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Random heat flow with phase change

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Abstract

Temperature distributions in structure with random material properties is investigated. Variational methodology is proposed for the analysis of heat flow with phase change using the enthalpy of the system. The solution procedure for phase change effect is discussed. A system of partial differential equations is obtained and solved for the first two probabilistic moments of the random temperature field. The finite element equations are derived. © 2000 Elsevier Science Ltd. All rights reserved.

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1. Introduction

The numerical methods, especially the finite elements, are widely used and its application in thermal analysis is universally accepted. The analysis of thermal problems subjected to external loads is developed under the assumption that the structure's parameters are deterministic quantities. For a significant number of circumstances, this assumption is not valid, and the probabilistic aspects of the thermal problem need to be taken into account. The literature on the probabilistic methods in mechanics is considerable (see Refs. [1,2], for instance). In this paper, we apply the finite element method with a probabilistic context called stochastic finite element method (see Refs. [3–6], for instance). This broad definition includes the first- and second-order moment methods. The main advantage of this non-statistical methodology is that only the first two probabilistic moments of random parameters (i.e. spatial expectations and cross-covariances or cross-correlation functions) are required on input, while in the statistical approach the whole probabilistic structure (probability density or probability distribution functions) and a large number of samples generated randomly are needed. In the paper a variational methodology is proposed for nonlinear transient heat transfer systems with phase change with random parameters defined by their first two probabilistic moments. The basic difficulty in the finite element modeling of heat transfer problems with phase changes lies in a temperature solution with discontinuous temperature gradients at the phase transition surface. A method that can directly be employed in conventional finite element computer programs is the procedure proposed by Morgan et al. [11] and Comini et al. [10]. However, this technique must be used with care, because for a given phase change temperature interval the time step used must be small enough that the change in temperature during one time step, in a region undergoing a change of phase, is less than phase change temperature interval. In this study we use a procedure to phase change problems proposed by Rolph and Bathe [14]. This procedure is relatively simple and restrictions on the time step size and mesh configurations are greatly reduced and no special con-

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Nomenclature

T	temperature	ϵ	surface emissivity
K_{ij}	thermal conductivity tensor	$\epsilon_{(r)}$	emissivity of the radiation source
Q	rate of heat generated per unit volume	c	specific heat of material
H	enthalpy	ρ	density of material
$\boldsymbol{x}$	position vector	L	Latent heat
t	time	T_s	solidus temperature
$\hat{T}$	boundary temperature	T_l	liquidus temperature
$\hat{q}$	boundary heat flux	η	Heaviside function
n_i	unit outward	ΔT_f	phase change interval
$\hat{T}_0$	initial temperature	T_f	phase change temperature ($T_f = T_s$)
q_i	heat flux vector	$\boldsymbol{b} = b_r$	random variable vector
$\xi_{(c)}$	convection coefficient	b_r^0	spatial expectation of $b_r(x_i)$
$\xi_{(r)}$	radiation coefficient	$\boldsymbol{T}$	nodal temperature vector
σ	Stefan–Boltzmann constant	$\mathbf{K}$	heat conductivity matrix
$T_{(r)}$	temperature of external radiation source	$\mathbf{C}$	specific heat matrix
V	radiation view factor	$\boldsymbol{Q}$	thermal load vector

ditions on the phase change temperature interval need be satisfied.

2. Heat flow equation

The governing equation of heat transfer in a thermally anisotropic 3D region Ω can be written in a differential form as follows ($i, j = 1, 2, 3$)

$$\left(k_{ij}T_{,j}\right)_{,j} + Q = \frac{\partial H}{\partial \tau} \quad (\boldsymbol{x}, \tau) \in \Omega \times t \tag{1}$$

with the boundary conditions imposed on the boundary surface temperature

$$T = \hat{T} \quad (\boldsymbol{x}, \tau) \in \partial\Omega_T \times t \tag{2}$$

and the boundary surface heat flux

$$-k_{ij}n_jT_{,i} = \hat{q} \quad (\boldsymbol{x}, \tau) \in \partial\Omega_q \times t \tag{3}$$

and the initial condition imposed on the initial temperature distribution

$$T_0 = \hat{T}_0 \quad (\boldsymbol{x}, \tau) \in \Omega \times \{0\} \tag{4}$$

where

- T is the temperature
- k_{ij} is the thermal conductivity tensor
- Q is the rate of heat generated per unit volume
- H is the enthalpy
- $\boldsymbol{x}$ is the position vector which identifies materials particles in the domain Ω
- t denotes the time domain
- $\hat{T}$ is the temperature acting on the boundary surface $\partial\Omega_T$
- $\hat{q}$ is the heat flux on the complementary boundary surface $\partial\Omega_q$
- n_i is the unit outward-drawn vector normal to $\partial\Omega$
- $\hat{T}_0$ is the initial temperature

and for any function g, the notation $g_{,i}$ stands for the partial differentiation of g with respect to the spatial coordinate x_i.

The Fourier's constitutive relation reads

$$q_i = -k_{ij}T_{,j} \tag{5}$$

q_i being the heat flux vector

Eq. (3) may be specified to include convection boundary conditions on a part $\partial\Omega q^{(1)}$ of $\partial\Omega q$

$$-k_{ij}n_jT_{,i} = \xi_{(c)}(T - T_\infty) \quad (\boldsymbol{x}, \tau) \in \partial\Omega q^{(1)} \times t \tag{6}$$

where $\xi_{(c)}$ is convection coefficient, and radiation boundary conditions on a part $\partial\Omega q^{(2)}$ of $\partial\Omega q$

$$-k_{ij}n_jT_{,i} = \xi_{(r)}\left(T^n - T^n_{(r)}\right) = \chi\left(T - T_{(r)}\right) \tag{7}$$

in which the coefficient $\xi_{(r)}$ is computed as

$$\xi_{(r)} = \sigma V\left(\frac{1}{\epsilon} + \frac{1}{\epsilon_{(r)}} - 1\right)^{-1} \tag{8}$$

and

$$\chi = \xi_{(r)}\left(T^2 + T^2_{(r)}\right)\left(T + T_{(r)}\right) \tag{9}$$

where σ is the Stefan–Boltzmann constant, $T_{(r)}$ is the temperature of known external radiation source, V is the radiation view factor, ϵ is the surface emissivity, and $\epsilon_{(r)}$ the emissivity of the radiation source.

Looking for an approximate temperature solution to the above initial-boundary value problem we usually form the residuals

$$r_1 = -\left(k_{ij}T_{,j}\right)_{,i} - Q + \frac{\partial H}{\partial \tau} \tag{10}$$

$$r_2 = \hat{q} + k_{ij}n_jT_{,i} \tag{11}$$

and then solve the problems (1)–(4) by determining the square integrable temperature field T satisfying the temperature boundary condition and zeroing the following weighted residual

$$R = \int_\Omega r_1\phi\,\mathrm{d}\Omega + \int_{\partial\Omega q} r_2\phi\,\mathrm{d}(\partial\Omega) = 0 \tag{12}$$

for all square integrable weighting functions $\phi(\boldsymbol{x})$ that vanish on $\partial\Omega_T$. The residual (12) can be transformed as follows

$$R = \int_\Omega\left[-\left(k_{ij}T_{,j}\right)_{,i}\phi + \left(\frac{\partial H}{\partial\tau} - Q\right)\phi\right]\mathrm{d}\Omega + \int_{\partial\Omega q}\left(\hat{q} + k_{ij}n_jT_{,j}\right)\phi\,\mathrm{d}(\partial\Omega)$$

$$= -\int_{\partial\Omega q} k_{ij}n_jT_{,i}\phi\,\mathrm{d}(\partial\Omega) + \int_\Omega\left[k_{ij}T_{,j}\phi_{,i} + \left(\frac{\partial H}{\partial\tau} - Q\right)\phi\right]\mathrm{d}\Omega + \int_{\partial\Omega q}\left(\hat{q} + k_{ij}n_jT_{,i}\right)\phi\,\mathrm{d}(\partial\Omega)$$

$$= \int_\Omega\left[k_{ij}T_{,j}\phi_{,i} + \left(\frac{\partial H}{\partial\tau} - Q\right)\phi\right]\mathrm{d}\Omega + \int_{\partial\Omega q}\hat{q}\phi\,\mathrm{d}(\partial\Omega) = 0 \tag{13}$$

The derivative of H with respect to time τ is given as

$$\frac{\partial H}{\partial\tau} = \left(\tilde{c} + s\frac{\partial L}{\partial T}\right)\frac{\partial T}{\partial\tau} \tag{14}$$

where $\tilde{c} = c\cdot\rho$, c is the specific heat of material, ρ is the density of material, L is the latent heat, and

$$s = \begin{cases} 1 & \text{for } T \in [T_\mathrm{s}, T_\mathrm{l}] \\ 0 & \text{for } T \in R - [T_\mathrm{s}, T_\mathrm{l}] \end{cases} \tag{15}$$

where T_s is the solidus temperature and T_l is the liquidus temperature.

By Eq. (14) we have

$$\frac{\partial H}{\partial\tau} = \tilde{c}\frac{\partial T}{\partial\tau} + s\frac{\partial L}{\partial T}\frac{\partial T}{\partial\tau} = \left(\tilde{c} + s\frac{\partial L}{\partial T}\right)\frac{\partial T}{\partial\tau} \tag{16}$$

We can also rewrite the above equation in the alternative manner which is applicable in the paper of Morgan et al.

$$\frac{\partial H}{\partial\tau} = \left\{\tilde{c} + \frac{\left[\eta(T-T_\mathrm{s}) - \eta(T-T_\mathrm{l})\right]L}{\Delta T}\right\}\frac{\partial T}{\partial\tau} \tag{17}$$

where η denotes the Heaviside function

$$\eta(\tau - a) = \begin{cases} 1 & (\tau > a) \\ 0 & (\tau \le a) \end{cases} \tag{18}$$

and $\Delta T = T_\mathrm{l} - T_\mathrm{s}$ is the phase change interval.

We rewrite Eq. (17) as

$$\frac{\partial H}{\partial\tau} = \left(\tilde{c} + \hat{S}L\right)\frac{\partial T}{\partial\tau} \tag{19}$$

where

$$\hat{S} = \hat{S}(T, T_\mathrm{s}, T_\mathrm{l}) = \frac{\left[\eta(T-T_\mathrm{s}) - \eta(T-T_\mathrm{l})\right]}{\Delta T} \tag{20}$$

The residual R in Eq. (13) takes the form

$$R = \int_\Omega\left\{k_{ij}T_{,j}\phi_{,i} + \left[\left(\tilde{c} + sL_{,T}\right)\frac{\partial T}{\partial\tau} - Q\right]\phi\right\}\mathrm{d}\Omega + \int_{\partial\Omega q}\hat{q}\phi\,\mathrm{d}(\partial\Omega) = 0 \tag{21}$$

At any given time instant τ, Eq. (21) is clearly nonlinear in T. To solve the equation for T we may use the iterative technique of Newton–Raphson which is based on zeroing the 'next' kth residual written as

$$R^{(k)} \cong R^{(k-1)} + R_T^{(k-1)} * \delta T^{(k)} = 0 \tag{22}$$

in which $R^{(k-1)} = R^{(k-1)}(T(\boldsymbol{x}, \tau,), \boldsymbol{x}, \tau,)$ corresponds to the 'last' $(k-1)$th approximation to the temperature field $T = T^{(k-1)}$ assumed known, $\delta T^{(k)}$ is the iterative correction to be determined from Eq. (22) such that

$$T^{(k)} = T^{(k-1)} + \delta T^{(k)} \tag{23}$$

and $R_T^{(k-1)} = \mathrm{d}R^{(k-1)}/\mathrm{d}T$ is the $(k-1)$th tangent operator defined by

$$R_T = \int_\Omega\left[\frac{\partial k_{ij}}{\partial T}T_{,j}\phi_{,i} + k_{ij}\phi_{,i}\frac{\partial}{\partial x_j} + \phi\left(\tilde{c}\frac{\partial}{\partial\tau} + \frac{\partial\tilde{c}}{\partial T}\frac{\partial T}{\partial\tau} + s\frac{\partial^2 L}{\partial T^2} - \frac{\partial Q}{\partial T_{,i}}\frac{\partial}{\partial x_i}\right)\right]\mathrm{d}\Omega + \int_{\partial\Omega_q}\phi\frac{\partial\hat{q}}{\partial T}\,\mathrm{d}(\partial\Omega) \tag{24}$$

The notation $R_T * \delta T$ should be clear from the context with $*$ indicating that δT multiplies the appropriate integrand rather than the whole integrand expression that defines R_T. The operator R_T depends nonlinearly on T, linearly on ϕ and acts linearly on δT; we shall use the notation

$$R_T[T;\phi] * \delta T = \hat{R}_T[T;\phi;\delta T] = \int_\Omega \left[\frac{\partial k_{ij}}{\partial T} T_{,j}\phi_{,i}\delta T + k_{ij}\phi_{,i}\delta T_{,j} + \phi\left(\tilde{c}\frac{\partial \delta T}{\partial \tau} + \frac{\partial \tilde{c}}{\partial T}\frac{\partial T}{\partial \tau}\partial T + s\frac{\partial^2 L}{\partial T^2} - \frac{\partial Q}{\partial T}\delta T - \frac{\partial Q}{\partial T_{,i}}\partial T_{,i} \right) \right] \mathrm{d}\Omega + \int_{\partial\Omega_q} \phi \frac{\partial \hat{q}}{\partial T}\delta T\, \mathrm{d}(\partial\Omega) \tag{25}$$

The iterative procedure can be seen more clearly for a time-discretized formulation in which we assume that:

(a) solution up to a typical time instant t has been obtained,
(b) solution $T_{t+\Delta t}$ at time $t+\Delta t$ is looked for,
(c) a finite difference scheme in time such as the one-step backward Euler scheme is employed so that

$$\dot{T}_{t+\Delta t} = \frac{1}{\Delta t}(T_{t+\Delta t} - T_t) \tag{26}$$

and consequently

$$\dot{T}^{(k)}_{t+\Delta t} = \frac{1}{\Delta t}\left(T^{(k)}_{t+\Delta t} - T_t\right),$$

$$\delta T^{(k)} = \delta T^{(k)}_{t+\Delta t} = \Delta t \delta \dot{T}^{(k)}_{t+\Delta t},$$

$$\frac{\partial}{\partial \tau}\delta T^{(k)} = \frac{\partial}{\partial \tau}\delta T^{(k)}_{t+\Delta t} = \frac{1}{\Delta t}\delta T^{(k)}_{t+\Delta t} = \frac{1}{\Delta t}\delta T^{(k)}.$$

Eq. (25) at $\tau = t+\Delta t$ becomes

$$R_T^{(k-1)}[T;\phi] * \delta T^{(k)} = \int_\Omega \left[\frac{\partial k_{ij}^{(k-1)}}{\partial T} T_{,j}^{(k-1)}\phi_{,i} + k_{ij}^{(k-1)}\phi_{,i}\frac{\partial}{\partial x_j} + \phi\left(\tilde{c}^{k-1}\frac{1}{\Delta t} + \frac{\partial \tilde{c}^{k-1}}{\partial T}\frac{1}{\Delta t}\left(T^{(k-1)} - T_t\right) + \frac{\partial^2 L}{S\partial T^2} - \frac{\partial Q}{\partial T} - \frac{\partial Q}{\partial T_{,i}}\frac{\partial}{\partial x_i} \right) \right] \delta T^{(k)}\, \mathrm{d}\Omega + \int_{\partial\Omega_q} \phi\frac{\partial \hat{q}}{\partial T}\delta T^{(k)}\, \mathrm{d}(\partial\Omega) \tag{27}$$

where all the functions (except for T_t!) are understood to be computed at time $t+\Delta t$ and the temperature value $T^{(k-1)}_{t+\Delta t}$. The operator equation (22) with the term $R_T^{(k-1)}\delta T^{(k)}$ given as Eq. (27) can be solved for $\delta T^{(k)}$ by any of the known techniques in use for solving partial differential equations (PDEs) with respect to space variables. It should be noted in this context that even though the operator R in Eq. (21) generates the symmetric finite element 'secant' stiffness matrix (dependent on T), the spatial discretization applied to Eq. (22) with (27) results in a non-symmetric tangent stiffness matrix which may unfavorably influence the efficiency of the solution procedure typically based on symmetric linear equations solvers. Therefore, different symmetric approximations to the non-symmetric tangent stiffness are used in practice with the non-symmetry effects accounted for in an iterative fashion.

3. Formulation of the problem

Let us denote by $\boldsymbol{b} = b_r = (b_1, \ldots, b_R)$ any random variable vector. The second-moment-second-order-perturbation methodology (see Refs. [5,6,9]) involves expanding in the power series in all the functions of the random variables $b_r(x_i)$ included in Eq. (13), i.e. temperature $T(b_r)$, latent heat $L(b_r)$, thermal conductivity $k_{ij}((b_r), T(b_r))$, material density $\rho((b_r); T(b_r))$, specific heat capacity $c((b_r); T(b_r))$, rate of heat generated per unit volume $Q(b_r)$ and boundary heat flow $\hat{q}((b_r), T(b_r))$ about the spatial expectations of $b_r(x_i)$, i.e. about $b_r^0 = b_r^0(x_i)$ and retaining up to the second-order terms. These expansion are expressed symbolically as

$$(\cdot) = (\cdot)^0 + \gamma(\cdot)^{;r}\Delta b_r + \frac{1}{2}\gamma^2(\cdot)^{;rs}\Delta b_r \Delta b_s \tag{28}$$

where

$$\gamma \Delta b_r = \delta b_r = \gamma\left(b_r - b_r^0\right) \tag{29}$$

is the first variation of b_r about b_r^0, and

$$\gamma^2 \Delta b_r \Delta b_s = \delta b_r \delta b_s = \gamma^2\left(b_r - b_r^0\right)\left(b_s - b_s^0\right) \tag{30}$$

is the mixed variation of b_r and b_s about b_r^0 and b_s^0 and γ is a small parameter. The symbol $(\cdot)^0$ denotes the value of the functions taken at the expectations b_r^0, while $(\cdot)^{;r}$ and $(\cdot)^{;rs}$, respectively, represent the first and second total derivatives with respect to b_r evaluated at b_r^0. The expansion (28) is now substituted into the principle (13). By equating the same order terms in the resulting expression, we obtain the hierarchical PDE system for the stochastic version of the transient virtual temperature principle as follows:

Zeroth-order

$$\int_{\Omega}\left(\tilde{c}^0 + sL^0_{,T}\dot{T}^0\phi + \chi^0_{ij}T^0_{,j}\phi_{,i}\right)\,\mathrm{d}\Omega = \int_{\Omega}\phi Q^0\,\mathrm{d}\Omega + \int_{\partial\Omega_q}\phi\hat{q}^0\,\mathrm{d}(\partial\Omega) \tag{31}$$

First-order

$$\int_{\Omega}\left(\tilde{c}^0 + sL^0_{,T}\dot{T}^{:r}\phi + \chi^0_{ij}T^{r}_{,j}\phi_{,i}\right)\,\mathrm{d}\Omega = \int_{\Omega}\phi Q^{:r}\,\mathrm{d}\Omega + \int_{\partial\Omega_q}\phi\hat{q}^{:r}\,\mathrm{d}(\partial\Omega) - \int_{\Omega}\left[\left(c^{:r} + sL^{:r}_{,T}\right)\dot{T}^0\phi + \chi^{:r}_{ij}T^{:r}_{ij}\phi_{,i}\right]\mathrm{d}\Omega \tag{32}$$

Second order

$$\int_{\Omega}\left(\tilde{c}^0 + sL^0_{,T}\dot{T}^{(2)}\phi + \chi^0_{ij}T^{(2)}_{,j}\phi_{,i}\right)\,\mathrm{d}\Omega = \int_{\Omega}\phi Q^{(2)}\,\mathrm{d}\Omega + \int_{\partial\Omega_q}\phi\hat{q}^{(2)}\,\mathrm{d}(\partial\Omega) - \int_{\Omega}\left[\left(c^{:rs} + sL^{:rs}_{,T}\right)\dot{T}^0 + \left(c^{:r} + sL^{r}_{,T}\right)\dot{T}^{:s}\right]S^{rs}\phi\,\mathrm{d}\Omega - \int_{\Omega}\left(\chi^{:rs}_{ij}T^0_{,j} + 2\chi^{:r}_{ij}T^{:s}_{,j}\right)S^{rs}\phi_{,i}\,\mathrm{d}\Omega \tag{33}$$

where $(\cdot)^{(2)}$ denotes the double sum $(\cdot)^{:rs}S^{rs}$, $r,\ s = 1, 2, \ldots, R$. The first two probabilistic moments for the random variable field $b_r = (b_1, \ldots, b_R)$ are defined as

$$E(b_r) \equiv b^0_r = \int_{-\infty}^{+\infty} b_r f(b_r)\,\mathrm{d}b_r \tag{34}$$

$$\mathrm{Cov}(b_r, b_s) = S^{rs} \quad \text{(no sum on } R\text{)}$$

$$= \int_{-\infty}^{+\infty}\left[b_r - b^0_r\right]\left[b_s - b^0_s\right] f(\boldsymbol{b})\,\mathrm{d}\boldsymbol{b} \tag{35}$$

The definition $(35)_2$ corresponds to

$$S^{rs} = \alpha_r\alpha_s b^0_r b^0_s \mu_{rs} \tag{36}$$

with

$$\alpha_r = \left[\frac{\mathrm{Var}(b_r)}{\left(b^0_r\right)^2}\right]^{1/2} \qquad \mu_{rs} = \int_{-\infty}^{+\infty} b_r b_s f(\boldsymbol{b})\,\mathrm{d}\boldsymbol{b} \tag{37}$$

where $E[b_r]$, $\mathrm{Cov}(b_r, b_s)$, $\mathrm{Var}(b_r)$, μ_{rs}, α_r and $f(b_r) = f(b_1,\ b_2, \ldots,\ b_R)$ are the spatial expectations, covariances, variances, correlation functions, coefficients of variation and R-variate probability density function, respectively.

Having solved the equation system (31)–(33) for the functions T^0, $T^{:r}$, $T^{(2)}$ the probabilistic distributions of the random temperature field $T(b_r(x_i),\ x_i,\ \tau)$ may, for a given γ, be computed from its power expansion using the definition of the first two probabilistic moments. (Setting $\gamma = 0$ yields the deterministic solution.) The solution can be obtained by setting $\gamma = 1$ which, of course, stipulates that the fluctuation of the random field variables b_r is small. Thus, by substituting the expanded equation (cf. Eq. (28))

$$T = T^0 + T^{:r}\Delta b_r + \frac{1}{2}T^{:rs}\Delta b_r\Delta b_s \tag{38}$$

into the definition of the first probabilistic moment

$$E\left[T(x_i, \tau)\right] = \int_{-\infty}^{+\infty} T(x_i, \tau) f(\boldsymbol{b})\,\mathrm{d}\boldsymbol{b} \tag{39}$$

the second-order accurate expectation for the random temperature field is written as

$$E\left[T(x_i, \tau)\right] = T^0(x_i, \tau) + \frac{1}{2}T^{(2)}(x_i, \tau) \tag{40}$$

since (cf. Eqs. (28) and (35))

$$E\left[T(b_r)\right] = \int_{-\infty}^{+\infty}\left[T^0\left(b^0_r\right) + T^{:s}\left(b^0_r\right)\Delta b_s + \frac{1}{2}T^{:st}\left(b^0_r\right)\Delta b_s\Delta b_t\right] f(\boldsymbol{b})\,\mathrm{d}\boldsymbol{b}$$

$$= T^0 \times 1 + T^{:r} \times 0 + \frac{1}{2}T^{:rs}S^{rs} = T^0 + \frac{1}{2}T^{(2)} \tag{41}$$

Clearly, if only the first-order accuracy of the temperature estimation is required, then Eq. (40) reduces to

$$E\left[T(x_i)\right] = T^0(x_i) \tag{42}$$

In the framework of the second-moment-second-order-perturbation methodology, the cross-covariances can be estimated with only the first-order accuracy. Introducing the second-order expansion of the random temperature field into the definition

$$\mathrm{Cov}(T^1, T^2) = \int_{-\infty}^{+\infty} [T^1 - E(T^1)][T^2 - E(T^2)] f(\boldsymbol{b})\, \mathrm{d}\boldsymbol{b} \tag{43}$$

we get the cross-covariances for the random temperatures at the spatial coordinates x_i^1, x_j^2 at any time instant τ as

$$\mathrm{Cov}(T^1, T^2) = T^{1,r}\left(x_i^{r,(1)}, \tau\right) T^{2,r}\left(x_j^{s(2)}, \tau\right) S^{rs} = T^{1,r} T^{2,r} S^{rs} \tag{44}$$

Eqs. (40) and (44) holds true for both the transient and the steady heat transfer systems. It is pointed out that in the above formulations the input random parameters b_r defined by Eq. (34) are random variables in space, i.e. uncertainties in b_r are assumed to be time-independent. Although problems with input data being random in space as well as in time are beyond the scope of the current second-moment-second-order-perturbation strategy, it turns out that the first two space-time probabilistic moments for the temperature field $T(b_r\tau)$ can be evaluated.

4. Finite element model

The incremental finite element interpolation is employed

$$T(b_r) = H_\alpha T_\alpha(b_\rho) = \boldsymbol{HT}$$
$$\alpha = 1, 2, \ldots, N,\ \rho = 1, 2, \ldots, \tilde{N},\ r = 1, 2, \ldots, R \tag{45}$$

The power expansions for the functions T, k, $\tilde{c}$, $Q(\tau)$ and $\hat{q}$ about the random variable expectations b_ρ^0 are written symbolically as

$$(\cdot) = (\cdot)^0 + \gamma(\cdot)^{;\rho}\Delta b + \frac{1}{2}\gamma^2(\cdot)^{;\rho\sigma}\Delta b_\rho \Delta b_\sigma \tag{46}$$

where, as before (cf. Eq. (28))

$$\gamma\Delta b_\rho = \delta b_\rho = \gamma\left(b_\rho - b_\rho^0\right) \tag{47}$$

is the first variation of b_ρ about b_ρ^0, and

$$T(b_r) = H_\alpha T_\alpha(b_\rho) = \boldsymbol{HT}$$

$$\gamma^2\Delta b_\rho \Delta b_\sigma = \delta b_\rho \delta b_\sigma = \gamma^2\left(b_\rho - b_\rho^0\right)\left(b_\sigma - b_\sigma^0\right) \tag{48}$$

is the mixed variation of b_ρ and b_σ about b_ρ^0 while $(\cdot)^0$, $(\cdot)^{;\rho}$ and $(\cdot)^{;\rho\sigma}$ are functions of the zeroth, first and second total derivatives with respect to b_ρ, respectively; the functions are evaluated at b_ρ^0.

Moreover, we assume

$$\hat{S}(T(b_r), T_s(b_r), T_l(b_r)) = \hat{S}\left(T^0, T_s^0, T_l^0\right) = \hat{S}^0 \tag{49}$$

By introducing the finite element approximations (45) and (46) into the zeroth-, first- and second-order variational statements (31)–(33) and using the arbitrariness of δT in Ω, we arrive at the following hierarchical ordinary differential equation system governing the transient heat transfer process:

Zeroth-order (γ^0) term

$$\mathbf{C}^0\dot{\boldsymbol{T}}^0 + \mathbf{K}^0\boldsymbol{T}^0 = \boldsymbol{Q}^0 \tag{50}$$

First-order (γ^1) terms

$$\mathbf{C}^0\dot{\boldsymbol{T}}^{,\rho} + \mathbf{K}^0\dot{\boldsymbol{T}}^{,\rho} = \boldsymbol{Q}^{,\rho} - \left(\mathbf{C}^{,\rho}\dot{\boldsymbol{T}}^0 + \mathbf{K}^{,\rho}\dot{\boldsymbol{T}}^0\right) \tag{51}$$

Second-order (γ^2) term

$$\mathbf{C}^0\dot{\boldsymbol{T}}^{(2)} + \mathbf{K}^0\boldsymbol{T}^{(2)} = \left[\boldsymbol{Q}^{,\rho\sigma} - 2\left(\mathbf{C}^{,\rho}\dot{\boldsymbol{T}}^{,\sigma} + \mathbf{K}^{,\rho}\boldsymbol{T}^{,\sigma}\right) - \left(\mathbf{C}^{,\rho\sigma}\dot{\boldsymbol{T}}^0 + \mathbf{K}^{,\rho\sigma}\boldsymbol{T}^0\right)\right]S^{\rho\sigma} \tag{52}$$

$b_\rho^0 = E[b_\rho]$ denotes the expectations of the random variable vector b_ρ, $S^{\rho\sigma} = \mathrm{Cov}(b_\rho, b_\sigma)$ is the covariance matrix for the entries of the vector b_ρ, while the vector of the second-order nodal temperatures is defined as

$$\boldsymbol{T}^{(2)}\left(\boldsymbol{b}^0\right) = \boldsymbol{T}^{,\rho\sigma}\left(\boldsymbol{b}^0\right)S^{\rho\sigma} \tag{53}$$

The right-hand side of Eq. (54) results from the relationship (cf. Eqs. (34) and (46))

$$T_{,i}^{(2)} = T_{,i}^{;rs}S^{rs} = \boldsymbol{H}_{,i}\boldsymbol{T}^{;\rho\sigma}S^{\rho\sigma} = \boldsymbol{H}_{,i}\boldsymbol{T}^{(2)} \tag{54}$$

In Eqs. (51)–(53), the zeroth-order heat capacity matrix $\mathbf{C}^0$, heat conductivity matrix $\mathbf{K}^0$, right-hand vector $\boldsymbol{Q}^0$ and first and second derivatives of $\mathbf{C}$, $\mathbf{K}$ and $\boldsymbol{Q}$ with respect to the random variables $\boldsymbol{b}$ are expressed as follows:

Zeroth-order functions

$$\mathbf{C}^0 = \int_\Omega \left(c^0 + \hat{S}^0 L^0\right)\boldsymbol{HH}\, \mathrm{d}\Omega$$

$$\mathbf{K}^0 = \int_\Omega k_{ij}^0 \boldsymbol{H}_{,i}\boldsymbol{H}_{,j}\, \mathrm{d}\Omega$$

$$\boldsymbol{Q}^0 = \int_\Omega Q^0 \boldsymbol{H}\, \mathrm{d}\Omega + \int_{\partial\Omega_q} \hat{q}^0 \boldsymbol{H}\, \mathrm{d}(\partial\Omega) \tag{55}$$

First derivatives

$$\mathbf{C}^{,\rho} = \int_\Omega \left(c^{,\rho} + \hat{S}^0 L^{\rho}\right) \boldsymbol{HH}\, \mathrm{d}\Omega$$

$$\mathbf{K}^{,\rho} = \int_\Omega k_{ij}^{,\rho} \boldsymbol{H}_{,i} \boldsymbol{H}_{,j}\, \mathrm{d}\Omega$$

$$\boldsymbol{Q}^{,\rho} = \int_\Omega Q^{,\rho} \boldsymbol{H}\, \mathrm{d}\Omega + \int_{\partial\Omega_q} \hat{q}^{,\rho} \boldsymbol{H}\, \mathrm{d}(\partial\Omega) \tag{56}$$

Second derivatives

$$\mathbf{C}^{,\rho\sigma} = \int_\Omega \left(c^{,\rho\sigma} + \hat{S}^0 L^{,\rho\sigma}\right) \boldsymbol{HH}\, \mathrm{d}\Omega$$

$$\mathbf{K}^{,\rho\sigma} = \int_\Omega k_{ij}^{,\rho\sigma} \boldsymbol{H}_{,i} \boldsymbol{H}_{,j}\, \mathrm{d}\Omega$$

$$Q^{,\rho\sigma} = \int_\Omega Q^{,\rho\sigma} \boldsymbol{H}\, \mathrm{d}\Omega + \int_{\partial\Omega_q} \hat{q}^{,\rho\sigma} \boldsymbol{H}\, \mathrm{d}(\partial\Omega) \tag{57}$$

All expressions evaluated at the expectations $\boldsymbol{b}^0$. Recalling the notation

$$(\,\cdot\,)^{,\rho} = \left.\frac{\mathrm{d}(\,\cdot\,)}{\mathrm{d}\boldsymbol{b}}\right|_{\boldsymbol{b}=\boldsymbol{b}^0} \qquad (\,\cdot\,)^{,\rho\sigma} = \left.\frac{\mathrm{d}^2(\,\cdot\,)}{\mathrm{d}b_\rho \mathrm{d}b_\sigma}\right|_{b_\rho=b_\rho^0;\ b_\sigma=b_\sigma^0} \tag{58}$$

the following differential operators are employed for **C** and **K**

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{b}} = \frac{\partial}{\partial \boldsymbol{b}} + \frac{\partial}{\partial \boldsymbol{T}} \frac{d\boldsymbol{T}}{d\boldsymbol{b}}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}b_\rho \mathrm{d}b_\sigma} = \frac{\partial^2}{\partial b_\rho \partial b_\sigma} + \frac{\partial^2}{\partial b_\rho \partial T_\alpha} \frac{\mathrm{d}T_\alpha}{\mathrm{d}b_\sigma} + \frac{\partial^2}{\partial b_\sigma \partial T_\alpha} \frac{\mathrm{d}T_\alpha}{\mathrm{d}b_\rho} + \frac{\partial^2}{\partial T_\alpha \partial T_\beta} \frac{\mathrm{d}T_\alpha}{\mathrm{d}b_\rho} \frac{\mathrm{d}T_\beta}{\mathrm{d}b_\sigma} + \frac{\partial}{\partial T_\alpha} \frac{\mathrm{d}^2 T_\alpha}{\mathrm{d}b_\rho \mathrm{d}b_\sigma} \tag{59}$$

Similarly, as for the continuous system the zeroth-order nodal temperatures $\boldsymbol{T}^0$ are to be solved iteratively.

We rewrite Eq. (49) in the residual form as

$$\boldsymbol{R}(\boldsymbol{T}) = \mathbf{C}^0 \dot{\boldsymbol{T}}^0 + \mathbf{K}^0 \boldsymbol{T}^0 - \boldsymbol{Q}^0 = 0 \tag{60}$$

The nodal random temperature field can now be expressed as (cf. Eq. (45))

$$\boldsymbol{T} = \boldsymbol{T}^0 + \boldsymbol{T}^{,\rho} \Delta b_\rho + \frac{1}{2} \boldsymbol{T}^{,\rho\sigma} \Delta b_\rho \Delta b_\sigma \tag{61}$$

By the definition of the expectations for any nodal temperatures $\boldsymbol{T}(\tau)$ at any time instant and cross-covariances for $\boldsymbol{T}(t_1)$ and $\boldsymbol{T}(t_2)$ we have, respectively (cf. Eqs. (36) and (42))

$$E(\boldsymbol{T}) = \int_{-\infty}^{+\infty} \boldsymbol{T} f(\boldsymbol{b})\, \mathrm{d}\boldsymbol{b}$$

$$\mathrm{Cov}\big(\boldsymbol{T}(t_1), \boldsymbol{T}(t_2)\big) = \int_{-\infty}^{+\infty} \big\{\boldsymbol{T}(t_1) - E\big[\boldsymbol{T}(t_1)\big]\big\}\big\{\boldsymbol{T}(t_2) - E\big[\boldsymbol{T}(t_2)\big]\big\} f(\boldsymbol{b})\, \mathrm{d}\boldsymbol{b} \tag{62}$$

in which $f(\boldsymbol{b})$ is the probability density (nodal) function. Similar relationships hold for the nodal temperature velocities $\dot{\boldsymbol{T}}$.

Introducing Eq. (61) into (62), observing in the resulting equation that the terms involving the first variation of Δb_ρ vanish (cf. Eq. (39)), and using Eq. (53) yields the second-order accurate spatial expectations for the nodal temperatures at any time instant as

$$E[\boldsymbol{T}] = \boldsymbol{T}^0 + \frac{1}{2} \boldsymbol{T}^{(2)} \tag{63}$$

and the first-order accurate space-time cross-covariances as

$$\mathrm{Cov}\big[\boldsymbol{T}(t_1), \boldsymbol{T}(t_2)\big] = \boldsymbol{T}^{,\rho}(t_1) \boldsymbol{T}^{,\sigma}(t_2) S^{\rho\sigma} \tag{64}$$

5. Solution procedure

The problem considered can be solved using the method of solution proposed by Comini et al. [10] and Morgan et al. [11]. In our example, we use the method proposed by Rolph and Bathe [14].

The essence of the procedure is to construct the latent heat flow vector using the enthalpy the system. The enthalpy for any time step $n+1$ (i.e. time $t+\Delta t$) can be written in an alternating manner as

$$H = \int_\Omega \left(\int_0^{t+\Delta t} \tilde{c} \dot{T}\, \mathrm{d}\tau + s \int_0^{t+\Delta t} \dot{L}\, \mathrm{d}\tau \right) \mathrm{d}\Omega \tag{65}$$

Typical relationships between the enthalpy and temperature are shown schematically in Fig. 1. The flow due to latent heat (index l) at node k at time step $n+1$ is denoted by $Q_{l,k}^{(k-1)}$ and by $T_k^{(i)}$ is the i the approximation of the total temperature increment at node k

and $Q^{*}_{l,k}$ is $L/\Delta t$ integrated over the contributory nodal volume. Consider Euler backward integration scheme. At the beginning of each time step $i = 1$, ${}^{n+1}Q^{(0)}_{l,k} = 0$.

For pure substances ($\Delta T_f = 0$), T_f is phase change temperature (Fig. 2), if temperature is outside phase change

$$ {}^{n}T_k < T_f \quad \text{and} \quad {}^{n+1}T^{(i)}_k < T_f \tag{66}$$

or

$$ {}^{n}T_k > T_f \quad \text{and} \quad {}^{n+1}T^{(i)}_k > T_f \tag{67}$$

then

$$\bar{T}^{(i)}_k = T^{(i)}_k$$

$$\Delta Q^{(i)}_{l,k} = 0 \tag{68}$$

If temperature passes through phase change temperature ${}^{n}T_k = T_f$ or

$$ {}^{n}T_k < T_f \quad \text{and} \quad {}^{n+1}T^{(i)}_k \geq T_f \quad \text{or} \quad {}^{n}T_k > T_f \quad \text{and}$$

$$ {}^{t+\Delta t}T^{(i)}_k \leq T_f$$

then

$$\bar{T}^{(i)}_k = T_f - {}^{n}T_k \tag{69}$$

$$\Delta Q^{(i)}_{l,k} = -\int_{\Omega_k} \frac{1}{\Delta t} \bar{c}^{n+1} \left(T^{(i)}_k - \bar{T}^{(i)}_k \right) d\Omega \tag{70}$$

$$\sum \Delta Q^{(i)}_{l,k} = \pm Q^{*}_{l,k} \tag{71}$$

where '+' is for solidification, and '−' for melting.

$$ {}^{n+1}T^{(i)}_k = {}^{n}T_k + \bar{T}^{(i)}_k \tag{72}$$

$$ {}^{n+1}Q^{(i)}_{l,k} = {}^{t+\Delta t}Q^{(i-1)}_{l,k} + \Delta Q^{(i)}_{l,k} \tag{73}$$

If $\Delta T_f > 0$ and temperature is outside phase change temperature interval

$$\begin{gathered} {}^{n}T_k < T_f \quad \text{and} \quad {}^{n+1}T^{(i)}_k < T_f \quad \text{or} \\ {}^{n}T_k > T_f + \Delta T_f \quad \text{and} \quad {}^{n+1}T^{(i)}_k > T_f + \Delta T_f \end{gathered} \tag{74}$$

then

$$\bar{T}^{(i)}_k = T^{(i)}_k$$

$$\Delta Q^{(i)}_{l,k} = 0 \tag{75}$$

If temperature passes through phase change temperature interval

$$T_f \leq {}^{n}T_k \leq T_f + \Delta T_f \tag{76}$$

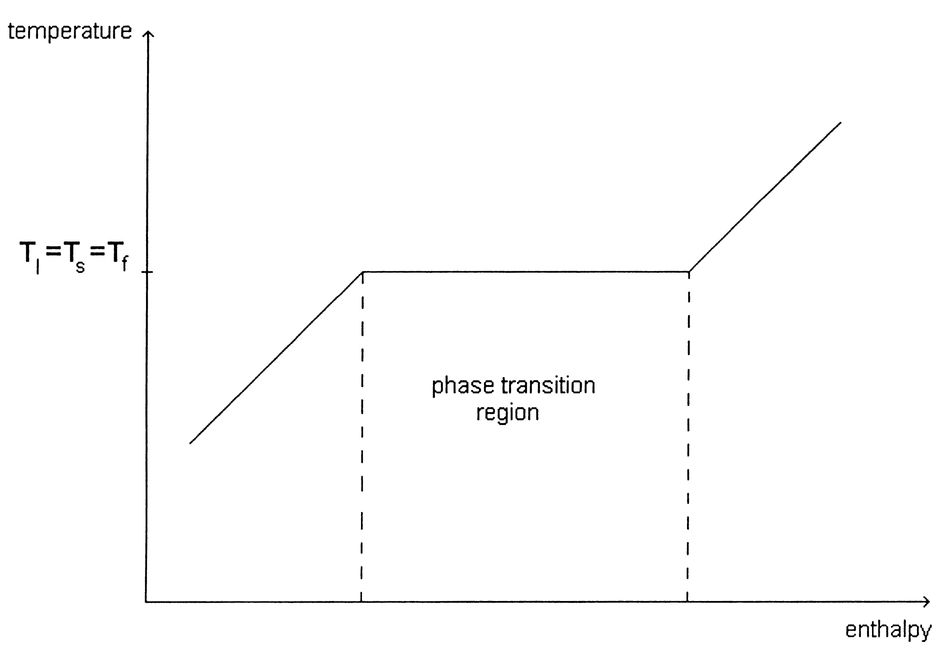

Fig. 1. Relation between enthalpy and temperature ($T_l = T_s = T_f$).

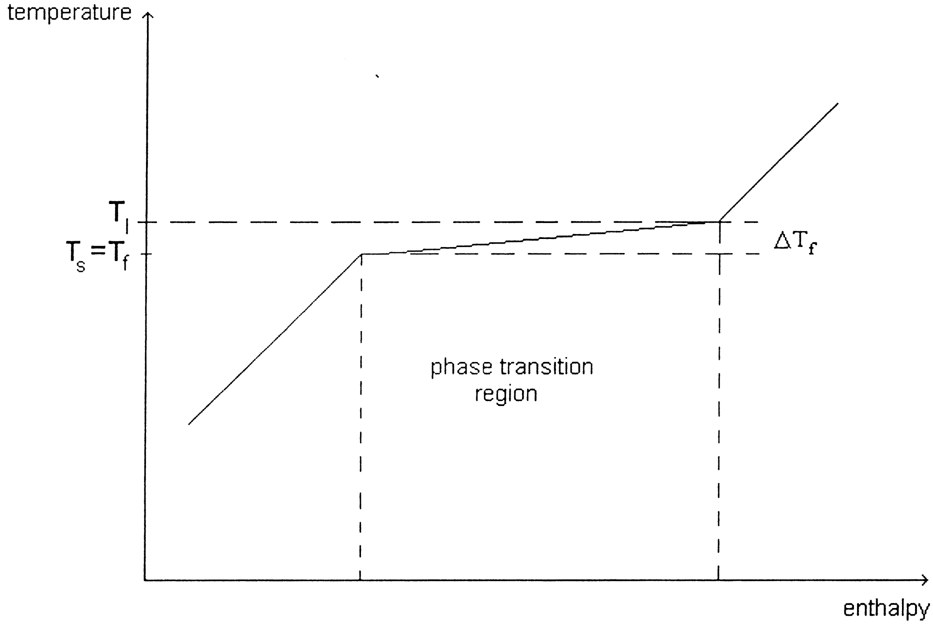

Fig. 2. Relation between enthalpy and temperature ($T_l > T_s$, $\Delta T_f > 0$).

or

$$ {}^{n}T_k < T_f \quad \text{and} \quad {}^{t+\Delta t}T_k^{(i)} \geq T_f \tag{77} $$

or

$$ {}^{n}T_k > T_f + \Delta T_f \quad \text{and} \quad {}^{n+1}T_k^{(i)} \leq T_f + \Delta T_f \tag{78} $$

then

$$ \Delta Q_{l,k}^{(i)} = -\int_{\Omega_k} \frac{1}{\Delta t}\tilde{c}^*\left(T_k^{(i)} - T_f + {}^{t}T_k\right) \mathrm{d}\Omega \tag{79} $$

where

$$ \tilde{c}^* = \frac{1}{(\Delta T_f/L) + \left(1/{}^{n+1}\tilde{c}\right)} \tag{80} $$

$$ \bar{T}_k^{(i)} = T_f - {}^{n}T_k + \left[\frac{\sum \Delta Q_{l,k}^{(i)}}{Q_{l,k}^*}\right]\Delta T_f \tag{81} $$

$$ \sum \Delta Q_{l,k}^{(i)} = \pm Q_{l,k}^* \tag{82} $$

6. Sample analysis

Solidification of a semi-infinite slab of liquid is considered initially at zero temperature (Fig. 3). At time $t = 0$ the temperature of the surface of the liquid is reduced to $-45°F$. The similar deterministic problem was considered earlier by Comini et al. [10], Morgan et al. [11] and Ichikawa and Kikucki [12,13]. The probabilistic data used in computations:

- random material properties:

$$ E(k) = 1.08 $$

$$ E(\tilde{c}) = 1.0 $$

$$ E(L) = 70.26 $$

$$ E(T_f) = -0.1 $$

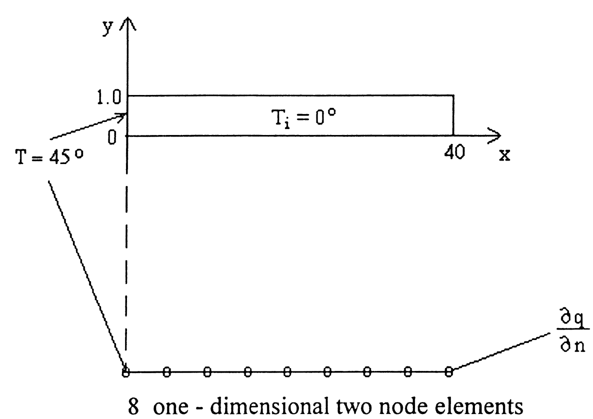

Fig. 3. Finite element model for solidification problem considered.

Table 1
Expectations of temperature and temperature deviations at $x = 1$

Time step	1	2	3	4
Expectation of temperature	−1.23	−11.21	−17.35	−20.01
Standard deviation	0.296	2.842	4.457	5.175

- cross-correlation functions

$$\mu(k^r, k^s) = \exp\left[-\text{abs}(x_i - x_j)/\xi_k\right]$$

$$\mu(\tilde{c}^r, \tilde{c}^s) = \exp\left[-\text{abs}(x_i - x_j)/\xi_{\tilde{c}}\right]$$

$$\mu(L^r, L^s) = \exp\left[-\text{abs}(x_i - x_j)/\xi_L\right]$$

- coefficient of variations

$$\xi_k = \xi_c = \xi_L = 1$$

- correlation lengths

$$\alpha_k^r = \alpha_{\tilde{c}}^r = \alpha_L^r = 0.15$$

Results of the analysis are given in Table 1 where assumed time step is $\Delta t = 1$ s.

7. Concluding remarks

The derivations presented in the paper show that heat flow with phase change in systems with spatially random parameters can be effectively carried out using the stochastic finite element technique.

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