A GENERALIZED FORM OF INTEGRAL-FINITE ELEMENT FORMULATIONS FOR DIFFUSION EQUATION

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Abstract

A physical problem such as diffusion can be described mathematically in two ways, i.e. by Differential Equation Formulation or Integral Formulation. An integral form is derived from its governing differential equation using the method of Variational Principle for a three-dimensional heat flow equation. The equivalent Integral Formulation will be a very useful and an inevitable tool in the formulation of finite element equation.

Introduction

Problems in engineering can be classified as steadystate, transient, and eigenvalue [4]. The field problems such as the transient behavior of heat conduction, saturated-unsaturated porous media flow, solute transport studies, and consolidation are the typical examples of those governed by parabolic type diffusion and diffusion with convection equations. Each of these problems can be described mathematically by differential equation formulation or by its equivalent intergal formulation.

In this paper the time-dependent heat flow problem is considered as an illustration to the derivation of integral and finite element formulation. The remaining types of diffusion problems will then follow in a similar manner.

Governing Diffusion Equation

The basic equation governing the 3-dimensional transient heat flow in solids (Carslaw and Jaeger, 1959) is

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial T}{\partial z}\right) + Q' = \rho c \frac{\partial T}{\partial t} \qquad (1)$$

in which T = temperature, ρ = density, c = specific heat, t = time, Q' = specified heat flux, and K_x, K_y, K_z = thermal conductivities in x, y, and z directions, respectively.

Initial Conditions: For timewise solution, initial conditions on T are required and can be stated as follows

$$T(x,y,z,o) = T_o(x, y, z) \qquad (2a)$$

Boundary Conditions (B.C.): For the heat flow domain shown in Fig. 1, the following general boundary conditions can occur in diffusion problems:

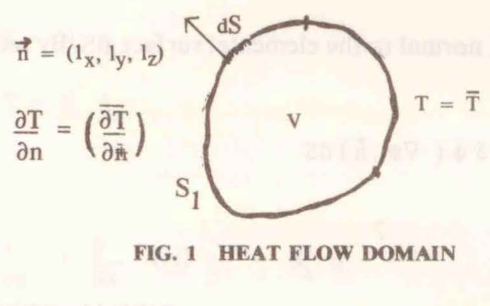

FIG. 1 HEAT FLOW DOMAIN

1. Temperature potential B.C.

$$T = \bar{T} \quad \text{on surface } S_1 \tag{2b}$$

2. Heat flux B.C.

$$\nabla T . \vec{n} = \frac{\partial T}{\partial n} = \overline{\left(\frac{\partial T}{\partial n}\right)} \quad \text{on surface } S_2 \tag{2c}$$

where $\vec{n}$ is the unit outward normal vector to the surface boundary. It represents the direction cosines of 1_x, 1_y, and 1_z and the overbar denotes a prescribed quantity.

Integral Formulation

The finite element equations can be derived by using either a variational principle or residual procedure. For problems with certain mathematical properties such as self-adjointness of heat flow, valid variational principles are available. For certain other problems, it may not be possible to establish a mathematically consistent variational principle. The Galerkin's residual procedure can be used to derive finite element equations for such problems [5].

Variational Principle

The integral equation will be derived from Eq. 1 using the variational principle. For simplicity the material in Eq. 1 is assumed thermodynamically isotropic and homogeneous, i.e., $K_x = K_y = K_z = K$, a constant that gives

$$K \nabla^2 T + Q' = \rho c \frac{\partial T}{\partial t} \tag{3}$$

in which $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ is the Laplacian of T. A quantity δT called "virtual temperature" is introduced which is an arbitrary temperature and has nothing to do with actual temperature T. With δT we construct Eq.3 by the following functional $\delta\pi$:

$$\delta\pi = \iiint_v \frac{\rho c}{K} \left(\frac{\partial T}{\partial t}\right) \delta T \, dv - \iiint_v \nabla^2 T \delta T dv - \iiint_v Q^* \delta T dv = 0 \tag{4}$$

in which $Q^* = \dfrac{Q'}{K}$, $\nabla^2 T = \nabla . \nabla T = \nabla . \left(\dfrac{\partial T}{\partial x} \vec{i} + \dfrac{\partial T}{\partial y} \vec{j} + \dfrac{\partial T}{\partial z} \vec{k} \right)$,

and $\vec{i}$, $\vec{j}$, and $\vec{k}$ are the vectors in x, y, and z directions, respectively.

Divergence Theorem: For the sake of approaching the required formulation we have to convert the second term of the volume integrals in Eq. 4 into surface integral [2]. It is succeeded by applying the divergence theorem of the form

$$\iiint_v \nabla . \vec{q} dv = \iint_S \vec{q} . \vec{n} dS \tag{5a}$$

in which $\vec{q}$, $\vec{n}$ are the heat flux and unit vector normal to the elemental surface dS. By setting $\vec{q} = (\nabla \phi)\, \delta \phi$ the theorem of Eq. 5a is modified to

$$\iiint_v \nabla . (\nabla\phi) \, \delta \phi dv = \iint_S \delta \phi (\nabla\phi . \vec{n}) \, dS \tag{5b}$$

If the LHS of Eq. 5b is expanded we get

$$\iiint_v (\nabla \cdot \nabla\phi)\,\delta\phi dv + \iiint_v \nabla\phi \cdot \nabla(\delta\phi)\,dv = \iint_S \delta\phi\,(\nabla\phi \cdot \vec{n})\,dS \quad (5c)$$

Replacing ϕ with T and equating Eq. 4 and Eq. 5c we obtain

$$\iiint_v \frac{\rho c}{K}\left(\frac{\partial T}{\partial t}\right)\delta T dv + \iiint_v \nabla T \cdot \nabla(\delta T)\,dv$$

$$-\iint_S \delta T\,(\nabla T \cdot \vec{n})\,dS - \iiint_v Q^*\delta T dv = 0$$

$$S = S_1 + S_2 \quad (6)$$

in which $(\nabla T.\vec{n}) = \left(\overline{\frac{\partial T}{\partial n}}\right)$ is the heat flux B.C. Expanding the third term of Eq. 6 into surface S_1 and surface S_2, setting $\delta T = O$ on S_1 where T is given, and apply B.C. $\frac{\partial T}{\partial n} = \left(\overline{\frac{\partial T}{\partial n}}\right)$ on S_2 gives

$$\iiint_v \frac{\rho c}{K}\left(\frac{\partial T}{\partial t}\right)\delta T dv + \iiint_v \nabla T \cdot \nabla(\delta T)\,dv$$

$$-\iiint_v Q^*\delta T dv - \iint_{S_2}\left(\overline{\frac{\partial T}{\partial n}}\right)\delta T dS = 0 \quad (7a)$$

This integral equation implies the heat conduction equation and in an expanded form Eq. 7a is written as

$$\iiint_v \frac{\rho c}{K}\left(\frac{\partial T}{\partial t}\right)\delta T dv + \iiint_v \left(\frac{\partial T}{\partial x}\frac{\partial \delta T}{\partial x} + \frac{\partial T}{\partial y}\frac{\partial \delta T}{\partial y} + \frac{\partial T}{\partial z}\frac{\partial \delta T}{\partial z}\right) dv$$

$$-\iiint_v Q^*\delta T dv - \iint_{S_2}\left(\overline{\frac{\partial T}{\partial n}}\right)\delta T\,dS = 0 \quad (7b)$$

Finite Element Formulation

Eq. 7 governs the integral formulation for transient heat flow through 3 — dimensional media; in fact there are a number of other penomena such as fluid flow in porous rigid media that are also governed by similar equations. The finite element equations can therefore be derived and there are some steps required in this approximations. Only a general element and shape function will be discussed herein, the specific form of discretization of the continuum and selection of certain shape function will depend on the type of problem and the interest of the worker. A more comprehensive discussion of the subject can be found in references [5], [8] and [10].

Element Equations

For each element an approximation function is selected to express the temperature within the element. In i — th element we assume

$$T = \underset{\sim}{N}\,\underset{\sim}{q}_i \quad (8a)$$

$$\dot{T} = \underset{\sim}{N}\,\dot{\underset{\sim}{q}}_i \quad (8b)$$

and

$$\frac{\partial T}{\partial x} = \frac{\partial}{\partial x}(\underset{\sim}{N})\,\underset{\sim}{q}_i = \underset{\sim}{B}_x\,\underset{\sim}{q}_i \quad (9a)$$

$$\frac{\partial T}{\partial y} = \frac{\partial}{\partial y} (\underset{\sim}{N}) \underset{\sim}{q_i} = \underset{\sim}{B_y} \underset{\sim}{q_i} \tag{9b}$$

$$\frac{\partial T}{\partial z} = \frac{\partial}{\partial z} (\underset{\sim}{N}) \underset{\sim}{q_i} = \underset{\sim}{B_z} \underset{\sim}{q_i} \tag{9c}$$

where $\underset{\sim}{N}$ is the shape function and dependent on the space coordinate x, y, and z, $\underset{\sim}{q_i}$ is the vector of nodal temperature, and T and $\dot{\underset{\sim}{q_i}}$ denotes the time derivative of temperature and nodal temperature, respectively. $\underset{\sim}{B_x}$, $\underset{\sim}{B_y}$ and $\underset{\sim}{B_z}$ incorporate the spatial derivatives of the shape function in x, y, and z directions, respectively. Substitution of Eqs. 8 and 9 into Eq. 7 leads to the formation of element heat capacitance matrix ($\underset{\sim}{C}^i$), conductivity matrix ($\underset{\sim}{K}^i$), and nodal heat flux vector ($\underset{\sim}{F}^i$). They are respectively obtained from the 1st. term, 2nd. term, and 3rd. and 4th. terms of Eq. 7 and are described below

$$\iiint_{v_i} \frac{\rho c}{K} \left(\frac{\partial T}{\partial t} \right) \delta T dv = \delta \underset{\sim}{q_i}^T \underset{\sim}{C}^i \dot{\underset{\sim}{q_i}} \tag{10a}$$

$$\iiint_{v_i} \nabla T . \nabla (\delta T) dv = \delta \underset{\sim}{q_i}^T \underset{\sim}{K}^i \underset{\sim}{q_i} \tag{10b}$$

$$\iiint_{v_i} Q^* \delta T dv + \iint_{S_{2_i}} \left(\overline{\frac{\partial T}{\partial n}} \right) \delta T dS = \delta \underset{\sim}{q_i}^T \underset{\sim}{F}^i \tag{10c}$$

where

$$\underset{\sim}{C}^i = \iiint_{v_i} \frac{\rho c}{K} \underset{\sim}{N}^T \underset{\sim}{N} dv \quad \text{(Capacitance Matrix)} \tag{11a}$$

$$\underset{\sim}{K}^i = \iiint_{v_i} (\underset{\sim}{B_x}^T \underset{\sim}{B_x} + \underset{\sim}{B_y}^T \underset{\sim}{B_y} + \underset{\sim}{B_z}^T \underset{\sim}{B_z}) dv \quad \text{(Conductivity Matrix)} \tag{11b}$$

$$\underset{\sim}{F}^i = \iiint_{v_i} \underset{\sim}{N}^T Q^* dv + \iint_{S_{2_i}} \underset{\sim}{L}^T \left(\overline{\frac{\partial T}{\partial n}} \right) dS \quad \text{(Flux Vector)} \tag{11c}$$

in which L represents the boundary function and $\underset{\sim}{L} = \underset{\sim}{N}$ on boundary S_{2_i}. The finite element equation is obtained by combining Eq. 10 and Eq. 11; assemblying the element equation over the whole region of the heat flow problem and assuming B.C. On S_1 has been applied, the following general equation is formed;

$$\underset{\sim}{C}\dot{\underset{\sim}{q}} + \underset{\sim}{K}\underset{\sim}{q} = \underset{\sim}{F} \tag{12}$$

Eq. 12 is the form of 1st order ordinary differential equation for $\underset{\sim}{q}$ and can be solved using certain available procedures on computer [9].

Other Field Problems

A number of other problems occur in various disciplines of engineering that involve the phenomenon of diffusion. This can include the saturated-unsaturated porous media flow and consolidation in soils. The governing differential equations for their respective fields are shown in Table 1. For saturated flow in porous media it applies to both confined and unconfined aquifer systems in groundwater [1]. In unsaturated flow, problems are frequently encountered in the soil-water studies which involve, for instance, infiltration or simultaneous transfer of heat and moisture. These governing differential equations can be used to simulate some important processes, particularly in the prediction of isothermal and non-isothermal evaporaton of soil water, gravity drainage without evaporation, and evaporation without drainage [7].

Also illustrated in Table 1 is a problem that governed by diffusion with convection type parabolic differential equation. It involves the transport through diffusion and convection of chemicals, pollutants, contaminants, and dissolved salts in water under saturated and unsaturated conditions. El-Damek [1983] used the Galerkin's 1-dimensional finite element models to solve simultaneously the moisture, heat, and solute transport in porous media.

TABLE 1: FIELD PROBLEMS OF PARABOLIC TYPE DIFFUSION EQUATIONS

Field Problem	Governing Differential Equation
1. 2-Dimensional Transient Saturated Flow in Porous Media.	$\frac{\partial}{\partial x}\left[K_x \frac{\partial \phi}{\partial x}\right] + \frac{\partial}{\partial y}\left[K_y \frac{\partial \phi}{\partial y}\right] + \overline{Q} = C \frac{\partial \phi}{\partial t}$
2. 2-Dimensional Transient Heat Flow in Solids.	$\frac{\partial}{\partial x}\left[K(T) \frac{\partial T}{\partial x}\right] + \frac{\partial}{\partial y}\left[K(T) \frac{\partial T}{\partial y}\right] + \overline{Q} = C \frac{\partial T}{\partial t}$
3. Infiltration Equation	$\frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z} + 1\right)\right] = C(\psi) \frac{\partial \psi}{\partial t}$ or $\frac{\partial}{\partial z}\left[D(\Theta) \frac{\partial \Theta}{\partial z}\right] + \frac{\partial K}{\partial z}(\Theta) = \frac{\partial \Theta}{\partial t}$
4. 1-Dimensional Consolidation in Soils.	$\frac{K}{\gamma_w} \frac{\partial^2 p^*}{\partial z^2} = m_v \frac{\partial p^*}{\partial t}$
5. 1-Dimensional Simultaneous Transfer of Moisture and Heat in Unsaturated Porous Media.	$\nabla(D_T \nabla T) + \nabla(D_\Theta \nabla \Theta) - \frac{\partial K}{\partial z} = \frac{\partial \Theta}{\partial t}$ and $\nabla \cdot (\lambda \nabla T) + \rho L' \nabla (D_{\Theta, v} \nabla \Theta) = C \frac{\partial T}{\partial t}$ where $\nabla = \frac{\partial}{\partial z}$
6.** 1-Dimensional Non-reacting Solute Transport in Porous Media	$\frac{\partial}{\partial x}\left(D_x \frac{\partial C^*}{\partial x}\right) - \frac{\partial}{\partial x}(\nu_x C^*) - \overline{Q} = \frac{\partial C^*}{\partial t}$

where

$\phi, T, \psi, \Theta, p^*, C^*$ = dependent variables, respectively as fluid potential, temperature, suction, moisture, excess porewater, and concentration of solute.

K, D, λ = material properties, conductivity and diffusivity.

$C, m_v, \gamma_w, \rho, L$ = diffusive agents (fluids) properties

ν_x = velocity.

$\overline{Q}$ = applied flux (fluid, heat, etc).

**diffusion with convection problem.

Conclusion

The integral formulation can therefore be used for the derivation of element equations and solves the heat conduction problem as well as other field problems, like sat-unsaturated porous media flow, solute transport studies, and consolidation. We may note, however, that the finite element formulation for all these problems will essentially be the same except for different relevance of material properties and meanings of the unknowns such as temperature and fluid head.

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