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CORRELATION OF FRACTURE TOUGHNESS WITH IMPURITY COMPONENTS

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1 Nomenclature

Girrens' Nomenclature.

A	Dufour coefficient
b_i	mixture body force vector
B	Soret coefficient
C	Green deformation tensor
c_α	concentration of the α constituent
D	diffusion coefficient
G	shear modulus
j_i	specific mass flux of constituent α
K	thermal conductivity
M	piezo diffusion coefficient
N	piezo thermal coefficient
q_i	heat flux due to thermal diffusion
s	mixture specific entropy
T_{ij}	mixture stress tensor
T	mixture temperature
T_0	reference temperature
α_c	coefficient of linear diffusive expansion
α_θ	coefficient of linear thermal expansion
β_c	$3[\lambda + (2/3)G]\alpha_c$
β_θ	$3[\lambda + (2/3)G]\alpha_\theta$
θ	mixture temperature
μ_α	chemical potential of constituent α
I_e	infinitesimal strain dilatation
λ	Lame's constant
ρ_0	undeformed mixture density
ρ	mixture density
ω	material constant relating concentration to entropy
ζ	material constant relating concentration to chemical potential

Aifantis' nomenclature

a	acceleration of the gas
b	external body force field
c_E	specific heat of the solid
e	energy supply per unit volume per unit time due to interaction with solid
e	infinitesimal strain tensor of the gas
E	Young's modulus of elasticity
F	deformation gradient of the elastic solid
m	specific entropy increase arising from interaction with solid
M, N, D	phenomenological constants
q	heat flux vector
s	stress tensor of the solid
T	stress tensor of the gas
t	time
u	velocity of the gas
v	velocity of the gas
ρ	density of the gas
ρ_1	density of the solid
α	coefficient of linear thermal expansion, also the ratio M/N
θ	temperature
θ_0	reference temperature
$\hat{p}$	diffusive force vector
ε	internal energy density of the gas
η	entropy of the gas
ψ	free energy function
λ	Lame's constant
μ	Lame's constant
ν	Poisson's ratio
σ	hydrostatic stress applied

Abstract

Work done on the extension of the existing 'Coupled Thermomechanical Diffusion' theory [1] to enable the prediction of diffusion of a solute species in stressed solids in the presence of cracks is presented here. Mathematical formalism is provided to support the intuitive notion that a singular solution for the concentration field can exist in crack tip neighborhoods driven by singular solutions for stresses that have been obtained within the framework of classical Linear Elastic Fracture Mechanics.

It has been shown that under certain limiting assumptions, a singular solution for the concentration profile of the kind $\frac{1}{\sqrt{r}}$ emerges from the governing equations. Both steady state and transient solutions were obtained. A numerical simulation using quarter point finite elements was carried out and the results obtained also indicated the presence of this singularity. A singular solution for the concentration profiles of diffusing species in crack tip neighborhoods was obtained by Gdoutos and Aifantis [4]. The order of the singularity obtained in their investigation was different from that discovered in the present work as were the governing differential equations and the underlying assumptions of their model.

In order to determine the reasons for the differences, a detailed study was undertaken comparing the two theories and their underlying assumptions, methodology and results. These comparisons also form part of the present work. A study of the boundary conditions will reveal if the admissible solutions obtained have significance in physical applications. If it turns out that physically meaningful boundary conditions can be realised by employing the singular solutions obtained here, a significant stride can be made in the direction of modeling physical problems. Ongoing research is directed towards the extension of the scope of these results and identifying new failure criteria and design parameters that would be useful in modeling physical structures operating in corrosive environments.

To enable numerical modeling of complex problems not amenable to analytical treatment, a finite element model incorporating the results of the present study will be built. An existing finite element code that employs an "assumed displacement hybrid finite element" that models the crack tip singularity exactly has been identified and tested. Software incorporating this model as well as the results of ongoing theoretical studies into the already existing code that models nonlinear coupled thermoelastic diffusion will become a useful and viable design tool in the analysis of structures. This work will be presented in a Ph.d dissertation.

2 Introduction

This final report presents the work done on the extension of the extant 'Coupled Thermomechanical Diffusion' theory [1] to enable the prediction of diffusion of a solute species in stressed solids in the presence of cracks. Earlier reports [2,3] are enclosed as appendices A and B. Their contents will not be reproduced in great detail but relevant synopses will be included in the present text to provide completeness of discussion.

In the first report [2], it was asserted that a singular behavior was expected to emerge in the concentration profiles of diffusing species in crack tip neighborhoods. The theoretical foundation for this assertion was established later and forms in part, the body of the second report [3]. It was also reported in [2], that an existing finite element code HDMSNG, which incorporates an "assumed displacement hybrid finite element" that models the crack tip singularity exactly and also provides directly the stress intensity factors associated with Mode I and II type failures, has been identified and tested in the local computing environment. The code PSTDIF which performs non-linear thermoelastic analysis of stress assisted diffusion was similarly modified and tested.

In the second report [3], mathematical formalism to support the earlier assertion that a singular solution can exist for the concentration field in crack tip neighborhoods was presented. Numerical simulation using quarter point finite elements to model the diffusion behavior indicates but does not confirm the presence of this singularity. In the mathematical analysis presented therein, to isolate the influence of the mechanical response on the concentration field, only the piezo diffusion coefficient M and the diffusion co-efficient D were retained. Isothermal conditions were assumed. All other coupling effects were ignored in an attempt to discover how the mechanical response drives the phenomenon of diffusion.

It was also mentioned in [3], that Gdoutos and Aifantis [4] established a relationship between concentration and the stress intensity factors in mixed mode fracture based on Aifantis' theory [5,6,7]. The order of the singularity obtained by them is, however, different from that obtained in [2] and [3] and is dependent on the ratio M/N . However, the governing differential equation they used for modeling diffusion in the isothermal case, in the presence of a crack, is also different. To enable a direct comparison, it became necessary to compare the fundamental assumptions and methodology of the two diffusion theories proposed by Aifantis and Girrens and further determine from this comparison the reasons for the difference in the order of the singularity.

2.1 Comparison of Girrens' and Aifantis' Theories

The methodology adopted in both investigations falls within the realm of modern rational and continuum mechanics and adopts procedures laid down by Coleman and Mizel, Truesdell, Noll and Eringen [8,9,10,11]. The continuum being modeled is required to obey the fundamental balance laws, conservation of mass, momentum and energy and is further restricted in its behavior by the second law of Thermodynamics.

In building the constitutive model of the continuum, (gas, solid or mixture), strict heed is paid to the axioms of material objectivity (frame indifference), and equipresence among others as outlined by Eringen [11] and insuring that they are not violated. The other axioms that are implicitly obeyed include those of causality, determinism, material invariance, neighborhood, memory and admissibility.

In spite of subscribing to similar philosophies and methodology, there exist several fundamental differences in the theories developed by Girrens and Aifantis, not all of which have been reported or amplified upon in the literature. First, the similarities (and differences) in the two approaches will be outlined. Next, the consequences of the underlying differences will be examined, with specific focus on the distribution of an infiltrating solute species in crack tip neighborhoods and the nature of the singular behavior of the concentration profiles as predicted by the two theories.

As the next step in the ongoing research, the issue of the existence (or absence) of physically meaningful boundary conditions that enable (or preclude) any significance in practical applications of the admissible singular solutions obtained from both the theories above, will be examined for the first time.

The most striking and fundamental difference between Girrens' and Aifantis' theories is that Girrens models the gas-solid mixture as a single continuous entity while Aifantis treats the diffusing gas and the parent solid as separate constitutive classes.

Aifantis further assumes that the thermo-mechanical response of the parent solid is not affected by the presence of the gas, and that the solid conforms to linear uncoupled thermoelastic behavior [5,6]. The presence of the solid is recognized by the gas by allowing selected thermomechanical variables of the solid to enter the constitutive equations of the gas in certain stipulated ways.

Specifically, Aifantis stipulates that the effects of the solid on the gas are fully captured by the introduction of three quantities, $\hat{p}$, e and m [5,6], where $\hat{p}$ is a 'diffusive force vector' postulated to exist as a body force that enters the momentum balance equation for the gas, e is the energy supply per unit volume per unit time due to the interaction with the solid which enters the energy equation of the gas, and m is the specific entropy increase arising from interaction with the solid.

2.2 Variables Employed by Aifantis

In his constitutive model of the gas [5], Aifantis chooses the following variables as independent; ρ , F , $D\rho$, ∇F , v , θ , $D\theta$ where, ρ is the density of the gas, $D\rho$ is the density gradient of the gas, F is the deformation gradient of the elastic solid, ∇F is gradient of the deformation gradient tensor, v is the velocity of the gas, θ is the temperature of the gas and $D\theta$ is the gradient of temperature. Both the solid and the gas have the same temperature at a given point in space.

The dependent variables that have a general functional dependence on the independent variables listed above, are further taken to be, ϵ , η , e , m , T , q , and $\hat{p}$, where, ϵ is the internal energy density of the gas, η is the entropy of the gas, e is the energy supply per unit volume per unit time due to the interaction with the solid,

m is the specific entropy increase arising from interaction with the solid, $\mathbf{T}$ is the stress tensor of the gas, $\mathbf{q}$ is the heat flux vector, and $\hat{\mathbf{p}}$ is the diffusive flux vector (body force as stipulated above).

2.3 Variables Employed by Girrens

Girrens [1], employs the following set of independent variables : θ the temperature of the mixture, $\nabla\theta$ the gradient of the temperature of the mixture, c_α the concentration of the alpha constituent, ∇c_α the gradient of the concentration, $\mathbf{C}$ the Green deformation tensor of the mixture $\nabla\mathbf{C}$ the gradient of the Green deformation tensor of the mixture.

The dependent variables in his constitutive model are : e the specific internal energy of the mixture, s the specific entropy of the mixture, ψ the specific free energy of the mixture, $\mathbf{T}_{ij}$ the stress tensor of the mixture, μ_α the chemical potential of the constituent, $j_{\alpha i}$ the specific mass flux vector of the constituent, and q_i the heat flux vector due to thermal diffusion,

The original nomenclature and symbols of the two theories have been preserved above and once this is noted, no confusion is anticipated in comparing the equations of the two theories with their original symbols. Specifically, in thermodynamic analyses, Aifantis employs e to represent the energy supply per unit volume per unit time to the gas due to the interaction with the solid, while Girrens uses e to represent the specific internal energy of the mixture. The meaning will be stated explicitly in all discussion below if a possibility of confusion is encountered.

In comparing the choice of variables of the two theories, two points are noteworthy.

1. Girrens determines an explicit expression for the mass flux of the constituent, $j_{\alpha i}$ while Aifantis retrieves this information by tracking the velocity of the gas diffusing in the solid.
2. Aifantis defines three new quantities e , m and $\hat{\mathbf{p}}$ and stipulates that the influence of the solid on the gas is captured by the introduction of these three quantities.

2.4 Balance Laws and Constitutive Structure of Aifantis

2.4.1 Gas

1. Conservation of Mass

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{u}) = 0 \quad (1)$$

where ρ is the density of the gas, $\mathbf{u}$ its velocity and t denotes time.

2. Conservation of momentum

$$\text{div} \mathbf{T} + \rho \mathbf{b} + \rho \hat{\mathbf{p}} = \rho \mathbf{a} \quad (2)$$

$$\mathbf{T} = \mathbf{T}^T \quad (3)$$

where $\mathbf{T}$ is the stress tensor of the gas, $\mathbf{b}$ is the external body force field, $\hat{\mathbf{p}}$ is the diffusive force vector and $\mathbf{a}$ is the acceleration defined by

$$\mathbf{a} = \frac{D\mathbf{u}}{Dt} \quad (4)$$

The operator $\frac{D}{Dt}$ is defined as

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \text{grad} \quad (5)$$

3. Conservation of energy

$$\rho \frac{D\varepsilon}{Dt} = \mathbf{T} \cdot \text{grad} \mathbf{u} - \text{div} \mathbf{q} + \rho r + e \quad (6)$$

where, ε is the specific internal energy of the gas, e its energy exchange with the solid per unit volume per unit time, $\mathbf{q}$ is the heat flux vector and r a heat supply density.

A linearized constitutive model with respect to the quantities $\nabla \rho$, $\nabla \theta$, $\mathbf{u}$, ∇tre (the gradient of the strain dilatation; $\mathbf{e}$ is the infinitesimal strain tensor [6]) is adopted and the constitutive structure of the gas is,

$$\varepsilon = \hat{\varepsilon}(\rho, \theta, \text{tre}) \quad (7)$$

$$\eta = \hat{\eta}(\rho, \theta, \text{tre}) \quad (8)$$

$$\psi = \hat{\psi}(\rho, \theta, \text{tre}) \quad (9)$$

$$\mathbf{T} = \rho^2 \hat{\psi}_\rho(\rho, \theta, \text{tre}) \quad (10)$$

$$\mathbf{q} = \alpha_0(\rho, \theta, \text{tre}) \nabla \rho + \alpha_1(\rho, \theta, \text{tre}) \nabla \theta + \alpha_2(\rho, \theta, \text{tre}) \mathbf{u} + \alpha_3(\rho, \theta, \text{tre}) \nabla \text{tre} \quad (11)$$

$$\hat{\mathbf{p}} = \beta_0(\rho, \theta, \text{tre}) \nabla \rho + \beta_1(\rho, \theta, \text{tre}) \nabla \theta + \beta_2(\rho, \theta, \text{tre}) \mathbf{u} + \beta_3(\rho, \theta, \text{tre}) \nabla \mathbf{e} \quad (12)$$

Here, the α_i and β_i coefficients are functions of ρ , θ , and tre as indicated. The constitutive modeling of the gas in Aifantis' theory [5], and that of the gas-solid mixture in Girrens' theory [1], follow similar routes in enforcing material objectivity and equipresence, and further deriving thermodynamic identities from the restrictions enforced by the second law of thermodynamics in accordance with the procedures used by Noll and Mizel [8].

2.4.2 Solid

Aifantis and Gerberich [6] further derive a separate constitutive model for the solid wherein the stress tensor for the solid is related to the strain tensor (of the solid-gas system; no separate strain tensor for the gas is defined) via the linear stress-strain relation of *uncoupled* thermoelasticity.

$$\mathbf{s} = \lambda \text{tre} \mathbf{1} + 2\mu \mathbf{e} - (3\lambda + 2\mu) \alpha (\theta - \theta_0) \mathbf{1} \quad (13)$$

Here, s and e are the stress and strain tensor respectively, λ and μ are Lamé constants, while α is the coefficient of linear thermal expansion. θ_0 represents a reference uniform temperature. No influence from the gas is conveyed to the solid here.

The energy equation satisfied by the solid is assumed to be that of *uncoupled* quasi-static linear thermoelastic theory, namely the heat conduction equation.

$$\frac{\partial \theta}{\partial t} = k \nabla^2 \theta \quad (14)$$

Here, t denotes time and the coefficient k is defined by

$$k = \frac{k^*}{\rho_1 c_E} \quad (15)$$

where, ρ_1 is the density of the solid, c_E the specific heat of the solid, and k^* its thermal conductivity.

At this stage, Aifantis argues that at an 'initial state' the diffusive force $\hat{p}$ in (12) becomes

$$\hat{p}|_0 = \beta_{03} \nabla t r e + \beta_{01} \nabla \theta \quad (16)$$

and that at the 'initial state' the force $-\rho_0 \hat{p}|_0$ acts as an external body force field on the solid constituent. This is the point at which *coupling* due to the influence of the gas on the solid is established by allowing the 'diffusive force vector' $\hat{p}$ appear in the equilibrium equation for the solid. The equilibrium equation for the solid then takes the form,

$$\text{div } s - \rho_0 \beta_{03} \nabla t r e - \rho_0 \beta_{01} \nabla t r \theta = 0 \quad (17)$$

Using the compatibility equations for a linear elastic solid and applying the *div* operator, to (17) and further neglecting the effect of the diffusive force on the equilibrium of the solid, Aifantis and Gerberich conclude that when the temperature distribution does not change with time, the following relation holds

$$\nabla^2 t r e = 0 \quad (18)$$

Finally, continuity of mass is stated in the form

$$\rho_1 = \rho_{01}(1 - t r e) \quad (19)$$

2.5 Balance Laws and Constitutive Structure of Girrens (Mixture)

The following summary of balance laws and constitutive equations model the problem of coupled thermomechanical diffusion of dilute mobile constituents in an immobile, elastic, isotropic solid. [1]

2.5.1 Balance Laws

1. Conservation of mass

$$\frac{\rho_0}{\rho} = 1 + I_\epsilon \quad (20)$$

Here, ρ and ρ_0 represent the mixture density and the undeformed mixture density respectively. I_ϵ is the first invariant of the strain tensor, ie its trace or the strain dilatation.

$$\dot{c} = -j_{\alpha i, i} \quad (21)$$

Here the dot denotes derivative with respect to time, α represents the constituent α .

2. Conservation of Momentum

$$T_{pji, j} + \rho b_i = 0 \quad (22)$$

$$T_{pij} = T_{pji} \quad (23)$$

3. Conservation of Energy

$$\rho T \dot{s} = -q_{i, i} - \rho j_{\alpha i} \mu_{\alpha, i} + \rho r \quad (24)$$

Since this energy equation is derived for the *mixture*, it permits implicitly, a more general behavior of the *solid* to be modeled with all coupling effects retained, while Aifantis and Gerberich assume that the solid obeys the energy equation of *uncoupled* thermoelasticity.

2.5.2 Constitutive Relations

The following are the constitutive relations of Girrens' theory.

$$T_{pij} = 2G\epsilon_{ij} + (\lambda I_\epsilon - \beta_\theta \theta - \beta_{c\alpha} c_\alpha) \delta_{ij} \quad (25)$$

where, T_{pij} is the parent stress tensor (the constituents are assumed dilute enough to support negligible stress; here p refers to 'parent', it is not an index), G and λ are elastic constants, β_θ and $\beta_{c\alpha}$ are material constants defined by multiplying the coefficients of linear thermal expansion and linear diffusive expansion respectively by, $3[\lambda + (2/3)G]$ [1]. ϵ_{ij} is the infinitesimal strain tensor

$$s = \frac{\beta_{theta}}{\rho} I_\epsilon + \frac{1}{T_0} (d)_{\epsilon, c} \theta - \omega c_\alpha \quad (26)$$

where, s is the mixture specific entropy, T_0 the reference temperature, $d_{\epsilon, c}$ the mixture specific heat, and ω is the material constant relating concentration to entropy.

$$\mu_\alpha = -\frac{\beta_{c\alpha}}{\rho} I_\epsilon + \zeta c_\alpha + \omega \theta \quad (27)$$

where, μ_α is the chemical potential of constituent α , and ζ is the material constant

relating concentration to chemical potential.

$$q_i = -(K\theta_{,i} + Bc_{\alpha,i} - NI_{\epsilon,i}) \quad (28)$$

where, q_i is the heat flux vector and K , B , and N are coupling coefficients tabulated in Appendix B (I).

$$j_{\alpha i} = -(Dc_{\alpha,i} + A\theta_{,i} - MI_{\epsilon,i}) \quad (29)$$

where, D , A , and M are coupling coefficients tabulated in Appendix B(I).

2.5.3 Kinematic Relationships

$$I_{\epsilon} = \epsilon_{kk} \quad (30)$$

$$\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \quad (31)$$

It is to be noted here, that Girrens' theory outlined above permits full coupling between the various thermomechanical and diffusion variables in modeling the behavior of the *mixture*; ie both the solid and the diffusing species affect each other and their effects are captured in the above model. This is visible in the constitutive relations outlined above and in keeping with the axiom of equipresence, no simplifying assumptions are made that result in partial uncoupling.

In the model of Aifantis and Gerberich, coupling effects are introduced in specific and stipulated ways by allowing selected thermomechanical variables of the solid to enter the constitutive model of the gas. As stated earlier, the solid is assumed to obey uncoupled thermoelasticity and the effects of the gas on the thermomechanical response of the solid are captured a-posteriori, if deemed necessary, via a perturbation calculation.

2.6 Direct Comparison in the Isothermal Case

Before proceeding to compare the singular solutions obtained from the above two theories, [3,4], it is noted that the most general diffusion equation (mass balance equation with constitutive relations embedded) derived by Aifantis for the gas in the isothermal case is

$$\frac{\partial \rho}{\partial t} = \text{div} [A_1 \nabla \rho + A_2 \nabla tre + A_3 (\mathbf{b} - \mathbf{a})] \quad (32)$$

where, A_1 , A_2 , A_3 are coefficients dependent on ρ , $\mathbf{e}$, and p , the thermodynamic pressure.

$$A_1 = \frac{1}{\beta_2} [\rho \beta_0 - \frac{\partial p}{\partial \rho}]_{tre}, A_2 = \frac{1}{\beta_2} [\rho \beta_3 - \frac{\partial p}{\partial tre}]_{\rho}, A_3 = \frac{1}{\beta_2 \rho}; \quad (33)$$

Under isothermal conditions, the diffusion equation (mass balance with constitutive relations substituted) derived by Girrens is, [1]

$$c_{,t} = Dc_{,ii} - Me_{,ii} \quad (34)$$

Here, e represents the strain dilatation or the trace of the strain tensor. Equations (32) and (34) derived by Aifantis and Girrens respectively, share close similarities. Girrens defines c_α as a ratio ρ_α/ρ where, ρ_α is the constituent density and ρ is the mixture density [1]. Thus equations (32) and (34) essentially convey the same information, namely, that the time rate of change of density/concentration is driven by the divergence of a 'gradient field' which includes the gradients of density, strain dilatation if the body forces are neglected. Aifantis further casts the above equation (32), in the following form (37) (below), which is then solved [4], to obtain singular solutions.

In arriving at (37), from (32), Aifantis makes the following assumptions. The external body force 'b' and the acceleration field 'a' are neglected. Only processes in which density gradients, velocities, and velocity gradients are small quantities of $O(\varepsilon)$ where $\varepsilon (\ll 1)$ is a small real parameter; [6] are considered. Then the coefficients in Eq (32) are expanded in a Taylor series and terms higher than those of $O(\varepsilon)$ are neglected. This yields the intermediate result,

$$\frac{\partial \rho}{\partial t} = c_1 \nabla^2 \rho + c_2 \nabla \text{tre} \cdot \nabla \rho + c_3 \text{tre} \nabla^2 \rho \quad (35)$$

where, c_1 , c_2 and c_3 are coefficients dependent on the uniform density ρ_0 . The following result of linear isothermal elasticity is employed in arriving at this result.

$$\nabla^2 \text{tre} = 0 \quad (36)$$

The use of this relation merits some mention of the restrictions it brings with its usage.

It can be shown [11] that the above relation (36) holds only when the components of the body forces appearing in the momentum balance equation are all either constant, or can be derived from a harmonic potential function. If such is the case, the first invariants (trace) of both the stress tensor and the strain tensor are harmonic.

In the present context, this implies that the 'diffusive force vector' as postulated by Aifantis must be derivable from a harmonic scalar potential function. A further consequence of this requirement is that the 'diffusive force vector' must be a conservative force field. This leads to the observation that if a diffusion process being modeled involves effects which do not possess a 'conservative' character in the above sense and involve a dissipative mechanism which precludes the derivation of the 'diffusive force vector' from a scalar harmonic potential, the above relation is not applicable and equation (37) cannot be employed.

Using the relation $\text{tre} = \frac{1-2\nu}{E} \sigma$, Aifantis transforms (35) to

$$\frac{\partial \rho}{\partial t} = \bar{D}^* \nabla^2 \rho - \bar{M} \nabla \sigma \cdot \nabla \rho \quad (37)$$

where, $\bar{D}^* = \bar{D} + \bar{N}\sigma$.

$\bar{D}$, $\bar{M}$, $\bar{N}$ are given in terms of c_1 , c_2 , c_3 , ν and E .

This equation models a cracked plate immersed in a corrosive environment. A solution to the steady state reached by (37) is given by Gdoutos and Aifantis [4] as

$$\rho = \rho_0(1 + \beta\sigma^0)^\alpha \quad (38)$$

where, ρ_0 is the concentration across the crack planes, $\alpha = \frac{M}{N}$, $\beta = \frac{N}{D}$. An estimate for β for hydrogen diffusion in iron, given by Aifantis et al [12] is $8.715 \times 10^{-10} \frac{m^2}{N}$, while a value of $\alpha = 4.2$ for a 4340 steel-hydrogen system. [13]

To obtain the concentration profile in crack tip neighborhoods, Aifantis introduces a solution for σ^0 obtained from classical Fracture Mechanics, free from the influence of any coupling effects into (2.2) above. For the case of an infinite plate, with uniaxial stress σ perpendicular to the crack, Gdoutos and Aifantis [4] obtain the solution

$$\rho = \rho_0[1 + \beta A \sigma (\sqrt{\frac{2a}{r}} \cos \frac{\theta}{2} - 1)]^\alpha \quad (39)$$

The solution above is clearly dependent on the parameter $\alpha = M/N$

A solution to the problem of isothermal diffusion driven by the mechanical response alone and ignoring all other coupling effects, within the framework of Girrens' theory was proposed in Report II [3]. Both steady state and transient solutions were obtained.

Under steady state conditions, the admissible concentration profile in crack tip neighborhoods for an infinite plate with biaxial load [3] was found to be,

$$c = \frac{MK_I}{D} \frac{1}{\sqrt{r}} F(\theta, \frac{\partial f_1}{\partial \theta}, \frac{\partial f_2}{\partial \theta}) \quad (40)$$

where, K_I is the mode I stress intensity factor, f_1 , f_2 , and F are dependent of the geometry and load configuration of the system. Here, r is the radial distance from the crack tip, M and N are phenomenological constants [1,3], c the concentration profile and ϵ the strain dilatation.

Clearly the singular behavior exhibited by the two admissible solutions obtained above within the framework of the two theories is different. A reality check that can be employed to explore the significance of these solutions in practical applications is to verify whether they satisfy physically meaningful boundary conditions. For instance, in the theory of Fracture Mechanics [13], several *admissible* singular solutions to the governing equations of stress in crack tip neighborhoods exist, but of the contending singularities, only the $\frac{1}{\sqrt{r}}$ kind insures that physically meaningful boundary conditions are satisfied. Thus, only this solution qualifies as a candidate to be *useful* in physical applications. Such an analysis will be carried out as the next step in currently ongoing research.

2.7 Summary and Conclusions

This report presents work done towards the extension of the extant coupled theory of thermomechanical diffusion [1] to enable analysis of diffusion in stressed solids in the presence of cracks. This investigation was sponsored by the Los Alamos National Laboratory in an effort to understand better the phenomenon of stress assisted diffusion in cracked structures operating in corrosive environments. This document constitutes the final report for that sponsored project.

Earlier project reports [2,3] included here as appendices A and B discuss the proof of existence of admissible singular solutions for concentration profiles in crack tip neighborhoods. Both transient and steady state solutions were obtained under certain limiting assumptions. Numerical simulation using quarter point finite elements supported the theoretical predictions. The nature of the singularity obtained differs from that obtained by Gdoutos and Aifantis [4], and in order to determine the reasons for this apparent discrepancy, a comparison of the two theories was undertaken.

Though the methodology of Girrens [1] and Aifantis [5,6,7] overlap to some degree, significant differences exist in the assumptions made at various stages of the formulation. These similarities and differences have been pointed out in the body of the this report.

Briefly, the fundamental differences include : (1) Girrens models the gas+solid combination as a single continuum or mixture and retains all possible coupling effects in modeling the mixture, thus implicitly, allowing both the diffusing species and the parent material to influence each other freely without external stipulations. (2) Aifantis introduces three new quantities, $\hat{p}$, e and m , and stipulates that the effects of the solid on the constitutive model of the gas are captured thereby. He further assumes that the solid is unaffected by the presence of the gas while certain thermomechanical variables of the solid are allowed to enter the constitutive model of the gas. Thus the rigor of modern continuum mechanics that is employed in deriving the constitutive class of the gas is not retained in the treatment of the solid.

A direct comparison of the governing partial differential equations proposed by the two theories was made for the isothermal case and as a direct consequence of the different approaches outlined above, different equations and solutions resulted. Mathematical details and step-by-step comparisons have been included in the body of the report above. The successful application of the admissible solutions obtained to physical problems hinges on their satisfying physically meaningful boundary conditions and this remains to be investigated.

In conclusion, an advance has been made in understanding the nature of solutions that can be obtained in predicting concentration profiles in stressed solids in the neighborhood of existing cracks. Further mathematical formalism to extend the results obtained and broaden the scope of application is underway. Work has also been initiated towards incorporating the results obtained from theoretical investigations into a viable design tool in the form of a finite element model.

The results and discussion presented in two earlier progress reports and the

present final report are a result of investigation that was begun under the sponsorship of Los Alamos National Laboratory in August 1990 and concluded in February 1992. The graduate student conducting the research was also pursuing fulltime coursework toward a Ph.d degree during this period. These and other results obtained from ongoing investigation will appear in a doctoral dissertation and are expected to be published in the open literature.

2.8 Plan for Remainder of Research

The existence of the singularity in concentration profiles in crack tip neighborhoods, when the diffusion is driven by the mechanical response alone, has been established as theoretically admissible. Both steady state and transient solutions have been obtained within the framework of the extant theory of 'Coupled Thermomechanical Diffusion of Mobile Constituents in a Deformable Solid'. The next step is to study the effects of other coupling effects outlined in Report II, Appendix I [3], and also determine if physically meaningful boundary conditions can be realised by employing the solution obtained. If this turns out to be the case, the existence of an extended class of coupled thermomechanical diffusion problems in the presence of cracks, all within the framework of the theory and assumptions of Girrens' theory will have been formally established.

To enable fruitful application of this extended theory to real world physical problems, a failure theory with criteria involving new parameters defined in this theory will have to be established. Following existing parallels with the classical theory of linear elastic Fracture Mechanics, it is proposed that a failure criterion akin to the Strain Energy Release Rate argument proposed by Irwin may exist and if it turns out that such is the case, it will be incorporated in the failure model. If not, an alternative failure theory with different failure criteria will have to be identified.

To further facilitate applications, a working finite element code incorporating modeling abilities and the design parameters identified in the above process will be developed. Some details of the proposed code development were outlined in Report II [3]. Such a design tool would find application in the analysis of structures with crack defects operating in corrosive environments.

2.9 References

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APPENDIX A

A Appendix A : Progress Report I

The research being conducted involves extension of the extant "*Coupled Thermomechanical Diffusion Theory*" [1], to enable prediction of diffusion in stressed solids, in the presence of cracks. From Fracture Mechanics, we know that stress singularities exist at the crack tip and this is expected to influence the diffusion behavior in the vicinity of the crack tip. To incorporate this in the existing finite element model [1], it is necessary to employ special elements that correctly model the singular behavior of the stresses. A singular behavior is also expected to emerge from the governing diffusion equations. The form of the equations is such that a singular solution is admissible but the theoretical foundation for this assertion needs to be established yet.

The initial step in conducting the research has been to assemble the building blocks needed to conduct coupled thermomechanical diffusion analyses in the neighborhood of crack tips. The Fall semester of 1990 was dedicated to conducting this step. Two elements of code were identified, assembled to operate in the CSU computing environment and run for test cases with known results. The following paragraphs describe what was done.

First, an existing finite element code HDMSNG was identified and made to operate in the CSU computing environment. It was necessary to translate this code from punch card format. The code was used to model the state of stress in a 2-D rectangular isotropic specimen with a double-edge crack, under a uniform tension loading [2]. The model employs eight-noded quadrilateral elements to generate the mesh except in the immediate vicinity of the crack tips. The crack tips are surrounded by special "assumed displacement hybrid elements" which contain proper singular displacement and stress fields [3,4]. Results for this sample problem are readily available in the literature and comparisons with the program run agreed closely [5]. HDMSNG in its present state does not model diffusion, so, as the research progresses, it will be necessary to formulate and implement a version of the singular element which does model diffusion.

Secondly, the code titled PSTDIF [1], was received electronically from LANL and successfully modified to operate in the CSU computing environment.

The existing code PSTDIF performs non linear thermoelastic analysis of stress assisted diffusion, transient in temperature and concentration, with inertia neglected. Results from a sample program run at CSU were identical to the sample output from an independent run at LANL. The sample problem modeled was a wedge-opening loaded plane strain compact tension specimen.

Thus the current status of the research is that the singular crack tip element code is operating correctly as is the coupled diffusion code.

The immediate objective is to incorporate the "assumed displacement hybrid finite element" in PSTDIF to enable it model stress singularities introduced in the presence of cracks. The next step would be to conduct a theoretical investigation into the behavior of the diffusion equations in the vicinity of the crack tip and implement this to enhance the present model. The validity of the model will then be tested on sample problems for which theoretical and /or experimental results are

available in the literature.

The project formally began in May 1990, and the graduate research assistant began work on August 10, 1990. The reported progress took place during the fall semester while the student was also pursuing course work.

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APPENDIX B

B Appendix B : Progress Report II

In a previous report [1], it was asserted that a singular solution was admissible for the concentration field as predicted by the " *Coupled Thermomechanical Diffusion Theory* " [2], in the immediate vicinity of crack tips. Mathematical formalism to support this assertion has now been established. Numerical simulation of plane problems using quarter point finite elements to model the diffusion behavior confirms the presence of this singularity. To better model the singular behavior in the crack neighborhood, a hybrid finite element similar to HDMSNG developed by Atluri et al [3,4], can be built. As noted in [1], HDMSNG currently, does not model diffusion. In light of evidence presented below, the new hybrid element when constructed, would become a powerful tool to model thermo-mechanically assisted diffusion in the presence of cracks.

B.1 Theory and Analysis

The fully coupled equations describing thermo-mechanical diffusion have been developed in [2]. A summary of the influence of the various coupling co-efficients is presented in tabular form in Appendix I.

In order to isolate the influence of the mechanical response on the concentration field, only the piezo diffusive co-efficient M and the diffusion co-efficient D are retained. Isothermal conditions are assumed. Specifically, the setting of β_c to zero assumes that the effect of the diffusion on the mechanical response is small. A closed form solution including this effect is permitted by the theory and will be attempted later. As pointed out in [2], the theory proposed by Aifantis and Gerberich ignores the effect of the concentration solution on the mechanical response and that of temperature on the diffusion.

Appendix II presents an admissible solution to the concentration field as determined by the governing equations simplified by the above assumptions. This solution is obtained by inspection and supports the intuition that the concentration field is driven by the strain dilatation field. Note that the relationship between concentration and strain dilatation is linear and the singularity in both is of the type $1/\sqrt{r}$. Recently, Gdoutos and Aifantis [10] established a relation between concentration and the stress intensity factors in modes I and II based on Aifantis' theory [11], however, the order of the singularity obtained therein is dependent on M/N .

Appendix III is a solution to the transient problem under the same assumptions as above using classical transform techniques. The singularity is embedded in a series solution and its effect must be studied by including sufficient terms from the series expansion.

B.2 Numerical Results

Results from a finite element simulation of a standard compact tension sample [5] with uniform initial concentration under isothermal conditions appear in Appendix IV. Quarter point elements are employed to model the singular behavior in the vicinity of the crack tip.

Comparison of figures (1) and (2) reveals that the concentration profile follows that of the normal stress σ_{yy} closely, indicating qualitatively that the two quantities have similar singular behavior close to the crack tip.

Figures (3) and (4) are log-log plots of the same concentration and stress profiles. A linear behavior (with slope -0.5) in the neighborhood of the crack tip reveals that the singularity modeled is in fact of the type $1/\sqrt{r}$.

Figures (5) and (6) are the mesh used and a contour plot of the concentration profile obtained.

The use of finite elements raises the issue of correct numerical modeling of the singular behavior of the variables of interest at the crack tip. An assessment of the use of quarter point elements in achieving this is presented in [8] and [9]. In this technique, parameters of primary interest in design, such as stress intensity factors and similar parameters describing the diffusion would have to be approximated a-posteriori by curve fitting techniques during post processing. The use of a hybrid element as described in [3,4], would yield such parameters directly in the solution vector (as Lagrange multipliers) with far greater accuracy.

B.3 Summary and Conclusions

The objective of establishing the singular behavior of concentration profiles in crack neighborhoods has been realised under certain limiting assumptions. Investigation of a broader class of problems within the framework of the fully coupled theory [2], is underway. Finite element simulations for test problems have yielded results that support both intuition and mathematical formulations at hand. Motivated by this, a more sophisticated modeling tool incorporating a hybrid finite element that will yield stress and concentration profiles and other parameters of interest will be built. A failure model to address the material degradation due to the diffusion of the solute species will also be proposed.

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B.4 Appendix I : Coupling Effects

No	Effect of (Response)	On (Response)	Controlled By	Co-efficient
1	Mechanical	Thermal	N	Piezo-thermal
2	Mechanical	Diffusive	M	Piezo-diffusive
3	Diffusive	Mechanical	β_c	Soret
4	Diffusive	Thermal	B	
5	Thermal	Mechanical	β_θ	Dufour
6	Thermal	Diffusive	A	

Other co-efficients that bear a direct influence on the themomechanical diffusion process include.

K = thermal conductivity

D = diffusion co-efficient

ω = material constant relating concentration to entropy

ζ = material constant relating concentration to chemical potential

B.5 Appendix II : A steady state solution

In order to discover the effect of the mechanical response alone on diffusion, all other coupling effects listed in Appendix I are ignored. Isothermal conditions are assumed. Thus, the following co-efficients are set to zero. $A, B, N, \beta_c, \beta_\theta = 0$. The governing equations then reduce to the following.

(a) Momentum Balance

$$[G(u_{i,j} + u_{j,i}) + (\lambda e - \beta_\theta \theta)]_{,j} + \rho f_i = 0 \quad (41)$$

(b) Mass Balance or 'Diffusion Equation'

$$Dc_{,ii} - Me_{,ii} = 0 \quad (42)$$

(c) The Energy equation is trivially satisfied if ω and ζ are zero. Rewriting (2) as

$$\left(C - \frac{M}{D}e\right)_{,ii} = 0 \quad (43)$$

by inspection, it is noted that $c = \gamma e + \text{constant}$ is a solution to (3) provided $e_{,ii}$ and $c_{,ii}$ are both not zero. Note that for M or D to have any effect on the solution, $e_{,ii}$ must hold. Whether $e_{,ii}$ holds in a given problem is determined by the solution of (1). e can be computed after (1) is solved for the displacements.

Example. An infinite plate with a crack is subjected to a biaxial stress as shown in figure (B) where the symbols have their usual meaning.

The boundary conditions are,

- (i) $\sigma_y = 0$; $-a < x < a$; $y = 0$
- (ii) $\sigma_y \rightarrow \infty$; $as x \rightarrow \pm\infty$
- (iii) $v = 0$; $|x| \geq a$, $y = 0$
- (iv) $\frac{\partial c}{\partial y} = 0$, $|x| \geq a$

Let the solution for u and v be of the form,

$$u = K_I \sqrt{r} f_1(\theta)$$

$$v = K_I \sqrt{r} f_2(\theta)$$

where,

$$r = \sqrt{(x-a)^2 + y^2}$$

$$\theta = \tan^{-1} \frac{y}{x-a}$$

Now,

$$e = e_{11} + e_{22} \text{ where } e_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$$

$$\text{or, } e = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}$$

Plugging for u and v from above, we have

$$e = \frac{\partial}{\partial x}[K_I \sqrt{r} f_1(\theta)] + \frac{\partial}{\partial y}[K_I \sqrt{r} f_2(\theta)]$$

$$\begin{aligned}
e &= K_I \left[\frac{1}{2\sqrt{r}} \frac{\partial r}{\partial x} f_1(\theta) + \sqrt{r} \frac{df_1(\theta)}{d\theta} \frac{\partial \theta}{\partial x} + \frac{1}{2\sqrt{r}} \frac{\partial r}{\partial y} f_2(\theta) + \sqrt{r} \frac{df_2(\theta)}{d\theta} \frac{\partial \theta}{\partial y} \right] \\
\text{Computing } \frac{\partial r}{\partial x}, \frac{\partial r}{\partial y}, \frac{\partial \theta}{\partial x}, \frac{\partial \theta}{\partial y}, \text{ and plugging into the above expression for } e, \text{ we have,} \\
e &= K_I \left[\frac{1}{2\sqrt{r}} \cos \theta f_1(\theta) + \sqrt{r} \frac{df_1(\theta)}{d\theta} \left(-\frac{\sin(\theta)}{r} \right) + \frac{1}{2\sqrt{r}} \sin \theta f_2(\theta) + \sqrt{r} \frac{df_2(\theta)}{d\theta} \left(-\frac{\cos(\theta)}{r} \right) \right] \\
e &= K_I \left[\underbrace{\frac{1}{\sqrt{r}} \left(f_1(\theta) \frac{\cos(\theta)}{2} - \sin(\theta) \frac{df_1(\theta)}{d\theta} \right)}_I + \underbrace{\frac{1}{\sqrt{r}} \left(f_2(\theta) \frac{\sin(\theta)}{2} + \cos(\theta) \frac{df_2(\theta)}{d\theta} \right)}_{II} \right] \\
e &= \frac{K_I}{\sqrt{r}} F \left(\theta, \frac{df_1}{d\theta}, \frac{df_2}{d\theta} \right) \tag{44}
\end{aligned}$$

where, $F(\theta, \frac{df_1}{d\theta}, \frac{df_2}{d\theta}) = (I) + (II)$

If $e_{,ii} \neq 0$, and $c_{,ii} \neq 0$, then, $c = \frac{M}{D} e$ is an admissible solution to (3)

$\Downarrow$, from (4)

$$c = \frac{MK_I}{D\sqrt{r}} F \left(\theta, \frac{\partial f_1}{\partial \theta}, \frac{\partial f_2}{\partial \theta} \right) \tag{45}$$

where, M is the piezo-diffusive co-efficient, N the diffusion co-efficient, and K_I the stress intensity factor (Mode I). For the Neumann boundary conditions considered, it can be shown from elementary theory of partial differential equations, that the uniqueness of this solution is guaranteed to within an additive constant.

ie, $c = \frac{M}{D} e + \text{an additive constant.}$

B.6 APPENDIX III : A transient singular solution

OBJECTIVE

To obtain an analytical solution to the following non homogeneous, boundary initial value problem.

Governing equation

$$c_{,t} - Dc_{,ii} = -Me_{,ii} \quad (46)$$

in $\Omega, t > 0$.

Boundary Conditions

$$\alpha_i \frac{\partial c}{\partial n_i} + \gamma_i c = g_i(x, y) \quad (47)$$

on $\Gamma_i, t > 0$

Initial condition

$$c = f(x, y) \quad (48)$$

in $\Omega, t > 0$.

Typical Geometries of Interest are sketched in figure (A). Assumptions

1. The mechanical problem has been solved using conventional techniques of Linear Elastic Fracture Mechanics. Therefore $e(x, y)$ in the governing equation (1) is known.
2. In obtaining the solution in (1) and all that follows, isothermal conditions prevail.

Integral Transform and Inversion Formula

The Fourier transform for a finite region, $0 \leq x \leq L$ and its inversion formula are defined as,

Integral transform

$$\bar{F}(\beta_m) = \int_0^L K(\beta_m, x) F(x) dx \quad (49)$$

Inversion formula

$$F(x) = \sum_{m=1}^{\infty} K(\beta_m, x) \bar{F}(\beta_m) \quad (50)$$

where, $K(\beta_m, x)$ is called the transform kernel and the β_m s are the eigen values. The type of kernels and eigenvalues to be used in (4) and (5) depends on the combination of boundary conditions at $x = 0$ and $x = L$. Two and three dimensional problems can be solved by repeated application of (4) and (5) for x , y , and z space variables in the bounded regions $0 \leq x \leq a$ and $0 \leq y \leq b$.

Essentially, (4) represents an arbitrary function $F(x)$ in the interval $0 \leq x \leq L$ in an infinite series of the eigenfunctions $K(\beta_m, x)$ all of which are orthogonal and the summation is taken over all the eigenvalues β_m .

The contribution of each eigenfunction to the expansion is given by $\bar{F}(\beta_m)$, ie, (5) the Fourier transform. For further details on the determination of $K(\beta_m, x)$ and the β_m s for various combination of boundary conditions, see Ozisik's 'Boundary Value Problems of Heat Conduction', [10].

Application to a 2-D Rectangular Domain

Consider the crack problem described by the geometry sketched in figure (A1). Assume that the mechanical boundary value problem has been solved. Thus, $e(x, y)$ is known.

$$Dc_{,ii} - Me_{,ii} = c_{,t} \quad (51)$$

in $-2a \leq x \leq 2a$, $-b \leq y \leq b$, $t > 0$. Here, c is the concentration and e the strain dilatation; D and M are phenomenological constants listed in Appendix I and [1].

The boundary conditions are given by,

$$\alpha_i \frac{\partial c}{\partial x} + \gamma_i c = g_i(y, t) \quad (52)$$

on Γ_i , where $i = 1, 2, 3, 4, 5$ as shown in the figure, $t > 0$

Initial condition is $c = f(x, y)$ in Ω , $t = 0$.

The double integral transform and the corresponding double inversion formula are defined respectively as,

$$\bar{c}(\beta_m, \nu_n, t) = \int_0^L \int_0^L K(\beta_m, x) K(\nu_n, y) \cdot c(x, y, t) dx dy \quad (53)$$

$$c(x, y, t) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} K(\beta_m, x) K(\nu_n, y) \cdot \bar{c}(\beta_m, \nu_n, t) \quad (54)$$

For the boundary conditions of the type specified in (7) through (11), the kernels $K(\beta_m, x)$ and $K(\nu_n, y)$ are given by

$$K(\beta_m, x) = \sqrt{2} \frac{\beta_m \cos \beta_m x + H_i \sin \beta_m x}{[(\beta_m^2 + H_i^2)(L + \frac{H_{i+1}}{\beta_m^2 + H_{i+1}^2}) + H_i]^{1/2}} \quad (55)$$

where, the β_m s are the roots of,

$$\tan \beta L = \frac{\beta(H_i + H_{i+1})}{\beta^2 - H_i H_{i+1}} \quad (56)$$

where $H_i = \frac{\gamma_i}{\alpha_i}$, and L = the range of the spatial variable. [10].

To get $K(\nu_n, y)$, replace β by ν and x by y in the above expressions.

Taking the double transform of the equation (6),

$$\underbrace{\int_{-2a}^{2a} \int_{-b}^b K(\beta_m, x) K(\nu_n, y) \cdot D \cdot \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) dx dy}_{I_1} - \underbrace{\int_{-2a}^{2a} \int_{-b}^b K(\beta_m, x) K(\nu_n, y) \cdot M \cdot \left(\frac{\partial^2 e}{\partial x^2} + \frac{\partial^2 e}{\partial y^2} \right) dx dy}_{I_2} = \frac{d\bar{c}}{dt} \quad (57)$$

where, $\bar{c}(\beta_m, \nu_n, t)$ is the double transform of c as defined above.

Evaluation of I_1 and I_2

It is first necessary to state that $K(\beta_m, x)$ are the normalised eigenfunctions which satisfy the following auxiliary eigenvalue problem. [Ozisik].

$$\nabla^2 K + \beta^2 K = 0 \quad (58)$$

$$0 \leq x \leq L,$$

$$\alpha_i \frac{\partial K}{\partial n_i} + \gamma_i K = 0 \quad (59)$$

on Γ_i

Similarly for $K(\nu_n, y)$.

I_1 may now be evaluated by applying Green's theorem as follows.

Evaluation of Integral I_1

Green's second identity may be stated as,

$$\int_{\Omega} (u \nabla^2 v - v \nabla^2 u) d\Omega = \int_S (u \frac{\partial v}{\partial n} - v \frac{\partial u}{\partial n}) dS$$

$$I_1 = \int_{-2a}^{2a} K(\beta_m, x) \cdot D \left(\int_{-b}^b K(\nu_n, y) \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) dy \right) dx \quad (60)$$

⇓

or,

$$I_1 = \int_{-2a}^{2a} K(\beta_m, x) \cdot D \cdot \left[\int_{-b}^b (I_3) \right] dx$$

$$\text{where, } I_3 = \int_{-b}^b K(\nu_n, y) \frac{\partial^2 c}{\partial x^2} dy + \int_{-b}^b K(\nu_n, y) \frac{\partial^2 c}{\partial y^2} dy$$

Applying Green's theorem,

$$I_3 = \int_{-b}^b c \frac{\partial^2 K}{\partial y^2} dy + \left[K(\nu_n, y) \frac{\partial c}{\partial y} - c \frac{\partial K(\nu_n, y)}{\partial y} \right]_{-b}^b + \left[\frac{\partial^2 c_y(\nu_n)}{\partial x^2} \right]_{-b}^b$$

The last term on the right hand side is the transform in the y direction of $\frac{\partial^2 c}{\partial x^2}$ in the interval (-b,b). The first integral on the right hand side can be evaluated by multiplying the auxiliary eigen equation (13) by c and integrating from -b to b. Therefore,

$$I_3 = -[\nu_n^2 \bar{c}_y(\nu_n)]_{-b}^b + \left[K(\nu_n, y) \frac{\partial c}{\partial y} - c \frac{\partial K(\nu_n, y)}{\partial y} \right]_{-b}^b + \left[\frac{\partial^2 c_y(\nu_n)}{\partial x^2} \right]_{-b}^b$$

and,

$$I_1 = \int_{-2a}^{2a} K(\beta_m, x) \cdot D \cdot \left(-\nu_n^2 \bar{c}_y(\nu_n) + \frac{\partial^2 c_y(\nu_n)}{\partial x^2} + \left[K(\nu_n, y) \frac{\partial c}{\partial y} - c \frac{\partial K(\nu_n, y)}{\partial y} \right]_{-b}^b \right) dx$$

The expressions in the box brackets may be evaluated using the boundary conditions (7) (i = 3, 4, 5) and (14) (check equation nos before final draft.) For example, after plugging for the partial derivatives,

$$\left[K(\nu_n, y) \frac{\partial c}{\partial y} - c \frac{\partial K(\nu_n, y)}{\partial y} \right]_{-b}^b = K(\nu_n, b) g_4(x, t) \frac{1}{\alpha_5} - K(\nu_n, -b) g_3(x, t) \frac{1}{\alpha_3}$$

Similarly, other terms (in box brackets above) can be evaluated. Thus, I_1 reduces to

$$I_1 = -D(\nu_n^2 + \beta_m^2) \bar{c}(\nu_n, \beta_m, t) + D \cdot [S_3]$$

where,

$$\begin{aligned} S_3 = & -\frac{K(\nu_n, -b)}{\alpha_3} \int_{-2a}^0 K(\beta_m, x) g_3(x, t) dx \\ & + \frac{K(\nu_n, b)}{\alpha_4} \int_{-2a}^0 K(\beta_m, x) g_4(x, t) dx \\ & + \frac{K(\nu_n, b)}{\alpha_4} \int_0^{2a} K(\beta_m, x) g_4(x, t) dx \\ & - \frac{K(\nu_n, -b)}{\alpha_3} \int_0^{2a} K(\beta_m, x) g_4(x, t) dx \\ & + \frac{K(\beta_m, -2a)}{\alpha_1} \int_{-b}^b K(\nu_n, y) g_1(y, t) dy \\ & - \frac{K(\beta_m, 2a)}{\alpha_2} \int_{-b}^b K(\nu_n, y) g_2(y, t) dy \end{aligned}$$

Evaluation of Integral I_2

$$I_2 = \int_{-2a}^{2a} \int_{-b}^b K(\beta_m, x) K(\nu_n, y) . M . \nabla^2 e \, dx \, dy$$

Since e has a singularity at the origin (0,0), the integral 'blows up' at the origin. The following integral, however, has meaning and is known as the Cauchy principal value (CPV) of I_2

$$CPV(I_2) = \lim_{\epsilon \rightarrow 0} [\int_{-2a}^{0-\epsilon} \int_{-b}^b K(\beta_m, x) K(\nu_n, y) . M . \nabla^2 e \, dx \, dy + [\int_{0+\epsilon}^{2a} \int_{-b}^b K(\beta_m, x) K(\nu_n, y) . M . \nabla^2 e \, dx \, dy]$$

Proceeding as in the case of I_1 and applying Green's second identity,

$$\int_{-2a}^{0-\epsilon} \int_{-b}^b K(\beta_m, x) K(\nu_n, y) M \nabla^2 e \, dx \, dy = \int_{-2a}^{0-\epsilon} K(\beta_m, x) M (-\nu_n^2 \bar{e}_y(\nu_n) + \frac{\partial^2 \bar{e}_y(\nu_n)}{\partial x^2}) + [K(\nu_n, y) \frac{\partial e}{\partial y} - e \frac{\partial K(\nu_n, y)}{\partial y}]_{-b}^b \, dx$$

Similarly for $\int_{0+\epsilon}^{2a} (\cdot)$ above.

The expression in the box bracket above can be evaluated since the solution for e is known in the entire domain, (e and $\frac{\partial e}{\partial y}$ are thus known), and by employing the boundary condition (14) and using orthogonality.

Thus, the Cauchy principal value of the integral can be evaluating by plugging these computed values back into the expression for CPV above and evaluating the limit as $\epsilon \rightarrow 0$ if it exists. Let this limit be L . Then, the CPV of I_2 may be written as,

$$CPV(I_2) = -M(\nu_n^2 + \beta_m^2) \bar{e}(\beta_m, \nu_n, t) + M.L \quad (61)$$

In view of this and the computed value of I_1 the transformed differential equation (12) reduces to the following.

$$\frac{d\bar{c}}{dt} + (\nu_n^2 + \beta_m^2) \bar{c} = D.(S_1) + M(\nu_n^2 + \beta_m^2) \bar{e} - M.L \quad (62)$$

The forcing term on the right hand side (R) is fully known and the solution is reduced to the transient solution of a first order ordinary differential equation.

Applying the double transform to the initial condition and denoting the transform of $f(x, y)$ by $f(\nu_n, \beta_m)$, using the theory of elementary ordinary differential equations, and the inversion formula (5), the solution may be written as

$$c = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} (K(\beta_m, x) K(\nu_n, y) . \exp[-(\nu_n^2 + \beta_m^2)t] . (\bar{f}(\nu_n, \beta_m) + A(t))) \quad (63)$$

where, $A(t) = \int_0^t \exp[(\nu_n^2 + \beta_m^2)t] \cdot R$

The singularity appears explicitly in R as $\bar{e}$. From Linear Elastic Fracture Mechanics, the singularity embedded in $\bar{e}$ is of the $\frac{1}{\sqrt{r}}$ kind.

(A1)

(A2)

Figure (A)

Figure (B)

APPENDIX - IV

SIGMA-y vs. DISTANCE (from crack tip)

Sigma-y x 1e04

Fig (1)

CONC vs. DISTANCE (from crack tip)

fig (2)

Log-log plot of Sigma-y vs Dist from crack tip

Log-log plot of Conc vs. Dist from crack tip

Y

CONCENTRATION DISTRIBUTION : 25 contours evenly spaced.

Fig (6)

Log(C-C0) vs Dist from crack tip

Y

X

SIGMA-y vs. DISTANCE (from crack tip)

Sigma-y x 10e-4

(Distance from Crack tip
+ 0.5)

CONC vs. DISTANCE (from crack tip)