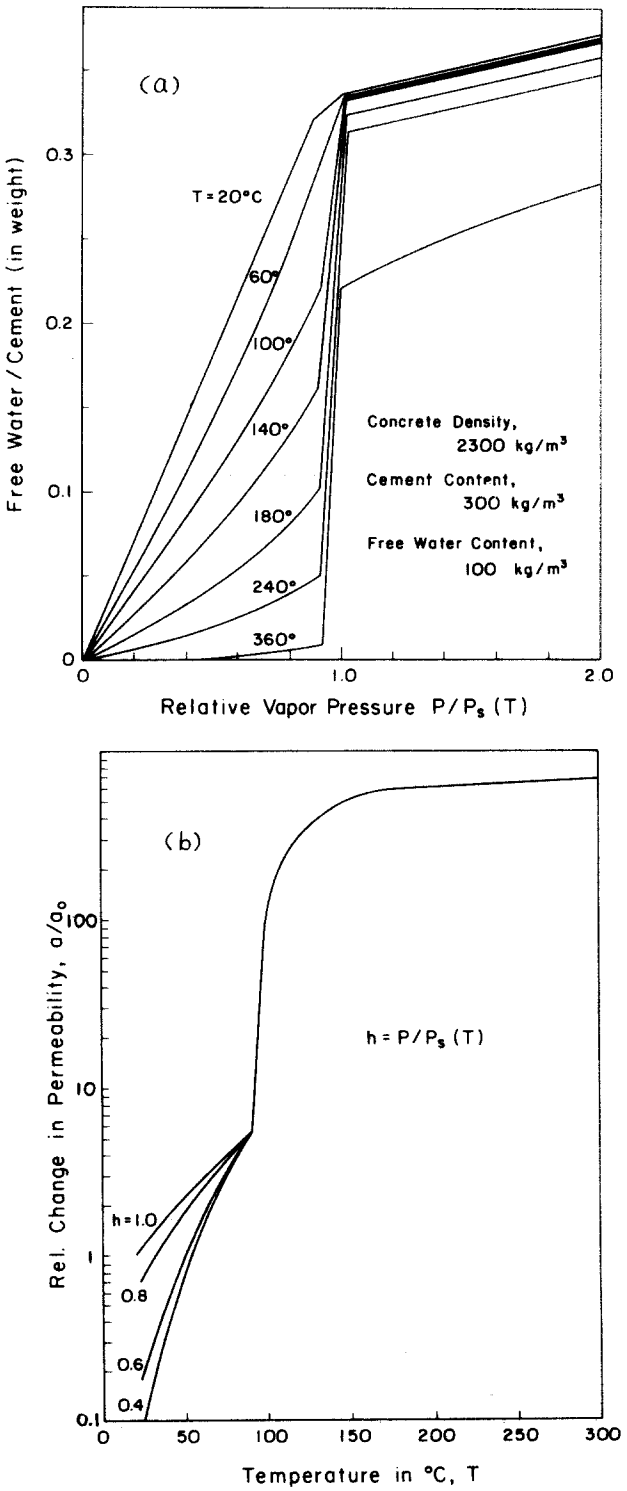

Fig. 1. (a) Sorption isotherms; (b) dependence of permeability on temperature and humidity.

state is described in terms of the sorption isotherms shown in fig. 1a.

Another very important factor is the permeability, which is highly dependent on temperature as well as pore pressure. The dependence on pore pressure is apparently due to the effect of adsorption phenomena and disappears at temperatures well over 100°C. As the temperature of 100°C is passed, permeability is found to exhibit a sharp upward jump, approximately a 200-times increase, which is explained by a transition to a flow that is controlled by steam viscosity rather than adsorption phenomena (fig. 1b). The sharp rise of permeability is a well confirmed fact, independently found by several investigators [1,3–6].

The aforementioned theoretical model, which is described in detail in refs. [1] and [2], has been calibrated with the help of available test data published in literature as well as some further drying tests conducted at Northwestern University. Comparisons with test data which support this model are given in refs. [1] and [2].

3. Capabilities of the program

Two versions of the program are available: one-dimensional and two-dimensional, both of them axisymmetric. The one-dimensional axisymmetric program can be used to analyze radial moisture diffusion and heat conduction through a wall of a cylindrical vessel. The two-dimensional version can be used to analyze arbitrary axisymmetric solids. The boundary conditions available are those of perfect moisture transfer from the surface to an environment of prescribed, possibly time-variable, relative vapor pressure, perfect sealing of the surface, perfect heat exchange with an environment of prescribed time-dependent temperature, and perfect thermal insulation. The boundary conditions for imperfect moisture or heat transmission at the surface can be also implemented. The two-dimensional finite element program utilizes triangular three-node elements, the unknowns being the value of temperature and pore pressure in the nodes. The finite element formulation is based on the Galerkin approach and utilizes a step-by-step algorithm for the integration in time, corresponding to the central difference Crank–Nicholson algorithm for the diffusion equation.

The program has been coded in FØRTRAN IV and has been tested and run on the CDC 170/730 Cyber computer at Northwestern University. The program is made available through the NISEE Center, University of California, Berkeley (Davis Hall, Division of Structural Engineering and Structural Mechanics, University of California, Berkeley, CA 94720, USA) [7]. The available package consists of the full FØRTRAN listing, a deck of cards or magnetic tape, and a complete user's manual, which includes description of the input, description of the output and a fully documented example problem. Numerous comments within the program listing make it possible to carry out various modifications of the program.

The example problem is that of a hot spot on a reactor vessel wall. A portion of the interior surface of the cylinder is subjected to a rapid heating, such that the temperature increases 32°C per min and then stops at the constant value of 800°C. The element mesh is shown in figs. 2a and 2b. The temperature distributions and the pore pressure distributions obtained with the program are plotted in figs. 2c and 2d.

As another example, we show in figs. 3a–d the temperature distributions, the pore pressure distributions, the water release and the peak value of pressure in a half-space subjected at its surface to a rapid temperature rise to 500°C.

4. Discussion of numerical aspects

Although the program appears to work satisfactorily, the user should not expect great accuracy in cases of rapid heating, cases which involve an interface between oversaturated and dried concrete, and cases of very high temperatures. The numerical modeling is in these situations tremendously complicated by the fact that the sorption isotherms exhibit an almost discontinuous jump [1,2] (which is somewhat smoothed out for the purpose of numerical modeling, see fig. 1a), and that permeability changes by orders of magnitude as the temperature of 100°C is passed (fig. 1b). Although the iterative scheme used in each time step of the program appears to converge, it often converges slowly in these situations. The spatial convergence as the size of the finite elements is decreased appears to be in these situations also rather slow. The output of pressure histories and distributions tends to exhibit in these situations often spurious oscillations which are diminished only slowly as the finite element mesh is refined. Decrease of the time-step does not reduce the spurious oscillations. The reason for the oscillation is that the peaks of the pore pressure distribution curves tend to be very sharp and cannot be accurately represented by the simple shape functions of finite elements, considered as linear distributions within the element in the present program. The temperature distribution, on the other hand, never exhibits such a sharp peak, and can be very closely

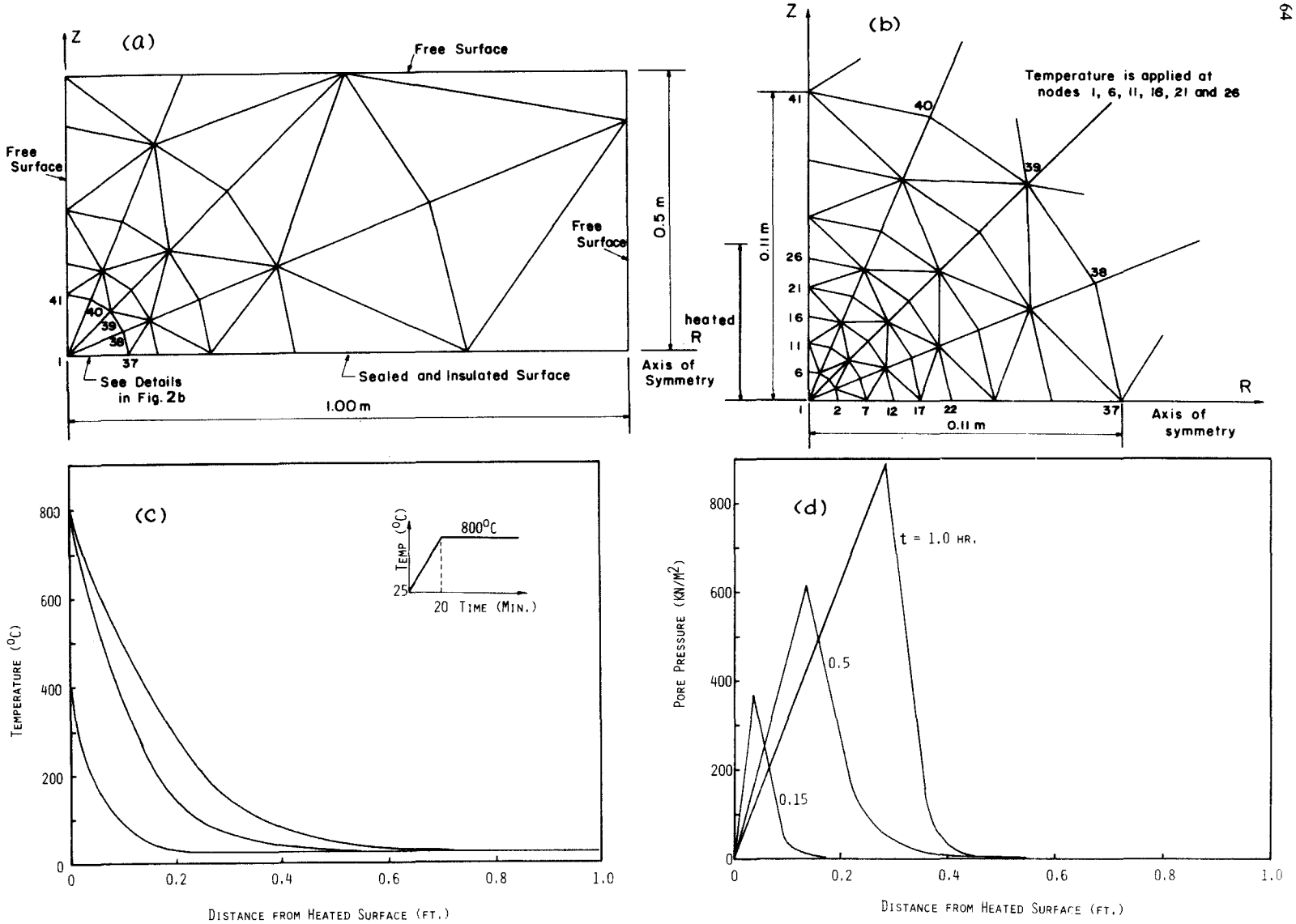

Fig. 2. (a), (b) Finite element mesh (2-D program); (c) temperature distributions in radial direction; (d) pore pressure distributions in radial direction.

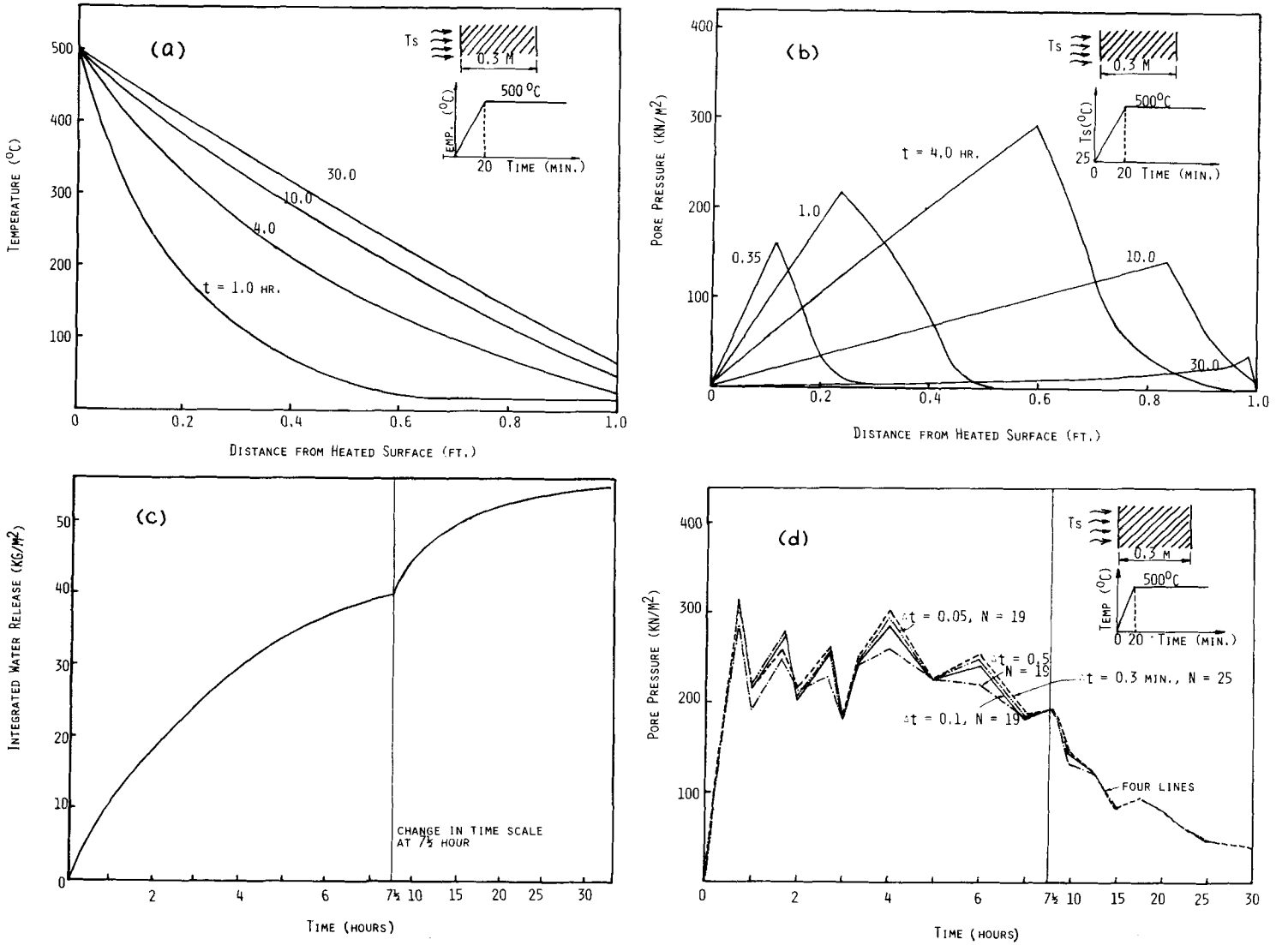

Fig. 3. Rapid heating of half-space to 500°C (1-D program); (a) temperature distributions; (b) pore water pressure distributions; (c) water release; (d) peak value of pore water pressure using different time increment and different mesh subdivisions.

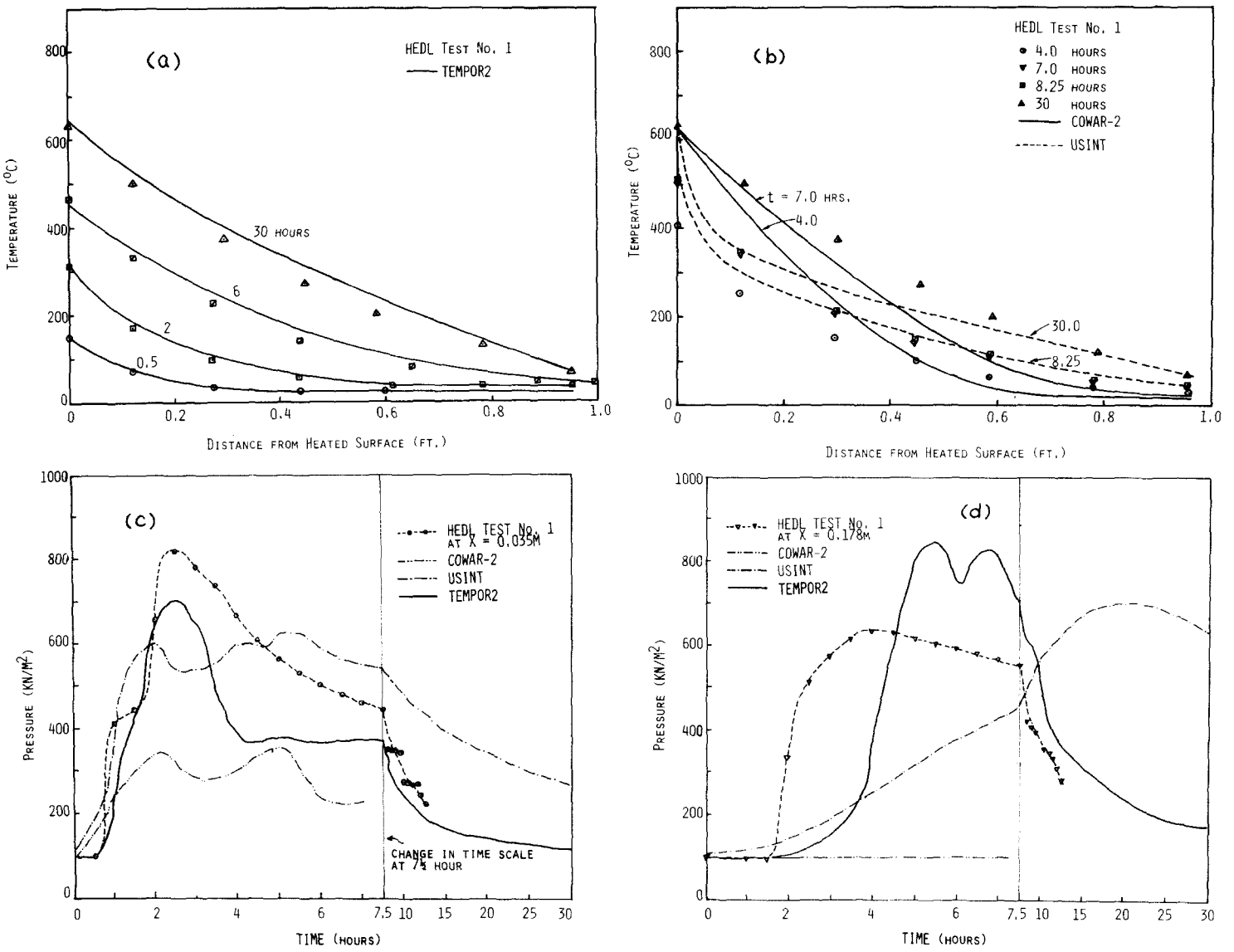

Fig. 4. Comparisons with HEDL test no. 1; (a) comparisons of temperature distributions with TEMPOR2 predictions; (b) comparisons of temperature distributions with USINT and COWAR-2 predictions; (c) comparisons of pore pressure at $x = 0.035$ m; (d) comparisons of pore pressure at $x = 0.177$ m; (e) comparisons of water release.

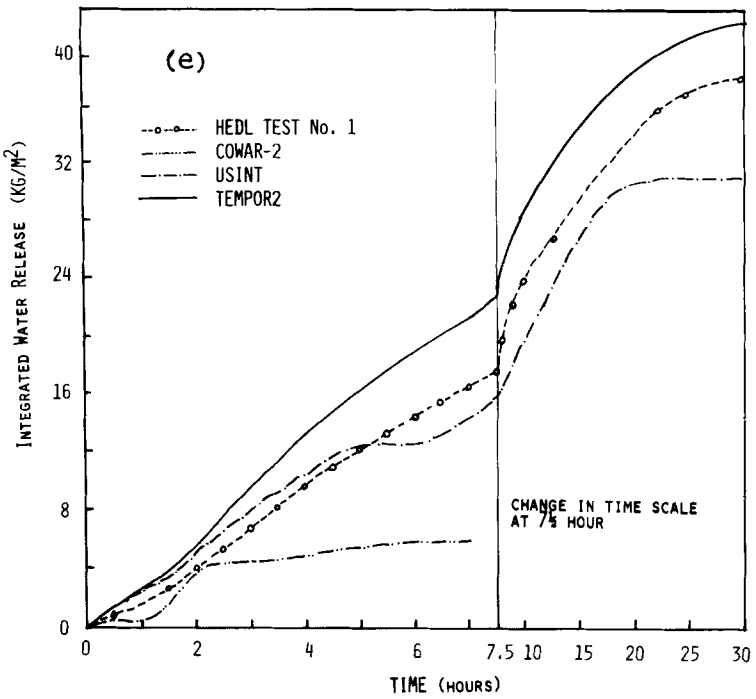

Fig. 4e.

represented by the linear shape functions even for relatively large finite elements. Note that if the finite element size is increased away from the heated face the spurious oscillations of peak pore pressure increase with the advance of pressure peak into the cruder elements. Examples of the oscillations which are probably spurious in nature, are seen in fig. 3d; these oscillations can be eliminated, but only at the expense of an extremely fine element mesh. Refined meshes are required in the following situations:

(a) Near the boundary where temperature is prescribed (hot face), very small elements are required to prevent the oscillation of the calculated spatial distributions. Near the surface, there should be few elements at least of the size 1/100 of the thickness of specimen.

(b) Likewise, the boundary condition of prescribed environmental vapor pressure may cause spurious oscillations of the calculated spatial distributions near the cold face. Small elements are then required near the cold face to get sufficiently accurate results for the weight loss of concrete.

(c) If the rate of heating is high, e.g., 50°C per min, many small elements are required near the heated surface.

(d) If the solution is required for long times, the sharp high pressure peak travels a long distance into the wall. Small finite elements must then be used through the whole thickness from the hot face to the cold region if accurate solution in the high pressure zone is desired. This leads to a very large number of elements.

Various approaches have been tried to reduce the aforementioned spurious oscillations and slow convergence. For example, a method analogous to that recently used by Matthies and Strang [8] for situations of a sudden change in stiffness in elastic-plastic programs has been tried. In this spirit, the iterations in each time step have been based on an assumed slope of the sorption isotherm, which may differ from the actual slope (fig. 1a). In particular, when the state point was in the vertical transition in fig. 1a, the much smaller slope of the sorption isotherm on either left or right of this transition region has been used in iterations (which corresponds to a higher stiffness in the sense of stress analysis). The correct term resulting from the difference between the actual and assumed slope has been treated as a prescribed fixed force term in the equation. However, this approach which corresponds to the initial strain method in elastic-plastic analysis, did not yield any improvement.

Even though the convergence at saturation–

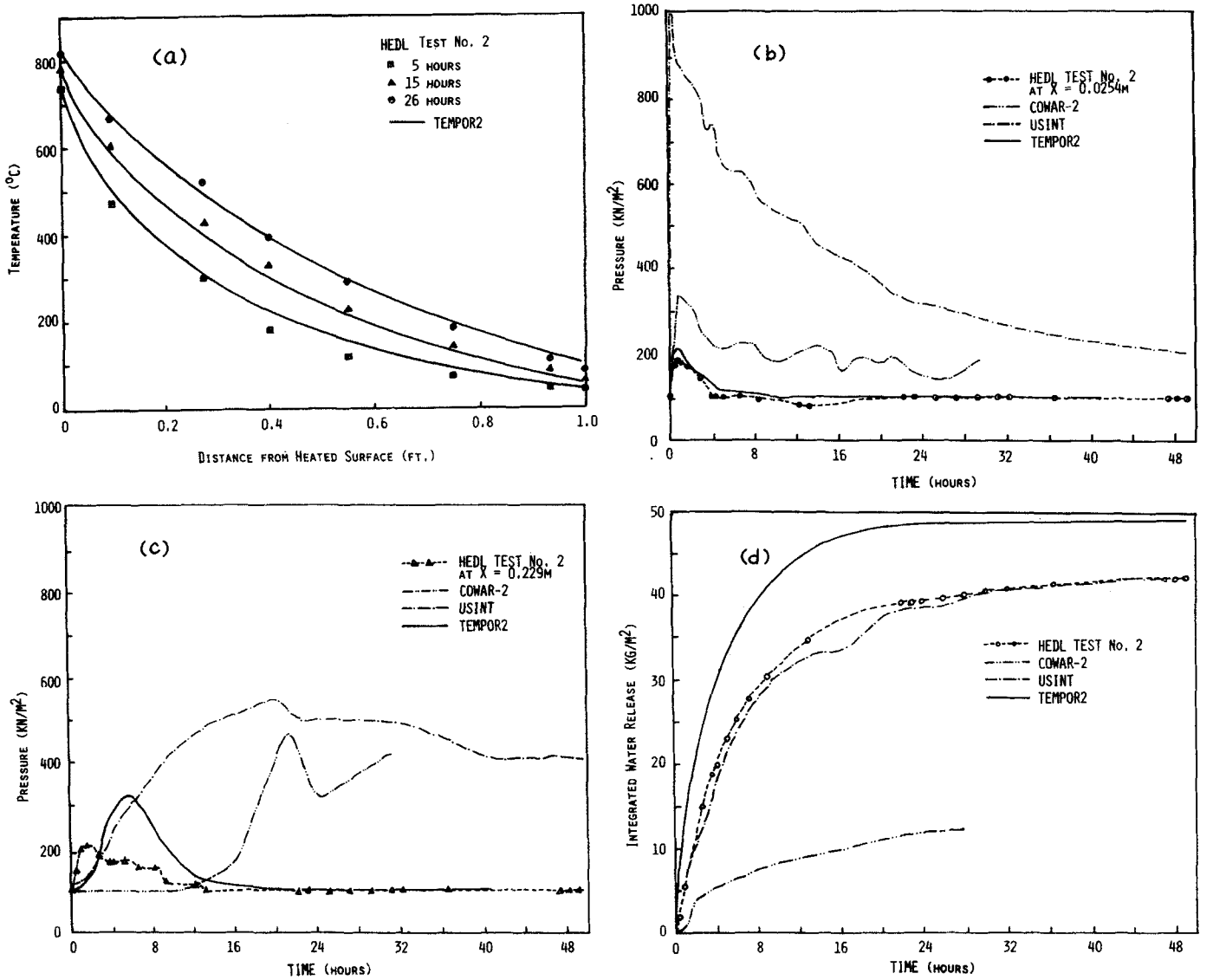

Fig. 5. Comparisons with HEDL test No. 2; (a) Comparisons of temperature distributions; (b) comparisons of pore pressure at $x=0.025$ m; (c) comparisons of pore pressure at $x=0.229$ m; (d) comparisons of water release with HEDL test no. 2.

Table 1
Summary of features of concrete water release codes

	COWAR-2 (GE)	USINT (SANDIA)	TEMPOR2 (Northwestern Univ.)
Geometry	1-D planar	1-D planar, cylindrical and spherical	1-D and 2-D axisymmetric
Species	Water, water vapor, air	Water, water vapor, CO_2 (not verified)	Water, water vapor in air
Energy transport	Diffusion and convection	Diffusion and convection	Diffusion and convection
Mass transport	Darcy and Fick's Law	Darcy's Law	Darcy's Law (extended)
Permeability and porosity	Constant parameters	– Porosity related linearly to mass releases	– Permeability depends on temperature (jump at 100°C), and below 100°C on pressure as well
		– Permeability and porosity related by Kozeny–Carmen equation	– Porosity related linearly to water released by dehydration
Equation of state and reaction kinetics	– Clausius–Clapeyron equation for wet-zone	– Modified Clausius–Clapeyron equation for saturated wet zone	– Thermodynamic properties of water (ASTM "Steam Tables") for saturated concrete
	– Dry zone; no liquid phase	– Kinetic eqs.: release of CO_2 and of free and chemically bound water	– Semiempirical sorption isotherms for non-saturated pores
	– Ideal gas law for vapor and air (and steam table)	– Ideal gas law for vapor and CO_2	– Hydration and dehydration of cement included in equation of state
			– Cold concrete also covered
Solution procedure	– Explicit finite difference in time	– Implicit finite difference in time	– Implicit finite difference in time
	– Finite difference in space	– Finite difference in space	– Finite elements in space
	– Δt controlled by stability criterion	– Δt arbitrary	
		– Equations linearized	– Equations linearized, iterated

Table 2
Material parameters used in computations

	Fig. 2	Fig. 3	Fig. 4	Fig. 5
Age of concrete (days)	42	42	42	42
Rel. humidity of concrete	0.95	0.95	0.95	0.95
Rel. humidity of environment before heating	0.70	0.70	0.70	0.70
Initial temperature (°C)	25	25	25	25
Saturation water content at 25°C (kg/m^3)	180	180	180	180
Cement content (kg/m^3)	380	380	400	400
Unit weight of concrete (kg/m^3)	2200	2400	2400	2400
Thermal conductivity (J/ms°C)	1.674	1.674	1.674	1.674
Permeability (m/s)	1×10^{-12}	1×10^{-11}	2×10^{-12}	1×10^{-11}
Thickness of concrete wall (m)	1.0	0.30	0.30	0.30
Water/cement ratio	0.50	0.50	0.50	0.50

nonsaturation transition and at permeability transitions is often very slow, it does appear to take place. This is demonstrated for example by the numerical results in fig. 3d, in which the values of the peak pore water pressure in the heated wall at various times after the start of heating are plotted for various numbers of finite elements and for various time steps.

5. Comparisons with test data and other codes

Comparisons of the present mathematical model with various test data available in the literature were given in preceding papers [1,2]. To further check the capability of the TEMPOR2 code, its predictions have been compared (figs. 4 and 5) to the results of water release demonstration tests [5,9,10] carried out by Hanford Engineering Development Laboratory (HEDL) as well as to the predictions of two other available codes, namely COWAR-2 (General Electric Co.) [11] and USINT (Sandia Laboratories) [12]. The principal characteristics of these codes are listed in table 1.

HEDL tests No. 1 and 2 were chosen for comparison due to their long transient periods and well defined boundary conditions. Since the material properties were not available from the literature, typical values listed in table 2 were assumed for the fitting of test data.

Although all of the codes give only rather crude predictions, figs. 4 and 5 show that the results obtained with TEMPOR2 appear to be relatively best.

6. Conclusion

Prediction of mass transport and pore pressure in heated concrete is a very complex problem. The computer program developed to solve this problem realistically reflects the known physics of the problem and appears to give predictions that are in an acceptable, albeit crude, agreement with measurements.

Acknowledgment

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