

Hygrothermal Fracture Analysis in Dissimilar Materials

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Abstract

This paper demonstrates an explicit-implicit, finite element analysis for linear as well as nonlinear hygrothermal stress problems. Additional features, such as moisture diffusion equation, crack element and virtual crack extension(VCE) method for evaluating J-integral are implemented in this program. The Linear Elastic Fracture Mechanics(LEFM) Theory is employed to estimate the crack driving force under the transient condition for an existing crack. Pores in materials are assumed to be saturated with moisture in the liquid form at the room temperature, which may vaporize as the temperature increases. The vaporization effects on the crack driving force are also studied. The ideal gas equation is employed to estimate the thermodynamic pressure due to vaporization at each time step after solving basic nodal values. A set of field equations governing the time dependent response of porous media are derived from balance laws based on the mixture theory. Darcy's law is assumed for the fluid flow through the porous media. Perzyna's viscoplastic model incorporating the Von-Mises yield criterion are implemented. The Green-Naghdi stress rate is used for the invariant of stress tensor under superposed rigid body motion. Isotropic elements are used for the spatial discretization and an iterative scheme based on the full Newton-Raphson method is used for solving the nonlinear governing equations.

Key Word : Hygrothermal Fracture, Dissimilar Materials, Vaporization

Nomenclature

Subscripts

s : solid constituent
 f : fluid constituent

Roman symbols

D_e, D_h, D_{vp} : elastic, hygrothermal, viscoplastic strain rates, respectively
 F, F_s, F_f : deformation gradient tensors
 f, f_f, f_s : body forces
 I_i : source(sink) of the component i

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j_{ic}	: convective component of mass flux of the component i
j_{id}	: conductive component of mass flux of the component i
J	: J-integral
k, k_f, k_s	: heat conduction coefficients
q	: heat flux vector
r, r_s, r_f	: specific energy supply rates
T, T_f, T_s	: Cauchy stresses
t, t_f, t_s	: surface tractions
t	: time
u, \hat{u}, u_0	: displacement vector and its boundary and initial values
v_s, v_f, v_r	: velocities
v_0, V_s	: volume, Darcy flow velocity
w	: weight function
W	: moisture content
Greek symbols	
β, β_s, β_f	: thermal expansion coefficients
γ	: viscosity constant of viscoplastic material
ε	: symmetric part of displacement gradient tensor
$\theta, \hat{\theta}, \theta_0$: temperature, its boundary and initial values
$\Omega, \partial\Omega$: domain and boundary
$\pi, \hat{\pi}, \pi_0$: pore pressure, its boundary and initial values
$\rho, \bar{\rho}$: true and apparent mass densities
$\sigma, \bar{\sigma}$: Cauchy and effective stresses, respectively
ϕ	: porosity

Introduction

Interface crack between composite(dissimilar) materials with a fluid-saturated porous media under thermal loading and permeation of moisture is a major problem in the manufacturing of ceramic composites and electronics devices, in particular, plastic encapsulated ICs. For instance, there have been numerous incidents reported in the area of interface cracking between the ceramic fibers and matrix in a ceramic composite.

This kind of interface cracking is mainly caused by the fact that there are mismatch of thermal properties and vapor pressure which may vaporize as the temperature increases.

The coefficient of thermal expansion(CTE) mismatches of the constituents of the package and permeation of moisture are the primary contributor to stresses. These stresses in concert with processing residual stresses can be sufficient to induce cracking and interfacial delamination in dissimilar materials. Delamination at these interface is a complicated function of the elastic moduli and CTEs etc..

Ceramic composites and IC packages are most often used in environments with high temperature gradients and permeation of moisture. Therefore, a better understanding of interface cracks under thermal loading and moisture conditions is needed to guide the judicious selection of materials and fabrication methods which do not lead to interfacial failure.

Recent trends pertinent to geological media have focused considerable attention on fluid-infiltrated and/or thermally induced responses. Following Terzaghi's work[1] on one-dimensional consolidation, Biot[2] has presented a generated three-dimensional consolidation. Nonisothermal finite-strain dynamic of a porous solid containing a viscous fluid was studied by Biot; he showed how the Lagrangian equation in the finite element methods were formulated. Rice

and Cleary[3] have reformulated Biot's equations relating strain and fluid mass content to stress and pore pressure in terms of revised material properties. McTigue et al[4] have extended fluid-saturated porosity with temperature effects. The variational principle for fluid-coupled problems in continuum mechanics was reported by Sandhu et al[5].

The variational principle applied to the coupled-fluid and thermoelastic problem was studied by Aboustit et.[6]. Kim[7] extended Aboustit's work by using the Perzyna model in his viscoplastic model but his work didn't include a finite element fracture model. Lewis and Schrefler[8] summarized investigations on coupled poroelastic and hygrothermomechanical response of geological media utilizing finite-element techniques.

The goal of this research is to develop a finite element fracture model through which the crack/delamination driving forces can be computed for representative failure mechanisms and loadings of composite materials.

Numerical Background

Pores in composite materials are assumed to be saturated with moisture in the liquid form at the room temperature, which may vaporize as the temperature increases. For study these phenomena, the following equations are used. From the theory of mixtures along with Darcy's flow laws for the porous media which effectively express momentum conservation, the governing balance laws are

$$\overline{\rho}_s + \overline{\rho}_s \operatorname{div}(V_s) = 0 \quad (1)$$

$$\text{where } \overline{\rho}_s = (1 - \phi) \rho_s$$

$$\overline{\rho}_f + \overline{\rho}_f \operatorname{div}(V_f) + V_r \operatorname{grad}(\overline{\rho}_f) = 0 \quad (2)$$

$$\text{where } \overline{\rho}_f = \phi \rho_f, \quad V_r = V_f - V_s$$

$$\operatorname{div}(T_s) + \overline{f}_s = \overline{\rho}_s \dot{V}_s \quad (3)$$

$$\operatorname{div}(T_f) + \overline{f}_f = \overline{\rho}_s \dot{V}_f + \overline{\rho}_s L_f V_r \quad (4)$$

$$\rho \dot{\varepsilon} + \overline{\rho}_f V_r \cdot \operatorname{grad}(\varepsilon_f) = \rho r - \operatorname{div}(q) + T_s \cdot D_s + T_f \cdot D_f \quad (5)$$

$$\text{where } \rho \dot{\varepsilon} = \overline{\rho}_s \dot{\varepsilon}_s + \overline{\rho}_f \dot{\varepsilon}_f \text{ and } \rho r = \overline{\rho}_s r_s + \overline{\rho}_f r_f$$

$$\frac{\partial W_i}{\partial t} = - \operatorname{div}(j_{ic} + j_{id}) + I_i \quad (6)$$

Equation(1) and (2) are the continuity equation which expresses mass conservation of solid and fluid, respectively, equation(3) and (4) are the equilibrium equation of solid and fluid, respectively, equation(5) is the energy conservation equation which expresses temperature transport and equation(6) describes the moisture diffusion. During the deformation, the mass densities, i.e., thermodynamic relationships giving material properties as functions of pressure and temperature, are updated as follows :

$$\rho_s = \rho_{s_0} \left[1 - 3\beta_s(\theta - \theta_0) - \frac{1}{3K_s} \operatorname{tr}(\sigma_s) \right]$$

$$\rho_f = \rho_{f_0} \left[1 - 3\beta_f(\theta - \theta_0) - \frac{1}{K_f} p \right]$$

In addition, the materials are assumed to be isotropic.

The constitutive equations for the time-temperature dependent elastic-viscoplastic fluid-saturated material are obtained by superposing the elastic, D_e , hygro-thermal, D_h , and time dependent viscoplastic, D_{vp} , strain rate components in the form

$$D = D_e + D_h + D_{vp} \quad (7)$$

$$\text{where } D = \frac{1}{2} \left[\frac{\partial v}{\partial x} + \frac{\partial v^T}{\partial x} \right], \quad D_h = \alpha \theta I + \beta \pi I$$

The viscoplastic strain rate is assumed to obey Perzyna's viscoplastic flow rule defined as

$$D_{vp} = \gamma \langle \Phi(F) \rangle \frac{\partial F}{\partial \sigma} \quad (8)$$

The total objective stress rate is defined by

$$\dot{T} = C \{ D - D_h - D_{vp} \} \quad (9)$$

where C is the conventional temperature dependent elasticity tensor.

From the weak formulations for the fluid thermal diffusion and the Lagrangian formulations for the solid deformation, the coupled algebraic system equations, in terms of the unknown increment and residual vectors are obtained in the form

$$\begin{bmatrix} K_{uw} & K_{u\theta} & K_{u\pi} & K_{uw} \\ M_{vu} & M_{v\theta} & M_{v\pi} + \Delta t K_{v\pi} & M_{vw} + \Delta t K_{vw} \\ 0 & M_{w\theta} & M_{w\pi} + \Delta t K_{w\pi} & M_{w\pi} + \Delta t K_{w\pi} \\ M_{\varphi u} & M_{\varphi\theta} & M_{\varphi\pi} + \Delta t K_{\varphi\pi} & M_{\varphi\pi} + \Delta t K_{\varphi\pi} \end{bmatrix}_{(i)}^{t+\Delta t} \begin{pmatrix} \Delta u \\ \Delta \theta \\ \Delta p \\ \Delta w \end{pmatrix}_{(i)} = \Delta L_{(i)}^{t+\Delta t} \quad (10)$$

where

$$\Delta L_{(i)}^{t+\Delta t} = \begin{pmatrix} \Delta R_{(i)}^{t+\Delta t} \\ Q_{(i)}^{t+\Delta t} \\ F_{(i)}^{t+\Delta t} \\ W_{(i)}^{t+\Delta t} \end{pmatrix} - \begin{bmatrix} M_{vu} & M_{v\theta} & M_{v\pi} & M_{vw} \\ 0 & M_{\varphi\theta} & M_{\varphi\pi} & M_{\varphi\pi} \\ M_{vu} & M_{v\theta} & M_{v\pi} & M_{vw} \\ 0 & M_{\varphi\theta} & M_{\varphi\pi} & M_{\varphi\pi} \end{bmatrix}_{(i)} \begin{pmatrix} \dot{u} \\ \dot{\theta} \\ \dot{p} \\ \dot{w} \end{pmatrix}_{(i)}^{t+\Delta t} \\ - \begin{bmatrix} K_{vu} & K_{v\theta} & K_{v\pi} & K_{vw} \\ K_{vu} & K_{v\theta} & K_{v\pi} & K_{vw} \\ 0 & K_{w\theta} & K_{w\pi} & K_{w\pi} \\ K_{\varphi u} & K_{\varphi\theta} & K_{\varphi\pi} & K_{\varphi\pi} \end{bmatrix}_{(i)} \begin{pmatrix} u \\ \theta \\ p \\ w \end{pmatrix}_{(i)}^{t+\Delta t}$$

Two point explicit time marching scheme with time rate steps and the full Newton-Raphson method are utilized. The unknown increments are solved using equation, and the total solution increments, mass densities and mesh configuration after i^{th} iteration are updated during each time step Δt .

For implicit time marching scheme, the following equations are used,

$$\begin{bmatrix} K_{uw} & K_{u\theta} & K_{u\pi} & K_{uw} \\ M_{vu} & M_{v\theta} & M_{v\pi} + \Delta t K_{v\pi} & M_{vw} + \Delta t K_{vw} \\ 0 & M_{w\theta} & M_{w\pi} + \Delta t K_{w\pi} & M_{w\pi} + \Delta t K_{w\pi} \\ M_{\varphi u} & M_{\varphi\theta} & M_{\varphi\pi} + \Delta t K_{\varphi\pi} & M_{\varphi\pi} + \Delta t K_{\varphi\pi} \end{bmatrix}_{(i)}^{t+\Delta t} \begin{pmatrix} \Delta u \\ \Delta \theta \\ \Delta p \\ \Delta w \end{pmatrix}_{(i)} = \Delta L_{(i)}^{t+\Delta t} \quad (11)$$

where

$$\Delta L_{(i)}^{t+\Delta t} = \Delta t \begin{pmatrix} (1-\beta)R'_{(i)} + \beta R_{(i)}^{t+\Delta t} \\ (1-\beta)Q'_{(i)} + \beta Q_{(i)}^{t+\Delta t} \\ (1-\beta)F'_{(i)} + \beta F_{(i)}^{t+\Delta t} \\ (1-\beta)W'_{(i)} + \beta W_{(i)}^{t+\Delta t} \end{pmatrix} - \begin{pmatrix} M_{vu} & M_{v\theta} & M_{v\pi} & M_{vw} \\ 0 & M_{\varphi\theta} & M_{\varphi\pi} & M_{\varphi\pi} \\ M_{vu} & M_{v\theta} & M_{v\pi} & M_{vw} \\ 0 & M_{\varphi\theta} & M_{\varphi\pi} & M_{\varphi\pi} \end{pmatrix}_{(i)}^{t+\Delta t} \\ + \beta \Delta t \begin{pmatrix} K_{vu} & K_{v\theta} & K_{v\pi} & K_{vw} \\ K_{vu} & K_{v\theta} & K_{v\pi} & K_{vw} \\ 0 & K_{w\theta} & K_{w\pi} & K_{w\pi} \\ K_{\varphi u} & K_{\varphi\theta} & K_{\varphi\pi} & K_{\varphi\pi} \end{pmatrix}_{(i)}^{t+\Delta t} \begin{pmatrix} u \\ \theta \\ p \\ w \end{pmatrix}_{(i)}^{t+\Delta t} + \begin{pmatrix} M_{vu} & M_{v\theta} & M_{v\pi} & M_{vw} \\ 0 & M_{\varphi\theta} & M_{\varphi\pi} & M_{\varphi\pi} \\ M_{vu} & M_{v\theta} & M_{v\pi} & M_{vw} \\ 0 & M_{\varphi\theta} & M_{\varphi\pi} & M_{\varphi\pi} \end{pmatrix}_{(i)} \\ - (1-\beta) \begin{pmatrix} K_{vu} & K_{v\theta} & K_{v\pi} & K_{vw} \\ K_{vu} & K_{v\theta} & K_{v\pi} & K_{vw} \\ 0 & K_{w\theta} & K_{w\pi} & K_{w\pi} \\ K_{\varphi u} & K_{\varphi\theta} & K_{\varphi\pi} & K_{\varphi\pi} \end{pmatrix}_{(i)}^t \begin{pmatrix} u \\ \theta \\ p \\ w \end{pmatrix}_{(i)}^t$$

The region, Ω occupied by the saturated solid is subjected to applied traction t , prescribed displacement \hat{u} . The boundary of Ω , $\partial\Omega$ may also be divided into portions of boundary of temperature $\partial\Omega_h$, moisture $\partial\Omega_w$, pore-pressure $\partial\Omega_p$. The domain $\bar{\Omega}$ is composed of the interior Ω and the boundary $\partial\Omega$. All of the functions defined in the domain are the product of the spatial domain with a non-negative time interval, i.e. $\bar{\Omega} \times [0, \infty)$.

The J-integral by virtual crack extension(VCE) method[9] is

$$J = - \int_{v_0} \left\{ w \frac{\partial p_n}{\partial x_i} - \sigma_{kl} \frac{\partial u_k}{\partial x_i} \frac{\partial p_n}{\partial x_i} + \sigma_{mm} \beta_t \frac{\partial T}{\partial x_i^n} p_n \right\} \mathcal{I} dV \quad (12)$$

In the influence of hygro-thermal stress, J-integral is

$$J = - \int_{v_0} \left\{ w \frac{\partial p_n}{\partial x_i} - \sigma_{kl} \frac{\partial u_k}{\partial x_i} \frac{\partial p_n}{\partial x_i} + \sigma_{kk} \beta_t \frac{\partial T}{\partial x_i^n} p_n + \sigma_{kk} \beta_w \frac{\partial W}{\partial x_i^n} p_n \right\} \mathcal{I} dV \quad (13)$$

where β_t and β_w are coefficients of thermal, hygral expansion, respectively, p_n is the element shape function.

Applications

A typical shape in half model of interface crack problem between two dissimilar materials is shown in Fig. 1. The system consists of a silicon bonded to an encapsulant substrate. A silicon is assumed to be viscoplastic, whereas an encapsulant is assumed to be stiffer than silicon and elastic isotropic. A long separation between these two materials is assumed to exist after exposure to the ambient environment. The initial moisture content, mass density and porosity of the encapsulating material are estimated to be $W=0.25\%$, $\rho_s=4.925(\text{kg}/\text{m}^3)$ and $\phi=0.005$, respectively.

Ideal gas equation($p\nu = RT$) is valid in this case, $R=461.6(\text{J}/\text{kg}^0\text{K})$ for vapor. Increased vapor pressure is due to the heating of entrapped moisture and only the encapsulant can absorb moisture.

This finite element analysis provides a computational capability for solving two-dimensional nonlinear hygrothermal problems under finite deformation. Time increment can be selected as basic factors in improving the accuracy of the solution in discretized system. Perzyna's model is chosen for evaluating the stress field with the Von-Mises yield criterion. Incremental formulation is used to compute the time dependent stress field equations. Full coupled as well as uncoupled analysis are chosen for analysis tool.

Initial conditions :

- Encapsulant with moisture $4.925(\text{kg}/\text{m}^3)$, $\phi=0.005$
- Initial temperature 26°C
- No strains and stresses
- This bimaterial has an initial crack length 2mm (1mm in the half meshed model) in the center

Boundary conditions :

- This bimaterial is heated from 26°C to 220°C in 1 sec. and maintained at 220°C for 200 sec. at the upper boundary
- No moisture flux at the boundaries

Results and Discussion

Two methods(coupled system and uncoupled system) of solving the heat and moisture transient problem are compared. Coupled solutions are obtained directly by solving the problem

with assumption that the displacements, temperature and moisture are fully coupled. Uncoupled solutions are obtained by solving each field separately. The solution sequence made in the uncoupled system is moisture, temperature, displacement and stresses. With such sequence, the vapor pressure is determined by the moisture content and current temperature($p_v=RT$).

The deformation of this model is influenced by the moisture, temperature and vapor pressure. For this case, the J-integral histories are shown in Fig. 2. As this figure shows, the energy release rates by these two schemes in consideration of hygrothermal or thermal effect are compared.

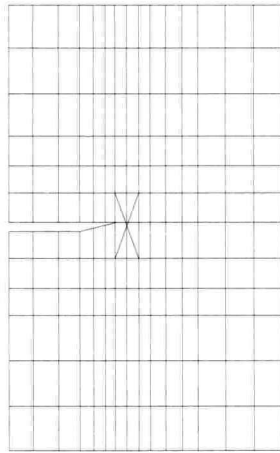


Fig. 1. Finite element discretization of the half meshed model

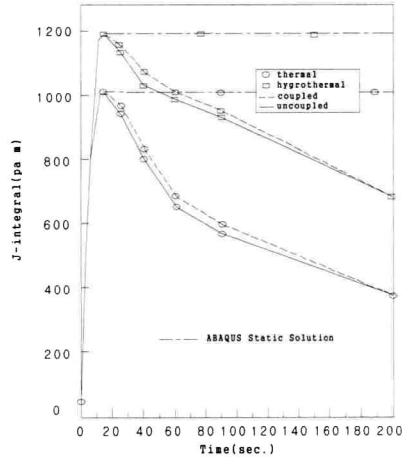


Fig. 2. J-integral histories of thermal and hygrothermal effect

From this comparison, we can see that the developed program is accurate because results between the coupled solution and uncoupled solution in Fig. 2 are almost similar and maximum values of these two results are almost equal to those of ABAQUS. Therefore, the use of uncoupled solution is recommended because the coupled case is expensive to run (5 times larger than uncoupled case). And the maximum J-integral value by the effect of vapor pressure(hygrothermal) is about 20% larger than that by the effect of thermal.

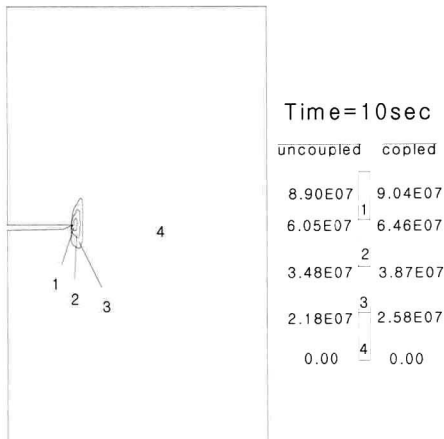


Fig. 3. Comparison of the principal stress by two schemes in consideration of hygrothermal effect(time=10sec.)

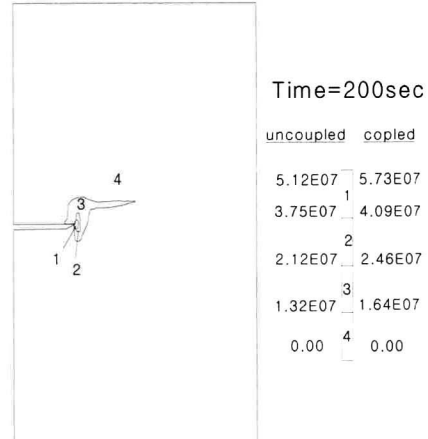


Fig. 4. Comparison of the principal stress by two schemes in consideration of hygrothermal effect(time=200sec.)

For the silicon/encapsulant dissimilar material treated in this study, it is seen that the interaction of moisture and heat can significantly alter the stress distribution in the dissimilar material.

The results of the principal stress distribution assumed hygrothermal effect by these schemes are shown in Fig. 3, Fig. 4 and Fig. 5 according to time 10sec., 200sec. and 1,418sec., respectively. Fig. 6 shows the representative principal stress distribution at time 10sec.

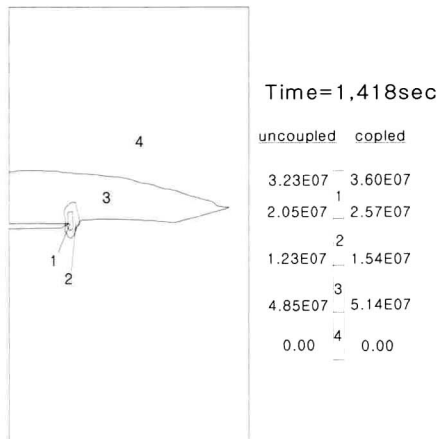


Fig. 5. Comparison of the principal stress by two schemes in consideration of hygrothermal effect(time=1,418sec.)

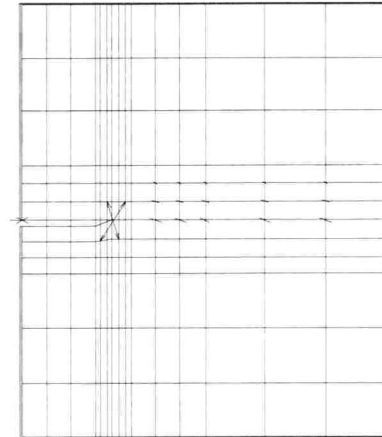


Fig. 6. The principal stress distributions(time=10sec.)

From these results, we can know the entrapped moisture and its vapor pressure(hygrothermal effect) create larger spreading force on the delamination surfaces causing quickly to the maximum principal stress value at time=10 sec. After this time, the principal stress is decreased to zero slowly.

Conclusions

Through the finite element analysis for hygrothermal fracture in dissimilar materials, this finite element program is very reasonable to apply to hygrothermal fracture analysis of composite materials and to predict J-integral accurately, the vaporization effect has to be considered because it is accelerate the crack driving force at an early stage. The use of uncoupled solution in this analysis is recommended because the result by this scheme is reasonable and CPU time is not costly and this procedure is also applicable to problems related to structure response evaluations associated with various porous materials, including ceramics, polymers, thin film and plastic encapsulated ICs etc..

References

1. K. Terzaghi, Theoretical Soil Mechanics, Wiley, New York, 1943.
2. M. A. Biot, Thermoelasticity and Irreversible Thermodynamics, J. Appl. Phys., 27, 240, 1956.
3. J. R. Rice and M. P. Cleary, Some Basic Stress Diffusion Solutions for Fluid-Saturated Elastic Porous Media Compressible Constituents, Rev. Geophys. Space Phys., 14, 227, 1976.
4. D. F. McTigue, Thermoelastic Response of Fluid-Saturated Porous Rock, J. Geophys.

Res., 91, 9533, 1986.

5. R. S. Sandhu and E. L. Wilson, Finite Element Analysis of Seepage in Elastic Media, J. Eng. Mech. Div. ASEC, (EM3), 95, pp.641-652, 1969.

6. B. L. Aboustit, S. H. Advani and J. K. Lee, Variational Principles and Finite Element Simulation for Thermoelastic Consolidation, Int. J. Numer. Anal. Meth. in Geomech., 9, 29, 1985.

7. C. S. Kim, T. S. Lee, S. H. Advani and J. K. Lee, Hygrothermomechanical Evaluation of Porous Media under Finite Deformation, Int. J. for Numer. Meth. in Engineering, Vol.36, pp.147-179, 1993.

8. R. W. Lewis, C. Majorana and B. Schrefler, A Coupled Finite Element Method for the Consolidation of Non-Isothermal Elastoplastic Porous Media, Trans. Porous Media, 1, 155, 1986.

9. C. F. Shih, B. Moran and T. Nakamura, Energy Release Rate Along a Three-dimensional Crack Front in a Thermally Stressed Body, Int. J. of Fracture, Vol.30, pp.79-102, 1986.