ON PROBLEMS OF HEAT AND MASS TRANSFER IN CONCRETE STRUCTURES

Introduction

Transport phenomena in porous media have recently received growing attention in light of the common usage of such media in various applications in the fields of energy technology [1, 2].

The physics of moisture transfer in porous media are usually explained by diffusion theory [3], capillary flow theory [4-7], and evaporation condensation theory [5, 8]. In a present work the evaporation mechanism was assumed with concentration and pressure gradient terms, because for examples presented i.e. concrete structure undergoing thermal loading this theory is generally accepted. Drying experiments at elevated temperatures revealed high pore pressure as a consequence of intensive water vaporization.

The measures pore pressure, determined under heating conditions, correspond to the sum of saturated water vapor pressure and ambient air pressure. The consequences of these phenomena are poroelastic and poroplastic stresses in porous structures [9-17].

Problems of heat and mass transfer in porous bodies are considered usually by deterministic theories. But many of these problems have stochastic character.

The literature on probabilistic methods in mechanics can be divided into two parts i.e. using statistical and nonstatistical approaches [18-21]. Non-statistical methods include for instance the stochastic finite element method [22, 23].

Stochastic methods can be an effective tool in solutions of heat and mass transfer problems. As the name suggests, these methods combine two crucial methodologies developed to deal with problems of heat and mass transfer: analytical or numerical analysis with the stochastic one.

The stochastic analysis in the broadest sense refers to the explicit treatment of uncertainty in any quantity entering the corresponding deterministic analysis.

1 Politechnika Częstochowska, Wydział Budownictwa, ul. Akademicka 3, 42-200 Częstochowa, e-mail: mkowalik@bud.pcz.czest.pl, mpomski@bud.pcz.czest.pl
The exact values of these quantities are usually unknown because they cannot be
precisely measured.

The stochastic approach to heat and mass transfer problems is important not only because of random material parameters, but particularly because of boundary problems appearing in these processes.

Existing uncertain variations in parameters may have significant effects on such fundamental final characteristics, as temperature distributions, and they must affect the final design. Useful analytical tools for performing analysis of element with uncertain properties are provided by the theory of random fields, which is an outgrowth of the probability theory.

This paper is limited to equations typical for heat and mass transfer. In analyzing of stochastic behavior of porous bodies in heating processes systems of equations are functions of random variables. The distinguishing feature of the stochastic methods, which are based on the perturbation approach, is treating probabilistic problems with deterministic computational techniques that take full advantage of the mathematical properties of linear or even nonlinear operators.

This offers a specific treatment of heat and mass transfer problems for which we can use the probabilistic numerical techniques. In the paper the so-called the stochastic finite difference method is applied which is a modification of the stochastic finite elements mentioned above. A system of partial differential equations is obtained and solved for first two probabilistic moments of the random temperature field.

1. Discretized random variable

Assume that the domain of interest $V$ is discretized. The basic idea of the mean-based, second-order, second-moment analysis in a stochastic discretized problem is to expand via Taylor series all the vector and matrix stochastic field variables about the mean values of random variables $b(x)$, to retain only up to second-order terms and to use in the analysis only the first two statistical moments. Equations for the expectations and cross-covariances (autocovariances) of the nodal temperatures can be obtained in terms of the nodal temperature derivatives with respect to the random variables.

In the stochastic numerical approach the fields $b(x)$ have to be represented by a set of basic random variables. To discretize $b(x)$ by expressing them in terms of point values the following approximation is used

$$b(x) = N_\pi(x) b_\pi$$

where $N_\pi$ are shape functions and $b_\pi$ is the matrix of random parameter nodal values.

The same shape functions as in Eq. (1) as used for temperature approximation

$$T(x) = N_\pi(x) T_\pi$$

(2)
where $T_\pi$ is the matrix of nodal temperatures. The matrix $T_\pi$ can be related to the nodal temperature vector $T_\alpha$ by the transformation

$$T_\pi = B_{\pi\alpha} T_\alpha$$

which substituted into Eq. (2) gives

$$T(x) = N_\alpha(x) T_\alpha$$

provided we denote

$$N_\alpha(x) = N_\pi(x) B_{\pi\alpha}$$

A vector of nodal random variables $b_\rho$ related to the matrix $b_\pi$ is introduced by an appropriate transformation

$$b_\pi = B_{\pi\rho} b_\rho$$

Then Eq. (1) is

$$b(x) = N_\pi(x) B_{\pi\rho} b_\rho = N_\rho(x) b_\rho$$

which may be regarded as the random variable counterpart of the temperature expansion Eq. (2).

By Eq. (1)

$$E(b(x)) = b_0(x) = N_\rho(x) b_\rho$$

$$\text{Cov}(b_\rho(x), b_\sigma(x)) = S_{\rho\sigma} = N_\rho(x) N_\sigma(x) S_{\rho\sigma}$$

and

$$\Delta b(x) = N_\rho(x) \Delta b_\rho$$

where

$$\Delta b_\rho = b_\rho - b_\rho^0$$

and $b_\rho^0$ and $S_{\rho\sigma}$ stand for the mean value vector and the covariance matrix of the nodal random variable vector $b_\rho$, respectively.

2. Equations of heat and mass transfer in porous body

Problems of heat and mass transfer in porous material are described by the following equations.
The conservation equations for mass can be written as

\[ \dot{\rho}_i = -\nabla (\rho_i w_i) + W_i \]  

(12)

where \( \rho_i \) is the density of species i, \( w_i \) is the velocity of species i and \( W_i \) is the production rate of species i. Since no movement of the liquid (subscript c) is assumed \( w_c = 0 \). Also, \( W = -W_v = -W_m \) (v = vapor, m = air-vapor mixture), since the rate of liquid evaporation is the same as the rate of vapor production, and since the air does not change phase, the rate of mixture production equals the rate of vapor production. The above equation thus simplifies to

\[ \dot{\rho}_c = -W_m \]  

(13)

The continuity equation for the air (subscript a) takes the form

\[ \dot{\rho}_a = -\nabla (\rho_a w_a) \]  

(14)

and for the vapor,

\[ \dot{\rho}_v = -\nabla (\rho_v w_v) + W_v \]  

(15)

The conservation of gas phase mass gives

\[ \dot{\rho}_m = -\nabla (\rho_m w_m) + W_m \]  

(16)

Fick’s law allows the fluxes to be presented in the forms of equation (17) and (18):

\[ j_a = \rho_a (w_a - w_m) = -\rho_m D \nabla \rho_{pa} \]  

(17)

where \( \rho_{pi} = \rho_i / \rho_m \) is the mass fraction of species i with respect to the density of the air-vapor mixture, and D is the diffusion coefficient for Fick’s law for the air-vapor mixture; and

\[ j_v = \rho_v (w_v - w_m) = -\rho_m D \nabla \rho_{pv} \]  

(18)

Finally, we get the following species equations:

\[ \rho_{m(pa)} + \rho_m w_m \nabla \rho_{pa} = \nabla (\rho_m D \nabla \rho_{pa}) - \rho_{pa} W_m \]  

(19)

and

\[ \rho_{m(pv)} + \rho_m w_m \nabla \rho_{pv} = \nabla (\rho_m D \nabla \rho_{pv}) - \rho_{pv} W_m \]  

(20)

– Thermal equations

The fluxes of heat \( q \) and flowing gases \( r \) can be expressed as

\[ q = -k \nabla T \]  

(21)
and

\[ r = \rho_s w_s h_s + \rho_v w_v h_v \]  \hspace{1cm} (22)

where \( k \) is the thermal conductivity, and \( h_i \) is the enthalpy of component \( i \) per unit mass of component \( i \). Equation (22) can be transformed to the form

\[ r = \rho_m w_m h_m - \rho_m D_h \nabla \rho_{fa} - \rho_m D_h \nabla \rho_{pv} \]  \hspace{1cm} (23)

or

\[ r = \rho_m w_m h_m + \rho_m D(h_v - h_s) \nabla \rho_{fa} \]  \hspace{1cm} (24)

Assuming that

\[ \rho e = \rho_s h_s + \rho_c h_c + \rho_m h_m - \rho_m R_m \theta \]  \hspace{1cm} (25)

where \( e \) is the thermal energy and \( R \) is the gas constant.

The thermal equations can be expressed as

\[
\begin{bmatrix}
\rho c_p T = \nabla k VT - \rho_m \left[ w_m h_m c_{pm} + D(h_{pv} - c_{pa}) \nabla \rho_{fa} \right] \nabla T \\
- \left[ (h_v - h_s) w_m - \rho_m R_m T \right]
\end{bmatrix}
\]  \hspace{1cm} (26)

with boundary conditions for \( T \)

\[ B_1(T) = T - T_w = 0 \quad \text{on } S_1 \]

\[ B_2(T) = k \frac{\partial T}{\partial n} + q_w = 0 \quad \text{on } S_2 \]

\[ B_3(T) = k \frac{\partial T}{\partial n} + \alpha(T - T_f) = 0 \quad \text{on } S_3 \]

where \( T_w \) is the temperature of the body surface, \( T_f \) is the fluid temperature, and where \( c_p \) is the specific heat at constant pressure.

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**Darcy’s law**

The velocity of the air-vapor mixture is given by

\[ w_m = -k_D \nabla p \]  \hspace{1cm} (27)

where \( k_D \) is Darcy’s coefficient and \( p \) is the pressure.

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**Thermodynamic relations**

Assuming that the vapor and air are ideal gases we have the following relations:
-- Ideal gas equation for the vapor
\[ p_v \overline{V}_v = \rho_v R_v T \]  
(28)

where \( \overline{V}_i = \rho_i / \rho_{ci} \) represents the volume occupied by component \( i \) per unit total volume; and

-- Ideal gas equation for the air
\[ p_a \overline{V}_a = \rho_a R_a T \]  
(29)

– Clausius-Clapeyron equation
Since the liquid and vapor are assumed to be in equilibrium,
\[ p_v = p_{sat}(T) \]  
(30)
in the presence of liquid water. An analytic expression for \( p_{sat} \) is
\[ p_{sat}(T) = CT^{-(\beta_v / R_v)} \exp \left( -\frac{A}{R_v T} \right) \]  
(31)

– State equation
Using the notations \( \rho_{\beta_i} \) and \( \overline{V}_i \), the state equation can be presented as
\[ p_v (\phi - \overline{V}_c) = \rho_m \rho_{\beta_v} R_v T = (1 - \rho_{\beta_a}) \rho_m R_v T \]  
(32)
and
\[ p_a (\phi - \overline{V}_a) = \rho_m \rho_{\beta_a} R_a T \]  
(33)
where \( \overline{V}_v = \overline{V}_a = (\phi - \overline{V}_c) \) and \( \phi \) is the porosity.
Combining the above equations we get
\[ p(\phi - \overline{V}_c) = \rho_m R_m T \]  
(34)
where
\[ R_m = \rho_{lv} R_v + \rho_{pa} R_a \]  
(35)

3. Numerical solution
The thermal equations (26) are of parabolic type and can be transformed to matrix equation using any standard finite difference procedure. As the result we get the matrix equation for temperature vector \( \mathbf{T} \) with components \( T_i \) of temperatures in nodes of the finite difference mesh as
where \( C \) is the heat capacity matrix, \( K \) is the thermal conductivity matrix and \( F \) is the load vector. Stochastic equations of the problem are given by considering matrix thermal equations (36) with all the variables \( C, K, F \) and \( T \) which are functions of the discretized random variable vector \( b = b(x) \), where \( x \) is the coordinate vector

\[
C(b)\dot{T}(b,t) + K(b)T(b,t) = F(b,t)
\]  

(37)

The random function \( b(x) \) is approximated using shape functions \( N_i(x) \) by

\[
b(x) = \sum_{i=1}^{q} N_i(x) b_i = Nb
\]  

(38)

where \( b_i \) are nodal values of \( b(x) \), that is the values of \( b \) at \( x_i \), \( i = 1, \ldots, q \).

The mean value of \( b \) denoted by \( E(b) \) is expressed as

\[
e(b) = \sum_{i=1}^{q} N_i E(b_i)
\]  

(39)

and the variance by

\[
V(b) = \alpha^2 E(b)^2
\]  

(40)

where \( \alpha \) is the coefficient of variation.

All the random functions are expanded about the mean value \( E(b) \) via a Taylor series and only up to second-order terms are retained. For any small parameter \( \gamma \) we have

\[
T(b,t) = E(T(t)) + \gamma \sum_{i=1}^{q} E(T_{b_i}(t)) \Delta b_i + \frac{1}{2} \gamma^2 \sum_{i,j=1}^{q} E(T_{b_i b_j}(t)) \Delta b_i \Delta b_j
\]  

(41)

where \( \Delta b_i \) represents the first-order variation of \( b_i \) about \( E(b_i) \) and for any function \( g \)

\[
e(g(x)) = g(x, E(b))
\]

\[
e(g_{,b_i}) = \frac{\partial g}{\partial b_i}
\]

\[
e(g_{,b_i b_j}) = \frac{\partial^2 g}{\partial b_i \partial b_j}
\]  

(42)

In a similar manner we can express \( C(b), K(b) \) and \( F(b,t) \) as
\[ C(b) = E(C) + \gamma \sum_{i=1}^{q} E(C_{b_i}) \Delta b_i + \frac{1}{2} \gamma^2 \sum_{i,j=1}^{q} E(C_{b_ib_j}) \Delta b_i \Delta b_j \] (43)

\[ K(b) = E(K) + \gamma \sum_{i=1}^{q} E(K_{b_i}) \Delta b_i + \frac{1}{2} \gamma^2 \sum_{i,j=1}^{q} E(K_{b_ib_j}) \Delta b_i \Delta b_j \] (44)

\[ F(b,t) = E(F) + \gamma \sum_{i=1}^{q} E(F_{b_i}(t)) \Delta b_i + \frac{1}{2} \gamma^2 \sum_{i,j=1}^{q} E(F_{b_ib_j}) \Delta b_i \Delta b_j \] (45)

Substitution of equations (41) and (43)-(45) into equation (37) and collecting terms of order 1, \( \gamma \) and \( \gamma^2 \) yields the following equations for \( E(T(t)) \), \( E(T_{b_i}(t)) \) and \( E(T_{b_ib_j}(t)) \)

zerth order

\[ E(C)E(T(t)) + E(K)E(T(t)) = E(F(t)) \] (46)

first order

\[ E(C)E(T_{b_i}(t)) + E(K)E(T_{b_i}(t)) = E(F_{b_i}(E(T),t)) \] (47)

where

\[ E(F_{b_i}(E(T),t)) = E(F_{b_i}(t)) - (E(C_{b_i})E(T(t)) + E(K_{b_i})E(T(t))) \] (48)

second order

\[ E(C)T_2(t) + E(K)T_2(t) = \hat{F}_2(E(T),E(T_{b_i}),t) \] (49)

\[ \hat{F}_2 = \sum_{i,j=1}^{q} \left\{ \left[ \frac{1}{2} E(F_{b_ib_j}(t)) \right] \text{cov}(b_i,b_j) \right\} + \right. \]
\[ \left. - \sum_{i,j=1}^{q} \left\{ \left[ \frac{1}{2} E(C_{b_ib_j}) E(T(t)) + \frac{1}{2} E(K_{b_ib_j}) E(T(t)) + \right. \right. \right. \]
\[ \left. \left. \left. \left. E(C_{b_i}) E(T_{b_i}(t)) + E(K_{b_i}) E(T_{b_i}(t)) \right] \text{cov}(b_i,b_j) \right\} \right\} \] (50)

and

\[ \hat{T}_2(t) = \frac{1}{2} \sum_{i,j=1}^{q} E(T_{b_ib_j}) \text{cov}(b_i,b_j) \] (51)
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\[ \text{Cov}(b_i, b_j) = \left[ V(b(x_i))V(b(x_j)) \right]^{1/2} R(b(x_i), b(x_j)) \]  

(52)

and \( R(b(x_i), b(x_j)) \) is the autocorrelation.

The definitions for the expectation and autocovariance of the temperature are given by

\[ E(T) = \int_{-\infty}^{\infty} T(b, t) f(b) \, db \]  

(53)

and

\[ \text{Cov}(T^i, T^j) = \int_{-\infty}^{\infty} \left( T^i - E(T^i) \right) \left( T^j - E(T^j) \right) f(b) \, db \]  

(54)

where \( f(b) \) is the joint probability density function. The second-order estimate of the mean value of \( T \) is obtained from equation (53) to give

\[ E(T) = T(E(b)) + \frac{1}{2} \left\{ \sum_{i,j=1}^{d} E(T_{b_i,b_j}) \text{Cov}(b_i, b_j) \right\} \]  

(55)

4. Numerical example - Heated concrete element with random liquid contents

Consider the stochastic problem of temperature distribution in the process of one-sided heating of concrete element with velocity of heating of surrounding air equals to 1°C/sec. The length of concrete element is assumed as 0.0540 m. The number of nodes in finite difference meshes is 18. Calculations proved that the increase of number of nodes in element does not influence on accuracy of results both for deterministic and stochastic problems. Therefore the results are described for 18-nodes mesh of finite differences.

The heat transfer coefficient on the boundary was assumed as 5.73491 J/sec m² K and the coefficient of mass transfer on the boundary 0.00570734 kg/sec·m², and the shape coefficient for the boundary is taken as 0.9. The initial temperature of element’s temperature is equal to 20°C. In presented model the liquid contents \( \rho_l \) is defined as the random variable nodes 1 to 17 of finite difference mesh. For outer surface it is assumed the constant liquid contents equal to 0. The total number of random variables appearing in the analysis is equal 17 \( \rho_i = \{ \rho_{1,1}, ..., \rho_{1,m} \} \) \( m = 17 \).

For each node \( I \) the temperature \( T_I \) is assumed as the random variable. The formula for expected values for temperature is

\[ E[T_I] = T_I(\rho_I^0) + \frac{1}{2} \sum_{\alpha,\beta=1}^{m} \text{Cov}(\rho_{I,\alpha}, \rho_{I,\beta}) \]  

(56)
and for covariance of temperatures

\[
\text{Cov}(T_i, T_j) = \frac{dT_i}{d\rho^\alpha} \frac{dT_j}{d\rho^\beta} \text{Cov}(\rho^\alpha, \rho^\beta)
\]

(57)

where \(m\) is the number of nodes, \(I, J = 1, 2, \ldots, n, \alpha, \beta = 1, 2, \ldots, m\).

<table>
<thead>
<tr>
<th>Node</th>
<th>Thermal conductivity [W/m·K]</th>
<th>Density [kg/m³]</th>
<th>Heat capacity for the Fick’s law [J/kg·K]</th>
<th>Heat capacity for constant pressure for air [J/kg·K]</th>
<th>Heat capacity for constant pressure for vapor [J/kg·K]</th>
<th>Pressure [N/m²]</th>
<th>Liquid density [kg/m³]</th>
<th>Temperature [K]</th>
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<td>101325.</td>
<td>15.</td>
<td>293.15</td>
</tr>
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</table>

It is assumed that the expected values, covariance and the variation coefficient are:

\[
E[\rho] = \rho^0 = 1274.2435 \text{ J/kg·K}
\]

\[
\text{Cov}(\rho^\alpha, \rho^\beta) = 9 \cdot \exp \left( -\frac{|x^\alpha - x^\beta|}{\vartheta} \right)
\]

where \(\vartheta = 10\) is the correlation length, and \(\lambda = 0.01\) is the value of diagonal of covariance.
The deviation of liquid contents is assumed 10%. The initial thermal parameters of concrete element assumed for the numerical calculations are presented in Table 1. Stochastic and deterministic results of temperature distributions in concrete element for heating time 800 sec are presented in Table 2. Covariance of temperatures are given in Figure 1. Standard deviation for 10% of unreliability in liquid contents is presented in Table 3.

### TABLE 2

<table>
<thead>
<tr>
<th>Node</th>
<th>Deterministic problem</th>
<th>Stochastic problem</th>
<th>Change [%]</th>
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Fig. 1. Covariance of temperatures for 10% of unreliability in liquid contents.
TABLE 3

Standard deviation for temperature for 10% of unreliability in liquid contents

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Final remarks

The development of stochastic finite difference method for thermal analysis in porous continua with random properties requires the unification of mechanics, probability and numerical methods. Its is an attractive tool for computation of thermal variables considering random changes in porous material and its boundary conditions. An application of stochastic finite difference method to discretization of the region with the heat flow equation in porous body is a convenient approach for the model presented.

References

On problems of heat and mass transfer in concrete structures

Abstract

A stochastic finite difference approach based on stochastic finite elements is proposed for heat and mass transfer modeling. Porous structure with random material properties is investigated. The theoretical formulation of the problem is described. A system of partial differential equations is obtained and solved for first two probabilistic moments of the random temperature field. Example of stochastic thermal analysis in concrete structure with random material parameters are given.

Keywords: concrete, heat and mass transfer, uncertainty, perturbation method

Metoda stochastycznych różnic skończonych w problemach przepływu ciepła i ruchu wilgoci w elemencie betonowym

Streszczenie


Słowa kluczowe: beton, przepływ ciepła i masy, losowość, metoda perturbacyjna