Modeling of Hygrothermal Behavior of Two-Dimensional Concrete Structures

Dariusz J. Gawin, D.Sc. Bernhard A. Schrefler, D.Sc.

ABSTRACT

Coupled heat, air, and moisture transfer in concrete structures is of great practical importance in many fields of civil engineering. Modeling these phenomena, especially in fresh concrete structures or concrete elements exposed to fire, is a complex problem. Several nonlinear phenomena, such as heat and mass sources associated with hydration or dehydration processes, phase changes, hysteresis of sorption isotherms, material properties dependent on moisture content, and temperature and gas pressure, should be taken into account. A new two-dimensional finite element model of coupled heat, moisture, and air transfer in deforming porous building materials HMTRA is briefly presented. Different physical mechanisms governing the liquid and gas transport in the pores of partially saturated porous materials are clearly distinguished. Phase changes, hydration-dehydration processes, and related heat effects are taken into account as well. Temperature and moisture content dependent properties of the fluids and of the solid phase are considered. Also, the effect of material damaging on its intrinsic permeability is taken into account. This finite element model allows for the simulation of the evolution of temperature, gas pressure, moisture content, the global kinetics of the concrete maturing process, as well as stress and strain behavior. Some examples of computer simulations concerning hygrothermal behavior of two-dimensional concrete structures in various conditions are presented. Hygrothermal behavior of a matured concrete element, taking into account the hysteresis of sorption isotherms, is modeled. Temperature and moisture distribution in a fresh concrete structure and their influence on hydration process evolution are analyzed. Performance of a concrete element exposed to fire is simulated.

INTRODUCTION

Coupled heat, air, and moisture transfer in concrete structures is of great practical importance in many fields of civil engineering. Modeling these phenomena, especially in fresh concrete structures or concrete elements exposed to fire, is a complex problem. Several nonlinear phenomena (e.g., heat and mass sources associated with hydration or dehydration processes, phase changes, hysteresis of sorption isotherms, as well as permeability, porosity, and other material properties variable in time and dependent on temperature, gas pressure, and moisture content) should be taken into account in the simulation.

Mathematical models of these complex phenomena are obtained in two different ways, usually called phenomenological and mechanistic approach. Using the first one, heat and mass transport is described by means of a coupled, differential equation set of the diffusive type. Its coefficients are usually obtained by solving appropriate inverse problems that often result in a rather time-consuming experimental procedure. The model parameters are usually nonlinear functions of state variables because several complex physical phenomena are lumped together. Models of this type, widely used in practice, are aimed at predicting moisture content and temperature fields without entering in details of particular physical phenomena involved. Accuracy of the phenomenological models’ predictions is good, as shown by many validation tests (Hens 1996). Examples of these types of models are the models by Bazant and Najjar (1972), TRATMO (Kohonen
MATHEMATICAL MODEL

Wet concrete is modeled as a multiphase material, which is assumed to be in thermodynamic equilibrium state locally. The voids of the skeleton are filled partly with liquid water and partly with a gas phase.

The liquid phase consists of bound water, which is present in the whole range of moisture content, and capillary water, which appears when water content exceeds the upper limit of the hygroscopic region $S_{swp}$. Moisture content is described here by the degree of saturation with water $S_w$ related to the mass moisture content $\mu_M$ (kg water/kg dry material) by the relation $S_w = (\mu_M \rho^w)/(n \rho^w)$, where $n$ denotes porosity and $\rho^w$ and $\rho$ denote the densities of water and the solid skeleton, respectively. The gas phase is a mixture of dry air and water vapor (condensable constituent) and is assumed to be an ideal gas. The chosen primary variables of the model are gas pressure $p^g$, capillary pressure $p^c = p^g - p^v$ ($p^w$ denotes water pressure), temperature $T$, displacement vector of the solid matrix $\mathbf{u}$, and degree of cement hydration $\Gamma_{hyd}$ (when hydration or dehydrolysis processes are analyzed). A physical explanation of our model, including the energy and mass transport mechanisms considered, can be found in Lewis and Schrefler (1998) and Gawin (2000).

The mathematical model consists of four balance equations. These equations were obtained in Lewis and Schrefler (1998) and Gawin (2000) by use of the volume averaging theory, also called hybrid mixture theory, developed by Hassanzadeh and Gray (1979a, 1979b, 1980). The mass balance of the dry air includes both diffusional and advective (pressure forced) components of the mass fluxes,

$$-n \frac{\partial S_w}{\partial t} - \beta_1(1-n)S_w \frac{\partial T}{\partial t} + S_g \rho^a \frac{\partial v^g}{\partial t} + \frac{1}{\rho^a} \frac{\partial}{\partial t} \rho^a \mathbf{J}_g + \frac{1}{\rho^s} \div(nS_g \rho^a \mathbf{v}^g) + \frac{(1-n)S_g \rho^a}{\rho^s} \frac{\partial \Gamma_{hyd}}{\partial t} = \frac{m_{hyd}}{\rho^s} \mathbf{S}_w,$$

and has been summed with the solid skeleton mass balance equation in order to eliminate the time derivative of porosity. Because of this, some terms related to thermal dilatation and mechanical deformation of the skeleton (the second and third terms on L.H.S.), as well as the mass source (sink) resulting from chemical reactions of the skeleton (hydration or dehydrolysis), appear in Equation 1. The symbol $t$ denotes time, $m_{hyd}$ denotes mass source (sink) related to the hydration (dehydration) process, $\beta_1$ is the cubic thermal expansion coefficient of the solid skeleton, $\mathbf{v}^g$ denotes gas velocity relative to the solid skeleton, $\mathbf{J}_g$ denotes diffusional flux of the dry air, and the subscripts and superscripts $s, w, a, v$ and $g$ are related to solid, liquid water, dry air, water vapor, and gas phase, respectively. According to the notation introduced by Hassanzadeh and Gray (1979a, 1979b, 1980), subscripts are used for physical quantities averaged in all phases of the medium, and superscripts for quantities averaged inside a single phase only.

The mass balances of liquid water and of vapor, summed together to eliminate the source term related to phase changes (evaporation-condensation or adsorption-desorption), form the mass balance equation of water species (Gawin 2000),

$$n(p^w - p^v) \frac{\partial S_w}{\partial t} - \beta_{sw} n \frac{\partial T}{\partial t} + (p^v S_w + p^w S_{sw}) \div \mathbf{v}^v + S_w \frac{\partial \phi^v}{\partial t}$$

$$+ \div(nS_g \rho^v \mathbf{v}^g) + \div(nS_w \rho^w \mathbf{v}^w) + \frac{(1-n)(S_g \rho^w + p^w S_{sw})}{\rho^s} \frac{\partial \Gamma_{hyd}}{\partial t} = \frac{\rho^v S_w + p^w S_{sw} - p^v}{\rho^s} m_{hyd},$$

where $\mathbf{v}^w$ denotes water velocity relative to the solid skeleton. As before, these balance equations are summed up with the solid phase mass conservation equation in order to eliminate the time derivative of porosity. As a result, several terms describing the skeleton deformations (hydrothermal and mechanical) and hydration (or dehydrolysis) process appear in Equation 2.
The enthalpy conservation equation of the multiphase medium, obtained from the sum of the appropriate balance equations of the constituents, includes the heat effects due to phase changes and the hydration (dehydration) process, as well as the advective and latent heat transfer,

\[
\frac{\partial T}{\partial t} + (\rho u C_p^T + \rho_s C_p^g g_s') \cdot \nabla T - \text{div}(\lambda_{eq} \nabla T) = -m_{vap} \Delta H_{vap} + m_{hyd} \Delta H_{hyd},
\]

where \((\rho C_p)_T\) is effective thermal capacity, \(C_p^T\) is isobaric specific heat, \(\lambda_{eq}\) is effective thermal conductivity, \(\Delta H_{vap}\) and \(\Delta H_{hyd}\) are specific enthalpies of the phase change and the hydration (dehydration) process, and \(m_{vap}\) is the mass source or sink of vapor related to the evaporation (desorption) or condensation (adsorption) process.

In the hygroscopic moisture range, \(S \leq S_{sup}\), the terms in Equations 2 and 3, which describe the liquid phase, concern the bound water and, thus, \(\Delta H_{sup}\) should be substituted by \(\Delta H_{ads}\) (i.e., enthalpy of adsorption). In Equation 3, the phase change term has been substituted using the liquid water mass balance equation.

Introducing Bishop’s stress tensor \(\sigma''\), also called effective stress tensor (Lewis and Schrefler 1998), responsible for all the deformations of a concrete, the linear momentum conservation equation of the whole medium is given by (Gawin 2000),

\[
div[\sigma'' - \mathbf{I}(p^s - p_{atm} - S_u p^c)] + \{(1 - n) \rho^s + n S_u \rho^w + n S_g \rho^g\} g = 0,
\]

where \(p_{atm}\) is atmospheric pressure, \(\mathbf{I}\) is the unit, second order tensor, and \(g\) is the acceleration of gravity.

The evolution equation for the degree of cement hydration appearing in Equation 2 has the form,

\[
\Gamma_{hydr} = \Gamma_{hydr}(t_{eq}),
\]

where the equivalent period of hydration, \(t_{eq}\), is given by (Bazant 1988):

\[
t_{eq}(t) = \int_0^t \beta_T(\tau) \beta_\phi(\tau) d\tau,
\]

with

\[
\beta_T(\tau) = \exp \left[-\frac{U_{hydr}}{R} \left(\frac{1}{T_o} - \frac{1}{T(\tau)}\right)\right],
\]

\[
\beta_\phi(\tau) = \{1 + \alpha' [1 + \phi(\tau)]^4\}^{-1}.
\]

When the dehydration process at high temperature is analyzed, because of its irreversible nature, one can assume that (Gawin et al. 1999)

\[
\Gamma_{hydr} = \Gamma_{hydr}(T_{max}),
\]

where \(T_{max}(t)\) is the highest temperature reached by the concrete till time instant \(t\).

The governing Equations 1 through 8 are completed by an appropriate set of constitutive and state equations, as well as some thermodynamic relationships.

The constitutive relationship for the solid skeleton in the following form,

\[
d \sigma'' = C_T (d \varepsilon - d \varepsilon_f - d \varepsilon_0),
\]

is assumed together with the definition of the strain matrix \(\mathbf{B}\) relating strain tensor \(\varepsilon\) and displacement vector \(\mathbf{u}\),

\[
\varepsilon = \mathbf{B} \mathbf{u},
\]

where \(C_T\) is the tangent matrix, \(d \varepsilon_f = \mathbf{1} \beta_f/3 dT\) is the strain caused by thermo-elastic expansion, and \(d \varepsilon_0\) represents the autogeneous strain increment and the irreversible part of the thermal strain. We would like to underline that Equations 4 and 10 also take into account effect of the hygral state changes (described by capillary pressure \(p^c\) and degree of saturation \(S_u\)) on deformations and stresses of the material.

Fresh concrete is modeled as a viscoelastic material using the solidification theory by Bazant and Prasannan (1989a, b). In this theory, concrete maturing is attributed to a growth of the volume fraction of load-bearing hydrated cement, which itself is considered as a non-aging viscoelastic material.

During analysis of concrete behavior at high temperature, the material damage caused by the development of cracks is considered following the theory of scalar isotropic damage by Mazars and Pijaudier-Cabot (1989). This theory defines a modified effective stress \(\tilde{\sigma}\) and takes into account the damage \(D(0 \leq D \leq 1)\) as a parameter measuring the reduction of resistant area due to the crack beginning and spreading,

\[
\tilde{\sigma} = \sigma^{\alpha A} = \frac{\sigma''}{1 - D}
\]

where damage depends on the value of equivalent strain reached by the medium, considering its irreversible character (Mazars and Pijaudier-Cabot 1989). \(A\) is the resistant area of the uncracked material, whereas \(\tilde{A}\) is the resistant area of the damaged material. The applied damage theory was obtained by use of a phenomenological approach. It is slightly inconsistent with the rest of our mechanistic model, but we have found this theory very suitable for numerical analyzing of the damage response of concrete.

As a constitutive equation for the capillary water, Darcy’s law is applied,
and similarly for the gas phase, i.e.,

$$v_{wg} = -\frac{k^{wg}}{\mu_g}[\nabla p^g - \rho^g \mathbf{g}].$$

(13)

where $\mathbf{k}$ is the intrinsic permeability tensor, and $k^{wg}$ and $k^{rw}$ are values of relative permeability of the gaseous and liquid phases, while $\mu^g$ and $\mu^w$ are their dynamic viscosities.

For the physically adsorbed water flow, the following constitutive law is applied,

$$v_{ws} = -\mathbf{D}_b \nabla S_w,$$

(14)

where $\mathbf{D}_b$ is the bound water diffusion tensor and $S_w$ is the degree of saturation with bound water, which is assumed to be constant in the capillary moisture range.

For the description of the diffusion process in the binary gas mixture of dry air and water vapor, Fick’s law is applied,

$$J^g = -\rho^g \frac{M_a M_g}{M_g^2} \mathbf{D}_g \nabla \left( \frac{p^g}{\rho^g} \right) = -\mathbf{J}^g,$$

(15)

where $M_a$, $M_g$, and $M_b$ are molar masses of dry air, water vapor, and the gas phase, and $D_g^e$ is the effective diffusivity tensor of vapor in the air.

The equation of state of perfect gases and Dalton’s law are assumed for dry air, water vapor, and their mixture (moist air):

$$p^a = p^a TR/M_a, \quad p^g = p^a + p^v,$$

(16)

$$p^v = \rho^v TR/M_v, \quad \rho^g = \rho^a + \rho^v,$$

where

$$M_g = \left( \frac{\rho^v 1}{\rho^a M_w} + \frac{1}{\rho^v M_g} \right)^{-1}.$$

(17)

Due to the curvature of the meniscus separating the liquid water from the gas phase inside the pores of the concrete, which is considered as a capillary porous body, the equilibrium water vapor pressure $p^v$ differs from the saturation pressure $p^{vs}$ and may be obtained from the Kelvin equation,

$$p^v = p^{vs}(T) \cdot \exp \left( \frac{c M_w}{\rho^v RT} \right).$$

(18)

where the water vapor saturation pressure $p^{vs}$, depending only upon temperature $T$, may be calculated from the Clausius-Clapeyron equation or from empirical correlations (e.g., the formula of Hyland and Wexler [ASHRAE 1997]). Equation 18 is valid both for the capillary and adsorbed water (Lewis and Schrefler 1998). In the latter case, the capillary pressure $p^c$ should be understood as a thermodynamic potential, referring to the bound water and cannot be identified to the pressure.

For model closure, it is further necessary to define the initial and boundary conditions. The initial conditions specify the full fields of gas pressure, capillary pressure, temperature, and displacements in the whole analyzed domain $\Omega$ and its boundary $\Gamma (\Gamma = \Gamma_\Omega \cup \Gamma_{\pi g}, \ pi = g, c, l, u)$:

$$p^g = p^g_0, \quad p^c = p^c_0, \quad T = T_0, \quad u = u_0, \quad \text{for } t = 0.$$

(19)

The boundary conditions can be of Dirichlet’s type on $\Gamma_g$:

$$p^g(t) = p^g_0 \text{ on } \Gamma_g,$$

$$p^c(t) = p^c_0 \text{ on } \Gamma_c,$$

(20)

or of Neumann’s (Equations 21a and 21d) and Robin’s (Equations 21b,c) type on $\Gamma_q^g$:

$$\rho^w \frac{k^{wg}}{\mu_w} (-\nabla p^g + \rho^g \mathbf{g}) + \rho^v \frac{k^{vw}}{\mu_v} (-\nabla p^v + \rho^v \mathbf{g}) - \rho^a \frac{M_a M_w}{M_g^2} \mathbf{D}_g \nabla \left( \frac{p^g}{\rho^g} \right) \cdot \mathbf{n} = q^w + q^v + \beta_1 (p^v - \rho^w), \quad \text{on } \Gamma_q^g,$$

(21a)

$$\rho^w \frac{k^{kw}}{\mu_w} (-\nabla p^g + \rho^g \mathbf{g}) - \rho^a \frac{M_a M_w}{M_g^2} \mathbf{D}_g \nabla \left( \frac{p^v}{\rho^v} \right) \cdot \mathbf{n} = q^w + q^v + \beta_1 (p^v - \rho^w), \quad \text{on } \Gamma_q^g,$$

(21b)

$$\rho^w \frac{k^{kw}}{\mu_w} (-\nabla p^g + \rho^g \mathbf{g}) \Delta H_{\text{cap}} - \lambda_{ef} \nabla T \cdot \mathbf{n} = q^w + q^v + \beta_1 (p^v - \rho^w), \quad \text{on } \Gamma_q^g,$$

(21c)

$$\sigma \cdot \mathbf{n} = \mathbf{t}, \quad \text{on } \Gamma_u^q,$$

(21d)

where $\mathbf{n}$ is the unit normal vector, pointing toward the surrounding gas; $q^a$, $q^v$, $q^c$, and $q^T$ are, respectively, the imposed fluxes of dry air, vapor, liquid water, and the imposed heat flux; $\mathbf{t}$ is the imposed traction; $\rho^w_{cap}$ and $T_{\text{w}}$ are the mass concentration of water vapor and the temperature in the far field of undisturbed gas phase; $\epsilon$ is emissivity of the interface; $\sigma_0$ is the Stefan-Boltzmann constant, and $\alpha$ and $\beta$ are convective heat and mass transfer coefficients.

The mathematical model (Equations 1 through 21) contains several material parameters, which should be determined experimentally. However, indispensable experimental effort in this case is smaller in comparison to similar phenomenological models because effect of moisture content (saturation degree) and/or temperature and/or gas pressure on most of the transport properties can be predicted theoretically (Lewis and Schrefler 1998; Gawin et al. 1999; Gawin 2000).
NUMERICAL SOLUTION

Discretization in space of the governing equations is carried out by means of the finite element method (e.g., Zienkiewicz and Taylor 1989, 1991). The unknown variables are expressed in terms of their nodal values as

\[ p^s(t) = N_p^s \tilde{p}^s(t), \quad p^c(t) = N_p^c \tilde{p}^c(t), \]

\[ T(t) = N_T \tilde{T}(t), \quad u(t) = N_u \tilde{u}(t). \]

(22)

The variational (weak) form of the heat and mass transfer equations, applying also the other ones required to complete the model, was obtained by means of Galerkin’s method (weighted residuals) and can be expressed in matrix form as

\[
\begin{bmatrix}
K_{gg} & K_{gc} & K_{g}\mu_0 \\
K_{cg} & K_{cc} & K_{c}\mu_0 \\
K_{g}\mu & K_{c}\mu & K_{\mu}\mu_0 \\
\end{bmatrix}
\begin{bmatrix}
\tilde{p}^g \\
\tilde{p}^c \\
\tilde{u} \\
\end{bmatrix}
= 
\begin{bmatrix}
\tilde{f}_g \\
\tilde{f}_c \\
\tilde{f}_\mu \\
\end{bmatrix}
\]

(23)

The matrices occurring in Equation 23 are listed in Gawin (2000). The above nonsymmetric, nonlinear, and coupled system of partial differential equations may be rewritten in compact form as

\[ \mathbf{K}(\mathbf{x})\mathbf{x} + \mathbf{C}(\mathbf{x})\frac{\partial \mathbf{x}}{\partial t} = \mathbf{f}(\mathbf{x}) \]

(24)

where \( \mathbf{x}^T = \left[ p^g, p^c, T, u \right] \) and the nonlinear (matrix) coefficients \( \mathbf{C}(\mathbf{x}), \mathbf{K}(\mathbf{x}), \) and \( \mathbf{f}(\mathbf{x}) \), obtained by assembling the submatrices indicated in Equation 23, are given in Gawin (2000).

The time discretization is accomplished through a fully implicit finite difference scheme (backward difference),

\[ C_{n+1} \frac{x_{n+1} - x_n}{\Delta t} + K_{n+1} x_{n+1} - f_{n+1} = 0 \]

(25)

where \( C_{n+1} = C(x_{n+1}), K_{n+1} = K(x_{n+1}), f_{n+1} = f(x_{n+1}), n \) is the time step number, and \( \Delta t \) is the time step length.

Because of the nonlinearity of Equation 25, the solution is obtained with a Newton-Raphson type procedure,
these inner curves have been created in an artificial way. More information about their modeling can be found in Gawin et al. (2001a) and physical phenomena related to sorption and hysteresis are described in Gregg and Sing (1982).

The following material data are used in computations: \( \rho_o = 2330 \, \text{kg/m}^3 \), \( n = 0.1 \), \( \lambda_{ef} = 1.67 \, \text{W/(m} \cdot \text{K)} \), \( C_{wp} = 940 \, \text{J/(kg} \cdot \text{K)} \), \( k = 10^{-19} \, \text{m}^2 \), and \( \beta_s = 0.9 \cdot 10^{-6} \, \text{1/K} \). Young’s modulus \( E = 14 \, \text{GPa} \), Poisson’s ratio \( \nu = 0.25 \), and Biot’s constant \( \alpha = 0.5 \) are assumed.

Initially, the element has temperature \( T_0 = 278.15 \, \text{K} \) and relative humidity \( \varphi_0 = 50\% \, \text{RH} \). The external surfaces of the cylinder are exposed to convective boundary conditions for heat and moisture exchange. Temperature and relative humidity of the surrounding air change harmonically with the period \( T = 168 \, \text{hours (one week)} \), temperature between \( T_{min} = 278.15 \, \text{K} \) and \( T_{max} = 298.15 \, \text{K} \), and relative humidity between \( \varphi_{min} = 50\% \, \text{RH} \) and \( \varphi_{max} = 90\% \, \text{RH} \). The corresponding convective heat and mass transfer coefficients are \( \beta_c = 0.02 \, \text{m/s} \) and \( \alpha_c = 23 \, \text{W/(m}^2\text{K)} \). The gas pressure of the air is assumed to be constant, \( p^g = 101325 \, \text{Pa} \). For all surfaces, except those exposed to convective heat and moisture exchange, all the normal fluxes and normal displacements are set to zero. The total simulation time comprised two full wetting-drying cycles.

One-quarter of the cylinder has been spatially discretized by use of 168 8-node serendipity elements (12 along the radius and 14 along the height, i.e., 557 nodes). During computations, various time steps (from 1 second up to 100 seconds) according to the stage of the process evolution are applied. The problem is solved for isotherms with and without hysteresis (for the main desorption curve). The resulting distributions of water saturation at time instant \( t = 168 \, \text{hours} \) for the two cases are presented in Figure 1. In Figure 2, the hysteresis loops for the first case (for the points in the corner and in the center of the cylinder), obtained using the saturation and relative humidity results for the same time instants, are shown. Additionally, the experimental data of the primary adsorption and

---

**Figure 1** The resulting distributions of water saturation at time instant \( t = 168 \, \text{hours} \) for the analyzed cases: a) with hysteresis and b) without hysteresis.

**Figure 2** The resulting relative humidity-water saturation changes for the analyzed case with hysteresis: a) in the corner and b) in the center of the concrete cylinder.
desorption curves (diamond points) are shown in the figure. The time evolutions of temperature and relative humidity in the center of the cylinder are compared in Figure 3. A small effect of the hysteresis on the temperature solution is obtained. This is caused by a relatively weak dependence of the thermal conductivity upon the concrete moisture content. Hence, some differences in the material moisture content (saturation degree) had a very small influence on the temperature solution.

Simulation of a UHPC Concrete Nuclear Waste Container at High Temperature

Hygrothermal behavior and material damage of a cylindrical UHPC concrete nuclear waste container (diameter of 100 cm, height of 150 cm, wall thickness of 12 cm) during fire is solved. The analyzed UHPC has the following material parameters: \( \rho_o = 2470 \text{ kg/m}^3, \lambda_{ef} = 2.32 \text{ W/(m} \cdot \text{K}, n = 0.044, k_o = 10^{-20} \text{ m}^2, f_c = 200 \text{ MPa}, E = 55.2 \text{ GPa}, \text{ and } \nu = 0.18. \)

Considering the shape of the sample, one-half of the container is discretized by 268 axisymmetric eight-node elements (10 × 14 for the bottom and 8 × 16 for the wall). Initially, the specimen is at capillary pressure \( p_c = 92.67 \text{ MPa} \) and at temperature \( T = 293.15 \text{ K}. \) The external temperature increases according to the standard ISO fire conditions, while the partial vapor pressure of the external air has constant value \( p_v = 1000 \text{ Pa}. \) The problem is solved for an unsealed heated surface, assuming the radiative boundary conditions for heat exchange with \( \sigma_o = 5.1 \times 10^{-8} \text{ W/(m}^2 \cdot \text{K}^4) \) and convection for mass exchange with \( \beta_c = 0.019 \text{ m/s}. \) For the inner, unheated surfaces of the container, the convective boundary conditions for heat and mass exchange with \( \alpha_c = 18 \text{ W/(m}^2 \cdot \text{K}) \) and \( \beta_c = 0.019 \text{ m/s} \) are assumed. The greatest changes are observed in the corner of the container where the gas pressure and temperature reach the highest values; hence, only results for this zone are presented in Figures 4 through 7.

Figures 4a and 4b show the distributions of temperature at time stations 4 minutes and 8 minutes (i.e., the final time of simulation). A front of the increasing temperature and decreasing saturation with liquid water, moving from the heated surface toward the internal surface, can be observed in Figures 5a and 5b. The vapor pressure distributions at the same time stations are shown in Figures 6a and 6b. The maximum vapor pressure is observed very close to the external corner, reaching at the end a very high value of \( p_v' = 14.4 \text{ MPa}. \) At the same time, this zone damage parameter reaches a value greater than 0.95 (Figure 7), which indicates a high probability of spalling phenomenon occurrence.

Simulation of Maturing Process of a Concrete Column

Hygrothermal behavior of a concrete column (60 cm × 40 cm) during the first 30 days of its maturing in ambient air of different relative humidities is simulated by use of the HMTTRA-HC code (Gawin 2000). The heat and mass sources related to the concrete maturing process are expressed as a function of the hydration degree \( \Gamma_{hydr/(t_{eq})}. \) Effect of the temperature and relative humidity on the time evolution of the cement hydration (Equations 5 through 7) is taken into account using experimental data for the cement type IV given in Neville (1995).

The following material data are used in computations: \( \rho_o = 1900 \text{ kg/m}^3, n = 0.1, \lambda_{ef} = 1.67 \text{ W/(m} \cdot \text{K}, C_{ap} = 940 \text{ J/(kg} \cdot \text{K}), k = 10^{-18} \text{ m}^2, \beta_c = 0.9 \cdot 10^{-6} \text{ 1/K}, E = 55 \text{ GPa}. \)
Figure 4  Resulting temperature distribution in the heated UHPC concrete nuclear waste container at different time instants: a) $t = 4$ min, b) $t = 8$ min.

Figure 5  Resulting saturation distribution in the heated UHPC concrete nuclear waste container at different time instants: a) $t = 4$ min, b) $t = 8$ min.

Figure 6  Resulting vapor pressure distribution in heated UHPC concrete nuclear waste container at different time stations: a) $t = 4$ minutes, b) $t = 8$ minutes.
Initially, the column has a temperature $T_0 = 293.15$ K and relative humidity $\varphi = 99.9\%$. It is assumed that the hydration process started 2.5 hours before; hence, the element already has a certain shape rigidity. The external surfaces of the column are exposed to convective boundary conditions for heat and moisture exchange. The temperature and relative humidity of the surrounding air are constant: $T_\infty = 293.15$ K and $\varphi = 95\%$ or 55\%. The convective heat and mass transfer coefficients are assumed as $\beta_c = 0.033$ m/s and $\alpha_c = 8.3$ W/(m$^2$K). For all surfaces, except those exposed to convective heat and moisture exchange, the normal displacements and normal fluxes are set to zero.

Because of the symmetry, only one-quarter of the column has been spatially discretized by use of 130 eight-node serendipity elements ($13 \times 10$, i.e., 437 nodes). During computations, various time steps (from 10 seconds up to 900 seconds) are used according to the stage of the process evolution. The resulting distributions of the temperature at time instant $t = 24$ hours and total displacements (negative values correspond to the element shrinkage) at $t = 720$ hours for the two analyzed cases of relative humidity are presented in Figures 8 and 9. In Figure 10, the time evolutions of the temperature, relative humidity, and hydration degree in the center and the corner of the cylinder are compared for the two cases. They show a considerable effect of the ambient relative humidity upon the kinetics of hydration process and hygrothermal state of the maturing concrete, especially during first hours of the process. Self-desiccation and self-heating phenomena, characteristics of fresh concrete, are clearly visible, influencing significantly the deformations of the column. For the analyzed column, the hydration degree and the relative humidity for both analyzed cases have almost the same value inside the element and close to its surfaces.

**CONCLUSIONS**

HMTRA, the finite element model of coupled heat, moisture, and air transfer in porous building materials has been presented. It takes into account all important mass and energy transport mechanisms, phase changes, capillary hysteresis, and material deformations. It allows for analysis of hygrothermal behavior of two-dimensional (also axisymmetric) concrete structures in various situations, including concrete maturing and performance at high temperature, as well as evaluation of material stresses, deformations, or damage (crack development). Three examples of application of the
Figure 9  The distributions of total displacements in concrete column maturing in ambient air having a) 95% RH, b) 55% RH, at time instant $t = 24$ hours.

Figure 10  Comparison of the time evolutions of the temperature, relative humidity, hydration degree, and total displacements in the center and in the corner of the concrete cylinder maturing in ambient with the two different values of the relative humidity.
model for analysis of the performance of concrete structures, including their hygrothermal state, deformations, and damage, show the versatility of the model.

ACKNOWLEDGMENTS

The first author’s research was partly supported by the Polish State Committee for Scientific Research (K.B.N.) grant No. 7 T07E 018 19.

REFERENCES


