THERMO-MECHANICAL CRACKING IN COATED MEDIA WITH A CAVITY BY A MOVING ASPERITY FRICTION

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Mechanical Engineering Department
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Technical Report No. ME-144(88)ONR-233-3

Work performed under ONR Grant No. 00014-84-K-0252

March 1988
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ACKNOWLEDGEMENT

The present research is performed under a grant from the Office of Naval Research, Grant No. N00014–84–K–0252. Dr. A. William Ruff was the program manager. Dr. Marshall Peterson is the program manager.
ABSTRACT

The research deals with the problem of asperity-excited thermomechanical field in a medium with a surface layer and a near surface void defect. The thermomechanical field governs the mode of cracking, which leads to failure in the wear surface. The presence and location of the void defect is most critical. This investigation obtained the solutions for the temperature distribution and the stress state in a layered medium with a rectangular cavity. This temperature distribution and stress state result when the solid medium is subjected to Coulomb frictional loading from an asperity moving at a moderately high speed (of approximately $10^{-15}$ m/s). In the analysis, the coated medium was represented by a solid half space, with a thin top surface-layer of solid wear material. The cavity defect required a mathematical model in terms of the material coordinates. The corresponding governing differential equations were time-explicit and transient. A general finite difference formulation was developed to calculate both the temperature and the stress fields. The energy balance method was applied at the corners of the rectangular cavity to resolve the problem of singularities in the temperature field. The stress singularity at each corner was represented by a special element that was introduced representing the behavior of the known stress singularity at the corner and its vicinity. The general equation of the stress field, including the dynamic term, is of the regular perturbation type. The small order dynamic term is demonstrated to be a higher order effect by perturbation method, thus negligible. Numerical solutions were carried out for the zeroth order approximation and the case of uniform asperity pressure distribution.

It was shown that, at moderately high asperity speed, the thermal stress effect dominates the combined thermo-mechanical stress field, which eventually leads to failure in the no-cavity case. When a defect, such as a cavity, exists, the stress state that determines the failure phenomenon is much more severe and can be quantified depending on the location of the cavity. These results are determined through a numerical computation based on the
material properties of Stellite III. However, the parametric effects of material variations in the coating and the substrate, including changes in both thermal and mechanical properties, were also considered. The study of the cavity location also established the existence of a critical cavity location for cracking by cohesive failure. This location is defined by the critical ligament thickness (thickness between the wear surface and the top edge of the cavity), at which the cavity-influenced thermal tensile stress reaches a maximum. This thickness is important to designers when cavities at coating/substrate interfaces are either unavoidable or too expensive to control in fabrication.
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<td>$a$</td>
<td>asperity width</td>
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<tr>
<td>$b$</td>
<td>substrate thickness</td>
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<td>$c_1$</td>
<td>The dilatational wave speed of the substrate</td>
</tr>
<tr>
<td>$c_2$</td>
<td>The shear wave speed of the substrate</td>
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<td>$c_{I}, c_{II}$</td>
<td>specific heat of the coating layer and the substrate, respectively</td>
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<td>$C(t)$</td>
<td>distance from $x_1$ origin to leading edge of the asperity</td>
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<td>$D$</td>
<td>dimensionless coating thickness ($=H/a$)</td>
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<td>$d$</td>
<td>half width of the cavity</td>
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<td>$e$</td>
<td>depth of the cavity</td>
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<td>$E_{I}, E_{II}$</td>
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<td>$H$</td>
<td>coating thickness</td>
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<td>$k_{I}, k_{II}$</td>
<td>thermal conductivity of the coating layer and the substrate, respectively</td>
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<td>$L'$</td>
<td>ligament thickness</td>
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<tr>
<td>$L$</td>
<td>dimensionless ligament thickness</td>
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<td>$M$</td>
<td>Mach number</td>
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<td>$P(i,j)$</td>
<td>center point of the finite difference cell</td>
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<td>$N, R, S, W$</td>
<td>surrounding points of $P(i,j)$</td>
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<td>$P'(x_1, t)$</td>
<td>pressure over the contact area</td>
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<td>$P_0$</td>
<td>average pressure over the contact area</td>
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<tr>
<td>$q(x_1, t)$</td>
<td>heat flux through the contact area</td>
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<tr>
<td>$q_0$</td>
<td>average heat flux through the contact area</td>
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<tr>
<td>$Q^*$</td>
<td>dimensionless heat flux through the contact area ($=q/q_0$)</td>
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heat flux from point S to point P

Péclet number of the coating layer and the substrate, respectively

temperature

displacement in \( x_1 \) and \( x_2 \) direction, respectively

dimensionless displacement in \( \xi \) and \( \eta \) direction

internal energy of the point \( P(i,j) \)

traverse speed of the asperity

material coordinates fixed to the cavity

width of the plate

half width of the plate

coefficient of the thermal expansion of the coating and the substrate, respectively

the material region: I for the coating layer; II for the substrate

mass density ratio \( \rho_\beta / \rho_1 \)

Kronecker delta

dimensionless coordinates \( = (x_1/a, x_2/a) \)

coordinates in transformed plane

thermal diffusivity of the coating layer and the substrate, respectively

Lamé constants

Coulomb coefficient of friction

thermal conductivity ratio \( = k_{II} / k_1 \)

thermal diffusivity ratio \( \Omega = k_{II} / \kappa_1 \)

stress field
\[ \sigma_{\xi\xi}, \sigma_{\eta\eta}, \sigma_{\xi\eta} \]

- Dimensionless stress field \(=\sigma_{11}/P_0, \sigma_{12}/P_0, \sigma_{22}/P_0\)

\[ \sigma^T \]

- Dimensionless thermal principal stress

\[ \sigma^M \]

- Dimensionless mechanical principal stress

\[ \sigma^C \]

- Dimensionless combined principal stress

\[ \phi \]

- Dimensionless temperature \(=Tk/q_0a\)

\[ \rho \]

- Mass density

\[ \tau \]

- Dimensionless time \(=Vt/a\)
CHAPTER 1

INTRODUCTION

1.1 Statement of Problem

This investigation studies the thermomechanical cracking in a coated medium with a near surface cavity. Such cavity generally occurs in the neighborhood of the coating/substrate interface, as a result of either inclusion or poor bonding during the coating process. A typical geometry of the cavity can be shown as in Figure 1.1. To facilitate the analysis, this research will first study the effect of a rectangular cavity. The general failure mechanism is caused by the frictional excitation of a moderately high speed asperity traversing over a coated surface. The understanding of this failure process will improve the design of the modified wear surface by alleviating the problem of friction cracking or delamination.

When two flat solids, which are placed in contact under heavy loads, slide relative to each other, the nominal design pressure between the mating surfaces is based upon the nominal design contact area. When the contact pressure is evenly distributed according to design, the service life of the solids is not a serious problem, even at a high rubbing speed. However, at high operating speed, the real contact area can be reduced by several orders of magnitude. As a result, a low design pressure may result in a very high interfacial pressure, thus a very high dry frictional force in the real contact area. Kennedy [1] showed that the size of the real contact area depends on operating speed and material parameters such as thermal
Figure 1.1 A layered medium with a cavity.
conductivity and wear resistance. He concluded that decreasing thermal conductivity, increasing wear resistance and increasing operating speed will reduce the real contact area. It was shown that, for a conservative areal ratio (contact area/nominal area) of $10^{-3}$ (Burton [2] considered $10^{-4}$ as a possible areal ratio), a low design pressure of 240 kPa (35 psi) could result in a 240 MPa (35,000 psi) local pressure in the contact zone. The high friction would generate locally an extremely high temperature, which was called "flash temperature" by Archard [3]. The local contact area is called "red banding" or "hot spot" [4], which has been experimentally demonstrated. In severe cases the temperature can be extremely high, leading to cracking of the surface [5]. This phenomenon is called "heat checking" or "thermocracking" [6]. It is frequently seen in seal rings, brakes, and rail-wheels [7,8,9,10,11,12] as shown in Figures 1.2 and 1.3. In general, it was observed that numerous radial cracks developed perpendicular to the sliding direction and almost periodically along the circumference. In order to understand these failures, in recent years, there has been increased emphasis in finding a solution of failure control, both experimentally and analytically.

1.2 Related Investigation in Progress

The phenomenon of high temperature "hot spot" was observed in the experiments by Archard [3]. A general survey of the problem of cracking through the development of a frictional hot spot was discussed by Burton [4]. Proof of the existence of hot patches of solid-to-solid contact was obtained experimentally by Bannerjee and Burton [13] in the case of metallic rings rotating against a non-metallic disk and, more recently, in actual operating face seals by Kennedy [14]. The latter
Figure 1.2 Radial hairline cracks on the metallic ring after running against a carbon ring at a high peripheral speed.

Figure 1.3 Thermal cracks on the brake shoe.
study made use of a new contact probe which enables the monitoring of contact patch sizes and locations in ring-on-ring or ring-on-disk configurations. It was proven to be quite effective in determining the geometry and movement of contact patches in dry operation of mechanical face seals. In his earlier experiment [15], Kennedy used a carbon ring against a metallic mating ring made from 440 C stainless steel, beryllium copper or 52100 bearing steel under both dry and liquid lubricated conditions. In these experiments, the existence of distinct spot asperities on the metallic ring was also observed. It was found that the spots tend to remain stationary with respect to the metallic mating ring of the seal, whether that ring is stationary or rotating. However, other investigations have shown hot patches moving relative to the mating ring and stationary on the primary ring [13,16]. Burton [17] also reported that, for an aluminum ring sliding on a glass disc, the hot spot precessed at a much lower speed than the rubbing speed. The uncertainty of this observed discrepancy on the speed of the moving asperities remains, but there is no doubt about the existence of the moving asperities due to thermoelastic instability on mechanical face seals. Several analytical studies of the failure due to the existence of the moving asperities have been developed. Surface displacements, temperature field and stress state of a convective elastic half space under an arbitrarily distributed fast-moving line heat source were obtained, using integral transform techniques, by Ling et al [18,19,20] and Mow and Cheng [21]. Kilaparti and Burton [22] have developed an exact Fourier series solution for a periodic strip heat input. Their series is rather unwieldy, but, at large Peclet number (R=Va/κ), it reduces to a form [23] that is simpler than that of Ling and Mow [18].
Recently, Barber [24] employed the Green's function for the problem of Kilaparti and Burton, and obtained the thermoelastic displacements and stresses due to a heat source moving over the surface of a half plane. A finite element analysis was developed by Kennedy [25] to study the surface temperatures resulting from frictional heating in sliding systems. He also applied finite element techniques to study the stresses in the mechanical face seals [6] and showed that the dominant stresses in the seal components are thermal stresses. The surface stress component (parallel to the surface) resulting from a periodic row of moving hot patches, with width $2a$ each, and a spacing of $2m$ was investigated by Tseng and Burton [26]. They concluded that the tensile stress would appear instantaneously with each passage of the heat source. Two-dimensional models of heat checking in the contact zone of a face seal were presented by Ju and Huang [27]. Because of the three-dimensional aspect of those observed "hot spots", Ju and Huang reformulated the problem in three-dimensional theory of thermoelasticity [28,29,30]. The investigation concluded that the highest tensile stress occurs, for an asperity speed of 10-15 m/s (400-600 in/s), at a depth of the order of one-tenth the asperity size. This depth defines the critical depth of the material. The physical depth is therefore 50-100 $\mu$m. At such a asperity speed, the stresses from the thermal effect of the asperity friction are an order of magnitude larger than those from its mechanical traction effect. Ju and Huang [31] also demonstrated that, when asperities excite the surface periodically in close intervals (a numerical example used a spacing of twelve asperity size), the thermomechanical effects accumulate, yet tending to a limiting magnitude, even though the
mechanical stress dissipates with no residue effect. The cumulative effect definitely depends on the interval of periodic excitations. At a relatively large interval of approximately 1000 asperity size, no cumulative effect is evident.

For improvement of the wear property of the surface, recent effort has been directed toward surface modifications. Research to understand the behavior of coated surfaces under asperity excitation, hence, has gained importance. Ju and Chen [32,33] first solved for the case of a moderately thick coating (thickness of the order of the asperity size). Later Ju and Liu [34] extended the general formulation of [32,33] to study the thickness effect of the coating layer for various mechanical and thermal impedance matchings between the surface coating layer and the substrate. It is concluded by Ju et al that: (i) a stiff surface layer would result in higher thermal stress; (ii) the stress state in layered media is influenced by the layer thickness, reaching a worst state when the coating layer thickness is in the neighborhood of the critical depth; (iii) a substrate of lower thermal expansion coefficient, higher Young's modulus, higher thermal conductivity and capacity will result in lower stresses in the coating layer; (iv) for the thin coating layer, the shearing stress at the coating/substrate interface is by no means trivial, depending again on the surface coating thickness. The interface shear reaches a maximum when the coating thickness is in the neighborhood of the thermal layer. These results are important for designing the bonding of the surface coating.

In the previous work on the moving asperity problem, the analyses dealt with basically uniform solid media; that is, the material and asperity properties are invariant in the direction of the asperity
motion. In such cases, since the time effect can be rendered implicit in the Fourier and the Navier equations by using a coordinate system fixed to the traversing asperity (called the convective coordinate system), the resulting solutions are steady-state. However, when the material has a cavity, uniformity in the direction of the asperity motion no longer exists. Consequently, a coordinate system fixed either to the cavity or to the material (referred to as the material coordinates) must be employed. The governing equations and their solutions, therefore, are transient. The present investigation not only obtains the temperature field solutions but also analyzes the stress field caused by the input of a moving heat source. In this study, since the Fourier and the thermoelastic Navier's equations in the material coordinates are time explicit, the finite difference method is considered more appropriate. Although a specific numerical solution does not show the effects of parameters, a general trend of the parameters effects can be obtained with adequate numerical solutions for a series of given parametric values.

1.3 General Theory

The phenomenon of thermomechanical cracking, as observed from experiments and operational damages, is connected with relatively hard materials; such as cast iron and Stellite III. Blau [35] and Ruff and Blau [36] demonstrated experimentally that the plastic wear and surface shear for hard wear material are restricted to a very thin surface layer (about 4–8μ). Ju et al [27,28,29,30,33,34] also proved that the critical depth is at a depth of an order of magnitude larger than plastic depth. Therefore, the linear thermoelastic theory holds. The basic mathematical formulation of uncoupled thermoelasticity consists
of the following equations:

\[ \mu V^2 u + (\lambda + \mu) \text{grad div } u - (3\lambda + 2\mu) \alpha \text{grad } T = \rho \ddot{u} \quad (1.1) \]

and \[ kV^2 T = \rho c \ddot{T} \quad (1.2) \]

where \( T \) and \( u \) are temperature and displacement fields, respectively, \( k \) is the thermal conductivity, \( \rho \) is the mass density, \( c \) is the specific heat, \( \lambda, \mu \) are the Lamé constants, and \( \alpha \) is the coefficient of thermal expansion. The coupling term is negligible except for conditions in which the temperature distributions have sharp variations in their time histories, which often occurs during the propagation of thermoelastic waves in the aftermath of thermal shocks [37, 38, 39, 40, 41, 42]. For the current problem, since the asperity speed under consideration is much slower than the elastic wave speed, the uncoupled thermoelastic theory is applied.

The dynamic effect may result from either a dynamic loading state or a non-steady thermal state in which the time rate of temperature change could keep up with the stress waves in the material. Duhamel [43] stated that the inertia term can be disregarded if the time rate of change of temperature is slow enough. Parkus [44] showed that the significant effect from the inertia term can arise only when there is an instantaneous change in the surface temperature or in the temperature of the surrounding medium. In fact, the dynamic effect is greatly reduced if the temperature change occurs in a very short, but finite, interval of time. This was confirmed by Danilovskaya [45, 46], who studied the dynamic effect due to a thermal shock on the surface of
a half-space and demonstrated that the maximum dynamic stress is reduced to 86% even for the extremely short duration heating of $10^{-12}$ seconds. In general, under usual conditions of heat exchange, the rate of temperature change is small in comparison with the speed of sound in the material. Thus, at any instant, the thermal stress state can be determined by the instantaneous values of the temperature field.

For the cavity problem, the effect of the dynamic term in Equation (1.1) will be studied quantitatively with a perturbation method. That is, the solution to Equation (1.1) can be expressed in an asymptotic series. Substituting this series into Equation (1.1) leads to a set of linear equations for $u$. Each set of linear equations represents a different order of solution of the asymptotic series. The details of the perturbation procedure will be addressed in Chapter 4.
CHAPTER 2

ANALYTICAL MODEL AND BASIC EQUATIONS

The experiments performed by Kennedy [47] have shown that contact between two flat conforming rings is concentrated in several (1 to 5) patches, with a few small solid-solid contact spots occurring within each patch. Each contact spot is identical and the contacts are equally spaced around the ring circumference. A ring could therefore be divided into as many sections as the number of contact spots and only one such section would have to be analyzed. Kennedy [15] also proved that the width of the contact spot (asperity) is about 0.1 to 1 mm (0.004 to 0.04 in.); however, the size of a typical mating ring is several orders of magnitude larger than the asperity size. Because of this size difference between the contact area and the mating rings, the analytical model is represented by a semi-infinite body with a thin coating layer and a rectangular cavity in the neighborhood of the coating layer/substrate interface. The half space surface is subjected to the frictional heating of a moving asperity over the wear surface (Figure 2.1), and the material coordinate system (fixed to the cavity) is used. As presented in Chapter 1, the linear thermoelastic theory applies for the current problem. The advantage of the linear theory is the application of the superposition principle, which allows a separation of the stress field to a contribution of the mechanical load of the pressure and friction from the moving asperity and another contribution of the heat input from the rate of the frictional energy dissipation. The combined effects will then determine the possibility
Figure 2.1 Two-dimensional model of a coated wear surface with a cavity.
of fracture initiation. The governing differential equations for the temperature and the stress fields are the Fourier equation and the thermoelastic Navier's equation, respectively.

2.1 Temperature Field

The governing equation for the temperature field is

$$\frac{\partial}{\partial x_1} \left( k \frac{\partial T}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left( k \frac{\partial T}{\partial x_2} \right) = \rho c \frac{\partial T}{\partial t} \quad (2.1)$$

where \( T \) is the temperature; \( k \) is the thermal conductivity; \( \rho \) is the mass density; \( c \) is the specific heat; and \( \beta \) denotes the layered region: I for the coating surface, II for the substrate.

The temperature field \( T \) must satisfy the initial condition,

$$T^B(x_1, x_2, 0) = 0, \quad (2.2)$$

and the boundary conditions:

(i) The regularity condition holds at infinity \((x_1^2 + x_2^2 = \infty)\),

$$T^B = 0. \quad (2.3)$$

(ii) In the asperity contact surface \((c(t) \leq x_1 \leq c(t) + a, x_2 = 0)\), the maximum heat input through the boundary is the rate of the frictional energy

$$-k_i \frac{\partial T^I}{\partial x_2} = q = \mu_f Vp'(x_1), \quad (2.4)$$

where \( \mu_f \) is the Coulomb coefficient of friction; \( V \) is the asperity
velocity; \( p'(x_1) \) is the pressure over the contact area; \( q \) is the heat flux through the contact area; and \( c(t) \) is the distance from \( x_1 \) origin to the leading edge of the asperity.

(iii) Outside the contact surface, \( x_1 < c(t) \) or \( x_1 > c(t)+a, x_2 = 0 \), the convective heat loss, being of small order, is neglected without loss of generality,

\[
- \frac{\partial T^I}{\partial x_2} = 0. 
\]  

(2.5)

(iv) At the coating layer/substrate interface, \( x_2 = H \), the continuity conditions hold

\[
T^I = T^{II}, 
\]  

(2.6)

\[
k_1 \frac{\partial T^I}{\partial x_2} = k_{II} \frac{\partial T^{II}}{\partial x_2},
\]  

(2.7)

where \( H \) is the layer thickness.

(v) Adiabatic conditions at cavity boundaries,

\[
\frac{\partial T^I}{\partial x_2} = 0, \text{ at } -d \leq x_1 \leq d, x_2 = L'
\]  

(2.8)

\[
\frac{\partial T^I}{\partial x_2} = 0, \text{ at } -d \leq x_1 \leq d, x_2 = L'+e
\]  

(2.9)

\[
\frac{\partial T^I}{\partial x_1} = 0, \text{ at } x_1 = d, L' \leq x_2 \leq L'+e
\]  

(2.10)

\[
\frac{\partial T^I}{\partial x_1} = 0, \text{ at } x_1 = -d, L' \leq x_2 \leq L'+e
\]  

(2.11)
where \( d \) is the half width of the cavity and \( e \) is the depth of the cavity. The region between the cavity and the wear surface, which is important in determining the magnitude of the temperature field and the stress state, shall be designated descriptively as the ligament region. The distance between the surface and the cavity top edge is therefore the ligament thickness \( L' \) (see Figure 2.1).

2.2 Mechanical stress field

The elastic Navier's equation and the Hooke's law equation are

\[
\frac{\partial}{\partial x_1} \left( \lambda \frac{\partial u^B}{\partial x_k} \right) + \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u^B}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u^B}{\partial x_j} \right) = \rho \frac{\partial^2 u^B}{\partial t^2}, \quad i, j, k = 1, 2 \tag{2.12}
\]

and

\[
\sigma^B_{ij} = \lambda \delta_{ij} \left( \frac{\partial u^B}{\partial x_k} \right) + \mu \left( \frac{\partial u^B}{\partial x_j} + \frac{\partial u^B}{\partial x_i} \right), \quad i, j, k = 1, 2 \tag{2.13}
\]

where \( u_1 \) and \( u_2 \) are the displacements in \( x_1 \) and \( x_2 \) direction, respectively; \( \sigma_{11}, \sigma_{12}, \sigma_{22} \) are stress components; \( \lambda \) and \( \mu \) are the Lamé constants; and \( \delta_{ij} \) is the Kronecker delta. The summation convention is used for all repeated indices of Roman minuscules.

The mechanical stress field is initially homogeneous.

The boundary conditions are:

(i) On the contact surface \((c(t) \leq x_1 \leq c(t) + a, \; x_2 = 0)\), tractions are prescribed by

\[
\sigma_{12} = \mu f'p'(x_1), \quad \sigma_{22} = -p'(x_1). \tag{2.14}
\]
(ii) Outside the contact area, the region given by \( x_1 < c(t) \) or \( x_1 > c(t) + a, x_2 = 0 \), the surface tractions are identically zero:

\[
\sigma_{12}^I = 0, \quad \sigma_{22}^I = 0. \tag{2.16}
\]

(iii) The regularity conditions hold at infinity \( (x_1^2 + x_2^2) \to \infty \),

\[
u_i^\beta = 0, \quad \sigma_{i j}^\beta = 0. \tag{2.18}
\]

(iv) At the coating layer/substrate interface, \( x_2 = H \), the continuity conditions are

\[
u_1^I = u_1^{II}, \quad \sigma_{12}^I = \sigma_{12}^{II}. \tag{2.20}
\]

(v) The cavity boundary is traction free; that is,

\[
\sigma_{12}^\beta = \sigma_{22}^\beta = 0, \text{ at } -d \leq x_1 \leq d, x_2 = L' \tag{2.22}
\]

\[
\sigma_{12}^\beta = \sigma_{22}^\beta = 0, \text{ at } -d \leq x_1 \leq d, x_2 = L'+e \tag{2.23}
\]

\[
\nu_{11}^\beta = \sigma_{12}^\beta = 0, \text{ at } x_1 = d, L' \leq x_2 \leq L'+e \tag{2.24}
\]
\[ \sigma_{11} = \sigma_{12} = 0, \text{ at } x_1 = -d, \quad L' \leq x_2 \leq L'+e \quad (2.25) \]

2.3 Thermal Stress Field

The thermoelastic Navier's equation is

\[
\frac{\partial}{\partial x_1} \left( \lambda_\beta \frac{\partial u^\beta}{\partial x_k} \right) + \frac{\partial}{\partial x_j} \left( \nu_\beta \frac{\partial u^\beta}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \nu_\beta \frac{\partial u^\beta}{\partial x_k} \right) - \\
- \frac{\partial}{\partial x_1} \left[ (3\lambda_\beta + 2\nu_\beta) a_\beta (T - T_0) \right] = \rho_\beta \frac{\partial^2 u^\beta}{\partial t^2}, \quad i, j, k = 1, 2 \quad (2.26)
\]

and the Hooke's law equation is

\[
\sigma_{ij} = \lambda_\beta \delta_{ij} \left( \frac{\partial u^\beta}{\partial x_k} \right) + \nu_\beta \left( \frac{\partial u^\beta}{\partial x_j} + \frac{\partial u^\beta}{\partial x_i} \right) - \\
- (3\lambda_\beta + 2\nu_\beta) a_\beta \delta_{ij} (T - T_0), \quad (2.27)
\]

where \( \alpha \) is the coefficient of thermal expansion, \( T \) and its derivatives are derived from the temperature field.

The initial conditions for the thermal stress field are

\[ u^\beta_i (x_1, x_2, 0) = 0, \quad (2.28) \]

\[ \sigma^\beta_{ij} (x_1, x_2, 0) = 0. \quad (2.29) \]

The boundary conditions are:

(1) The surface, \( x_2 = 0 \), is traction free, i.e.

\[ \sigma^T_{12} = 0, \quad (2.30) \]
\( \sigma_{22}^I = 0. \) \hfill (2.31)

(ii) The regularity conditions hold at infinity, \( x_1^2 + x_2^2 \to \infty \), i.e.

\[ u_1^\beta = 0, \] \hfill (2.32)

\[ \sigma_{1j}^\beta = 0. \] \hfill (2.33)

(iii) Continuity conditions hold at the interface, \( x_2 = H \), i.e.

\[ u_1^I = u_1^{II}, \] \hfill (2.34)

\[ \sigma_{12}^I = \sigma_{12}^{II}. \] \hfill (2.35)

(iv) The cavity boundary is traction free, i.e.

\[ \sigma_{12}^\beta = \sigma_{22}^\beta = 0, \text{ at } -d \leq x_1 \leq d, x_2 = L' \] \hfill (2.36)

\[ \sigma_{12}^\beta = \sigma_{22}^\beta = 0, \text{ at } -d \leq x_1 \leq d, x_2 = L'+e \] \hfill (2.37)

\[ \sigma_{11}^\beta = \sigma_{12}^\beta = 0, \text{ at } x_1 = d, L' \leq x_2 \leq L'+e \] \hfill (2.38)

\[ \sigma_{11}^\beta = \sigma_{12}^\beta = 0, \text{ at } x_1 = -d, L' \leq x_2 \leq L'+e \] \hfill (2.39)

The solution techniques and the numerical results of the temperature and the stress fields shall be given in Chapters 3 and 4.
CHAPTER 3

TEMPERATURE SOLUTIONS

Since a high temperature and its gradients are the source of the high thermal stresses, which can lead to the thermocracking of the wear medium. Therefore, it is of primary importance that a temperature solution is available. The governing equations in the dimensionless form are as follows:

In the coating layer, $0 < \eta < D$, denoted by the superscript I,

$$\frac{\partial^2 \Phi^I}{\partial \xi^2} + \frac{\partial^2 \Phi^I}{\partial \eta^2} = R^I \frac{\partial \Phi^I}{\partial \tau},$$

(3.1)

In the substrate region, $D < \eta < \infty$, denoted by superscript II,

$$\frac{\partial^2 \Phi^{II}}{\partial \xi^2} + \frac{\partial^2 \Phi^{II}}{\partial \eta^2} = R^{II} \frac{\partial \Phi^{II}}{\partial \tau},$$

(3.2)

where $\Phi^\beta = \frac{T^\beta - T^0}{q_0 a}$ is the dimensionless temperature; $(\xi, \eta) = (x_1/a, x_2/a)$ are the dimensionless coordinates in the direction opposed to the asperity motion and the depth direction, respectively (as shown in Figure 2.1); $\tau = (V t/a)$ is the dimensionless time; $D = H/a$ is the dimensionless coating thickness; $R_\beta = (Va/\kappa_\beta)$ are the Peclet numbers in the coating layer ($\beta = I$) and in the substrate ($\beta = II$); $q_0$ is the average heat flux through the contact area; and $T$, $K$, $\kappa$, $x_1$, $x_2$, $V$, $t$, $H$ are the same as defined in Chapter 2.

3.1 Difference Formulation

Because of the analytical complexity of the mathematical model, the
explicit finite difference method is employed to solve the current problem [48,49,50,51,52,53,54,55]. A brief discussion of the finite difference method is given in Appendix I. In the finite difference method, the semi-infinite body is replaced by a sufficiently large rectangular region (Figure 3.1). A central difference is used for the space derivatives, and a two-point forward difference is used for the time derivative of the first time step, then a three-point forward difference is employed for the following time steps. The reason for using the three-point forward difference after the first time step is that it is more accurate than the two-point forward difference. But, for the first time step, we have information only on one previous time line (initial condition), and, therefore, only the two-point difference formula may be used.

The governing differential equations in the difference form are:

In the coating layer

\[ \phi^I(i,j,n) = r_1 \phi^I(i-1,j,n-1) + [1 - 2(r_1 + r_2)]\phi^I(i,j,n-1) + \\
+ r_1 \phi^I(i+1,j,n-1) + r_2 \phi^I(i,j-1,n-1) + \\
+ r_2 \phi^I(i,j+1,n-1), \quad n=1 \quad (3.3a) \]

and

\[ \phi^I(i,j,n) = \frac{1}{3} [-\phi^I(i,j,n-2) + 2r_1 \phi^I(i-1,j,n-1) + \\
+ 4(1 - r_1 - r_2)\phi^I(i,j,n-1) + 2r_1 \phi^I(i+1,j,n-1) + \]

-20-
\[ + 2r_2 \phi^I(i,j-1,n-1) + 2r_2 \phi^I(i,j+1,n-1) \], \quad n > 1 \quad (3.3b) \]

In the substrate

\[ \phi^{II}(i,j,n) = \Omega^2 r_1 \phi^{II}(i-1,j,n-1) + [1 - (2\Omega^2 r_1 + 2\Omega^2 r_2)] \phi^{II}(i,j,n-1) + \]
\[ + \Omega^2 r_1 \phi^{II}(i+1,j,n-1) + \Omega^2 r_2 \phi^{II}(i,j-1,n-1) + \]
\[ + \Omega^2 r_2 \phi^{II}(i,j+1,n-1), \quad n = 1 \quad (3.4a) \]

and

\[ \phi^{II}(i,j,n) = \frac{1}{3} [-\phi^{II}(i,j,n-2) + 2\Omega^2 r_1 \phi^{II}(i-1,j,n-1) + \]
\[ + 4(1 - \Omega^2 r_1 - \Omega^2 r_2) \phi^{II}(i,j,n-1) + 2\Omega^2 r_1 \phi^{II}(i+1,j,n-1) + \]
\[ + 2\Omega^2 r_2 \phi^{II}(i,j,n-1) + 2\Omega^2 r_2 \phi^{II}(i,j+1,n-1)], \quad n > 2 \quad (3.4b) \]

where \( r_1 = \Delta t / (R_{11} \Delta \xi^2) \), \( r_2 = \Delta t / (R_{11} \Delta \eta^2) \), \( \Omega^2 = \kappa_{11}/\kappa_1 \), and \((i,j,n)\) denotes the two spatial indices and the time step, respectively. For the explicit scheme, the time step \( \Delta t \) must satisfy a stability criterion. The most commonly used method of stability analysis is Von Neumann's method [48,50,54,55]. In this method, a finite Fourier series expansion of the solution to a model equation is made, and the decay or amplification of each mode is considered separately to determine stability or instability, as we now demonstrate.

Consider first the difference form of Equation (3.1) of the
coating layer

\[
\Phi^I(i,j,n) = \Phi^I(i,j,n-1) + r_1[\Phi^I(i-1,j,n-1) - 2\Phi^I(i,j,n-1) + \\
+ \Phi^I(i+1,j,n)] + r_2[\Phi^I(i,j-1,n-1) - 2\Phi^I(i,j,n-1) + \\
+ \Phi^I(i,j+1,n-1)] .
\] (3.5)

Each Fourier component of the solution is written as

\[
\Phi^I(i,j,n) = V^n e^{i\xi(i\Delta\xi) + i\eta(i\Delta\eta)} .
\] (3.6a)

where \(V^n\) is the amplitude function at time-level \(n\) of the particular component whose wave numbers are \(K_{\xi}\) and \(K_{\eta}\) in \(\xi\) and \(\eta\) directions and \(J = e^{\sqrt{-1}T}\). If \(\theta = K_{\xi}\) and \(\phi = K_{\eta}\) we obtain

\[
\Phi^I(i,j,n) = V^n e^{j(\theta + j\phi)} .
\] (3.6b)

Substituting Equation (3.6b) into Equation (3.5) gives

\[
V^n e^{j(\theta + j\phi)} = V^{n-1} e^{j(\theta + j\phi)} + r_1[V^{n-1} e^{j[(i-1)\theta + j\phi]} - 2V^{n-1} e^{j(\theta + j\phi)} + \\
+ V^{n-1} e^{j[(i+1)\theta + j\phi]} + r_2[V^{n-1} e^{j(\theta + (j-1)\phi)} - \\
- 2V^{n-1} e^{j(\theta + j\phi)} + V^{n-1} e^{j(\theta + (j+1)\phi)}] .
\] (3.7)

Canceling the common term \(e^{j(\theta + j\phi)}\) gives
\[ V^n = V^{n-1} \{1 + r_1(e^{j\theta} + e^{-j\theta} - 2) + r_2(e^{j\phi} + e^{-j\phi} - 2)\} . \quad (3.8) \]

Using the identity \( e^{j\theta} + e^{-j\theta} = 2\cos\theta \) and \( 2\sin^2(\theta/2) = 1 - \cos\theta \), Equation (3.8) becomes

\[ V^n = GV^{n-1} = [1 - 4r_1\sin^2(\frac{\theta}{2}) - 4r_2\sin^2(\frac{\phi}{2})]V^{n-1} . \quad (3.9) \]

where \( G \) is the amplification factor. Equation (3.9) shows clearly that, if solutions are to remain bounded, we must have \(|G| < 1\) for all \( \theta \) and \( \phi \). This is the stability criterion for the heat conduction equation.

For \(|G| < 1\), we have

\[ |1 - 4r_1\sin^2(\frac{\theta}{2}) - 4r_2\sin^2(\frac{\phi}{2})| \leq 1 , \quad (3.10) \]

which is true only if

\[ 4r_1\sin^2(\frac{\theta}{2}) + 4r_2\sin^2(\frac{\phi}{2}) \leq 2 , \quad \text{for all } \theta, \phi \quad (3.11) \]

The stability requirement is then

\[ r_1 + r_2 \leq \frac{1}{2} , \quad (3.12) \]

or

\[ \frac{\Delta r}{R_1} \left( \frac{1}{\Delta \xi^2} + \frac{1}{\Delta \eta^2} \right) \leq \frac{1}{2} . \quad (3.13) \]
Similarly, the equation for the stability criterion for the substrate is

\[ \Omega^2(r_1 + r_2) \leq \frac{1}{2} \]  \hspace{1cm} (3.14)

or

\[ \frac{\Omega^2 \Delta \tau}{R_1} \left( \frac{1}{\Delta \xi^2} + \frac{1}{\Delta \eta^2} \right) \leq \frac{1}{2} \]  \hspace{1cm} (3.15)

If \( \Omega^2 \) is less than 1, Equation (3.13) is the stability criterion; otherwise Equation (3.15) is the stability criterion for the current problem.

Based on previous results in references [28,29,30,31,33,34,35], we know that high temperature and high thermal stresses occur in the region near the asperity. Therefore, in that region and in the region near the cavity, a very fine mesh must be used to calculate accurate solutions. In the regions far away from the asperity and the cavity, a relatively coarse mesh can be used to save computing time. This non-uniform mesh can be transformed to a uniform mesh by using the general coordinate transformation proposed in references [54,55,56]. The non-uniform mesh and general coordinate transformation are discussed in Appendix II.

The heat conduction equation (3.1) and (3.2) in the transformed plane \((\xi, \eta)\) can be written as

\[ \left( A_1 \phi_{\xi \xi}^\beta + 2A_2 \phi_{\xi \eta}^\beta + A_3 \phi_{\eta \eta}^\beta + A_4 \phi_{\xi}^\beta + A_5 \phi_{\eta}^\beta \right) / J^2 = R_\beta \phi^\beta, \; \beta=I,II \]  \hspace{1cm} (3.16)
where $J = \delta_{m,n} - \delta_{m,n}$ is the Jacobian of the transformation, the subscripts $(\xi, \eta, \zeta, \eta, \tau)$ denote partial derivatives in those coordinates and time, respectively, and

\[
A_1 = \frac{\xi^2 + \eta^2}{\eta}, \quad (3.17)
\]

\[
A_2 = \frac{\xi \xi + \eta \eta}{\xi \eta}, \quad (3.18)
\]

\[
A_3 = \frac{\xi^2 + \eta^2}{\xi}, \quad (3.19)
\]

\[
A_4 = (\xi A_7 - \eta A_6)/J, \quad (3.20)
\]

\[
A_5 = (\eta A_6 - \xi A_7)/J, \quad (3.21)
\]

\[
A_6 = A_3 \xi \eta - 2A_2 \xi \eta + A_3 \xi \eta, \quad (3.22)
\]

\[
A_7 = A_1 \xi \eta + 2A_2 \xi \eta + A_3 \xi \eta. \quad (3.23)
\]

In the coating layer, the transformed heat conduction equation (3.16) in the difference form is

\[
\phi^I(1,j,n) = \phi^I(1,j,n-1) + \frac{\Delta \tau}{R_1} AA, \quad n=1 \quad (3.24a)
\]

\[
\phi^I(1,j,n) = \frac{1}{3} [-\phi^I(1,j,n-2) + 4\phi^I(1,j,n-1) + \frac{2\Delta \tau}{R_1} AA], \quad n>1 \quad (3.24b)
\]

where
\[ AA = \left( A_1/\Delta \alpha^2 \right) \left[ \phi^I(i-1,j,n-1) - 2\phi^I(i,j,n-1) + \phi^I(i+1,j,n-1) \right] - \]
\[ - \left( A_2/2\Delta \alpha \Delta n \right) \left[ \phi^I(i+1,j+1,n-1) - \phi^I(i+1,j-1,n-1) - \phi^I(i-1,j+1,n-1) + \phi^I(i-1,j-1,n-1) \right] + (A_3/\Delta n^2) \left[ \phi^I(i,j-1,n-1) - 2\phi^I(i,j,n-1) + \phi^I(i,j+1,n-1) \right] + \]
\[ + \phi^I(i,j+1,n-1) \right] + (A_4/2\Delta \alpha) \left[ \phi^I(i+1,j,n-1) - \phi^I(i-1,j,n-1) \right] + \]
\[ + (A_5/2\Delta \alpha) \left[ \phi^I(i,j+1,n-1) - \phi^I(i,j-1,n-1) \right] \right]/J^2. \tag{3.25} \]

In the substrate, the corresponding difference form of Equation (3.16) is given by

\[ \phi^I(i,j,n) = \phi^I(i,j,n-1) + \frac{\Delta \tau}{R_{II}} \cdot AA, \quad n=1 \tag{3.26a} \]

\[ \phi^I(i,j,n) = \frac{1}{3} \left[ -\phi^I(i,j,n-2) + 4\phi^I(i,j,n-1) + \right. \]
\[ + \frac{2\Delta \tau}{R_{II}} \cdot AA \right], \quad n>1 \tag{3.26b} \]

where

\[ AA = \left( A_1/\Delta \alpha^2 \right) \left[ \phi^I(i-1,j,n-1) - 2\phi^I(i,j,n-1) + \phi^I(i+1,j,n-1) \right] - \]
\[ - \left( A_2/2\Delta \alpha \Delta n \right) \left[ \phi^I(i+1,j+1,n-1) - \phi^I(i+1,j-1,n-1) - \phi^I(i-1,j+1,n-1) + \phi^I(i-1,j-1,n-1) \right] + \]
\[ + \phi^I(i,j,n-1)\right] + (A_3/\Delta n^2) \left[ \phi^I(i,j-1,n-1) - 2\phi^I(i,j,n-1) + \phi^I(i,j+1,n-1) \right] + \]

\[ + (A_4/2\Delta \alpha) \left[ \phi^I(i+1,j,n-1) - \phi^I(i-1,j,n-1) \right] + \]
\[ + \phi^{II}(i,j+1,n-1) + (A_q/2\Delta x) [\phi^{II}(i+1,j,n-1) - \phi^{II}(i-1,j,n-1)] + \]
\[ + (A_s/2\Delta y) [\phi^{II}(i,j+1,n-1) - \phi^{II}(i,j-1,n-1)]/J^2. \quad (3.27) \]

At the outer boundaries of the rectangular region (excluding the surface), \( \phi^\beta(i,j,n) = 0 \) is the nominal value. The remaining conditions, on the surface, the cavity boundaries and at the interface, will be incorporated with an energy balance scheme.

### 3.2 Energy Balance

The cavity boundaries, the moving asperity and the interface of the medium are taken care of with the use of the energy balance method [57].

(1) Energy balance at the interface (see Figure 3.2)

For material I (coating layer), the heat fluxes toward the central point \( P \) of the element at the interface from material points \( W, R \) and \( S \) in the coating layer are

\[ Q_{W+P} = k_1 (\Delta y/2) \frac{T(i-1,j) - T(i,j)}{\Delta x_1}, \quad (3.28) \]
\[ Q_{R+P} = k_1 (\Delta y/2) \frac{T(i+1,j) - T(i,j)}{\Delta x_2}, \quad (3.29) \]
\[ Q_{S+P} = k_1 (\frac{\Delta x_1 + \Delta x_2}{2}) \frac{T(i,j-1) - T(i,j)}{\Delta y}, \quad (3.30) \]

where \( Q \) is the heat flux, indexed by the direction.

For material II (substrate), the heat fluxes toward the point \( P \) from material points \( W, R \) and \( N \) in the substrate region are
Figure 3.2 Energy balance at the interface.
The total heat flux going to the interface point \( P(i,j) \) is

\[
Q_{\text{sum}} = (k_1 + k_{II})(\Delta y/2)[\frac{T(i-1,j) - T(i,j)}{\Delta x_1} + \frac{T(i+1,j) - T(i,j)}{\Delta x_2}]
\]

\[+ \frac{\Delta x_1 + \Delta x_2}{2} \frac{T(i,j-1) - T(i,j)}{\Delta y} + \frac{\Delta x_1 + \Delta x_2}{2} \frac{T(i,j+1) - T(i,j)}{\Delta y}\]  

(3.34)

The rate of change of internal energy \( \dot{U} \) in the time interval \( \Delta t \) at the point \( P(i,j) \) is

\[
\dot{U}_P = \dot{U}_{1P} + \dot{U}_{2P}
\]

\[
\dot{U}_P = (\rho_1 c_1 + \rho_{II} c_{II})[(\Delta x_1 + \Delta x_2) \frac{\Delta y}{4}] \frac{T(i,j,n) - T(i,j,n-1)}{\Delta t}, \quad n=1 \quad (3.35a)
\]

\[
\dot{U}_P = (\rho_1 c_1 + \rho_{II} c_{II})[(\Delta x_1 + \Delta x_2) \frac{\Delta y}{4}] \frac{3T(i,j,n) - 4T(i,j,n-1) + T(i,j,n-2)}{2\Delta t} \quad n>1 \quad (3.35b)
\]

Conservation of energy requires that the algebraic sum of the heat flowing into the point \( P \) is equal to the rate of change of internal energy at the same point \( (Q_{\text{sum}} = \dot{U}_P) \). From conservation of energy, one
can obtain the equation for the continuity condition at the interface point \( P(i, j) \) at the time step \( n \).

\[
T(i, j, n) = T(i, j, n-1) + AA_1 , \quad n=1 \quad (3.36a)
\]

\[
T(i, j, n) = \frac{1}{3} \left[ -T(i, j, n-2) + 4T(i, j, n-1) + 2AA_1 \right] , \quad n>1 \quad (3.36b)
\]

where

\[
AA_1 = \frac{\Delta t}{\rho_1 c_1 + \rho_1 c_{II}} \left[ \frac{2(k_1 + k_{II})}{\Delta x_1^2 + \Delta x_1 \Delta x_2} \left[ T(i-1, j, n-1) - T(i, j, n-1) \right] + \right.
\]

\[
+ \frac{2(k_1 + k_{II})}{\Delta x_1 \Delta x_2 + \Delta x_2^2} \left[ T(i+1, j, n-1) - T(i, j, n-1) \right] + \frac{2k_{II}}{\Delta y^2} \left[ T(i, j-1, n-1) - 
\]

\[
- T(i, j, n-1) \right] + \frac{2k_{II}}{\Delta y^2} \left[ T(i, j+1, n-1) - T(i, j, n-1) \right] . \quad (3.37)
\]

Equations (3.36a,b) in dimensionless form are given by

\[
\phi(i, j, n) = \phi(i, j, n-1) + AA_2 , \quad n=1 \quad (3.38a)
\]

\[
\phi(i, j, n) = \frac{1}{3} \left[ -\phi(i, j, n-2) + 4\phi(i, j, n-1) + 2AA_2 \right] , \quad n>1 \quad (3.38b)
\]

where

\[
AA_2 = \frac{2\Delta t}{R_1 + \eta R_{II}} \left[ \frac{(1+\eta)k_1}{\Delta x_1^2 + \Delta x_1 \Delta x_2} \left[ \phi(i-1, j, n-1) - \phi(i, j, n-1) \right] + \right.
\]

\[
+ \frac{(1+\eta)k_{II}}{\Delta x_1 \Delta x_2 + \Delta x_2^2} \left[ \phi(i+1, j, n-1) - \phi(i, j, n-1) \right] + \frac{1}{\Delta y^2} \left[ \phi(i, j-1, n-1) - 
\]

\[
- \phi(i, j, n-1) \right] .
\]
\[ -\Phi(i,j,n-1) + \frac{\kappa_k}{\Delta n^2} [\Phi(i,j+1,n-1) - \Phi(i,j,n-1)] , \quad (3.39) \]

where \( \kappa_k = k_{II}/k_I \).

Details of the energy balance method on the other boundary conditions are given in Appendix III. The dimensionless form of these boundary conditions are listed below.

(ii) Energy balance on the cavity boundaries (see Figure 3.3)

On face AB:

\[ \Phi^I(i,j,n) = \Phi^I(i,j,n-1) + AA_3 , \quad n=1 \quad (3.40a) \]

\[ \Phi^I(i,j,n) = \frac{1}{3} [-\Phi^I(i,j,n-2) + 4\Phi^I(i,j,n-1) + 2AA_3] , \quad n>1 \quad (3.40b) \]

where

\[ AA_3 = \frac{\Delta \tau}{R_I} \left[ \left( \Phi^I(i-1,j,n-1) - 2\Phi^I(i,j,n-1) + \Phi^I(i+1,j,n-1) \right) / \Delta \xi^2 + \right. \]

\[ \left. + 2(\Phi^I(i,j-1,n-1) - \Phi^I(i,j,n-1)) / \Delta n^2 \right] . \quad (3.41) \]

On face AC:

\[ \Phi^{II}(i,j,n) = \Phi^{II}(i,j,n-1) + AA_4 , \quad n=1 \quad (3.42a) \]

\[ \Phi^{II}(i,j,n) = \frac{1}{3} [-\Phi^{II}(i,j,n-2) + 4\Phi^{II}(i,j,n-1) + 2AA_4] , \quad n>1 \quad (3.42b) \]

where

\[ \]
Figure 3.3 Energy balance on the cavity boundary.
\[ AA_4 = \frac{2\Delta t}{R_{II}} \left\{ \frac{1}{\Delta x^2} \left[ \phi_{II}^{i-1,j,n-1} - \phi_{II}^{i,j,n-1} \right] + \frac{1}{\Delta n_1^2 + \Delta n_1 \Delta n_2} \left[ \phi_{II}^{i-1,j,n-1} - \phi_{II}^{i,j,n-1} \right] + \frac{1}{\Delta n_2^2 + \Delta n_1 \Delta n_2} \left[ \phi_{II}^{i,j+1,n-1} - \phi_{II}^{i,j,n-1} \right] \right\} \] 

(3.43)

On face BD:

\[ \phi_{II}^{i,j,n} = \phi_{II}^{i,j,n-1} + AA_5, \quad n=1 \] 

(3.44a)

\[ \phi_{II}^{i,j,n} = \frac{1}{3} \left[ -\phi_{II}^{i,j,n-2} + 4\phi_{II}^{i,j,n-1} + 2AA_5 \right], \quad n \geq 1 \] 

(3.44b)

where

\[ AA_5 = \frac{2\Delta t}{R_{II}} \left\{ \frac{1}{\Delta x^2} \left[ \phi_{II}^{i+1,j,n-1} - \phi_{II}^{i,j,n-1} \right] + \frac{1}{\Delta n_1^2 + \Delta n_1 \Delta n_2} \left[ \phi_{II}^{i,j-1,n-1} - \phi_{II}^{i,j,n-1} \right] + \frac{1}{\Delta n_2^2 + \Delta n_1 \Delta n_2} \left[ \phi_{II}^{i,j+1,n-1} - \phi_{II}^{i,j,n-1} \right] \right\} \] 

(3.45)

On face CD:

\[ \phi_{II}^{i,j,n} = \phi_{II}^{i,j,n-1} + AA_6, \quad n=1 \] 

(3.46a)

\[ \phi_{II}^{i,j,n} = \frac{1}{3} \left[ -\phi_{II}^{i,j,n-2} + 4\phi_{II}^{i,j,n-1} + 2AA_6 \right], \quad n \geq 1 \] 

(3.46b)
where

\[
A_{A_6} = \frac{\Delta t}{R_{II}} \left[ \phi^{II}(i-1,j,n-1) - 2\phi^{II}(i,j,n-1) + \phi^{II}(i+1,j,n-1) \right]/\Delta \xi^2 + \\
+ 2[\phi^{II}(i,j+1,n-1) - \phi^{II}(i,j,n-1)] .
\]  

(3.47)

(iii) Energy balance at the corner of the cavity (Figure 3.3)

The points at the four corners of the cavity are singularities, because at each of those four points there are two boundary conditions, \( \partial T/\partial x_1 = \partial T/\partial x_2 = 0 \), with only one unknown \( T \). However, by applying an energy balance scheme, one can resolve such problems at the corners. The dimensionless form for the corner points are:

Corner A:

\[
\phi(i,j,n) = \phi(i,j,n-1) + AA_a , \quad n=1 \]  

\[
\phi(i,j,n) = \frac{1}{3} \left[ -\phi(i,j,n-2) + 4\phi(i,j,n-1) + 2AA_a \right] , \quad n>1
\]  

(3.48a)

(3.48b)

where

\[
AA_a = \frac{\Delta t}{R_{II}/2 + \eta R_{II}/4} \left[ \frac{1+\eta_k}{2} \left[ \phi(i-1,j,n-1) - \phi(i,j,n-1) \right]/\Delta \xi^2 + \\
+ \frac{1}{2} \left[ \phi(i+1,j,n-1) - \phi(i,j,n-1) \right]/\Delta \xi^2 + \frac{\eta_k}{2} \left[ \phi(i,j+1,n-1) - \\
- \phi(i,j,n-1) \right]/\Delta \eta^2 + \left[ \phi(i-1,j,n-1) - \phi(i,j,n-1) \right]/\Delta \eta^2 \right] .
\]  

(3.49)
Corner B:

\[
\psi(i,j,n) = \psi(i,j,n-1) + AA_8, \quad n=1 \quad (3.50a)
\]

\[
\psi(i,j,n) = \frac{1}{3} \left[ -\psi(i,j,n-2) + 4\psi(i,j,n-1) + 2AA_8 \right], \quad n>1 \quad (3.50b)
\]

where

\[
AA_8 = \frac{\Delta t}{R_{11}^2 + n \xi / 4 \left[ \frac{1}{2} \left[ \psi(i-1,j,n-1) - \psi(i,j,n-1) \right]/\Delta \xi^2 + + \frac{1+n_k}{2} \left[ \psi(i+1,j,n-1) - \psi(i,j,n-1) \right]/\Delta \xi^2 \right] + \frac{\eta_k}{2} \left[ \psi(i,j+1,n-1) - \psi(i,j,n-1) \right]/\Delta \eta^2 + \right] \quad (3.51)
\]

Corner C:

\[
\psi^{\prime \prime}(i,j,n) = \psi^{\prime \prime}(i,j,n-1) + AA_9, \quad n=1 \quad (3.52a)
\]

\[
\psi^{\prime \prime}(i,j,n) = \frac{1}{3} \left[ -3\psi^{\prime \prime}(i,j,n-2) + 4\psi^{\prime \prime}(i,j,n-1) + 2AA_9 \right], \quad n>1 \quad (3.52b)
\]

where

\[
AA_9 = \frac{2 \Delta t}{3 R_{11}} \left[ \left[ 2\psi^{\prime \prime}(i-1,j,n-1) - 3\psi^{\prime \prime}(i,j,n-1) + \psi^{\prime \prime}(i+1,j,n-1) \right]/\Delta \xi^2 + + \left[ \psi^{\prime \prime}(i,j-1,n-1) - 3\psi^{\prime \prime}(i,j,n-1) + 2\psi^{\prime \prime}(i,j+1,n-1) \right]/\Delta \eta^2 \right] \quad (3.53)
\]

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Corner D:

\[ \Phi^{II}(i,j,n) = \Phi^{II}(i,j,n-1) + AA_{10}, \quad n=1 \quad (3.54a) \]

\[ \Phi^{II}(i,j,n) = \frac{1}{3} \left[ -\Phi^{II}(i,j,n-2) + 4\Phi^{II}(i,j,n-1) + 2AA_{10} \right], \quad n>1 \quad (3.54b) \]

where

\[ AA_{10} = \frac{2}{3} \frac{\Delta \tau}{R_{II}} \left[ \left( \Phi^{II}(i-1,j,n-1) - 3\Phi^{II}(i,j,n-1) + 2\Phi^{II}(i+1,j,n-1) \right) / \Delta z^2 + 
\]

\[ + \left( \Phi^{II}(i,j-1,n-1) - 3\Phi^{II}(i,j,n-1) + 2\Phi^{II}(i,j+1,n-1) \right) / \Delta \eta^2 \right]. \quad (3.55) \]

(iv) Energy balance on the surface boundary (the moving asperity)

The dimensionless form for the surface boundary condition is:

\[ \Phi^{I}(i,1,n) = \Phi^{I}(i,1,n-1) + \left( \Delta \tau \frac{\Delta z}{R_{I} \Delta \eta} \right) \Phi^{I}(i,1,n) + AA_{11}, \quad n=1 \quad (3.56a) \]

\[ \Phi^{I}(i,1,n) = \frac{1}{3} \left[ -\Phi^{I}(i,1,n-2) + 4\Phi^{I}(i,1,n-1) + \left( \Delta \tau \frac{\Delta \eta}{R_{I} \Delta \eta} \right) + 2AA_{11} \right], \quad n=2 \quad (3.56b) \]

where \( h' = h / (\Delta x / 2) \), \( h \) is defined in Appendix III, and

\[ AA_{11} = \frac{\Delta \tau}{R_{I}} \left[ \left( \Phi^{I}(i-1,1,n-1) - 2\Phi^{I}(i,1,n-1) + \Phi^{I}(i+1,1,n-1) \right) / \Delta z^2 + 
\]

\[ + 2\Phi^{I}(1,2,n-1) - \Phi^{I}(1,1,n-1) \right) / \Delta \eta^2 \right]. \quad (3.57) \]

Equations (3.24, 3.26, 3.38, 3.40, 3.42, 3.44, 3.46, 3.48, 3.50,
3.52, 3.54, 3.56) constitute the general formulation of the problem with a complete set of difference equations for the solutions of the discrete temperature field $f(i,j,n)$ at some specific time. The computer programs which are used to compute the temperature field solutions are given in Appendix IV.

3.3 Numerical Results

Numerical results are obtained by using the non-uniform rectangular mesh corresponding to different cases of material properties and geometry. For the surface layer of silicon carbide, $k_1 = 1.047$ J/cm·°C·s, $\kappa_1 = 0.49$ cm²/s, and $c_1 = 712$ J/kg·°C. For the substrate of aluminum, $k_{II} = 2.02$ J/cm·°C·s, $\kappa_{II} = 0.961$ cm²/s, and $c_{II} = 917$ J/kg·°C. The other numerical parameters on the asperity and the cavity are: $v=15$ m/s, $w=10a$, $H=1.2a$, $b=1.9a$, $d=0.3a$, $e=0.5a$, $a=1mm$, the smallest $\Delta e$ and $\Delta n$ are 0.02 and 0.01 respectively, and $\Delta r=0.01$. In the limiting case of no cavity, the maximum dimensionless temperature at the surface of the coated media was found to be 0.124 by using the Fourier transform method [33, 34]. The result at the same point by the current finite difference formulation is 0.123. The error is less than 1%. The numerical scheme is therefore confirmed by the benchmark problem.

The solutions for a single material with and without a cavity would then be compared with two limiting cases. For the first case, the cavity is located entirely in the surface layer, Figure 3.4a. In the second case, the top edge of the cavity is at the layer/substrate interface, Figure 3.4b. The solutions for the single material without and with a cavity are designated as the third and the fourth cases, respectively, included for the purpose of comparison. Different cases of the temperature field solutions are given in Table 1. In Case 1,
* Base materials for the coating layer and the substrate are silicon carbide and aluminum, respectively.

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<th>$k_{II}$</th>
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<th>$(pc)_{II}$</th>
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<td>$2k_{II}$</td>
<td>$1(pc)_I$</td>
<td>$1(pc)_{II}$</td>
<td>$1k_1$</td>
<td>$1k_{II}$</td>
<td>0.04</td>
<td>Interface</td>
</tr>
<tr>
<td>2C</td>
<td>$1k_1$</td>
<td>$\frac{1}{2}k_{II}$</td>
<td>$1(pc)_I$</td>
<td>$\frac{1}{2}(pc)_{II}$</td>
<td>$1k_1$</td>
<td>$1k_{II}$</td>
<td>0.04</td>
<td>Interface</td>
</tr>
<tr>
<td>2D</td>
<td>$1k_1$</td>
<td>$1k_{II}$</td>
<td>$1(pc)_I$</td>
<td>$\frac{1}{2}(pc)_{II}$</td>
<td>$1k_1$</td>
<td>$2k_{II}$</td>
<td>0.04</td>
<td>Interface</td>
</tr>
<tr>
<td>2E</td>
<td>$1k_1$</td>
<td>$2k_{II}$</td>
<td>$1(pc)_I$</td>
<td>$1(pc)_{II}$</td>
<td>$1k_1$</td>
<td>$2k_{II}$</td>
<td>0.04</td>
<td>Interface</td>
</tr>
<tr>
<td>3</td>
<td>$1k_1$</td>
<td></td>
<td>$1(pc)_I$</td>
<td></td>
<td>$1k_1$</td>
<td></td>
<td></td>
<td>No cavity</td>
</tr>
<tr>
<td>4</td>
<td>$1k_1$</td>
<td></td>
<td>$1(pc)_I$</td>
<td></td>
<td>$1k_1$</td>
<td></td>
<td>0.04</td>
<td>Single material</td>
</tr>
</tbody>
</table>
Figure 3.4 Numerical examples with different cavity position.
three different values of the ligament thickness: 0.04 (Case 1A), 0.06 (Case 1B), and 0.1 (Case 1E), are used to illustrate the effect of the ligament volume. The temperature fields at two depths, for all three Cases 1A, 1B and 1E are shown in Figure 3.5. In the figure, the cavity width is from $\xi=1.6$ to 2.2. The asperity position, at the dimensionless time $\tau=1.04$, representing the worst case, is from $\xi=1.2$ to 2.2. The relative positions of the asperity and the cavity is shown in Figure 3.6.

The Case 1A then is compared with Case 2 of the same ligament thickness for which the top edge of the cavity is at the layer/substrate interface. The effect of the relative position of the cavity to the interface is shown in Figure 3.7. It is noticed that when the top edge of the cavity is at the interface, the temperature field in the region immediately on the trailing edge of the asperity will be affected by the substrate material.

The effect of the heat capacity and thermal conductivity of the surface layer for Case 1A is shown in Figure 3.8. The figure shows the original value as Case 1A. Case 1C represents a reduction of thermal capacity of the surface layer by half. Case 1D shows the result of an increase in thermal conductivity of the surface layer by 75%. The thermal conductivity of the surface layer is shown to have little effect on the nondimensional surface temperature. But the real temperature field, $T=q_0\phi/k_I$, is lowered with increasing thermal conductivity $k_I$.

Figures 3.9 and 3.10 illustrate the effect of a cavity on the direction of heat flux. The figures show the nondimensional heat flux components in $\xi$ and $\eta$ directions of a single material without a cavity.
Figure 3.5 Dimensionless temperature field (cases 1A, 1B, 1E, 3).
Figure 3.6 The relative positions of the cavity and the asperity at $\tau = 1.04$. 
Figure 3.8  Dimensionless temperature field (cases 1A, 1C, 1D).
Figure 3.10 Dimensionless heat flux in η direction (cases 1A, 3).
(Case 3) and a layered medium with a cavity (Case 1A). From the figures, it is observed that, with no cavity, the heat flux at $\xi=2.2$, and $\eta=0.04$ has a magnitude of 0.7 at an angle of 82° to the wear surface. With a cavity, at the same location, the magnitude is increased to 1.5 at an angle 23° to the wear surface. Hence, the existence of the cavity will increase the heat flux tremendously, especially in the $\xi$ direction near the upper trailing corner of the cavity. Figures 3.9 and 3.10 demonstrate not only an increase in magnitude of the heat flux, hence the temperature gradient, but also the flux at a more oblique angle to the wear surface.

Ju [28] has studied the effect of thermal properties of a single material subjected to the high-speed asperity excitation. It was pointed out that thermal conductivity ($k$) and thermal capacity ($pc$) are the parameters controlling the temperature field. For layered media, a similar effect was found by Ju and Liu [35]. For the case of a layered medium with a cavity, the thermal property variation in the coating layer can be accordingly extrapolated. It is the effect of the substrate in the neighborhood of the cavity that would be influential in determining the temperature field in the critical region. The effect of thermal property variation for the substrate is therefore studied numerically for the Case 2, for which the coating/substrate interface is at the top edge of the cavity. For this case, the thermal properties of the substrate will be of immediate influence to the temperature field in the vicinity of the top trailing corner of the cavity. For the purpose of demonstrating the individual effect, a benchmark case is chosen for comparison in which both the coating and the substrate are of silicon carbide, $(k_1=k_2=1.047 \text{ J/cm.}^\circ\text{C.s.)}$.
\( \kappa_{II} = 0.49 \text{ cm}^2/\text{s}, \rho_{II} c_{II} = 2.137 \text{ J/cm}^3/\text{C}, \) designated as Case 4. Figure 3.11 illustrates the temperature field near the top surface and at the coating/substrate interface for cases with marked changes in thermal properties from those given in Case 4. Case 2B shows no change in the substrate diffusivity, but both the thermal conductivity and the thermal capacity are doubled. The ensuing improved conductivity and capacity in the substrate allow a significant heat flow into the substrate; thus a high temperature gradient is also found. The Case 2C, at the same diffusivity, but with both the thermal conductivity and the thermal capacity halved, shows a reduced heat flow into the substrate, with a corresponding low temperature gradient. Cases 2D and 2E, with doubled diffusivity, but with half capacity and double conductivity, respectively, showed reduced and increased heat flow into the substrate, respectively. The heat flux, being proportional to the temperature gradient, is illustrated in Figures 3.12 and 3.13 for the surface region and at the interface.

Figure 3.14 shows the transient temperature for Case 1A (cavity in the coating and ligament thickness of 0.04) in comparison to the case of a single material without cavity (Case 3). The dimensionless temperature, \( \phi = T_k / q_0 a, \) plotted against dimensionless time, \( \tau = vt/a, \) at the surface and at the ligament depth, \( \eta = 0.04, \) for the position \( \xi = 2.2, \) where the temperature is maximum in the vicinity of the cavity. It is shown that, before the asperity reaches the point, the temperature is low. Then the surface temperature increases and reaches a maximum when the asperity just passes over the trailing edge of the cavity. After the passing of the asperity, the temperature at the trailing corner of the cavity drops again.
Figure 3.11 Dimensionless temperature field (cases 2B, 2C, 2D, 2E, 4)
Figure 3.12 Dimensionless heat flux in \( \xi \) direction (cases 2B, 2C, 2D, 2E, A), \( \eta = 0 \) for all cases.
Figure 3.13 Dimensionless Heat flux in \( \xi \) direction (cases 2B, 2C, 2D, 2E, 4), \( \eta = 0.04 \) for all cases.
Figure 3.14 Dimensionless temperature field (cases 1A, 3).
CHAPTER 4  
STRESS SOLUTION

Ju et al [28,29,30,31,32,33,34] established that, for a moderately high-speed asperity excitation, the thermal stress effect dominates the stress field and eventually leads to failure in the no-cavity case. Liu [58] in his thesis also showed that, if the asperity speed is larger than 0.127 m/s (5 in/s), the thermal stress dominates the failure, and the mechanical stress becomes less important. However, the mechanical stress may not be trivial when a cavity exists. Therefore, both the mechanical and thermal stress field will be presented in this chapter.

The thermoeelastic Navier's equations and the Hooke's law in dimensionless form are:

\[
\frac{\partial}{\partial \xi} \left( N_1 \frac{\partial \phi}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( N_2 \frac{\partial \phi}{\partial \eta} \right) + \frac{\partial}{\partial \xi} \left( N_3 \frac{\partial \phi}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( N_3 \frac{\partial \phi}{\partial \eta} \right) - \\
- \frac{\partial}{\partial \xi} \left( \frac{b^2 \gamma \beta}{c^2} \phi \right) = \delta M^2 \frac{\partial^2 \phi}{\partial \xi^2}, \quad (4.1)
\]

\[
\frac{\partial}{\partial \xi} \left( N_1 \frac{\partial \phi}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( N_2 \frac{\partial \phi}{\partial \eta} \right) + \frac{\partial}{\partial \xi} \left( N_3 \frac{\partial \phi}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( N_1 \frac{\partial \phi}{\partial \eta} \right) - \\
- \frac{\partial}{\partial \eta} \left( \frac{b^2 \gamma \beta}{c^2} \phi \right) = \delta M^2 \frac{\partial^2 \phi}{\partial \eta^2}, \quad (4.2)
\]

\[
\sigma_{\xi \xi} = \frac{\mu_2}{P_0} \delta \left( N_1 \frac{\partial \phi}{\partial \xi} + N_2 \frac{\partial \phi}{\partial \eta} - \frac{b^2 \gamma \beta}{c^2} \phi \right), \quad (4.3)
\]

\[
\sigma_{\xi \eta} = \frac{\mu_2}{P_0} \delta N_3 \left( \frac{\partial \phi}{\partial \eta} + \frac{\partial \phi}{\partial \xi} \right), \quad (4.4)
\]

and
where $u^B$ and $v^B$ are respectively the dimensionless stress modulated by the average pressure $P_0$; $M=(v/c^2)$ is the Mach number; $V$ is theasperity speed; $N_1=(\lambda_\beta + 2\mu_\beta)/\rho_{II}c^2$; $N_2=\lambda_\beta/\rho_{II}c^2$; $N_3=\mu_\beta/\rho_{II}c^2$; $b^2=(3\lambda_\beta+2\mu_\beta)/\rho_{II}$; $\gamma_\beta=(\alpha_0\alpha_\beta)/k_1$; $\delta=\rho_\beta/\rho_{II}$, $c_1=[(\lambda_\beta + 2\mu_\beta)/\rho_{II}]^{1/2}$, $c_2=(\rho_{II}/\rho_{II})^{1/2}$ are the dilatational and shear wave speed, respectively; $\xi, \eta, \tau, \lambda, \mu_\beta, \alpha_\beta, \rho_{II}$ and $\phi^B$ were defined in Chapters 2 and 3.

Equations for the mechanical stress field are the same as the thermal stress field except that there is no temperature effect.

4.1 Perturbation Method

For hard wear materials, such as Stellite III, the Mach number $M$ is of the order of $10^{-3}$. Since $M^2$ is a parameter which is sufficiently small, Equations (4.1) and (4.2) can be solved by the perturbation method.

Let the solutions to (4.1) and (4.2) be expressed as a power series of $\epsilon=M^2$; that is

$$u^B(\xi,\eta,\tau,\epsilon) = u^B_0(\xi,\eta,\tau) + \epsilon u^B_1(\xi,\eta,\tau) + \epsilon^2 u^B_2(\xi,\eta,\tau) + \ldots, \quad (4.6)$$

$$v^B(\xi,\eta,\tau,\epsilon) = v^B_0(\xi,\eta,\tau) + \epsilon v^B_1(\xi,\eta,\tau) + \epsilon^2 v^B_2(\xi,\eta,\tau) + \ldots, \quad (4.7)$$

when equations (4.6) and (4.7) are substituted into equations (4.1) and (4.2), the terms with the same power of $\epsilon$ are grouped, leading to a set of equations for $u^B_0, u^B_1, u^B_2, \ldots$ and $v^B_0, v^B_1, v^B_2, \ldots$, as
follows:

For the terms of the zeroth order in $\epsilon$,

$$\frac{a}{\partial \xi} \left( N_1 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_2 \frac{\partial \phi}{\partial \eta} \right) + \frac{a}{\partial \eta} \left( N_3 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_4 \frac{\partial \phi}{\partial \eta} \right) =$$

$$= \frac{\partial}{\partial \xi} \left( \frac{b_2 \phi}{c_2^2} \right), \quad (4.8)$$

For the terms of the first order in $\epsilon$,

$$\frac{a}{\partial \xi} \left( N_1 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_2 \frac{\partial \phi}{\partial \eta} \right) + \frac{a}{\partial \eta} \left( N_3 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_4 \frac{\partial \phi}{\partial \eta} \right) =$$

$$= \frac{\partial}{\partial \eta} \left( \frac{b_2 \phi}{c_2^2} \right). \quad (4.9)$$

For the higher order solutions, it is evident that the equations are recursive. Accordingly, the recurrence formulas can be written as:

$$\frac{a}{\partial \xi} \left( N_1 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_2 \frac{\partial \phi}{\partial \eta} \right) + \frac{a}{\partial \eta} \left( N_3 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_4 \frac{\partial \phi}{\partial \eta} \right) =$$

$$= \frac{\partial}{\partial \xi} \left( \frac{b_2 \phi}{c_2^2} \right), \quad (4.10)$$

$$\frac{a}{\partial \xi} \left( N_1 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_2 \frac{\partial \phi}{\partial \eta} \right) + \frac{a}{\partial \eta} \left( N_3 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_4 \frac{\partial \phi}{\partial \eta} \right) =$$

$$= \frac{\partial}{\partial \eta} \left( \frac{b_2 \phi}{c_2^2} \right). \quad (4.11)$$

For the higher order solutions, it is evident that the equations are recursive. Accordingly, the recurrence formulas can be written as:

$$\frac{a}{\partial \xi} \left( N_1 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_2 \frac{\partial \phi}{\partial \eta} \right) + \frac{a}{\partial \eta} \left( N_3 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_4 \frac{\partial \phi}{\partial \eta} \right) =$$

$$= \delta \frac{\partial^2 \phi}{\partial \xi^2}, \quad (4.10)$$

$$\frac{a}{\partial \xi} \left( N_1 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_2 \frac{\partial \phi}{\partial \eta} \right) + \frac{a}{\partial \eta} \left( N_3 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_4 \frac{\partial \phi}{\partial \eta} \right) =$$

$$= \delta \frac{\partial^2 \phi}{\partial \eta^2}. \quad (4.11)$$

For the higher order solutions, it is evident that the equations are recursive. Accordingly, the recurrence formulas can be written as:

$$\frac{a}{\partial \xi} \left( N_1 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_2 \frac{\partial \phi}{\partial \eta} \right) + \frac{a}{\partial \eta} \left( N_3 \frac{\partial \phi}{\partial \xi} \right) + \frac{a}{\partial \eta} \left( N_4 \frac{\partial \phi}{\partial \eta} \right) =$$

$$= \delta_{10} \frac{\partial}{\partial \xi} \left( \frac{b_2 \phi}{c_2^2} \right) + (1-\delta_{10}) \delta \frac{\partial^2 \phi}{\partial \xi^2}, \quad (4.12)$$
\[
\frac{\partial}{\partial \xi} \left( N_3 \frac{\partial \nu^\beta}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( N_2 \frac{\partial \nu^\beta}{\partial \eta} \right) + \frac{\partial}{\partial \xi} \left( N_3 \frac{\partial \omega^\beta}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( N_1 \frac{\partial \omega^\beta}{\partial \eta} \right) = \\
= \delta_{10} \frac{\partial}{\partial \eta} \left( \frac{b^2 \gamma \beta}{c_2^2} \phi^\beta \right) + (1-\delta_{10}) \frac{\partial^2 \nu^\beta - 1}{\partial \xi^2}, \quad (4.13)
\]

where \( \delta_{10} \) is Kronecker delta.

Similarly, we can obtain a set of equations for the stress field as follows:

For the terms of the zeroth order in \( \epsilon \),

\[
\sigma^\beta_{\xi \xi} = \frac{\mu_2}{P_0} \delta \left( N_1 \frac{\partial \nu^\beta}{\partial \xi} + N_2 \frac{\partial \omega^\beta}{\partial \eta} - \frac{b^2 \gamma \beta}{c_2^2} \phi^\beta \right), \quad (4.14)
\]

\[
\sigma^\beta_{\xi \eta} = \frac{\mu_2}{P_0} \delta N_3 \left( \frac{\partial \nu^\beta}{\partial \xi} + \frac{\partial \omega^\beta}{\partial \eta} \right), \quad (4.15)
\]

\[
\sigma^\beta_{\eta \eta} = \frac{\mu_2}{P_0} \delta \left( N_2 \frac{\partial \nu^\beta}{\partial \xi} + N_1 \frac{\partial \omega^\beta}{\partial \eta} - \frac{b^2 \gamma \beta}{c_2^2} \phi^\beta \right). \quad (4.16)
\]

For the terms of the first order in \( \epsilon \),

\[
\sigma^\beta_{\xi \xi} = \frac{\mu_2}{P_0} \delta \left( N_1 \frac{\partial \nu^\beta}{\partial \xi} + N_2 \frac{\partial \omega^\beta}{\partial \eta} - \frac{b^2 \gamma \beta}{c_2^2} \phi^\beta \right), \quad (4.17)
\]

\[
\sigma^\beta_{\xi \eta} = \frac{\mu_2}{P_0} \delta N_3 \left( \frac{\partial \nu^\beta}{\partial \xi} + \frac{\partial \omega^\beta}{\partial \eta} \right), \quad (4.18)
\]

\[
\sigma^\beta_{\eta \eta} = \frac{\mu_2}{P_0} \delta \left( N_2 \frac{\partial \nu^\beta}{\partial \xi} + N_1 \frac{\partial \omega^\beta}{\partial \eta} - \frac{b^2 \gamma \beta}{c_2^2} \phi^\beta \right). \quad (4.19)
\]

The recurrence formulas for the stress field are

\[
\sigma^\beta_{\xi \xi} = \frac{\mu_2}{P_0} \delta \left( N_1 \frac{\partial \nu^\beta}{\partial \xi} + N_2 \frac{\partial \omega^\beta}{\partial \eta} - \frac{b^2 \gamma \beta}{c_2^2} \phi^\beta \right), \quad (4.20)
\]
\[ \sigma_{\xi \eta}^0 = \frac{\nu_2}{P_0} \delta N_3 \left( \frac{\partial u_0^\beta}{\partial \eta} + \frac{\partial v_0^\beta}{\partial \xi} \right), \]  \(4.21\)

\[ \sigma_{\eta \eta}^0 = \frac{\nu_2}{P_0} \delta \left( N_2 \frac{\partial u_0^\beta}{\partial \xi} + N_1 \frac{\partial v_0^\beta}{\partial \eta} - \frac{b^2 v_0^\beta}{c_2^2} \phi^\beta \right). \]  \(4.22\)

The boundary conditions are as follows:

For the zeroth order solutions,

(i) the surface \( (c(t)/a \leq \xi \leq [c(t)/a + 1], \eta = 0) \) is traction prescribed

\[ o_{\xi \eta}^I = \mu_f G, \]  \(4.23\)

\[ o_{\eta \eta}^I = -G, \]  \(4.24\)

where

\[ G = \begin{cases} P'(\xi), & \text{for the mechanical stress field} \\ 0, & \text{for the thermal stress field} \end{cases} \]

(ii) the regularity conditions at infinity, \( \xi^2 + \eta^2 \to \infty \), are

\[ u_0^\beta, v_0^\beta, o_{\xi \xi}^0, o_{\eta \eta}^0, o_{\xi \eta}^0 = 0, \]  \(4.25\)

(iii) the continuity conditions, at \( \eta = 0 \), are

\[ u_0^I = u_0^{II}, \quad v_0^I = v_0^{II}, \]  \(4.26\)

\[ o_{\xi \eta}^I = o_{\xi \eta}^{II}, \quad o_{\eta \eta}^I = o_{\eta \eta}^{II}. \]  \(4.27\)
(iv) the cavity boundary conditions are traction free.

For the nth order solutions, the surface is traction free and the remaining boundary conditions are the same as for the zeroth order solutions. The solutions of each perturbative order can be obtained by applying the finite difference method.

4.2 Difference Formulation

Because of the complexity of the geometry and the boundary conditions, the finite difference method is considered more appropriate than the transform method, which was used in the cases without a cavity. In this section, only the zeroth order solutions of the thermal stress field will be discussed in detail, the solutions of higher order and the mechanical stress field can be obtained similarly.

In the finite difference method, the semi-infinite body is replaced by a sufficiently large rectangular region (Figure 4.1), and a non-uniform mesh must be used as we stated in Chapter 3. The non-uniform mesh is transformed to the uniform mesh by applying the general coordinate transformation (Appendix II). The stress field can then be solved in the transformed plane (computational plane) \((\tilde{\xi}, \tilde{\eta})\). The finite difference form of the thermoelastic Navier's equations (4.8) and (4.9) in the computational plane \((\tilde{\xi}, \tilde{\eta})\) can be written as:

\[
\begin{align*}
& a_1 \phi(i-1,j-1,n) + a_2 \phi(i-1,j,n) + a_3 \phi(i-1,j+1,n) + a_4 \phi(i,j-1,n) + \\
& + a_5 \phi(i,j,n) + a_6 \phi(i,j+1,n) + a_7 \phi(i+1,j-1,n) + a_8 \phi(i+1,j,n) + \\
& + a_9 \phi(i+1,j+1,n) = \frac{\partial}{\partial \xi} \left[ \frac{b^2 \psi}{c^2} \phi(i,j,n) \right],
\end{align*}
\]

(4.28)
Figure 4.1 Numerical model for the stress field.
and

\[
a_{10} u^\beta(i-1,j-1, n) + a_{11} v^\beta(i-1,j, n) + a_{12} u^\beta(i-1,j+1, n) + \\
+ a_{13} v^\beta(i,j-1, n) + a_{14} v^\beta(i,j, n) + a_{15} v^\beta(i,j+1, n) + a_{16} u^\beta(i+1,j-1, n) + \\
+ a_{17} v^\beta(i+1,j, n) + a_{18} u^\beta(i+1,j+1, n) = \frac{\partial}{\partial n} \left[ \frac{b^2 \gamma^2}{c_2^2} \Phi(1,j,n) \right], \quad (4.29)
\]

where

\[
a_1 = \frac{[N_2(i-1,j) + N_3(i,j-1)]/(4\xi - \eta - \Delta \xi \Delta \eta)}{\xi \eta}, \quad (4.30)
\]

\[
a_2 = \frac{N_1(i-\frac{1}{2},j)/(\xi^2 \Delta \xi^2) + N_1(i,j)\xi - \eta/(2\xi^2 \Delta \xi)}{\xi \xi}, \quad (4.31)
\]

\[
a_3 = -[N_2(i-1,j) + N_3(i,j+1)]/(4\xi - \eta - \Delta \xi \Delta \eta), \quad (4.32)
\]

\[
a_4 = \frac{N_3(i,j-\frac{1}{2})/(\eta^2 \Delta \eta^2) + N_3(i,j)\eta - \eta/2\eta^2 \Delta \eta}{\eta \eta}, \quad (4.33)
\]

\[
a_5 = -[N_1(i+\frac{1}{2},j) + N_1(i-\frac{1}{2},j)]/(\xi^2 \Delta \xi^2) - \\
- [N_3(i,j+\frac{1}{2}) + N_3(i,j-\frac{1}{2})]/(\eta^2 \Delta \eta^2), \quad (4.34)
\]

\[
a_6 = \frac{N_3(i,j+\frac{1}{2})/(\eta^2 \Delta \eta^2) - N_3(i,j)\eta - \eta/2\eta^2 \Delta \eta}{\eta \eta}, \quad (4.35)
\]

\[
a_7 = -[N_2(i+1,j) + N_3(i,j-1)]/(4\xi - \eta - \Delta \xi \Delta \eta), \quad (4.36)
\]

\[
a_8 = \frac{N_1(i+\frac{1}{2},j)/(\xi^2 \Delta \xi^2) - N_1(i,j)\xi - \eta/(2\xi^2 \Delta \xi)}{\xi \xi}, \quad (4.37)
\]
\[ a_9 = \frac{N_2(i+1,j) + N_3(i,j+1)}{(4\xi - \eta - \Delta\xi \Delta\eta)}, \quad (4.38) \]

\[ a_{10} = \frac{N_2(i,j-1) + N_3(i-1,j)}{(4\xi - \eta - \Delta\xi \Delta\eta)}, \quad (4.39) \]

\[ a_{11} = \frac{N_3(1-\frac{i}{2},j)}{(\xi - \Delta\xi^2)} + \frac{N_3(1,j-1)\xi}{(2\xi - 3\Delta\xi)}, \quad (4.40) \]

\[ a_{12} = -\frac{N_2(1,j+1) + N_3(i-1,j)}{(4\xi - \eta - \Delta\xi \Delta\eta)}, \quad (4.41) \]

\[ a_{13} = \frac{N_1(i,j-\frac{1}{2})}{(\eta - \Delta\eta^2)} + \frac{N_1(i,j)\eta}{(2\eta - 3\Delta\eta)}, \quad (4.42) \]

\[ a_{14} = -\frac{N_3(1-\frac{i}{2},j) + N_3(1+\frac{i}{2},j)}{(\xi - \Delta\xi^2)} - \frac{N_1(i,j+\frac{1}{2}) + N_1(i,j-\frac{1}{2})}{(\eta - \Delta\eta^2)}, \quad (4.43) \]

\[ a_{15} = \frac{N_1(i,j+\frac{1}{2})}{(\eta - \Delta\eta^2)} - \frac{N_1(i,j)\eta}{(2\eta - 3\Delta\eta)}, \quad (4.44) \]

\[ a_{16} = -\frac{N_2(i+1,j) + N_3(i,j-1)}{(4\xi - \eta - \Delta\xi \Delta\eta)}, \quad (4.45) \]

\[ a_{17} = \frac{N_3(1+\frac{i}{2},j)}{(\xi - \Delta\xi^2)} - \frac{N_3(1,j-1)\xi}{(2\xi - 3\Delta\xi)}, \quad (4.46) \]

\[ a_{18} = \frac{N_2(1,j+1) + N_3(i+1,j)}{(4\xi - \eta - \Delta\xi \Delta\eta)}. \quad (4.47) \]

The traction surface boundary conditions are expressed in terms of the displacements:

\[-v_1(i-1,i,n)/(2\xi - \Delta\xi) - 3u_1(i,1,n)/(2\eta - \Delta\eta) + 2u_1(1,2,n)/(\eta - \Delta\eta) - \]

-62-
\[-u^I(i,3,n)/(2\eta_\Delta\bar{\eta}) + v^I(i+1,1,n)/(2\xi_\Delta\bar{\xi}) = 0, \quad (4.48)\]

and

\[\left[-N_2(i,1)u^I(i-1,1,n)/(2\xi_\Delta\bar{\xi}) - 3N_1(i,1)v^I(i,1,n)/(2\eta_\Delta\bar{\eta}) +
+ 2N_1(i,1)v^I(i,2,n)/(\eta_\Delta\bar{\eta}) - N_1(i,1)v^I(i,3,n)/(2\eta_\Delta\bar{\eta}) +
+ N_2(i,1)u^I(i+1,1,n)/(2\xi_\Delta\bar{\xi}) = \frac{b_2^2y_1}{c_2^2} \Phi^I(i,1,n) \right]. \quad (4.49)\]

The traction free boundary conditions on the cavity (Figure 3.3) are:

On face AB:

\[-v^I(i-1,j,n)/(2\xi_\Delta\bar{\xi}) + u^I(i,j-2,n)/(2\eta_\Delta\bar{\eta}) - 2u^I(i,j-1,n)/(\eta_\Delta\bar{\eta}) +
+ 3u^I(i,j,n)/(2\eta_\Delta\bar{\eta}) + v^I(i+1,j,n)/(2\xi_\Delta\bar{\xi}) = 0, \quad (4.50)\]

and

\[\left[-N_2(i,j)u^I(i-1,j,n)/(2\xi_\Delta\bar{\xi}) + N_1(i,j)v^I(i,j-2,n)/(2\eta_\Delta\bar{\eta}) -
- 2N_1(i,j)v^I(i,j-1,n)/(\eta_\Delta\bar{\eta}) + 3N_1(i,j)v^I(i,j,n)/(2\eta_\Delta\bar{\eta}) +
+ N_2(i,j)u^I(i+1,j,n)/(2\xi_\Delta\bar{\xi}) = \frac{b_2^2y_1}{c_2^2} \Phi^I(i,j,n) \right]. \quad (4.51)\]
On face AC:

\[- N_1(i,j)u^{II}(i-1,j,n)/(\xi \Delta \xi) - N_2(i,j)v^{II}(i,j-1,n)/(2\eta \Delta \eta) +
\]

\[+ N_1(i,j)u^{II}(i,j,n)/(\xi \Delta \xi) + N_2(i,j)v^{II}(i,j+1,n)/(2\eta \Delta \eta) =
\]

\[= \frac{b^2_{II} \gamma_{II}}{c_2^2} \phi^{II}(i,j,n), \tag{4.52}\]

and

\[- v^{II}(i-1,j,n)/(\xi \Delta \xi) - u^{II}(i,j-1,n)/(2\eta \Delta \eta) + v^{II}(i,j,n)/(\xi \Delta \xi) +
\]

\[+ u^{II}(i,j+1,n)/(2\eta \Delta \eta) = 0, \tag{4.53}\]

On face BD:

\[- N_2(i,j)v^{II}(i,j-1,n)/(2\eta \Delta \eta) - N_1(i,j)u^{II}(i,j,n)/(\xi \Delta \xi) +
\]

\[+ N_2(i,j)v^{II}(i,j+1,n)/(2\eta \Delta \eta) + N_1(i,j)u^{II}(i+1,j,n)/(\xi \Delta \xi) =
\]

\[= \frac{b^2_{II} \gamma_{II}}{c_2^2} \phi^{II}(i,j,n), \tag{4.54}\]

and

\[- u^{II}(i,j-1,n)/(2\eta \Delta \eta) - v^{II}(i,j,n)/(\xi \Delta \xi) +
\]

\[+ u^{II}(i,j+1,n)/(2\eta \Delta \eta) + v^{II}(i+1,j,n)/(\xi \Delta \xi) = 0, \tag{4.55}\]

\[-64-\]
On face CD:

\[- \nu^\Pi(i-1,j,n)/(2\xi_\Delta^\xi) - 3\nu^\Pi(i,j,n)/(2\eta_\Delta^\eta) +
\]
\[+ 2\nu^\Pi(i,j+1,n)/(\eta_\Delta^\eta) - \nu^\Pi(i,j+2,n)/(2\eta_\Delta^\eta) +
\]
\[+ \nu^\Pi(i+1,j,n)/(2\xi_\Delta^\xi) = 0, \quad (4.56)
\]

and

\[- \eta^\Pi(i,j)\nu^\Pi(i-1,j,n)/(2\xi_\Delta^\xi) - 3\phi^\Pi(i,j)\nu^\Pi(i,j,n)/(2\eta_\Delta^\eta) +
\]
\[+ 2\phi^\Pi(i,j)\nu^\Pi(i,j+1,n)/(\eta_\Delta^\eta) - \phi^\Pi(i,j)\nu^\Pi(i,j+2,n)/(2\eta_\Delta^\eta) +
\]
\[+ \phi^\Pi(i+1,j,n)/(2\xi_\Delta^\xi) = \frac{b^2 y_{\Pi}}{c_2^2} \phi^\Pi(i,j,n), \quad (4.57)
\]

where \( \phi^\Pi(i,j,n) \), \( \partial \phi^\Pi(i,j,n)/\partial \xi \), and \( \partial \phi^\Pi(i,j,n)/\partial \eta \) are input data obtained from the temperature field solutions (re: Chapter 3).

4.3 Cavity Corners Singularities

When values of a solution of a boundary-value problem or its derivatives approach infinity at points, lines, or surfaces in the domain, the solution is said to possess singularities at these places. The approximation of functions with singularities presents some serious numerical difficulties. Nevertheless, calculation of solutions with singularities is extremely important; such problems arise in fracture mechanics, various flow phenomena, heat conduction problems, and in
fact, in any boundary-value problem in which strong irregularities occur in one or more of the following: (a) the geometry of the domain, (b) the coefficients in the governing differential equation, or (c) the prescribed functions, and so on.

Despite the difficulties, numerical methods can be devised that yield excellent results for singular problems. Basically, there are two general ways the problem can be approached:

**Nonuniform Meshes:** This means that a finer gradation of the mesh is used in the neighborhood of singular points in order to capture large changes in the gradients of the solution nearby. This is often a straightforward and effective way to handle singularities and it requires no special modification of the code or special elements, but it may be expensive owing to the necessity of a large number of grid points.

**Special Singular Elements:** The scheme in this case is to devise special elements in which the approximation simulates the diverging rate in elements in the vicinity of the singular point. However, this method can be used only when the behavior of the singularity is known. The procedure of this method is to assume a series which consists of both the regular terms and the singular terms. For thermomechanical problems, the series form of the asymptotic expansion can be written in the form [59, 60, 61, 62, 63]:

\[ u(r, \theta) = \text{regular term} + \sum A_n r^{n m/\zeta} f(\theta), \]  

where \( r, \theta, \) and \( \zeta \) are defined in Figure 4.2. Indeed, when \( n/\zeta \) is not an integer, the derivatives of the leading term in the singular part of
Figure 4.2 Polar coordinates for a domain with a corner at p.

Figure 4.3 Special elements.
u may become unbounded. The order of the singularity increases as $\zeta$ increases. If $\pi/\zeta < 1$, $P$ is referred to as a reentrant corner and the first derivatives of $u$ are then unbounded as $r \to 0$. For the present problem, $\zeta = 3\pi/2$.

For the current problem, the stress singularity at the cavity corner can be resolved by using the results of Williams [64] and Sih [65]. The series form for the displacements in the neighborhood of the cavity corner are:

$$u(r, \theta) = a_1 r^{2/3} \cos(2\theta/3) + a_2 r^{2/3} \sin(2\theta/3) + a_3 r^{2/3} \cos(4\theta/3) +$$

$$+ a_4 r^{2/3} \sin(4\theta/3) + a_5 r^{4/3} \cos(4\theta/3) + a_6 r^{4/3} \sin(4\theta/3) +$$

$$+ \text{regular term}, \hspace{1cm} (4.59)$$

and

$$v(r, \theta) = b_1 r^{2/3} \cos(2\theta/3) + b_2 r^{2/3} \sin(2\theta/3) + b_3 r^{2/3} \cos(4\theta/3) +$$

$$+ b_4 r^{2/3} \sin(4\theta/3) + b_5 r^{4/3} \cos(4\theta/3) + b_6 r^{4/3} \cos(4\theta/3) +$$

$$+ \text{regular term}. \hspace{1cm} (4.60)$$

In the special elements, parts of the coefficients of the series can be determined by substituting equations (4.59) and (4.60) into Navier's Equations (4.8) and (4.9) and the traction free conditions on the cavity. The remaining coefficients can then be solved by using the difference form (4.28) and (4.29). As illustrated in Figure 4.3...
for one specific corner, one can use Equations (4.8) and (4.9) at points 3 and 7 and the traction free condition at point 5 incorporating the singular behavior; then one can use the difference form (4.28) and (4.29) at points 1, 2, 4, 6 to determine the other coefficients of the series.

Equations (4.28, 4.29, 4.48, 4.49, 4.50, 4.51, 4.52, 4.53, 4.54, 4.55, 4.56, 4.57) and the special elements compose a complete set of difference equations for finding the stress field. For the zeroth order solutions, we have to solve a set of simultaneous algebraic equations, which can be separated into two groups, depending on whether the coefficient matrix is dense (few zero elements) or the coefficient matrix is sparse (many zero elements). The two commonly used methods of solving simultaneous algebraic equations include the direct method and the iterative method [66, 67, 68, 69, 70, 71].

Figure 4.4 shows the element pattern of the matrix for the zeroth order solutions. It is a large, banded, but unsymmetric matrix. Because of the dimension of the matrix (≈ 4400x4400), it is almost impossible (too expensive) to store all of the elements. Fortunately, the matrix is banded, therefore we can only store the elements inside the bandwidth by using the one-dimensional array as shown in Figure 4.5, and then using Gauss elimination to solve the system. The computer programs for solving the thermal stress field are given in Appendix IV.

4.4 Numerical Results

For the numerical examples, Stellite III is used as the base material. The mechanical and thermal properties of stellite III are:

\[
E=240\times10^3 \text{ Mpa, } v=0.285, \rho=8.3\times10^3 \text{ kg/m}^3, K=9.7 \text{ J/m}^\circ\text{K}, \kappa=2.77\times10^{-6}
\]
Figure 4.4 Banded matrix for the stress field.
Figure 4.5 One-dimensional array to store banded matrix.
\( \text{m}^2/\text{s}, \ a=11.3 \times 10^{-6} \ \text{m/} \cdot \text{K}, \ \text{and} \ \mu_r=0.5. \) For this problem, the smallest \( \Delta \xi \) and \( \Delta \eta \) in the stress field are 0.02 and 0.006, respectively. The total grid points in \( \xi \) and \( \eta \) directions are 67 and 35. The other important numerical parameters are: \( V=15 \ \text{m/s}, \ \omega=30a, \ d=0.3a, \ e=0.5a, \) and \( a=1 \ \text{mm}. \)

In the numerical results, the effect of the cavity location and the effects of the mechanical and thermal properties on the stress field are also studied. All figures (Figures 4.7 through 4.24) are plotted for the worst case of the asperity position, that is when the asperity is right over the cavity or when the trailing edges of the asperity and the cavity are aligned as shown in Figure 4.6 (asperity position in from \( \xi=-0.7 \) to \( \xi=0.3 \); cavity location is from \( \xi=-0.3 \) to \( \xi=0.3 \)).

When the cavity is located entirely in the surface layer, because the coating layer is thick, the effect is similar to the effect of a single material [33,34,35]. Figures 4.7 to 4.12 plot the thermal principal stresses along the asperity traverse direction at the critical depth for the cases of a single material with a cavity. Different cases of a single material with a cavity are tabulated in Table 2. Figure 4.7 compares the dimensionless principal thermal stress of the single material with (case 1A) and without (case 2) a cavity. The maximum dimensionless tensile thermal stress is 0.98 for no-cavity case occurring at a depth \( \eta=0.16 \), while it is 5.9 at a depth of 0.088 for the medium with a cavity at a ligament thickness 0.094.

The location of the cavity from the wear surface, as indicated by the ligament thickness, influences the temperature field in the total volume available for heat content generated by frictional heating. As a consequence, the thermal stress state is strongly affected. Figure
### Table 2

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<th>Case</th>
<th>k</th>
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<th>E</th>
<th>α</th>
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* Base material is Stellite III.*
Figure 4.7 Thermal principal stress (cases 1A, 2).
4.8 shows the effect of various cavity locations on the thermal stress field. Ju et al [27,32,58] showed that, without a cavity, the critical depth at which the tensile thermal stress reaches a maximum is $\eta=0.16$ for a moving line asperity excitation over Stellite III. However, with a near-surface cavity, both the temperature distribution and its gradients are different, thus changing the critical depth. The maximum tensile stress is optimized with respect to various ligament thickness. The worst case for the maximum tensile stress for Stellite III is obtained when the top edge of the cavity is at $\eta=0.094$.

Figure 4.9 presents the effect of the thermal conductivity. Case 1A is of Stellite III. Case 3A shows the effect that the thermal conductivity is reduced by half, while case 3B demonstrates the effect that the thermal conductivity is twice that of Stellite III. Figure 4.9 establishes that the principal thermal stress increases with decreasing thermal conductivity. In Figure 4.10, cases 4A and 4B show the results of doubling and halving the thermal capacity, respectively. We observe that decreasing heat capacity will increase thermal stress. Figures 4.11 and 4.12 demonstrate the effects of Young's modulus and the coefficient of thermal expansion. In Figure 4.11, Young's moduli for cases 5A and 5B are, respectively, three times and one-half that of Stellite III. In Figure 4.12, the thermal expansion coefficients for cases 6A and 6B are, respectively, twice and one-half that of Stellite III. These two figures clearly show that increasing either Young's modulus or the thermal expansion coefficient induces higher thermal stress.

When the top edge of the cavity is at the interface, both the coating layer and the substrate will influence the stress field.
Figure 4.8 Thermal principal stress (cases 1A, 1B, 1C, 1D). $\eta=0.06$ above the top edge of the cavity for all cases.
Figure 4.9 Thermal principal stress (cases 1A, 3A, 3B). L=0.094, and \( \eta=0.06 \) above the top edge of the cavity for all cases.
Figure 4.10 Thermal principal stress (cases 1A, 4A, 4B). L=0.094, and η=0.06 above the top edge of the cavity for all cases.
Figure 4.11 Thermal principal stress (cases 1A, 5A, 5B). L=0.094, and η=0.06 above the top edge of the cavity for all cases.
Figure 4.12 Thermal principal stress (cases 1A, 6A, 6B). $L=0.094$, and $\eta=0.06$ above the top edge of the cavity for all cases.
Figures 4.13 to 4.24 show the results of the cases in which the top edge of the cavity is at the interface. Different cases of a layered medium with a cavity are listed in Table 3.

In the case of a medium with no-cavity, the effect of the mechanical stress field is small enough to be neglected. When a cavity exists, the effect of the mechanical stress field is no longer negligible. Figure 4.13 plots the principal thermal stress field (case 7A), mechanical stress field (case 7B), and combined stress field (case 7C). In this figure, the material of the substrate is Stellite III, and the material properties of the coating layer are the same as Stellite III except that Young's modulus is twice that of Stellite III. This figure establishes that the tensile thermal stress is larger than the tensile mechanical stress. However, the mechanical stress field is not so small that we can neglect it as indicated in the no-cavity case.

The effect of the cavity location on the thermal stress field for a layered medium is presented in Figure 4.14. From this figure, one can see that the maximum tensile stress occurs when the ligament thickness $L=0.094$, which is the same value as in the case of a single material with a cavity. Figures 4.15 and 4.16 present the effects of Young's modulus of the coating layer and the substrate, respectively. In Figure 4.15, the material of the substrate is Stellite III for all cases. Young's modulus of the surface layer for different cases is: case 1A is the same as Stellite III; case 7A is twice that of Stellite III, case 9A and case 9B are, respectively, three times and one-half that of Stellite III. From this figure, one can see that the principal thermal stress field is strongly influenced by the Young's modulus of the coating layer; increasing Young's modulus of the coating layer will
### Table 3

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<th>$E_I$</th>
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<th>$a_{II}$</th>
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<td>$E_{II}$</td>
<td>$2a_I$</td>
<td>$a_{II}$</td>
<td>0.094</td>
<td>Yes thermal stress</td>
</tr>
<tr>
<td>12B</td>
<td>$k_I$</td>
<td>$k_{II}$</td>
<td>$E_I$</td>
<td>$E_{II}$</td>
<td>$\frac{1}{2}a_I$</td>
<td>$a_{II}$</td>
<td>0.094</td>
<td>Yes thermal stress</td>
</tr>
</tbody>
</table>

* Base materials for both the coating layer and the substrate are Stellite III.
Figure 4.13 Thermal, mechanical, and combined principal stress (cases 7A, 7B, 7C).

L=0.094, and \( \eta=0.06 \) above the top edge of the cavity for all cases.
Figure 4.14 Thermal principal stress (cases 7A, 8A, 8B, 8C, 8D). $\eta = 0.06$ above the top edge of the cavity for all cases.
Figure 4.15 Thermal principal stress (cases 1A, 7A, 9A, 9B). L=0.094, and η=0.06 above the top edge of the cavity for all cases.
increase the principal thermal stress. In Figure 4.16, the material of
the coating layer is Stellite III for all cases. Young's modulus of
the substrate is one-fifth (case 10A), one-half (case 10B), and five
times (case 10C) that of Stellite III. This figure shows that
decreasing Young's modulus in the substrate will result in increasing
the thermal stress field, but the influence from the substrate is
weaker than from the coating layer. Figure 4.17 compares the effect of
Young's modulus on the thermal stress field from a single material and
from a layered medium. In the figure, dashed lines represent the case
of a single material with a cavity, while solid lines represent the
case of a layered medium with a cavity. From this figure, we observe
that thermal stress increases linearly in proportion to Young's modulus
for the single material case. For the layered medium case, however,
increasing by the same amount Young's modulus in the coating layer will
result in higher thermal stress than in the case of a single material.
This is because we will have a relative softer substrate by increasing
Young's modulus in the coating layer. The effects from thermal
conductivity and the coefficient of thermal expansion are presented in
Figures 4.18 and 4.19. These effects are similar to those found in the
case of a single material with a cavity.

From the failure specimen for the case of a single material with no-
cavity (Figures 1.1 and 1.2), we observe that the thermomechanical
cracking is perpendicular to the wear surface. However, Ju and Liu
[34] showed that, in the case of a layered medium with no-cavity, shear
delamination (cracking is parallel to the wear surface) may occur
caused by the changing of principal directions (larger angle of
principal direction), therefore, it is important to understand what
Figure 4.18 Thermal principal stress (1A, 11A, 11B). $L=0.094$, and $\eta=0.06$ above the top edge of the cavity for all cases.
Figure 4.19 Thermal principal stress (cases 1A, 12A, 12B). L=0.094, and \( \eta = 0.06 \) above the top edge of the cavity for all cases.
will affect principal directions. Figure 4.20 shows the effect of the
ligament thickness (cavity location) on principal directions at the
point \( \xi = 0.3 \) and \( \eta = 0.006 \) above the cavity top edge. From this figure,
we observe that increasing the ligament thickness will result in larger
angle of principal direction, and the angle of principal direction
changes drastically when \( L = 0.094 \), the value which gives the maximum
tensile stress. Figures 4.21 and 4.22 compare the effect of Young's
modulus on principal directions for the case of a single material with
a cavity (dashed line) and for the case of a layered medium with a
cavity (solid line). These two figures establish that decreasing
Young's modulus in the coating layer (\( E_I \)) or increasing Young's modulus
in the substrate (\( E_{II} \)) will increase the angle of principal direction.
Nevertheless, changing Young's modulus in the case of a single material
with a cavity will not affect the principal directions. Figures 4.23
and 4.24 illustrate the effects of the thermal conductivity and the
coefficient of thermal expansion on principal directions for the case
of a single material with a cavity (dashed line) and the case of a
layered medium with a cavity (solid line). From these two figures, one
can see that thermal conductivity and the coefficient of thermal
expansion will not influence principal directions significantly.
Figure 4.20 The effect of the ligament thickness on the angle of principal direction of the thermal stress field.
Figure 4.21 The effect of Young's modulus of the coating layer on the angle of principal direction of the thermal stress field. \( E = 0.094 \), and \( n = 0.06 \) above the top edge of the cavity for all cases.
Figure 4.22 The effect of Young's modulus of the substrate on the angle of principal
direction of the thermal stress field. $L=0.094$, and $\eta=0.06$ above the top
dge of the cavity for all cases.
Figure 4.23 The effect of thermal conductivity of the coating layer on the angle of principal direction of the thermal stream field. L=0.094, and η=0.06 above the top edge of the cavity for all cases.
Figure 4.24 The effect of the coefficient of thermal expansion of the coating layer on the angle of principal direction of the thermal stress field. L=0.094, and η=0.06 above the top edge of the cavity for all cases.
CHAPTER 5

DISCUSSION AND CONCLUSIONS

The present investigation demonstrates the effect of a near-surface rectangular cavity on the temperature and stress fields caused by the frictional excitation of a moving asperity. The effects of a coating layer are demonstrated by the material parameter variations in the coating layer and the substrate, including changes on both thermal and mechanical properties. The mathematical model, because of the geometry, is time explicit. Since the transient solution to a multiple-boundary problem is always complex, numerical solutions become necessary for analyses in specific cases. In the present problem, it has been demonstrated that: (i) the transient governing differential equations (2.1, 2.12, and 2.26), can be formulated in difference forms; (ii) the nonuniform mesh (ξ,η), which must be employed due to strong local effects, can be transformed into a uniform mesh (ξ,η); (iii) boundary conditions in temperature and/or heat flux can be expressed through the energy balance method, thus avoiding the singularity problem at the cavity corner; (iv) the stress singularity at each corner of the cavity can be taken care of by embedding a known stress singularity in the vicinity of the corner; (v) the numerical solution can be tested by comparing with a known analytical solution, showing a satisfactory accuracy; and (vi) the numerical scheme can be extended to compute the solution for other geometries, such as those including cracks and circular cavities, using proper coordinate transformations.

Like most numerical solutions, functional relationships can not be
obtained without voluminous computations. However, significant conclusions can be reached through a careful selection of pertinent cases for the numerical results. The conclusions for the present problem are:

**Temperature field**

1. Because of the discontinuity in heat transfer across the cavity, temperature will rise higher in the ligament region than the no-cavity case.

2. The temperature rise is inverse to the ligament volume, represented by the ligament thickness.

3. Increasing the thermal conductivity and heat capacity of the coating layer, will decrease the surface temperature.

4. When the coating/substrate interface is at the ligament depth, the thermal property of the substrate will influence the temperature field in the region on the trailing edge of the asperity.

5. Because of the necessary heat transfer in the lateral direction, the heat flux will be at a large oblique angle to the wear surface. In the case of a layered medium without a cavity, the near surface heat flux at the critical position is in a direction approximately 90° to the wear surface. With the presence of a cavity, not only the magnitude of the temperature gradient increases, but also the direction of the temperature gradient is rotated to a more oblique angle to the wear surface. This will affect principal directions in the thermal stress field.

**Stress field**

1. In the governing differential equation, the small order coefficients of the dynamic terms would have required an extremely
small time step for the consideration of stability and truncation error. This difficulty was circumvented by using the perturbation method. The solutions of the differential equations (4.12) and (4.13) of the various perturbation orders are well-behaved. The magnification, \((u_{i+1}/u_i)\), is of order \(10^2\). Since \(\epsilon = \frac{H^2}{N}\) is of the order \(10^{-6}\), each perturbation term in equations (4.12) and (4.13) is of order \(10^{-4}\) of its preceding term. Because the series converges rapidly, all computations are deemed adequate by using only one term.

2. When a cavity exists, the stress state that determines the failure phenomenon is much more severe than in the no-cavity case. This will lead to earlier failure of the mechanism.

3. The mechanical effect, which can be neglected in the no-cavity case, is not negligible when cavities exist.

4. The effects of the mechanical and thermal properties on the stress field are consistent with those obtained in the no-cavity case in reference [32]. These effects may be summarized as follows: thermal stress can be reduced by decreasing Young's modulus in the coating layer, increasing Young's modulus in the substrate, increasing thermal conductivity and thermal capacity of the coating layer, and decreasing the coefficient of thermal expansion of the coating layer.

5. For a thin coated medium, the cavity location and the material properties matching (especially Young's modulus) will influence the principal directions of the thermal stress field. When the angle of principal direction becomes larger, shear stress at the coating/substrate interface becomes dominant, leading toward delamination of the coating.

6. The location of the cavity influences the critical depth at
which the thermal tensile stress reaches a maximum. When the cavity occurs closer to the wear surface, not only the critical depth is reduced but also a higher stress results, which reaches its maximum at a critical ligament thickness. Further reduction of the ligament thickness would increase the ligament temperature, resulting in an extension of the thermal compressive region therein. Correspondingly, the thermal tensile stress decreases near the ligament region. The illustration for Stellite III shows that the critical thickness is at \( L_{cr}=0.094 \) for both cases of a single material and a layered medium with a thickness of approximately 40% of the critical depth of the no-cavity case. For the normal design of coating thickness, the critical depth of the specific coating material can function as a guide. However, if cavities are either unavoidable or too expensive to control, the design thickness should avoid the critical ligament thickness.
APPENDIX I

INTRODUCTION TO THE FINITE DIFFERENCE METHOD

The use of numerical methods for solving problems is a result of the complexity of the analytical solutions associated with practical engineering problems. Often times, analytical solutions are impossible. In engineering problems, factors that bring about the use of numerical methods are complex geometry, nonlinearity, nonuniform boundary conditions, time-dependent boundary conditions, temperature-dependent properties, and so on. In some cases, analytical solutions are possible, in principle, but the mechanics of obtaining the exact solution may be much more difficult than the task of solving the problem numerically. For example, in the problem of finding the stress solution of a composite multilayered body with nonhomogeneous boundary conditions, it is relatively easy to set up the differential equations. The solution, however, is extremely complex, because it is necessary to deal with simultaneous partial differential equations. In all such cases and many others, if one is equipped with the knowledge of numerical methods and computer programming, the required solution can be successfully obtained.

Finite difference approximations for derivatives were already in use by Euler in 1768. The simplest finite difference procedure for dealing with the problem \( \frac{dx}{dt} = f(x) \), \( x(0) = a \) is obtained by replacing \( (dx/dt)_{n-1} \) with the crude approximation \( (x_n - x_{n-1})/\Delta t \). This leads to the recurrence relation \( x_0 = a \), \( x_n = x_{n-1} + \Delta t \cdot f(x_{n-1}, t_{n-1}) \) for \( n > 0 \). This procedure is known as Euler's method. Thus we see
that, for one-dimensional systems, the finite difference approach has been deeply ingrained in computational algorithms for quite some time.

1.1 Finite Difference Approximation of Derivatives Through Taylor's Series

The derivative of a function at a given point can be represented by a finite difference approximation using a Taylor series expansion of the function about that point. Let \( f(x) \) be a function that can be expanded in a Taylor series. Then a Taylor series expansion of the functions \( f(x+h) \) and \( f(x-h) \) about \( x \), as illustrated in Figure I.1, is given by

\[
\begin{align*}
    f(x+h) &= f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \ldots, \\
    f(x-h) &= f(x) - h f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \ldots,
\end{align*}
\]

where primes denote derivatives with respect to \( x \). The first- and second-order derivatives \( f'(x) \) and \( f''(x) \) can be represented in the finite difference form in many different ways by utilizing Taylor series expansions given by equations (I.1) and (I.2) as now described.

First Derivatives

To obtain expressions for the finite difference form of the first-order derivative \( f'(x) \), equations (I.1) and (I.2) are solved for \( f'(x) \). We, respectively, obtain

\[
\begin{align*}
    f'(x) &= \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(x) + \frac{h^2}{6} f'''(x) + \ldots, \\
    f'(x) &= \frac{f(x) - f(x-h)}{h} + \frac{h}{2} f''(x) + \frac{h^2}{6} f'''(x) + \ldots.
\end{align*}
\]
Figure 1.1 Nomenclature for a Taylor series representation.

Figure 1.2 Nomenclature for finite difference representation of $f(x)$.
Subtracting equations (1.1) and (1.2) and solving for $f'(x)$ we obtain

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(x) + \ldots,$$

(1.5)

From equations (1.3) to (1.5), the following approximations can be written respectively for the first derivative of a function $f(x)$ about the point $x$.

$$f'_x = \frac{f_{i+1} - f_i}{h}, \text{ forward difference}$$

(1.6)

$$f'_x = \frac{f_i - f_{i-1}}{h}, \text{ backward difference}$$

(1.7)

$$f'_x = \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2), \text{ central difference}$$

(1.8)

here the notation $O(h)$ is used to show that the truncation error involved is of the order of $h$; similarly $O(h^2)$ is for the truncation error of the order of $h^2$, and

$$x = ih, \quad x+h = (i+1)h, \quad x-h = (i-1)h, \quad \text{etc},$$

(1.9)

$$f(x) = f_i, \quad f(x+h) = f_{i+1}, \quad f(x-h) = f_{i-1}, \quad \text{etc},$$

(1.10)

as illustrated in Figure 1.2. We note that forward and backward differences are accurate to the order $h$ whereas the central difference expression is accurate to the order $h^2$. More accurate expressions can be obtained for the forward and backward difference representation of the first-order derivative as will be discussed later.
Second Derivatives

We now proceed to the finite difference representation of the second derivative \( f''(x) \) of a function \( f(x) \) about the point \( x \). To obtain such results we consider a Taylor series expansion of functions \( f(x+2h) \) and \( f(x-2h) \) about \( x \) as

\[
4 f(x+2h) = f(x) + 2h f'(x) + 2h^2 f''(x) + \frac{4}{3} h^3 f'''(x) + \ldots, \quad (1.11)
\]

\[
4 f(x-2h) = f(x) - 2h f'(x) + 2h^2 f''(x) - \frac{4}{3} h^3 f'''(x) + \ldots, \quad (1.12)
\]

Eliminating \( f'(x) \) between equations (1.1) and (1.11) we obtain

\[
f'''(x) = \frac{f(x) + f(x+2h) - 2f(x+h)}{h^2} - h f'''(x) + \ldots, \quad (1.13)
\]

Similarly, eliminating \( f'(x) \) between equations (1.2) and (1.12), we find

\[
f'''(x) = \frac{f(x-2h) + f(x) - 2f(x-h)}{h^2} + h f'''(x) + \ldots, \quad (1.14)
\]

Eliminating \( f'(x) \) between equations (1.1) and (1.2) we obtain

\[
f'''(x) = \frac{f(x-h) + f(x+h) - 2f(x)}{h^2} - \frac{1}{12} h^2 f'''(x) + \ldots, \quad (1.15)
\]

Using the subscript notation defined by equations (1.9) and (1.10), various forms of the finite difference representation of the second-order derivative \( f''(x) \) about the point \( x \) given by equations (1.13) to
(I.15) are written, respectively, as

\[ f_i'' = \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} + O(h), \quad \text{forward difference} \quad (I.16) \]

\[ f_i'' = \frac{f_{i-2} - 2f_{i-1} + f_i}{h^2} + O(h), \quad \text{backward difference} \quad (I.17) \]

\[ f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + O(h^2), \quad \text{central difference} \quad (I.18) \]

We note that the central difference representation is accurate to \( O(h^2) \) whereas the forward and backward differences to \( O(h) \).

**More Accurate Finite Difference Representations**

The forward and backward finite difference representations given above are accurate to \( O(h) \). More accurate expressions can be obtained as now described. Suppose \( f'(x) \) is to be represented in forward difference to \( O(h^2) \). Equation (I.13) is introduced into equation (I.3) and \( f''(x) \) is eliminated. We obtain

\[ f'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} + \frac{1}{3} h^2 f'''(x) + \ldots, \quad (I.19) \]

which is written more compactly in the form

\[ f_i' = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + O(h^2), \quad \text{forward difference} \quad (I.20) \]

Similarly, introducing equation (I.14) into equation (I.4) to eliminate \( f'''(x) \), we find

\[ f_i' = \frac{f_{i-2} - 4f_{i-1} + 3f_i}{2h} + O(h^2), \quad \text{backward difference} \quad (I.21) \]
The above procedure can be extended to obtain more accurate expressions for the first and second derivatives. Such expressions are presented in reference [47] for various order derivatives.

The derivative of a function in non-uniform spacing (Figure 1.3) can also be approximated by finite difference using a Taylor series expansion. A summary of the finite difference representation of the first- and second-order derivatives of a function \( f(x) \) in non-uniform spacing is given below

\[
\begin{align*}
f'_1 &= \frac{2h_1 + h_2}{h_1 (h_1 + h_2)} f_i + \frac{h_1 + h_2}{h_1 h_2} f_{i+1} - \frac{h_1}{h_2 (h_1 + h_2)} f_{i+2}, \quad \text{forward difference} \\
f'_i &= \frac{h_2}{h_1 (h_1 + h_2)} f_{i-2} - \frac{h_1 + h_2}{h_1 h_2} f_{i-1} + \frac{h_1 + 2h_2}{h_2 (h_1 + h_2)} f_i, \quad \text{backward difference} \\
f'_i &= -\frac{h_2}{h_1 (h_1 + h_2)} f_{i-1} + \frac{h_2 - h_1}{h_1 h_2} f_i + \frac{h_1}{h_2 (h_1 + h_2)} f_{i+1}, \quad \text{central difference} \\
f''_i &= \frac{2}{h_1 (h_1 + h_2)} f_{i-1} - \frac{2}{h_1 h_2} f_i + \frac{2}{h_2 (h_1 + h_2)} f_{i+1}, \quad \text{central difference}
\end{align*}
\]

Using equations (I.22) to (I.25) is very cumbersome, and it may lead to loss of accuracy. A more elegant method, general coordinates transformation, can be employed in the non-uniform mesh to avoid these problems. This transformation will be discussed in detail later.

1.2 Errors Involved in Numerical Solutions

In numerical solutions using the method of finite differences, the partial differential equation is approximated with finite difference
expressions at each nodal point, and as a result the solution of the differential equation is transformed to the solution of a set of algebraic equations. We have seen that, whenever a derivative is approximated by finite difference using a Taylor series expansion, an error is involved. Such an error is called the truncation error or the discretization error. These errors appear because a continuous operator such as the first, or the second-order derivative, is replaced by a finite difference approximation. In addition, numerical calculations are carried out only to a finite number of decimal places or significant figures; as a result, at each step in the calculation, some error is introduced due to this rounding-off, called the round-off error.

Clearly, if the finite difference approximation is made by using formulas having truncation errors of high order, the truncation error at each step is minimum. Also, by decreasing the step size, the truncation error is reduced for each step; however, a limit also is reached at which further reduction in step size increases the total number of calculations and as a result the round-off error may become dominant.

Ideally, if it were possible to carry out the finite difference calculations with extremely small steps and to perform the calculations to an infinite number of decimal places, the resulting solution would be exact. However, due to the cumulative effects of the rounding off error and the discretization errors, the solutions obtained by the finite difference method is expected to deviate from the exact result; therefore, the solution computed is the numerical solution but not the exact result. It is very difficult to determine the cumulative
departure of the numerical solution from the exact result due to the cumulative effects of such errors. Comparison of numerical solutions with exact analytic solutions reveals that, for most cases, the results are very close indeed. After some experience with different methods and different step sizes, a suitable combination can be chosen for the numerical solution of a given problem.

1.3 Time Dependent Problem

The stability consideration plays an important role in the finite difference solution of time dependent problems. There are several schemes available to express the time dependent problems in finite difference form. Each of these differencing schemes has its advantages and limitations. We now discuss some of them by using the one-dimensional time-dependent heat conduction equation as examples.

Explicit Method

The one-dimensional, time-dependent heat conduction equation for a finite region $0 \leq x \leq L$ is

$$\frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2}, \quad (I.26)$$

If $\frac{\partial^2 T}{\partial x^2}$ and $\frac{\partial T}{\partial t}$ are replaced by the central and forward differences, respectively, and using a uniform mesh size $\Delta x$ in the $x$ domain and $\Delta t$ for the time step, equation (I.26) can be rewritten in the finite-difference form as

$$\frac{T(i, n+1) - T(i, n)}{\Delta t} = k \frac{T(i-1, n) - 2T(i, n) + T(i+1, n)}{\Delta x^2}, \quad (I.27)$$

with a truncation error of $O(\Delta t) + O(\Delta x^2)$. Where $T(x, t)$ is
represented by \( T(x,t) = T(i\Delta x, n\Delta t) = T(i,n) \). Solving equation (1.27) for \( T(i,n+1) \) one obtains

\[
T(i,n+1) = rT(i-1,n) + (1-2r)T(i,n) + rT(i+1,n),
\]

(1.28)

where \( r = \frac{k\Delta t}{\Delta x^2} \).

The equation is called the explicit form because the unknown temperature \( T(i,n+1) \) at the time step \( n+1 \) can be directly determined from the temperatures \( T(i-1,n), T(i,n), \) and \( T(i+1,n) \) at the previous time step. The explicit scheme provides a relatively straightforward expression for the determination of the unknown \( T(i,n+1) \). The only disadvantage of this method is that once \( k \) and \( \Delta x \) are fixed, there is a maximum permissible step size \( \Delta t \), which, by instability considerations should not be exceeded. For example, when the boundary conditions at \( x=0 \) and \( x=L \) are both of the first kind (i.e., specified temperature), the restriction imposed on the parameter \( r \) is

\[
0 \leq r \leq \frac{1}{2}.
\]

(1.29)

That is, for given values of \( k \) and \( \Delta x \), if the time step \( \Delta t \) exceeds the limit imposed by the above criteria, the numerical calculations become unstable, as a result of the amplification of errors. Figure 1.4 illustrates what happens to the numerical calculations when the above stability criteria is violated. In this figure, the numerical calculations performed with a time step satisfying the condition

\[
r = \frac{5}{11} < \frac{1}{2}
\]

is in good agreement with the exact solution; whereas the numerical solution of the same problem with slightly larger time step,
Figure 1.3 Nonuniform mesh.

Figure 1.4 Effects of parameter $r=\Delta t/(\Delta x)^2$ on the stability of finite difference solution.
which violates the above stability criteria, i.e., \( r = \frac{\Delta t}{2} \), results in an unstable solution.

**Implicit Method**

The explicit method discussed above is simple computationally, but very small time step should be used because of stability considerations. Therefore, a prohibitively large number of time steps may be required if solutions are to be computed over a large period of time. It is for this reason that other finite difference forms, found to be less restrictive to the size of time step \( \Delta t \), have been developed. One such scheme is the fully implicit method. We illustrate this method by considering the finite difference representation of the heat conduction equation (1.26). The partial derivative \( \frac{\partial^2 T}{\partial x^2} \) is represented in finite difference form using the central difference formula, whereas the time derivative \( \frac{\partial T}{\partial t} \) is represented in the finite difference form using the backward difference expression.

Then, the finite difference form of equation (1.26) becomes

\[
\frac{T(i,n+1) - T(i,n)}{\Delta t} = k \frac{T(i-1,n+1) - 2T(i,n+1) + T(i+1,n+1)}{\Delta x^2}, \tag{1.30}
\]

This is called an implicit form of the finite difference representation, because to determine the unknowns \( T(i,n+1) \), a set of simultaneous algebraic equations are to be solved. The advantage of the implicit method is that it is stable for all sizes of time step \( \Delta t \). Thus, there is no size restriction on \( \Delta t \). The only size restriction on \( \Delta t \) is due to the consideration of the truncation error.

The truncation errors for both explicit and implicit forms of the
finite difference representations of the heat conduction equation is of the order \((\Delta x^2) + (\Delta t)\). But the actual accumulated error in both methods need not be the same. Depending on the nature of the problem, one of the methods may be preferred to the other.

**Crank-Nicolson Method**

Crank and Nicolson [47] suggested a modified implicit method. In this method, the heat conduction equation (1.26) is represented in finite difference form by taking the arithmetic average of the right-hand sides of the explicit form (1.26) and the implicit form (1.30). Then, equation (1.26) becomes

\[
\frac{T(i,n+1) - T(i,n)}{\Delta t} = \frac{k}{2} \left[ \frac{T(i-1,n+1) - 2T(i,n+1) + T(i,n+1)}{\Delta x^2} + \frac{T(i-1,n) - 2T(i,n) + T(i+1,n)}{\Delta x^2} \right].
\] (1.31)

The advantage of this method is that, for given values of the space and time steps \(\Delta x\) and \(\Delta t\), the resulting solution involves less truncation error due to \(\Delta t\) than the explicit and the implicit forms discussed above. On the other hand the Crank-Nicolson form involves additional computation.

To provide a better insight to the physical significance of the Crank-Nicolson representation, equation (1.31) can be written in a more general form by taking a weighted average of the two terms in the brackets

\[
\frac{T(i,n+1) - T(i,n)}{\Delta t} = k \left( \frac{T(i-1,n+1) - 2T(i,n) + T(i+1,n)}{\Delta x^2} \right). \] (1.32)

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where $0 < \eta < 1$ is called the degree of implicitness. Clearly, equation (1.32) reduces to the explicit form given by equation (1.27) for $\eta = 0$, to the implicit form given by equation (1.30) for $\eta = 1$ and the Crank-Nicolson form (1.31) for $\eta = \frac{1}{2}$.

Alternating-Direction Implicit Method

The implicit methods discussed above are advantageous to us because of the superior stability properties. On the other hand, because a large number of simultaneous equations need to be solved at each time step, the computational problems become enormous when they are applied to the solution of time dependent problems involving two or three space dimensions. For example, for a three-dimensional problem with $N$ interior nodal points in each direction, there are a total of $N^3$ nodes, hence $N^3 \times N^3$ matrix equations must be solved for each time increment.

The alternating-direction implicit (A.D.I.) method introduced by Peaceman and Rachford [48], provides an efficient method for solving problems involving large number of nodes. To illustrate the procedure, a two-dimensional, time dependent heat conduction equation is considered

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = \frac{1}{\kappa}\frac{\partial T}{\partial t}, \quad \text{in the region } R \quad (1.33)$$

To represent the space derivatives in finite difference form, the central difference formula is used with an implicit and explicit difference approximation alternatively for $\frac{\partial^2 T}{\partial x^2}$ and $\frac{\partial^2 T}{\partial y^2}$. For example, if $\frac{\partial^2 T}{\partial x^2}$
is represented in the implicit form, the derivative $\frac{\partial^2 T}{\partial y^2}$ is represented by an explicit approximation. Then, the finite difference form of equation (I.33), to proceed the solution from the (n)th step to (n+1)th step, becomes

$$\frac{1}{\kappa} \frac{T(i,j,n+1) - T(i,j,n)}{\Delta t} = \frac{\Delta t}{\Delta x^2} \left[ T(i-1,j,n+1) + 2T(i,j,n+1) + T(i+1,j,n+1) \right]$$

$$+ \frac{T(i,j-1,n) - 2T(i,j,n) + T(i,j+1,n)}{\Delta y^2}. \quad (I.34)$$

The finite difference form of equation (I.33), to proceed the solution from the (n+1)th step to the (n+2)th step, is written using an explicit form for $\frac{\partial^2 T}{\partial x^2}$ and implicit form for $\frac{\partial^2 T}{\partial y^2}$ as

$$\frac{1}{\kappa} \frac{T(i,j,n+2) - T(i,j,n+1)}{\Delta t} = \frac{\Delta t}{\Delta x^2} \left[ T(i-1,j,n+1) + 2T(i,j,n+1) + T(i+1,j,n+1) \right]$$

$$+ \frac{T(i,j-1,n+2) - 2T(i,j,n+2) + T(i,j+1,n+2)}{\Delta y^2}. \quad (I.35)$$

The procedure is repeated alternately in the subsequent time steps.

The advantage of the A.D.I. method over the implicit method results from the fact that it reduces the number of equations to be solved simultaneously for each time step. Consider for example a two-dimensional, time dependent problem with N internal nodes along the x-axis and N nodes along the y-axis. The A.D.I. method requires the solution of N simultaneous equation N times for each time step, whereas the implicit method requires the solution of $N^2$ equation at each time step. There are other methods, for example, the alternating direction...
explicit (A.D.E) method [49], the Douglas-Rachford implicit scheme [48], ..., etc. The reader should consult these references for further discussion of these methods.
APPENDIX II

NON-UNIFORM MESH AND GENERAL COORDINATES TRANSFORMATION

The solution of a system of partial differential equations can be greatly simplified by a well-constructed grid. On the other hand, a grid which is not well suited to the problem can lead to an unsatisfactory result. In some applications, improper choice of grid point locations can lead to an apparent instability or lack of convergence. For many applications, a non-uniform mesh must be used in order to obtain an accurate solution and to save computing time. One can solve the problem in the physical plane (original plane) by applying the difference formulas on the non-uniform mesh directly, or transform the non-uniform mesh to a uniform mesh and solve the problem in the computational plane. Generally, the coordinate transformation gives a more accurate solution than mesh changes.

II.1 Non-Uniform Mesh

The simplest variation of the rectangular mesh system is obtained by simply changing the mesh spacing in one direction at some point. This would be done for the purpose of obtaining higher resolution (and hopefully higher accuracy) in some region where the gradients were expected to change rapidly. To illustrate this technique, we consider the obvious method of changing from $\Delta x_1$ to $\Delta x_2$ between node points at some node $i=m$, as shown in Figure II.1.

Expanding a function in a Taylor series forward and backward from $i=m$ gives
\[ f_{m+1} = f_m + \frac{\partial f}{\partial x} \Delta x_2 + \left( \frac{1}{2} \frac{\partial^2 f}{\partial x^2} \right) \Delta x_2^2 + \left( \frac{1}{6} \frac{\partial^3 f}{\partial x^3} \right) \Delta x_2^3 + O(\Delta x_2^4), \tag{11.1} \]

\[ f_{m-1} = f_m - \frac{\partial f}{\partial x} \Delta x_1 + \left( \frac{1}{2} \frac{\partial^2 f}{\partial x^2} \right) \Delta x_1^2 - \left( \frac{1}{6} \frac{\partial^3 f}{\partial x^3} \right) \Delta x_1^3 + O(\Delta x_1^4), \tag{11.2} \]

The expression for \( \frac{\partial f}{\partial x} \) is obtained by subtracting equation (11.2) from (11.1)

\[ f_{m+1} - f_{m-1} = \frac{\partial f}{\partial x} (\Delta x_1 + \Delta x_2) + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} (\Delta x_2^2 - \Delta x_1^2) + O(\Delta x^3), \tag{11.3} \]

where by \( O(\Delta x^3) \) we mean the largest of \( O(\Delta x_1^3) \) or \( O(\Delta x_2^3) \). Solving for \( \frac{\partial f}{\partial x} \) gives

\[ \frac{\partial f}{\partial x} = \frac{f_{m+1} - f_{m-1}}{\Delta x_1 + \Delta x_2} - \frac{1}{2} \frac{\partial^2 f}{\partial x^2} \left( \frac{\Delta x_2^2 - \Delta x_1^2}{\Delta x_1 + \Delta x_2} \right) + O(\Delta x^2), \tag{11.4} \]

This means that the form

\[ \frac{\partial f}{\partial x} = \frac{f_{m+1} - f_{m-1}}{\Delta x_1 + \Delta x_2}, \tag{11.5} \]

is second-order accurate only if

\[ O \left( \frac{\Delta x_2^2 - \Delta x_1^2}{\Delta x_1 + \Delta x_2} \right) \leq O(\Delta x_1^2). \tag{11.6} \]

Note that, for \( \Delta x_2 \) very small, the accuracy deteriorates to first order in \( \Delta x_1 \).

The expression for the second derivative is obtained by multiplying equation (11.2) by \( s^2 = (\Delta x_2/\Delta x_1)^2 \) and adding the result to (11.1).
\[
f_{m+1} + (1+s^2)f_m + s^{2}f_{m-1} = \frac{\partial f}{\partial x} \Delta x_2 (1-s) + \frac{\partial^2 f}{\partial x^2} \Delta x_2^2 + \frac{1}{6} \frac{\partial^3 f}{\partial x^3} \Delta x_2^2 \left( \Delta x_2 - \Delta x_1 \right) + O(\Delta x^4),
\]

(II.7)

\[
\frac{\partial^2 f}{\partial x^2} \bigg|_m = \frac{f_{m+1} + (1+s^2)f_m + s^{2}f_{m-1} - \frac{\partial f}{\partial x} \left( \frac{1 - s}{\Delta x_2} \right) + O(\Delta x_2^2 - \Delta x_1^2, \Delta x^2)}{\Delta x_2^2}.
\]

(II.8)

The resulting expression now requires \( s = O(1-\Delta x_1^2) \) just to be first-order accurate at \( i=m \).

It is clear from the above equations that, unless the mesh spacing is changed slowly, the formal truncation error is actually degraded, rather than improved.

II.2 Coordinates Transformations

Early work using finite difference methods was restricted to problems where suitable coordinate systems could be selected in order to solve the governing equations in that base system. As experience in computing complex problems was gained, general mappings were employed to transform the physical plane into a computational domain. Numerous advantages accrue when this procedure is followed. For example, when the untransformed equations are differenced in the expanding mesh, the result is a deterioration of formal accuracy, as we have seen; but the transformed equations may be differenced in a regular mesh (such as constant \( \Delta x, \Delta y \)) with no deterioration in the formal order of truncation error, except that it will now be \( O(\Delta y^2) \) rather than \( O(\Delta y^2) \), also, the body surface can be selected as a
boundary in the computational plane permitting easy application of
surface boundary conditions. In general, transformations are used
which lead to a uniform space grid in the computational plane while
points in physical space may be unequally spaced. This situation is
shown in Figure II.2. When this procedure is used, it is necessary to
include the derivatives of the mapping in the differential equation.

II.2.1 Simple Transformations

In this section, simple independent variable transformations are
used to illustrate how the governing equations are transformed. As a
first example, the problem of clustering grids near a wall is
considered. Figure II.3a shows a mesh above a flat plate in which
grid points are clustered near the plate in the normal direction (y).
While the spacing is not uniform in the y direction, it is convenient
to apply a transformation to the y coordinate so that the governing
equations can be solved on a uniformly spaced grid in the
computational plane (ξ, η) as seen in Figure II.3b. A suitable
transformation for a two-dimensional problem is given by

Transformation 1:

\[ \bar{x} = x , \quad (II.9) \]

\[ \bar{y} = 1 - \frac{\ln(\frac{\beta + 1 - (y/h)}{\beta - 1 + (y/h)})}{\ln(\frac{\beta + 1}{\beta - 1})} , \quad 1 < \beta < \infty \quad (II.10) \]

This stretching transformation clusters more points near \( y = 0 \) as the
stretching parameter \( \beta \) approaches 1.

In order to apply this transformation to the governing equations,
the following partial derivatives are formed
Figure II.1 Nonuniform spacing.

Figure II.2 Mapping to compute
Figure II.3 Grid clustering near a wall.
\[
\frac{\partial}{\partial x} = \frac{\partial \bar{x}}{\partial x} + \frac{\partial \bar{y}}{\partial x}, \quad \frac{\partial}{\partial y} = \frac{\partial \bar{x}}{\partial y} + \frac{\partial \bar{y}}{\partial y},
\]

where

\[
\frac{\partial \bar{x}}{\partial x} = 1, \quad \frac{\partial \bar{y}}{\partial y} = 0, \quad \frac{\partial \bar{x}}{\partial y} = 0,
\]

and \[
\frac{\partial \bar{y}}{\partial y} = \frac{2\beta}{h[\beta^2 - (1 - (y/h))^2] \ln((\beta + 1)/(\beta - 1))}.
\]

As a result, the partial derivatives simplify to

\[
\frac{\partial}{\partial x} = \frac{\partial \bar{x}}{\partial x}, \quad \frac{\partial}{\partial y} = \frac{\partial \bar{y}}{\partial y},
\]

If we now apply this transformation to the following equation

\[
\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} = 0,
\]

the following transformed equation is obtained

\[
\frac{\partial \bar{u}}{\partial \bar{x}} + \left(\frac{\partial \bar{y}}{\partial y}\right) \frac{\partial \bar{u}}{\partial \bar{y}} = 0.
\]

This transformed equation can now be differenced on the uniformly spaced grid in the computational plane. We note that the expression
for the derivative $\frac{\partial \bar{y}}{\partial y}$ contains $y$ so that we must be able to express $y$ as a function of $\bar{y}$. This is referred to as the inverse of the transformation. For the present transformation, given by equations (II.9) and (II.10), the inverse can be readily found as

$$x = \bar{x},$$

$$y = \frac{(\beta + 1) - (\beta - 1)\left\{(\beta + 1)/(\beta - 1)\right\}^{1-\bar{y}}}{\{\beta + 1)/(\beta - 1)\}^{1-\bar{y}} + 1}. \quad (II.18)$$

Transformation 2:

$$\bar{x} = x, \quad (II.19)$$

$$\bar{y} = \alpha + (1 - \alpha) \frac{\ln\left\{\beta + [(2\alpha + 1)/h] - 2\alpha]/[\beta - [(2\alpha + 1)/h] + 2\alpha]\right\}}{\ln\{\beta + 1)/(\beta - 1)\}}. \quad (II.20)$$

For this transformation, if $\alpha = 0$ the mesh will be refined near $y = h$ only, whereas, if $\alpha = \frac{1}{2}$ the mesh will be refined equally near $y = 0$ (Figure II.4). It has been shown that the stretching parameter $\beta$ is related (approximately) to the nondimensional thickness ($\delta/h$) by

$$\beta = \frac{1}{(1 - \delta/h)^{1/2}}, \quad 0 < \delta/h < 1 \quad (II.21)$$

where $h$ is the height of the mesh. For the transformation given by equations (II.19) and (II.20), the derivative $\frac{\partial \bar{y}}{\partial y}$ is

$$\frac{\partial \bar{y}}{\partial y} = \frac{2\beta(1 - \alpha)(2\alpha + 1)}{h[\beta^2 - [(2\alpha + 1)/h - 2\alpha]^2]ln\{\beta + 1)/(\beta - 1)\}}, \quad (II.22)$$
Figure II.4 Grid clustering in a duct.
and the inverse transformation becomes

\[ x = \tilde{x} , \quad (11.23) \]

\[ y = \frac{(\beta + 2\alpha)[(\beta + 1)/(\beta - 1)](y - a)/(1 - a) - \beta + 2\alpha}{(2\alpha + 1)[1 + [(\beta + 1)/(\beta - 1)](y - a)/(1 - a)} . \quad (11.24) \]

A useful transformation for refining the mesh above some interior point \( y_c \) (see Figure II.5) is given by

Transformation 3:

\[ \tilde{x} = x , \quad (11.25) \]

\[ \tilde{y} = B + \frac{1}{\tau} \sinh^{-1} \left[ \left( \frac{y}{y_c} - 1 \right) \sinh(\tau B) \right] , \quad (11.26) \]

where

\[ B = \frac{1}{2\tau} \ln \left[ \frac{1 + (e^\tau - 1)(y_c/h)}{1 + (e^{-\tau} - 1)(y_c/h)} \right] . \quad 0 < \tau < \infty \quad (11.27) \]

In this transformation, \( \tau \) is the stretching parameter which varies from zero (no stretching) to large values which produce the most refinement near \( y = y_c \). The metric \( \frac{\partial \tilde{y}}{\partial y} \) and \( y \) become

\[ \frac{\partial \tilde{y}}{\partial y} = \frac{\sinh(\tau B)}{y_c \{1 + [(y/y_c) - 1]^2 \sinh^2(\tau B)]^{1/2}} . \quad (11.28) \]

\[ y = y_c \left[ 1 + \frac{\sinh[\tau(\tilde{y} - B)]}{\sinh(\tau B)} \right] . \quad (11.29) \]

For our final transformation, a simple transformation which can be
Figure II.5 Grid clustering near an interior point.
used to transform a nonrectangular region in the physical plane into a rectangular region in the computational plane, as seen in Figure 11.6, will be examined. The required transformation is

Transformation 4: (Figure 11.6)

\[
\bar{x} = x, \tag{11.30}
\]

\[
\bar{y} = \frac{y}{h(x)}. \tag{11.31}
\]

The known distance between the lower boundary and the upper boundary (measured along a \(x=\text{constant}\) line) is designated by \(h(x)\). The required partial derivatives are

\[
\frac{\partial}{\partial x} = \frac{\partial}{\partial \bar{x}} - \bar{y} \frac{h'(x)}{h(x)} \frac{\partial}{\partial \bar{y}}, \tag{11.32}
\]

\[
\frac{\partial}{\partial y} = \frac{1}{h(x)} \frac{\partial}{\partial \bar{y}}, \tag{11.33}
\]

where \(h'(x) = dh(x)/dx\). Hence, equation (11.15) is transformed to

\[
\frac{\partial u}{\partial \bar{x}} - \bar{y} \frac{h'(\bar{x})}{h(x)} \frac{\partial u}{\partial \bar{y}} + \frac{1}{h(x)} \frac{\partial u}{\partial \bar{y}} = 0. \tag{11.34}
\]

11.2.2 Generalized Transformation

In the preceding section, the simple independent variable transformations which make it possible to solve the governing equations on a uniformly spaced computational grid were examined. Let us now consider a completely general transformation of the form
(a) physical plane

(b) computational plane

Figure II.6 Rectangularization of computational grid.
\[ \xi = \xi(x, y, z), \quad \eta = \eta(x, y, z), \quad \zeta = \zeta(x, y, z), \]

which can be used to transform the governing equations from the physical domain \((x, y, z)\) to the computational domain \((\xi, \eta, \zeta)\). Using the chain rule of partial differentiation, the partial derivatives become

\[ \frac{\partial}{\partial x} = \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta} + \zeta_x \frac{\partial}{\partial \zeta}, \]

\[ \frac{\partial}{\partial y} = \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta} + \zeta_y \frac{\partial}{\partial \zeta}, \]

\[ \frac{\partial}{\partial z} = \xi_z \frac{\partial}{\partial \xi} + \eta_z \frac{\partial}{\partial \eta} + \zeta_z \frac{\partial}{\partial \zeta}. \]

The derivatives \((\xi_x, \eta_x, \zeta_x, \xi_y, \eta_y, \zeta_y, \xi_z, \eta_z, \zeta_z)\) appearing in these equations can be determined in the following manner. We first write the differential expressions

\[ d\xi = \xi_x dx + \xi_y dy + \xi_z dz, \]

\[ d\eta = \eta_x dx + \eta_y dy + \eta_z dz, \]

\[ d\zeta = \zeta_x dx + \zeta_y dy + \zeta_z dz. \]
which in matrix form become

\[
\begin{pmatrix}
\frac{d\xi}{d\eta} & \frac{d\xi}{d\zeta}
\end{pmatrix}
= \begin{pmatrix}
\xi_x & \xi_y & \xi_z
\end{pmatrix}
\begin{pmatrix}
\eta_x & \eta_y & \eta_z
\end{pmatrix}
= \begin{pmatrix}
\xi_x & \xi_y & \xi_z
\end{pmatrix}
\begin{pmatrix}
\zeta_x & \zeta_y & \zeta_z
\end{pmatrix}
\begin{pmatrix}
\frac{d\eta}{d\zeta} & \frac{d\xi}{d\zeta}
\end{pmatrix},
\]

(II.44)

In a like manner we can write

\[
\begin{pmatrix}
\frac{dx}{dy} & \frac{dx}{dz}
\end{pmatrix}
= \begin{pmatrix}
x_x & x_y & x_z
\end{pmatrix}
\begin{pmatrix}
y_x & y_y & y_z
\end{pmatrix}
\begin{pmatrix}
z_x & z_y & z_z
\end{pmatrix}
\begin{pmatrix}
\frac{dy}{d\zeta} & \frac{dx}{d\zeta}
\end{pmatrix},
\]

(II.45)

Therefore,

\[
\begin{pmatrix}
\xi_x & \xi_y & \xi_z
\end{pmatrix}
\begin{pmatrix}
\eta_x & \eta_y & \eta_z
\end{pmatrix}
\begin{pmatrix}
\zeta_x & \zeta_y & \zeta_z
\end{pmatrix}
= \begin{pmatrix}
x_x & x_y & x_z
\end{pmatrix}
\begin{pmatrix}
y_x & y_y & y_z
\end{pmatrix}
\begin{pmatrix}
z_x & z_y & z_z
\end{pmatrix}
\begin{pmatrix}
\frac{d\xi}{d\eta} & \frac{d\eta}{d\zeta}
\end{pmatrix}
\begin{pmatrix}
\frac{d\xi}{d\zeta} & \frac{d\eta}{d\zeta}
\end{pmatrix}
\begin{pmatrix}
\frac{dx}{dy} & \frac{dx}{dz}
\end{pmatrix}
\begin{pmatrix}
\frac{dy}{d\zeta} & \frac{dx}{d\zeta}
\end{pmatrix}
\begin{pmatrix}
\frac{dx}{dy} & \frac{dy}{dy}
\end{pmatrix}
\begin{pmatrix}
\frac{dx}{dz} & \frac{dy}{dz}
\end{pmatrix}
\begin{pmatrix}
\frac{dz}{dz}
\end{pmatrix}
\]

(II.46)

Thus, the derivatives are:

\[
\xi_x = J(\gamma_{\eta\zeta} - \gamma_{\zeta\eta}),
\]

(II.47)
\[ \xi_y = -J(x_\eta z_\zeta - x_\zeta z_\eta), \] (II.48)

\[ \xi_z = J(x_\eta y_\zeta - x_\zeta y_\eta), \] (II.49)

\[ n_x = -J(y_\xi z_\zeta - y_\zeta z_\xi), \] (II.50)

\[ n_y = J(x_\xi y_\zeta - x_\zeta y_\xi), \] (II.51)

\[ n_z = -J(x_\xi y_\zeta - x_\zeta y_\xi), \] (II.52)

\[ \zeta_x = J(y_\xi z_\eta - y_\eta z_\xi), \] (II.53)

\[ \zeta_y = -J(x_\xi z_\eta - x_\eta z_\xi), \] (II.54)

\[ \zeta_z = J(x_\xi y_\eta - x_\eta y_\xi). \] (II.55)

where \( J \) is the Jacobian of the transformation

\[
J = \frac{\partial(x, y, z)}{\partial(x, y, z)} = \begin{pmatrix} \xi_x & \xi_y & \xi_z \\ n_x & n_y & n_z \\ \zeta_x & \zeta_y & \zeta_z \end{pmatrix},
\] (II.56)

which can be evaluated in the following manner

\[
J = 1/J^{-1} = 1/\left( \frac{\partial(x, y, z)}{\partial(\xi, \eta, \zeta)} \right) = \begin{pmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{pmatrix}^{-1},
\] (II.57)
The coordinate derivatives can be readily determined if analytical expressions are available for the inverse of the transformation:

\[ x = x(\xi, \eta, \zeta), \quad (11.59) \]

\[ y = y(\xi, \eta, \zeta), \quad (11.60) \]

\[ z = z(\xi, \eta, \zeta), \quad (11.61) \]

For a two-dimensional problem, the derivatives of a function \( f(x, y) \) in the transformed plane \((\xi, \eta)\) are:

\[ f_x = (y_{\xi}f_{\xi} - y_{\eta}f_{\eta})/J, \quad (11.62) \]

\[ f_y = (x_{\eta}f_{\eta} - x_{\xi}f_{\xi})/J, \quad (11.63) \]

\[ f_{xx} = (y_{\eta}^2f_{\xi\xi} - 2y_{\xi\eta}f_{\xi\eta} + y_{\xi}^2f_{\eta\eta})/J^2 + \]

\[ + \left[ (y_{\eta}^2f_{\xi\xi} - 2y_{\xi\eta}f_{\xi\eta} + y_{\xi}^2f_{\eta\eta})\right] f_{\eta\eta} \]

\[ + \left[ (y_{\eta}^2f_{\xi\xi} - 2y_{\xi\eta}f_{\xi\eta} + y_{\xi}^2f_{\eta\eta})\right] f_{\xi\eta} \]

\[ + \left[ (y_{\eta}^2f_{\xi\xi} - 2y_{\xi\eta}f_{\xi\eta} + y_{\xi}^2f_{\eta\eta})\right] f_{\xi\eta} \]

\[ f_{xy} = \left[ (x_{\xi}y_{\eta} + x_{\eta}y_{\xi})f_{\xi\eta} - x_{\xi}y_{\xi}f_{\eta\eta} - x_{\eta}y_{\xi}f_{\eta\xi} \right]/J^2 + \]

\[ + \left[ (x_{\xi}y_{\eta} + x_{\eta}y_{\xi})f_{\xi\eta} - x_{\xi}y_{\xi}f_{\eta\eta} - x_{\eta}y_{\xi}f_{\eta\xi} \right]/J^2 + \]

\[ + \left[ (x_{\xi}y_{\eta} + x_{\eta}y_{\xi})f_{\xi\eta} - x_{\xi}y_{\xi}f_{\eta\eta} - x_{\eta}y_{\xi}f_{\eta\xi} \right]/J^2 + \]
\[ f_{yy} = \frac{(x^2 f_{\xi \xi} - 2x_x f_{\xi} + x^2 f_{\eta \eta})}{J^2} + \]
\[ + [(x^2 f_{\xi \eta} - 2x_x f_{\xi \eta} + x^2 f_{\eta \eta})y_{\xi \eta} + x^2 f_{\eta \eta}y_{\eta \eta}](x_x f_{\xi} - x_x f_{\eta}) + \]
\[ + (x^2 f_{\xi \xi} - 2x_x f_{\xi \eta} + x^2 f_{\eta \eta})(y_{\xi \eta} - y_{\eta \xi})/J^3. \quad (11.66) \]

The Laplacian is given by

\[ \nabla^2 f = \frac{(A_1 f_{\xi \xi} - 2A_2 f_{\xi \eta} + A_3 f_{\eta \eta})}{J^2} + \]
\[ + [(A_1 f_{\xi \eta} - 2A_2 f_{\xi \eta} + A_3 f_{\eta \eta})(x_x f_{\xi} - x_x f_{\eta})])J^3, \quad (11.67) \]

or

\[ \nabla^2 f = \frac{(A_1 f_{\xi \xi} - 2A_2 f_{\xi \eta} + A_3 f_{\eta \eta} + A_4 f_{\eta} + A_5 f_{\xi})}{J^2}. \quad (11.68) \]

where

\[ A_1 = x_x^2 + y_{\eta \eta}^2, \quad (11.69) \]
\[ A_2 = x_x x_{\eta} + y_{\xi} y_{\eta}, \quad (11.70) \]
\[ A_3 = x_x^2 + y_{\xi \xi}^2, \quad (11.71) \]
\[ A_4 = (y_{\xi} A_6 - x_x A_7)/J, \quad (11.72) \]
\[ A_3 = \left( x\xi \eta - y\eta \xi \right) / J, \]  
(11.73)

\[ A_6 = A_1 x\xi \xi - 2 A_2 x\xi \eta + A_3 x\eta \eta, \]  
(11.74)

\[ A_7 = A_1 y\xi \xi - 2 A_2 y\xi \eta + A_3 y\eta \eta. \]  
(11.75)

Likewise, the Gradient is given by

\[ \nabla f = \left( y f_\xi - y f_\eta \right) e_1 + \left( x f_\xi - x f_\eta \right) e_2 / J. \]  
(11.76)

and the Divergence is expressed by

\[ \nabla \cdot F = \left( y (F_1)_\xi - y (F_1)_\eta \right) + \left( x (F_2)_\xi - x (F_2)_\eta \right) / J. \]  
(11.77)

where \( F = F_1 e_1 + F_2 e_2 \).

Finally, the Curl may be written as

\[ \text{Curl } F = e_3 \left( y (F_2)_\xi - y (F_2)_\eta \right) + \left( x (F_1)_\eta - x (F_1)_\xi \right) / J. \]  
(11.79)

where \( J = x_\xi y_\eta - x_\eta y_\xi \) is the Jacobian of the transformation, and the subscripts \((x,y,\xi,\eta)\) denotes partial derivatives in those coordinates, respectively.

For cases where the transformation is the direct result of a grid generation scheme, the metrics can be computed numerically using central difference in the computational plane.

The general coordinate transformation can be employed to transform very complicated curvilinear coordinates to simple
rectangular coordinates. Some examples which transform the problem in physical domain to computational domain are given in Figures II.7,8,9.

The detail and more complicated transformations are found in [49,50].
Figure 11.7 Rectangularization of computational grid.
(a) physical plane

(b) computational plane

Figure II.8 Rectangularization of computational grid.
Figure 11.9 Three-dimensional coordinates transformation.
APPENDIX III

ENERGY BALANCE METHOD

The subjects of thermodynamics and heat transfer are highly complementary. For example, heat transfer is an extension of thermodynamics in that it considers the rate at which energy is transported. Moreover, in many heat transfer analyses the first law of thermodynamics (the law of conservation of energy) plays an important role. In our application of the conservation laws, we first need to identify the control volume, a fixed region of space bounded by a control surface through which energy and matter may pass. With respect to a control volume, a form of the energy conservation requirement that is most useful for heat transfer analyses may be stated as follows.

"The rate at which thermal and mechanical energy enters a control volume minus the rate at which this energy leaves the control volume must equal the rate at which this energy is stored in the control volume."

If the inflow of energy exceeds the outflow, there will be an increase in the amount of energy stored (or accumulated) in the control volume; if the converse is true, there will be a decrease in energy storage. If the inflow of energy equals the outflow, then a steady state condition must prevail in which there will be no change in the amount of energy stored in the control volume. For the heat conduction problem, the inflow and outflow energy of the control volume is the heat flux \( Q = -k \nabla T \). The law of conservation of energy is the key concept of the energy balance method.
III.1 Energy Balance on the Cavity Boundaries (Figure 3.3)

On face AB (Figure III.1). Let us examine an arbitrary node P(i, j), on the face AB, surrounded by nodes R, S, and W. When heat conduction from the boundary nodes R or W to P is examined, we observe that the area available for heat flow is only \((\Delta y/2)\cdot \Delta x\), although the distance across which heat is conducted is still \(\Delta x\). Thus we have

\[
Q_{S \to P} = k_1 (\Delta x) \frac{T^I(i,j-1) - T^I(i,j)}{\Delta y}, \quad (III.1)
\]

\[
Q_{W \to P} = k_1 (\Delta y/2) \frac{T^I(i-1,j) - T^I(i,j)}{\Delta x}, \quad (III.2)
\]

\[
Q_{R \to P} = k_1 (\Delta y/2) \frac{T^I(i+1,j) - T^I(i,j)}{\Delta x}. \quad (III.3)
\]

The rate of change of internal energy \(\dot{U}_P\) in the time interval \(\Delta t\) at P(i, j) is

\[
\dot{U}_P = \rho c_I (\Delta x \cdot \Delta y/2) \frac{T^I(i,j,n) - T^I(i,j,n-1)}{\Delta t}, \quad n=1 \quad (III.4a)
\]

\[
\dot{U}_P = \rho c_I (\Delta x \Delta y/2) \frac{3T^I(i,j,n)-4T^I(i,j,n-1)+T^I(i,j,n-2)}{2\Delta t}. \quad n>1 \quad (III.4b)
\]

From conservation of energy, \(\dot{U}_P = Q_{sum}\), we obtain

\[
T^I(i,j,n) = T^I(i,j,n-1) + AB_1, \quad n=1 \quad (III.5a)
\]

\[
T^I(i,j,n) = \frac{1}{3} [-T^I(i,j,n-2) + 4T^I(i,j,n-1) + 2AB_1], \quad n>1 \quad (III.5b)
\]

where
Figure III.1 Energy balance on face AB.
\[ AB_1 = \frac{\Delta t k}{\rho c} \left\{ 2[T^I(i,j-1,n-1) - T^I(i,j,n-1)]/\Delta y^2 \right\} \]

\[ + [T^I(i+1,j,n-1) - 2T^I(i,j,n-1) + T^I(i-1,j,n-1)]/\Delta x^2 \]. (III.6)

The dimensionless forms were given in Equations (3.40a,b).

On face AC (Figure III.2)

\[ Q_{W+P} = k \frac{\Delta y_1 + \Delta y_2}{2} \frac{T^{II}(i-1,j) - T^{II}(i,j)}{\Delta x} \],  (III.7)

\[ Q_{S+P} = k \frac{\Delta x}{2} \frac{T^{II}(i,j-1) - T^{II}(i,j)}{\Delta y_1} \],  (III.8)

\[ Q_{N+P} = k \frac{\Delta x}{2} \frac{T^{II}(i,j+1) - T^{II}(i,j)}{\Delta y_2} \].  (III.9)

and

\[ \dot{U}_P = \rho c [\Delta x \cdot (\Delta y_1 + \Delta y_2)/4] \frac{T^{II}(i,j,n)-T^{II}(i,j,n-1)}{\Delta t} \],  n=1 (III.10a)

\[ \dot{U}_P = \rho c [\Delta x \cdot (\Delta y_1 + \Delta y_2)/4] \frac{3T^{II}(i,j,n)-4T^{II}(i,j,n-1)+T^{II}(i,j,n-2)}{2\Delta t} \]  

n>1 (III.10b)

\[ \dot{U}_P = Q_{sum} \] gives

\[ T^{II}(i,j,n) = T^{II}(i,j,n-1) + AB_2 \],  n=1 (III.11a)

\[ T^{II}(i,j,n) = \frac{1}{3} [\frac{1}{2} - T^{II}(i,j,n-2)+4T^{II}(i,j,n-1)+2AB_2], \]  n>1 (III.11b)

where
Figure III.2  Energy balance on face AC.
\[ AB_z = \frac{2 \Delta t k_{\text{II}}}{\rho_{\text{II}} c_{\text{II}}} \frac{[T^{\text{II}}(i-1, j, n-1) - T^{\text{II}}(i, j, n-1)]}{\Delta x^2} \]

\[ + \left[ T^{\text{II}}(i, j-1, n-1) - T^{\text{II}}(i, j, n-1) / (\Delta y_1^2 + \Delta y_1 \Delta y_2) \right] \]

\[ + \left[ T^{\text{II}}(i, j+1, n-1) - T^{\text{II}}(i, j, n-1) / (\Delta y_1 \Delta y_2 + \Delta y_2^2) \right] . \] (III.12)

The dimensionless forms were given in Equations (3.42a,b).

**On face BD (Figure III.3)**

\[ Q_{R \rightarrow P} = k_{\text{II}} \frac{\Delta y_1 + \Delta y_2}{2} \frac{T^{\text{II}}(i+1, j) - T^{\text{II}}(i, j)}{\Delta x}, \] (III.13)

\[ Q_{S \rightarrow P} = k_{\text{II}} (\Delta x / 2) \frac{T^{\text{II}}(i, j-1) - T^{\text{II}}(i, j)}{\Delta y_1}, \] (III.14)

\[ Q_{N \rightarrow P} = k_{\text{II}} (\Delta x / 2) \frac{T^{\text{II}}(i, j+1) - T^{\text{II}}(i, j)}{\Delta y_2}. \] (III.15)

and

\[ \dot{U}_P = \rho_{\text{II}} c_{\text{II}} [\Delta x \cdot (\Delta y_1 + \Delta y_2)/4] \frac{T^{\text{II}}(i, j+1, n) - T^{\text{II}}(i, j, n-1)}{\Delta t}, \] n=1 (III.16a)

\[ \dot{U}_P = \rho_{\text{II}} c_{\text{II}} [\Delta x \cdot (\Delta y_1 + \Delta y_2)/4] \frac{3T^{\text{II}}(i, j, n) - 4T^{\text{II}}(i, j, n-1) + T^{\text{II}}(i, j, n-2)}{2\Delta t}, \] n>1 (III.16b)

\[ \dot{U}_P = Q_{\text{sum}} \text{ gives} \]

\[ T^{\text{II}}(i, j, n) = T^{\text{II}}(i, j, n-1) + AB_3, \] n=1 (III.17a)

\[ T^{\text{II}}(i, j, n) = \frac{1}{3} [-T^{\text{II}}(i, j, n-2) + 4T^{\text{II}}(i, j, n-1) + 2AB_3], \] n>1 (III.17b)

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Figure III.3  Energy balance on face BD.
where

\[
AB_3 = \frac{2\Delta t k_{II}}{\rho_{II} c_{II}} \left\{ \frac{[T^{II}(i+1,j,n-1) - T^{II}(i,j,n-1)]}{\Delta x^2} + \frac{[T^{II}(i,j-1,n-1) - T^{II}(i,j,n-1)]}{\Delta y_1^2 + \Delta y_1 \Delta y_2} + \frac{[T^{II}(i,j+1,n-1) - T^{II}(i,j,n-1)]}{\Delta y_2^2 + \Delta y_1 \Delta y_2} \right\}. \quad (III.18)
\]

The dimensionless forms were given in Equations (3.44a,b).

On face CD (Figure III.4)

\[
Q_{N+P} = k_{II} \frac{T^{II}(i+1,j) - T^{II}(i,j)}{\Delta x}, \quad (III.19)
\]

\[
Q_{W+P} = k_{II} \frac{T^{II}(i-1,j) - T^{II}(i,j)}{\Delta y}, \quad (III.20)
\]

\[
Q_{R+P} = k_{II} \frac{T^{II}(i+1,j) - T^{II}(i,j)}{\Delta x}, \quad (III.21)
\]

and

\[
\dot{U}_p = \rho_{II} c_{II} \frac{(\Delta x \cdot \Delta y/2)}{\Delta t} \frac{T^{II}(i,j,n) - T^{II}(i,j,n-1)}{\Delta t}, \quad n=1 \quad (III.22a)
\]

\[
\dot{U}_p = \rho_{II} c_{II} \frac{3T^{II}(i,j,n) - 4T^{II}(i,j,n-1) + T^{II}(i,j,n-2)}{2\Delta t}. \quad n>1 \quad (III.22b)
\]

\[
\dot{U}_p = Q_{\text{sum}} \quad \text{gives}
\]

\[
T^{II}(i,j,n) = T^{II}(i,j,n-1) + AB_4, \quad n=1 \quad (III.23a)
\]
Figure III.4 Energy balance on face CD.
\[ T^{II}(i,j,n) = \frac{1}{3} [ -T^{II}(i,j,n-2) + 4T^{II}(i,j,n-1) + 2AB_q ] \quad n > 1 \text{ (III.23b)} \]

where

\[ AB_q = \frac{\Delta t \kappa_{II}}{\rho_{II} c_{II}} \frac{[T^{II}(i-1,j,n-1) - 2T^{II}(i,j,n-1) + T^{II}(i+1,j,n-1)]}{\Delta x^2} + 2[T^{II}(i,j+1,n-1) - T^{II}(i,j,n-1)] \text{ . (III.24)} \]

The dimensionless forms were given in Equations (3.46a,b).

III.2 Energy Balance at the Corner of the Cavity (Figure 3.3)

If one has a two-dimensional configuration that looks like the cross section of two walls meeting at a corner, the nodal point at the corner so formed is called a reentrant corner.

Corner A. The node P in Figure III.5 is located at a reentrant corner. The nodes N, R, S, and W are called exterior corner nodes. Observing that the areas available for the flow of heat from N to P and from R to P are \( \frac{\Delta x}{2} \cdot 1 \) and \( \frac{\Delta y}{2} \cdot 1 \), respectively. The heat fluxes toward the corner point P(i,j) are:

\[ Q_{W+P} = \left( -\frac{k_{I+II}}{2} \right) (\Delta y) \frac{T(i-1,j) - T(i,j)}{\Delta x} \text{, (III.25)} \]

\[ Q_{N+P} = k_{II} (\Delta x/2) \frac{T(i,j+1) - T(i,j)}{\Delta y} \text{, (III.26)} \]

\[ Q_{R+P} = k_{I} (\Delta y/2) \frac{T(i+1,j) - T(i,j)}{\Delta x} \text{, (III.27)} \]

\[ Q_{S+P} = k_{I} (\Delta x) \frac{T(i,j-1) - T(i,j)}{\Delta y} \text{, (III.28)} \]
Figure III.5  Energy balance at corner A.
and the rate of change of internal energy is

\[ \dot{U}_p = \left( \rho_{I1} c_{I1} / 2 + \rho_{II} c_{II} / 4 \right) (\Delta x \cdot \Delta y) \frac{T(i,j,n) - T(i,j,n-1)}{\Delta t}, \quad n=1 \quad (\text{III.29a}) \]

\[ \dot{U}_p = \left( \rho_{I1} c_{I1} / 2 + \rho_{II} c_{II} / 4 \right) (\Delta x \cdot \Delta y) \frac{3T(i,j,n) - 4T(i,j,n-1) + T(i,j,n-2)}{2\Delta t}, \quad n>1 \quad (\text{III.29b}) \]

From conservation of energy, \( \dot{U}_p = Q_{\text{sum}} \), one obtains

\[ T(i,j,n) = T(i,j,n-1) + AB_3, \quad n=1 \quad (\text{III.30a}) \]

\[ T(i,j,n) = \frac{1}{3} \left[ -T(i,j,n-2) + 4T(i,j,n-1) + 2AB_3 \right], \quad n>1 \quad (\text{III.30b}) \]

where

\[ AB_3 = \frac{\Delta t/2}{\left( \rho_{I1} c_{I1} / 2 + \rho_{II} c_{II} / 4 \right)} \left\{ \left( k_I + k_{II} \right) \left[ T(i-1,j,n-1) - T(i,j,n-1) \right] / \Delta x^2 \right. \]

\[ + k_{II} \left[ T(i,j+1,n-1) - T(i,j,n-1) \right] / \Delta y^2 + k_I \left[ T(i+1,j,n-1) - T(i,j,n-1) \right] / \Delta x^2 \]

\[ - T(i,j,n-1) / \Delta x^2 + 2k_I \left[ T(i-1,j,n-1) - T(i,j,n-1) \right] / \Delta y^2 \}. \quad (\text{III.31}) \]

Corner B (Figure III.6)

\[ Q_{W+P} = k_I (\Delta y/2) \frac{T(i-1,j) - T(i,j)}{\Delta x} \], \quad (\text{III.32}) \]

\[ Q_{N+P} = k_{II} (\Delta x/2) \frac{T(i,j+1) - T(i,j)}{\Delta y} \], \quad (\text{III.33}) \]

\[ Q_{R+P} = \left( \frac{k_I + k_{II}}{2} \right) (\Delta y) \frac{T(i+1,j) - T(i,j)}{\Delta x} \], \quad (\text{III.34}) \]

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Figure III.6 Energy balance at corner B.
\[ Q_{S \rightarrow P} = k_I (\Delta x) \frac{T(i, j-1) - T(i, j)}{\Delta y}, \quad (III.35) \]

and

\[ \dot{U}_p = (\rho c_1 /2 + \rho c_{II} c_{II} /4)(\Delta x \cdot \Delta y) \frac{T(i, j, n) - T(i, j, n-1)}{\Delta t}, \quad n=1 (III.36a) \]

\[ \dot{U}_p = (\rho c_1 /2 + \rho c_{II} c_{II} /4)(\Delta x \cdot \Delta y) \frac{3T(i, j, n) - 4T(i, j, n-1) + T(i, j, n-2)}{2\Delta t}, \quad n>1 (III.36b) \]

\[ \dot{U}_p = Q_{sum} \text{ gives} \]

\[ T(i, j, n) = T(i, j, n-1) + AB_6, \quad n=1 (III.37a) \]

\[ T(i, j, n) = \frac{1}{3} [-T(i, j, n-2) + 4T(i, j, n-1) + 2AB_6], \quad n>1 (III.37b) \]

where

\[ AB_6 = \frac{\Delta t/2}{(\rho c_1 /2 + \rho c_{II} c_{II} /4)} \left\{ k_I [T(i-1, j, n-1) - T(i, j, n-1)]/\Delta x^2 \right. \]

\[ + k_{II} [T(i, j+1, n-1) - T(i, j, n-1)]/\Delta y^2 + (k_I + k_{II}) [T(i+1, j, n-1) \right. \]

\[ - T(i, j, n-1)]/\Delta x^2 + 2k_I [T(i, j-1, n-1) - T(i, j, n-1)]/\Delta y^2 \} \quad (III.38) \]

Corner C (Figure III.7)

\[ Q_{N \rightarrow P} = k_{II} (\Delta y) \frac{T^{II}(i-1, j) - T^{II}(i, j)}{\Delta x}, \quad (III.39); \]

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Figure III.7 F
\[ Q_{N+p} = k_{II} (\Delta x) \frac{T^{II}(i,j+1) - T^{II}(i,j)}{\Delta y}, \quad (III.40) \]

\[ Q_{R+p} = k_{II} (\Delta y/2) \frac{T^{II}(i+1,j) - T^{II}(i,j)}{\Delta x}, \quad (III.41) \]

\[ Q_{S+p} = k_{II} (\Delta x/2) \frac{T^{II}(i,j-1) - T^{II}(i,j)}{\Delta y}, \quad (III.42) \]

and

\[ \dot{u}_p = \rho_{II} c_{II} \left( \frac{3}{4} \Delta x, \Delta y \right) \frac{T^{II}(i,j,n) - T^{II}(i,j,n-1)}{\Delta t}, \quad n=1 \quad (III.43a) \]

\[ \dot{u}_p = \rho_{II} c_{II} \left( \frac{3}{4} \Delta x, \Delta y \right) \frac{3T^{II}(i,j,n)-4T^{II}(i,j,n-1)+T^{II}(i,j,n-2)}{2\Delta t}, \quad n>1 \quad (III.43b) \]

\[ \dot{u}_p = Q_{sum} \text{ gives} \]

\[ T^{II}(i,j,n) = T^{II}(i,j,n-1) + AB_\gamma, \quad n=1 \quad (III.44a) \]

\[ T^{II}(i,j,n) = \frac{1}{3} \left[ -T^{II}(i,j,n-2) + 4T^{II}(i,j,n-1) + 2AB_\gamma \right], \quad n>1 \quad (III.44b) \]

where

\[ AB_\gamma = \frac{2\Delta t k_{II}}{3\rho_{II} c_{II}} \left\{ \frac{[2T^{II}(i-1,j,n-1) - 3T^{II}(i,j,n-1) + T^{II}(i+1,j,n-1)]}{\Delta x^2} \right. \]

\[ + \left. [T^{II}(i,j-1,n-1) - 3T^{II}(i,j,n-1) + 2T^{II}(i,j+1,n-1)]}{\Delta y^2} \right\}, \quad (III.45) \]
Corner D (Figure III.8)

\[ Q_{N \rightarrow P} = k_{\text{II}}(\Delta y/2) \frac{T^{\text{II}}(i-1,j) - T^{\text{II}}(i,j)}{\Delta x}, \]  

(III.46)

\[ Q_{W \rightarrow P} = k_{\text{II}}(\Delta x) \frac{T^{\text{II}}(i,j+1) - T^{\text{II}}(i,j)}{\Delta y}, \]  

(III.47)

\[ Q_{R \rightarrow P} = k_{\text{II}}(\Delta y) \frac{T^{\text{II}}(i+1,j - T^{\text{II}}(i,j)}{\Delta x}, \]  

(III.48)

\[ Q_{S \rightarrow P} = k_{\text{II}}(\Delta x/2) \frac{T^{\text{II}}(i,j-1) - T^{\text{II}}(i,j)}{\Delta y}, \]  

(III.49)

and

\[ \dot{U}_p = \rho_{\text{III}}c_{\text{III}} \left( \frac{3}{4} \Delta x \cdot \Delta y \right) \frac{T^{\text{II}}(i,j,n) - T^{\text{II}}(i,j,n-1)}{\Delta t}, \quad n=1 \]  

(III.50a)

\[ \dot{U}_p = \rho_{\text{III}}c_{\text{III}} \left( \frac{3}{4} \Delta x \cdot \Delta y \right) \frac{3T^{\text{II}}(i,j,n) - 4T^{\text{II}}(i,j,n-1) + T^{\text{II}}(i,j,n-2)}{2\Delta t}, \]  

n > 1 \]  

(III.50b)

\[ \dot{U}_p = Q_{\text{sum}} \text{ gives} \]

\[ T^{\text{II}}(i,j,n) = T^{\text{II}}(i,j,n-1) + AB_g, \quad n=1 \]  

(III.51a)

\[ T^{\text{II}}(i,j,n) = \frac{1}{3} [ -T^{\text{II}}(i,j,n-2) + 4T^{\text{II}}(i,j,n-1) + 2AB_g], \quad n > 1 \]  

(III.51b)

where

\[ AB_g = \frac{2\Delta t k_{\text{II}}}{3\rho_{\text{III}} c_{\text{III}}} \left\{ \frac{[T^{\text{II}}(i-1,j,n-1) - 3T^{\text{II}}(i,j,n-1) + 2T^{\text{II}}(i+1,j,n-1)]}{\Delta x^2} \right. \]

\[ + \left. \frac{T^{\text{II}}(i,j,n-1) - 3T^{\text{II}}(i,j,n-1) + 2T^{\text{II}}(i+1,j,n-1)]}{\Delta y^2} \right\}. \]  

(III.52)
Figure III.8 Energy balance
The dimensionless forms for the corner points A, B, C, and D were given in Equations (3.48a,b, 3.50a,b, 3.52a,b, 3.54a,b), respectively.

III.3 Energy Balance on the Surface Boundary (Figure III.9)

For the explicit scheme, the time step is limited by the stability criterion. As a result, the moving asperity at some time may not be right above the grid points. To alleviate this situation, one can also use the energy balance method to describe the surface boundary condition.

The heat fluxes toward P(i,j) from material points N, R, and W are

\[ Q_{W\rightarrow P} = k_I (\Delta y/2) \frac{T^I(i-1,1) - T^I(i,1)}{\Delta x} \]  

\[ Q_{N\rightarrow P} = k_I (\Delta x) \frac{T^I(i,2) - T^I(i,1)}{\Delta y} \]  

\[ Q_{R\rightarrow P} = k_I (\Delta y/2) \frac{T^I(i+1,1) - T^I(i,1)}{\Delta x} \]

The exterior heat which is conducted into the neighborhood surface of the boundary point P(i,j), which is under the asperity, is

\[ Q_{\text{ext.}} = q(0.5\Delta x + h)/\text{unit thickness} \]

where h is less than \( \Delta x/2 \). The formulation thus takes care of all cases when the asperity end points do not fall on the grid point. The rate of change of the internal energy \( \dot{U}_P \) in the interval \( \Delta t \) at P(i,j) is

\[ \dot{U}_P = \rho_I c_I (\Delta x \cdot \Delta y/2) \frac{T^I(i,j,n) - T^I(i,j,n-1)}{\Delta t}, \quad n=1 \]
Figure III.9 Energy balance on
\[ \dot{U}_p = \rho_i c_i (\Delta x \cdot \Delta y / 2) \frac{3T_i(i,j,n) - 4T_i(i,j,n-1) + T_i(i,j,n-2)}{2\Delta t} \]

\[ n > 1 \quad (III.57b) \]

From conservation of energy, \( \dot{U}_p = Q_{\text{sum}} \), one obtains

\[ T_i(i,1,n) = T_i(i,1,n-1) + \frac{2q(\Delta x/2+h)\Delta t}{\rho_i c_i \Delta x \Delta y} + AB_y, \quad n = 1 \quad (III.58a) \]

\[ T_i(1,1,n) = \frac{1}{3} \left[ -T_i(1,1,n-2) + 4T_i(1,1,n-1) + \frac{2q(\Delta x/2+h)\Delta t}{\rho_i c_i \Delta x \Delta y} + 2AB_y \right], \quad n > 1 \quad (III.58b) \]

where

\[ AB_y = \frac{\Delta t k_i}{\rho_i c_i} \left[ \frac{[T_i(i-1,1,n-1) - 2T_i(i,1,n-1) + T_i(i+1,1,n-1)]}{\Delta x^2} + 2[T_i(i,2,n-1) - T_i(i,1,n-1)]/\Delta y^2 \right]. \quad (III.59) \]

The dimensionless forms for the surface boundary were given in Equations (3.56a,b).
APPENDIX IV

THE PROGRAMS TO COMPUTE THE TEMPERATURE AND THE STRESS

FIELDS SOLUTIONS
MAIN PROGRAM

TEMPERATURE FIELD OF A LAYERED MEDIUM WITH A CAVITY, THE TOP
EDGE OF THE CAVITY IS AT THE INTERFACE

IMPLICIT REAL*8 (A-H,O-Z)

T,TT,TTT = TEMPERATURE IN THE CURRENT, PREVIOUS ONE, AND
PREVIOUS TWO TIME STEPS
FX & FY = HEAT FLUX IN X & Y DIRECTION, RESPECTIVELY
Q = SURFACE HEAT INPUT
X & Y = COORDINATES IN PHYSICAL PLANE
XS,YE,XSS,YEE,... = THE DERIVATIVES OF THE COORDINATES IN
PHYSICAL PLANE WITH RESPECT TO THE COORDINATES IN COMPUTATIONAL.

DIMENSION T(145,33),TT(145,33),TTT(145,33),FX(145,33),FY(145,33),
AQ(145),X(145,33),Y(145,33),XS(145,33),YE(145,33)

DA,DG,SIG,TAU = THE COEFFICIENTS DEFINED IN TEMPERATURE EQUATION

DIMENSION XSS(145,33),YEE(145,33),DA(145,33),DG(145,33),
ASIG(145,33),TAU(145,33)

TS,FXS,FYS = TEMPERATURE AND ITS GRADIENTS IN THE CORRESPONDING
POINTS IN STRESS FIELD

DIMENSION TS(67,35),FXS(67,35),FYS(67,35)

COMMON /AS4/ RL1,RL2,RLI,RLC,RMU1,RMU2,RMUI,RMUC,EX1,EX2,
AEXI,EXC,HAK,RHC
COMMON /AS5/ DV,DL,DIFF1,DIFF2,COND1,COND2,BETA,R1,R2,
AALPHS,DX,DY1,DY2,DT,R11,R12,R21,R22,A1,A2,A3,A4,A5,A,A6,A7,A8
COMMON /AS6/ DTR1,DTR2,M1,M2,N1,N2,MM1,MM2,NN1,NN2,NA1,NA2,
AM1,AM2,K1,K2,K3,NTE,M122,M222,M12,M212,M121
COMMON /AS7/ ID2,ID21,ID3,ID31,ID,J2,J3,J3,J4

I1 & J1 = TOTAL GRID POINTS OF THE TEMPERATURE FIELD IN X & Y
DIRECTION, RESPECTIVELY

I1=145
J1=33

L11 & K11 = TOTAL GRID POINTS OF THE STRESS FIELD IN X & Y
DIRECTION, RESPECTIVELY

L11=67
K11=35
I2=I1-1
I3=I1-2
J2=J1-1
J3=J1-2
I4=I1-3
J4=J1-3

M1 & M2 = X COORDINATES OF THE CAVITY CORNERS
M1=33
M2=64

N1 & N2 = Y COORDINATES OF THE CAVITY CORNERS

N1=14
N2=24
MM1=M1-1
MM2=M2+1
NM1=N1-1
NM2=N2+1
NA1=N1+1
NA2=N2-1
MA1=M1+1
MA2=M2-1
M122=M1+2
M222=M2+2
M112=M1-2
M212=M2-2
N121=N1+1

K1 = LAYERED THICKNESS

K1=N1
K2=K1-1
K3=K1+1
ID2=8
ID21=ID2+1
ID3=140
ID31=ID3-1

NTE = FINAL TIME STEP

NTE=121

DV = TRAVERSE SPEED OF ASPERITY

DV=6.D2

DL = ASPERITY WIDTH

DL=1.D-2

COND = THERMAL CONDUCTIVITY

COND1=1.213D0
COND2=1.213D0
COND1=(COND1+COND2)/2.D0
COND1=(2.D0*COND1+COND2)/3.D0

DIFF = THERMAL DIFFUSIVITY

DIFF1=4.29D-3
DIFF2=4.29D-3
DIFFI=(DIFF1+DIFF2)/2.DO
DIFFC=(2.DO*DIFF1+DIFF2)/3.DO

RNU = POISSON'S RATIO

RNU1=0.285D0
RNU2=0.285D0
RNU=(RNU1+RNU2)/2.DO
RNU=(2.DO*RNU1+RNU2)/3.DO

E = YOUNG'S MODULUS

E1=3.6D7
E2=3.6D7
EI=(E1+E2)/2.DO
EC=(2.DO*E1+E2)/3.DO

RHO = MASS DENSITY

RHO1=9.31D-3
RHO2=9.31D-3
RHO=(RHO1+RHO2)/2.DO
RHO=(2.DO*RHO1+RHO2)/3.DO

EX = THE COEFFICIENT OF THERMAL EXPANSION

EX1=6.29D-6
EX2=6.29D-6
EX=(EX1+EX2)/2.DO
EX=(2.DO*EX1+EX2)/3.DO

RMUF = COULOMB COEFFICIENT OF FRICTION

RMUF=0.5D0

RMU & RL = LAME CONSTANTS

RMU1=E1/(2.DO*(1.DO+RNU1))
RMU2=E2/(2.DO*(1.DO+RNU2))
RMU=(E1/(2.DO*(1.DO+RNU1))
RMU=(2.DO*E1+RNU1)/3.DO
RL1=2.DO*RNU1*RNU1/(1.DO-2.DO*RNU1)
RL2=2.DO*RNU2*RNU2/(1.DO-2.DO*RNU2)
RL=2.DO*RNU1*RNU1/(1.DO-2.DO*RNU1)
RLC=2.DO*RNU*RNUC/(1.DO-2.DO*RNU)
C2=DSQRT(RNU2*1.2D1/RHO2)
HAK=RMUF*DV*DL/COND1
RHC=RHO2*C2**2
BETA=COND2/COND1
R1=DV*DL/DIFF1
R2=DV*DL/DIFF2
ALPHS=DFF2/DIFF1
DX=0.2D-1
DY1 = 0.6D-2
DY2 = 0.2D-1

C
DT = TIME STEP
C
DT = 0.1D-1
R11 = DT / (R1 * DX * DX)
R12 = DT / (R1 * DY1 * DY1)
R21 = DT / (R2 * DX * DX)
R22 = DT / (R2 * DY2 * DY2)
A1 = 1.0D + BETA / ALPHS
A2 = 1.0D + BETA
A3 = A2 / A1
A4 = 1.0D - 2.0D * A3 * R11 - 2.0D * A3 * R12
A5 = 0.5D0 + 0.25D0 * BETA / ALPHS
A = 1.0D - 2.0D * R21 - 2.0D * R22
AA = 1.0D - 2.0D * R11 - 2.0D * R12
A6 = 0.5D0 * A2 * R11 + 0.5D0 * BETA * R12 + 0.5D0 * R11 + R12
A7 = R1 + BETA * R2
A8 = A2 / A7
DTR1 = DT / R1
DTR2 = DT / R2

C
CALL XYLCT(X, Y, XS, YE, XSS, YEE, DA, DG, SIG, TAU, I1, J1)
C
NC = 1
NT = 1
100 NC = NC + 1
NT = NT + 1
TIME = (NT - 1) * DT
C
CALL QIN(DX, DT, NT, I1, O, I1, JJ)
C
CALL TEMP(T, TT, TTT, Q, FX, FY, X, Y, XS, YE, XSS, YEE, DA, DG, SIG, TAU,
AII, JJ, NT, I1, J1)
C
NC = NC + 1
IF (NT .NE. NTE) GO TO S
C
CALL MAP(TS, FXS, FYS, T, FX, FY, I1, J1, I11, KJ1)
C
DO 31 J = NN1, NA1
WRITE(6, *) J
WRITE(6, *) (T(I, J), I = MM1, MA1)
WRITE(6, *) (FX(I, J), I = MM1, MA1)
31 WRITE(6, *) (FY(I, J), I = MM1, MA1)
DO 32 J = NN1, NA1
WRITE(6, *) J
WRITE(6, *) (T(I, J), I = MM2, MA2)
WRITE(6, *) (FX(I, J), I = MM2, MA2)
32 WRITE(6, *) (FY(I, J), I = MM2, MA2)
DO 33 J = NA2, NN2
WRITE(6, *) J
WRITE(6, *) (T(I, J), I = MM1, MA1)
WRITE(6, *) (FX(I, J), I = MM1, MA1)
33 WRITE(6,*) (FY(I,J),I=MM1,MA1)
DO 34 J=NA2,NN2
WRITE(6,*) J
WRITE(6,*) (T(I,J),I=MA2,MM2)
WRITE(6,*) (FX(I,J),I=MA2,MM2)
34 WRITE(6,*) (FY(I,J),I=MA2,MM2)
WRITE(6,101)
101 FORMAT(/,SX,'TS',/)
DO 20 J=1,KJ1
20 WRITE(6,90) (TS(I,J),I=1,L11)
WRITE(6,102)
102 FORMAT(/,SX,'FXS',/)
DO 21 J=1,KJ1
21 WRITE(6,90) (FXS(I,J),I=1,L11)
WRITE(6,103)
103 FORMAT(/,SX,'FYS',/)
DO 22 J=1,KJ1
22 WRITE(6,90) (FYS(I,J),I=1,L11)
90 FORMAT(S(IX,D14.7))
5 IF(NT .LT. NTE) GO TO 100
STOP
END
SUBROUTINE XYLCT(X,Y,XS,YE,XSS,YEE,DA,DG,SIG,TAU,I1,J1)
IMPLICIT REAL*8 (A-H,O-Z)

X & Y = COORDINATES IN PHYSICAL PLANE
XS, YE, XSS, YEE = THE DERIVATIVES OF THE COORDINATES IN
PHYSICAL PLANE WITH RESPECT TO THE COORDINATES IN
COMPUTATIONAL PLANE
DA, DG, SIG, TAU = COEFFICIENTS DEFINED IN TEMPERATURE EQUATION

DIMENSION X(I1,J1),Y(I1,J1),XS(I1,J1),YE(I1,J1),XSS(I1,J1)
DIMENSION YEE(I1,J1),DA(I1,J1),DG(I1,J1),SIG(I1,J1),TAU(I1,J1)
I2=I1-1
J2=J1-1
I3=I1-2
J3=J1-2

DO 90 J=1,J1
DO 91 I=1,I1
X(I,J)=0.D0
Y(I,J)=0.D0
XS(I,J)=0.D0
YE(I,J)=0.D0
XSS(I,J)=0.D0
YEE(I,J)=0.D0
DA(I,J)=0.D0
DG(I,J)=0.D0
SIG(I,J)=0.D0
TAU(I,J)=0.D0
91 CONTINUE
90 CONTINUE

DO 1 J=1,J1

DO 5 I=1,4
5 X(I,J)=(I-1)*0.5D0

DO 6 I=5,9
6 X(I,J)=1.5D0+(I-4)*0.1D0

DO 7 I=10,134
7 X(I,J)=2.0D0+(I-9)*0.02D0

DO 8 I=135,138
8 X(I,J)=4.5D0+(I-134)*0.05D0

DO 9 I=139,145
9 X(I,J)=4.7D0+(I-138)*0.1D0

1 CONTINUE

DO 3 I=1,I1

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\[ Y(I,1) = 0.023 \]
\[ Y(I,2) = 0.031 \]
\[ Y(I,3) = 0.04 \]
\[ Y(I,4) = 0.059 \]
\[ Y(I,5) = 0.075 \]
\[ Y(I,6) = 0.094 \]
\[ Y(I,7) = 0.115 \]
\[ Y(I,8) = 0.137 \]
\[ Y(I,9) = 0.151 \]
\[ Y(I,10) = 0.167 \]
\[ Y(I,11) = 0.185 \]
\[ Y(I,12) = 0.205 \]
\[ Y(I,13) = 0.225 \]
\[ Y(I,14) = 0.245 \]
\[ Y(I,15) = 0.266 \]
\[ Y(I,16) = 0.287 \]
\[ Y(I,17) = 0.308 \]
\[ Y(I,18) = 0.330 \]
\[ Y(I,19) = 0.480 \]
\[ Y(I,20) = 0.580 \]
\[ Y(I,21) = 0.680 \]
\[ Y(I,22) = 0.780 \]
\[ X(I,23) = 0.880 \]
\[ X(I,24) = 0.980 \]
\[ X(I,25) = 1.080 \]

\[ XS(I,J) = (X(I+1,J) - X(I-1,J)) / 2.0 \]
\[ YE(I,J) = (Y(I,J+1) - Y(I,J-1)) / 2.0 \]
\[ XSS(I,J) = X(I,J) - 2.0 * X(I,J) + X(I+1,J) \]
\[ YEE(I,J) = Y(I,J) + 2.0 * Y(I,J) + Y(I,J+1) \]
CONTINUE
C
I=I1
DO 21 J=2,J2
XS(I,J)=(X(I-2,J)-4.DO*X(I-1,J)+3.DO*X(I,J))/2.DO
YE(I,J)=(Y(I,J+1)-Y(I,J-1))/2.DO
21 CONTINUE
C
J=J1
DO 22 I=2,I2
XS(I,J)=(X(I+1,J)-X(I-1,J))/2.DO
YE(I,J)=(Y(I,J-2)-4.DO*Y(I,J-1)+3.DO*Y(I,J))/2.DO
22 CONTINUE
C
XS(1,1)=XS(1,2)
XS(1,J1)=XS(1,2)
XS(I1,1)=XS(I1,2)
XS(I1,J1)=XS(I1,2)
YE(1,1)=YE(2,1)
YE(1,J1)=YE(2,J1)
YE(I1,1)=YE(I1,2)
YE(I1,J1)=YE(I1,2)
C
DO 25 J=1,J1
DO 26 I=1,I1
DA(I,J)=1.DO/XS(I,J)**2
DG(I,J)=1.DO/YE(I,J)**2
SIG(I,J)=-YEE(I,J)/YE(I,J)**3
TAU(I,J)=-XSS(I,J)/XS(I,J)**3
IF(DABS(SIG(I,J)) .LT. 1.D-10) SIG(I,J)=0.DO
IF(DABS(TAU(I,J)) .LT. 1.D-10) TAU(I,J)=0.DO
26 CONTINUE
25 CONTINUE
C
RETURN
END
THIS SUBROUTINE INPUTS THE SURFACE B.C.

SUBROUTINE QIN(DX, DT, NT, I1, Q, I2, JJ)
IMPLICIT REAL*8 (A-H, O-Z)

Q = SURFACE HEAT INPUT

DIMENSION Q(I1)

NR2 = DX/DT, NR1 = NR2/2

NR1 = 1
NR2 = 2

DO 24 I = 1, I1
Q(I) = 0.D0
24 CONTINUE

IF (NT .GT. 2) GO TO 21
NC1 = 0
NC2 = 0
NC3 = 0
NTT = 1
ND1 = NR1
ND2 = NR2
ND3 = 0
NNT = 1

21 NC1 = NC1 + 1
NC2 = NC2 + 1
IF (NC1 .EQ. NR1) GO TO 1
GO TO 4

1 NC3 = NC3 + 1
IF (NC3 .EQ. 1) GO TO 6
NC3 = 0
GO TO 7

6 NTT = NTT + 1

7 NC1 = 0

4 I1 = 74 - NTT + 1
IF (NC2 .GE. NR1) GO TO 2
PB = 0.D0
GO TO 5

2 IF (NC2 .LT. NR2) GO TO 3
PB = 0.5D0
NC2 = 0
GO TO 5

3 PB = 0.D0
5 Q(I2) = PB + DT*NC1/DX
ND1 = ND1 - 1
ND2 = ND2 - 1
IF (ND1 .EQ. 0) GO TO 11
GO TO 12

11 ND3 = ND3 + 1
IF (ND3 .EQ. 1) GO TO 13
ND3 = 0
GO TO 14
13 NNT=NNT+1
14 ND1=NR1
12 JJ=124-NNT+1
   IF(ND2 .LE. NR1) GO TO 15
   PF=0.D0
   GO TO 16
15 IF(ND2 .GT. 0) GO TO 17
   ND2=NR2
   PF=0.D0
   GO TO 16
17 PF=0.5D0
16 Q(JJ)=PF+DT*ND1/DX
   II1=II+1
   JJ1=JJ-1
C
   DO 23 I=II1,JJ1
      Q(I)=1.D0
   23 CONTINUE
C
RETURN
END
THIS SUBROUTINE SOLVED A LAYERED MEDIUM WITH A CAVITY. THE TOP EDGE OF THE CAVITY IS AT THE INTERFACE.

SUBROUTINE TEMP(T,TT,TTT,Q,FX,FY,XS,YS,XSS,YSS,DA,DG,
ASIG,TAU,I,J,NT,II,JI)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION T(II,JI),TT(II,JI),TTT(II,JI),FX(II,JI),
AFY(II,JI),Q(II),X(II,JI),Y(II,JI),XS(II,JI),YS(II,JI),
ASIG(II,JI),TAU(II,JI)
COMMON /ASS/ RL1,RL2,RLI,RLC,RM1U1,RMU2,RMU3,RMU4,EX1,EX2,
AEX1,EXC,HACK,RHC
COMMON /ASS/ DV,DL,DIF1,DIF2,COND1,COND2,BETA,R1,R2,
AALPHS,DX,DY1,DY2,DT,R11,R12,R21,R22,A1,A2,A3,A4,A5,A6,A7,A8
COMMON /ASS/ DTR1,DTR2,M1,M2,N1,N2,M11,M22,N11,N22,NA1,NA2,
AMA1,MA2,K1,K2,K3,NTE,M122,M222,M112,M212,N121
COMMON /ASS/ ID2,ID2I,ID3,ID3I,ID32,I2,I3,J3,I4,J4
IF(NT .GT. 2) GO TO 100
DO 1 J=1,JI
DO 2 I=1,II
T(I,J)=0.DO
TT(I,J)=0.DO
TTT(I,J)=0.DO
CONTINUE
CONTINUE
C COMPUTE TEMPERATURE OF THE COATING LAYER
DA, DG, SIG, TAU = THE COEFFICIENTS DEFINED IN THE TEMPERATURE EQUATION
C
100 DO 3 I=2,II
DO 4 J=2,II
AA1=DA(I,J)*TT(I,J-1)-2.DO*TT(I,J)+TT(I,J+1))
AA2=DG(I,J)*TT(I,J-1)-2.DO*TT(I,J)+TT(I,J+1))
AA3=SIG(I,J)*TT(I,J-1)-TT(I,J-1))/2.DO
AA4=TAU(I,J)*TT(I,J-1)-TT(I,J-1))/2.DO
AAA=AA1+AA2+AA3+AA4
IF(NT .GT. 2) GO TO 5
C 2 POINTS BACKWARD DIFFERENCE IN TIME DERIVATIVE
C T(I,J)=TT(I,J)+AAA*DT/R1
GO TO 4
C 3 POINTS BACKWARD DIFFERENCE IN TIME DERIVATIVE
5 T(I,J)=(2.DO*AAA*DT/R1+4.DO*TT(I,J)-TTT(I,J))/3.DO
4 CONTINUE
3 CONTINUE
C COMPUTE TEMPERATURE OF THE SUBSTRATE
C DO 6 I=2,II
DO 7 J=K3,J2
AA1=DA(I,J)*(TT(I-1,J)-2.0*TT(I,J)+TT(I+1,J))
AA2=DG(I,J)*(TT(I,J-1)-2.0*TT(I,J)+TT(I,J+1))
AA3=SIG(I,J)*(TT(I,J-1)-TT(I,J-1))/2.0
AA4=TAU(I,J)*(TT(I+1,J)-TT(I-1,J))/2.0
AAA=AA1+AA2+AA3+AA4
IF(NT .GT. 2) GO TO 8

2 POINTS BACKWARD DIFFERENCE IN TIME DERIVATIVE

T(I,J)=TT(I,J)+AAA*DT/R2
GO TO 7

3 POINTS BACKWARD DIFFERENCE IN TIME DERIVATIVE

8 T(I,J)=(2.0*AAA*DT/R2+4.0*TT(I,J)-TTT(I,J))/3.0
7 CONTINUE
6 CONTINUE

DO 9 J=NI,N2
DO 10 I=HI,M2
T(I,J)=0.0
10 CONTINUE
9 CONTINUE

COMPUTE TEMPERATURE OF THE CORNER POINTS

IF(NT .GT. 2) GO TO 12

2 POINTS BACKWARD DIFFERENCE IN TIME DERIVATIVE

CORNER A

T(M1,N1)=TT(M1,N1)+(0.5D0*R11*TT(M1-1,N1)-
AA6*TT(M1,N1)+0.5D0*BETA*R12*TT(M1,N1+1)+0.5D0*R11*TT(M1+1,N1)+
AR12*TT(M1,N1-1))/AS

CORNER B

T(M2,N1)=TT(M2,N1)+(0.5D0*R11*TT(M2-1,N1)-A6
A*TT(M2,N1)+0.5D0*BETA*R12*TT(M2,N1+1)+0.5D0*R11*TT(M2+1,N1)
A+R12*TT(M2,N1-1))/AS

CORNER C

T(M1,N2)=A*TT(M1,N2)+4.0*(R21*(TT(M1-1,N2)+
A0.5D0*TT(M1+1,N2)+TT(M1,N2+1)))/3.0

CORNER D

T(M2,N2)=A*TT(M2,N2)+4.0*(R21*(0.5D0*TT(M2-1,N2)
A*TT(M2+1,N2)+R22*(0.5D0*TT(M2,N2-1)+TT(M2,N2+1)))/3.0

GO TO 14
3 POINTS BACKWARD DIFFERENCE IN TIME DERIVATIVE

CORNER A

\[ T(M1,N1) = \left( -TTT(M1,N1) + 4.0 \times TT(M1,N1) + 2.0 \times \right. \]
\[ \left( 0.5 \times A2R1 \times TT(M1-1,N1) - A6 \times TT(M1,N1) + 0.5 \times \right. \]
\[ \left( 0.5 \times A1 \times TT(M1,N1-1) + 0.5 \times TT(M1-1,N1) + \right. \]
\[ \left( 0.5 \times TT(M1-2,N1) \right) / A5 \right) / 3.0 \]

CORNER B

\[ T(M2,N1) = \left( -TTT(M2,N1) + 4.0 \times TT(M2,N1) + 2.0 \times \right. \]
\[ \left( 0.5 \times A2R1 \times TT(M2-1,N1) - A6 \times TT(M2,N1) + 0.5 \times \right. \]
\[ \left( 0.5 \times A1 \times TT(M2,N1-1) + 0.5 \times TT(M2-1,N1) + \right. \]
\[ \left( 0.5 \times TT(M2-2,N1) \right) / A5 \right) / 3.0 \]

CORNER C

\[ T(M1,N2) = \left( -TTT(M1,N2) + 4.0 \times TT(M1,N2) + 2.0 \times \right. \]
\[ \left( 1.5 \times A2R1 \times TT(M1-1,N2) - 1.5 \times TT(M1,N2) + \right. \]
\[ \left( 1.5 \times TT(M1-2,N2) \right) / 3.0 \]

CORNER D

\[ T(M2,N2) = \left( -TTT(M2,N2) + 4.0 \times TT(M2,N2) + 2.0 \times \right. \]
\[ \left( 1.5 \times A2R1 \times TT(M2-1,N2) - 1.5 \times TT(M2,N2) + \right. \]
\[ \left( 1.5 \times TT(M2-2,N2) \right) / 3.0 \]

COMPUTE TEMPERATURE ON THE LEFT & RIGHT HAND EDGE OF THE CAVITY

\[ 14 \ DO \ 15 \ J=NA1,NA2 \]
\[ I=M1 \]
\[ DDY1=Y(I,J)-Y(I,J-1) \]
\[ DDY2=Y(I,J+1)-Y(I,J) \]
\[ YY1=DDY1**2+DDY2**2 \]
\[ YY2=DDY1*DDY2+DDY2**2 \]
\[ EE1=DT*((TT(I-1,J)-TT(I,J))/DX**2+(TT(I,J-1)-TT(I,J))/YY1+ \]
\[ A*(TT(I,J+1)-TT(I,J))/YY2)/R2 \]
\[ IF(DABS(EE1) .LT. 1.D-65) EE1=0.0 \]
\[ I=M2 \]
\[ EE2=DT*((TT(I+1,J)-TT(I,J))/DX**2+(TT(I,J-1)-TT(I,J))/YY1+ \]
\[ A*(TT(I,J+1)-TT(I,J))/YY2)/R2 \]
\[ IF(DABS(EE2) .LT. 1.D-65) EE2=0.0 \]
\[ IF(NT .GT. 2) GO \ TO \ 16 \]

2 POINTS BACKWARD DIFFERENCE IN TIME DERIVATIVE

\[ I=M1 \]
\[ T(I,J)=TT(I,J)+2.0*EE1 \]
\[ I=M2 \]
\[ T(I,J)=TT(I,J)+2.0*EE2 \]

GO TO 15

3 POINTS BACKWARD DIFFERENCE IN TIME DERIVATIVE
DO 15 I=M1
T(I,J)=(-TTT(I,J)+4.DO*TT(I,J)+4.DO*EE1)/3.DO
I=M2
T(I,J)=(-TTT(I,J)+4.DO*TT(I,J)+4.DO*EE2)/3.DO
15 CONTINUE
C
C COMPUTE THE TEMPERATURE ON THE TOP & BOTTOM EDGE OF THE CAVITY
C
DO 17 I=MA1,MA2
IF(NT.GT.2) GO TO 18
C
2 POINTS BACKWARD DIFFERENCE IN TIME DERIVATIVE
C
J=N1
T(I,J)=A*TT(I,J)+R11*(TT(I+1,J)+TT(I-1,J))+2.DO*R12*TT(I,J-1)
J=N2
T(I,J)=A*TT(I,J)+R21*(TT(I-1,J)+TT(I+1,J))+2.DO*R22*TT(I,J+1)
C
GO TO 17
C
3 POINTS BACKWARD DIFFERENCE IN TIME DERIVATIVE
C
18 J=N1
T(I,J)=(-TTT(I,J)+4.DO*TT(I,J)+4.DO*(R11*(0.5DO*TT(I+1,J)-
ATT(I,J)+0.5DO*TT(I-1,J))*R12*(TT(I,J-1)-TT(I,J))))/3.DO
J=N2
T(I,J)=(-TTT(I,J)+4.DO*TT(I,J)+4.DO*(R21*(0.5DO*TT(I-1,J)
A-ATT(I,J)+0.5DO*TT(I+1,J))*R22*(TT(I,J+1)-TT(I,J))))/3.DO
17 CONTINUE
C
C COMPUTE THE TEMPERATURE AT THE INTERFACE
C
DO 19 IJ=1,2
IF(IJ.EQ.1) GO TO 20
MN1=MN2
MN2=12
GO TO 21
C
20 MN1=2
MN2=MN1
21 DO 22 I=MN1,MN2
J=K1
DDX1=X(I,J)-X(I-1,J)
DDX2=X(I+1,J)-X(I,J)
XX1=DDX1**2+DDX1*DDX2
XX2=DDX1*DDX2+DDX2**2
EE3=2.DO*A8*DT*(TT(I-1,J)-TT(I,J))**2
ATT(I,J)=XX2+2.DO*DT*(TT(I-1,J)-TT(I,J))**2
ABETA*DT*(TT(I-1,J)+TT(I,J)**2
IF(NT.GT.2) GO TO 29
C
2 POINTS BACKWARD DIFFERENCE
C
T(I,J)=TT(I,J)+EE1
GO TO 61
57 EF121=(3.D0*RLC+2.D0*RMUC)*1.2D1*EXC*HAK/RHC
58 IF (I .LT. MA1 .OR. I .GT. MM2) GO TO 62
59 IF (I .GT. MA1 .AND. I .LT. MM2) GO TO 63
60 IF (I .EQ. MA1 .OR. I .EQ. MM2) GO TO 64
61 EF111=(3.D0*RLI+2.D0*RMUI)*1.2D1*EXI*HAK/RHC GO TO 65
62 IF (I .LT. MI .OR. I .GT. Ml2) GO TO 63
63 EF111=(3.D0*RLI+2.D0*RMUI)*1.2D1*EXI*HAK/RHC GO TO 65
64 EF111=(3.D0*RLC+2.D0*RMUC)*1.2D1*EXC*HAK/RHC
65 IF (I .LT. M1 .OR. I .GT. MM2) GO TO 66
66 IF (I .GT. MA1 .AND. I .LT. MI2) GO TO 67
67 IF (I .EQ. MA1 .OR. I .EQ. M12) GO TO 68
68 EF11=(3.D0*RL1+2.D0*RMUI)*1.2D1*EXI*HAK/RHC GO TO 70
69 EF11=(3.D0*RL1+2.D0*RMUI)*1.2D1*EXI*HAK/RHC GO TO 70
70 IF (I .LT. Ml1 .OR. I .GT. M12) GO TO 71
71 IF (I .GT. M11 .AND. I .LT. M12) GO TO 72
72 IF (I .EQ. M11 .OR. I .EQ. M12) GO TO 73
73 EF211=(3.D0*RL1+2.D0*RMUI)*1.2D1*EXI*HAK/RHC GO TO 74
74 EF211=(3.D0*RL1+2.D0*RMUI)*1.2D1*EXI*HAK/RHC GO TO 74
75 IF (I .LT. M11 .OR. I .GT. M12) GO TO 76
76 IF (I .GT. M11 .AND. I .LT. M12) GO TO 77
77 IF (I .EQ. M11 .OR. I .EQ. M12) GO TO 78
78 EF221=(3.D0*RL1+2.D0*RMUI)*1.2D1*EXI*HAK/RHC GO TO 79
79 CONTINUE
80 CONTINUE
C
DO 32 J=2,J3
DO 33 I=1,11
IF(J .LT. NNI) GO TO 83
IF(J .EQ. NNI) GO TO 84
IF(J .GE. N1) GO TO 85
83 ES121=(3.D0*RL1+2.D0*RUMU1)*1.2D1*EX1*HAK/RHC
GO TO 86
84 IF(I .EQ. M1 .OR. I .EQ. M2) GO TO 87
IF(I .GT. M1 .AND. I .LT. M2) GO TO 88
ES121=(3.D0*RL1+2.D0*RUMU1)*1.2D1*EX1*HAK/RHC
GO TO 86
87 ES121=(3.D0*RLC+2.D0*RUMUC)*1.2D1*EXC*HAK/RHC
GO TO 86
88 ES121=(3.D0*RL1+2.D0*RUMU2)*1.2D1*EX1*HAK/RHC
GO TO 86
85 ES121=(3.D0*RL2+2.D0*RUMU2)*1.2D1*EX2*HAK/RHC
86 IF(I .LE. N1) GO TO 91
IF(J .EQ. N121) GO TO 92
IF(J .GT. N121) GO TO 93
91 ES111=(3.D0*RL1+2.D0*RUMU1)*1.2D1*EX1*HAK/RHC
GO TO 94
92 ES111=(3.D0*RL1+2.D0*RUMU1)*1.2D1*EX1*HAK/RHC
GO TO 94
93 ES111=(3.D0*RL2+2.D0*RUMU2)*1.2D1*EX2*HAK/RHC
94 FY(I,J)=(ES121*T(I,J+1)-ES111*T(I,J-1))/(2.D0*YE(I,J))
33 CONTINUE
32 CONTINUE
C
J=1
DO 34 I=1,11
FY(I,J)=-Q(I)
34 CONTINUE
C
DO 37 J=NA1,NA2
DO 38 I=M1,M2
FX(I,J)=0.DO
38 CONTINUE
37 CONTINUE
C
DO 39 J=N1,N2
DO 40 I=NA1,NA2
FY(I,J)=0.DO
39 CONTINUE
40 CONTINUE
C
DO 41 I=2,I2
DO 42 J=1,J2
TTT(I,J)=TT(I,J)
42 CONTINUE
41 CONTINUE
RETURN
END
THIS SUBROUTINE MAPS TEMPERATURE AND ITS GRADIENTS IN THE TEMPERATURE FIELD TO THE CORRESPONDING POINTS IN THE STRESS FIELD

SUBROUTINE MAP(TS, FXS, FYS, T, FX, FY, I1, J1, LI1, KJI)
IMPLICIT REAL*8 (A-H, O-Z)

T, FX, FY = TEMPERATURE AND ITS GRADIENTS IN TEMPERATURE FIELD
TS, FXS, FYS = TEMPERATURE AND ITS GRADIENTS IN STRESS FIELD

DIMENSION T(I1, J1), FX(I1, J1), FY(I1, J1), TS(LI1, KJI),
AFXS(LI1, KJI), FYS(LI1, KJI)

DO 1 J = 1, KJI
DO 2 I = 1, LI1
TS(I, J) = 0.0
FXS(I, J) = 0.0
FYS(I, J) = 0.0
CONTINUE
CONTINUE

DO 3 J = 1, J1
ITI = 1

DO 4 I = 7, 10
TS(I, J) = T(ITI, J)
FXS(I, J) = FX(ITI, J)
FYS(I, J) = FY(ITI, J)
ITI = ITI + 1

IT2 = 9
DO 5 I = 13, 15
TS(I, J) = T(IT2, J)
FXS(I, J) = FX(IT2, J)
FYS(I, J) = FY(IT2, J)
IT2 = IT2 + 5

IT3 = 22
DO 6 I = 16, 19
TS(I, J) = T(IT3, J)
FXS(I, J) = FX(IT3, J)
FYS(I, J) = FY(IT3, J)
IT3 = IT3 + 3

IT4 = 38
DO 7 I = 22, 30
TS(I, J) = T(IT4, J)
FXS(I, J) = FX(IT4, J)
FYS(I, J) = FY(IT4, J)
IT4 = IT4 + 3

ITS = 69
DO 8 I = 33, 39
TS(I, J) = T(ITS, J)

CONTINUE
CONTINUE
CONTINUE
CONTINUE
CONTINUE
FXS(I,J)=FX(ITS,J)
FYS(I,J)=FY(ITS,J)

8
ITS=ITS+3

C
IT6=91
DO 9 I=40,42
TS(I,J)=T(IT6,J)
FXS(I,J)=FX(IT6,J)
FYS(I,J)=FY(IT6,J)
9
IT6=IT6+4

C
IT7=104
DO 10 I=43,49
TS(I,J)=T(IT7,J)
FXS(I,J)=FX(IT7,J)
FYS(I,J)=FY(IT7,J)
10
IT7=IT7+5

C
IT8=136
DO 11 I=50,54
TS(I,J)=T(IT8,J)
FXS(I,J)=FX(IT8,J)
FYS(I,J)=FY(IT8,J)
11
IT8=IT8+2

C
TS(11,J)=T(6,J)
FXS(11,J)=FX(6,J)
FYS(11,J)=FY(6,J)
TS(12,J)=T(8,J)
FXS(12,J)=FX(8,J)
FYS(12,J)=FY(8,J)
TS(20,J)=T(33,J)
FXS(20,J)=FX(33,J)
FYS(20,J)=FY(33,J)
TS(21,J)=T(35,J)
FXS(21,J)=FX(35,J)
FYS(21,J)=FY(35,J)
TS(31,J)=T(64,J)
FXS(31,J)=FX(64,J)
FYS(31,J)=FY(64,J)
TS(32,J)=T(66,J)
FXS(32,J)=FX(66,J)
FYS(32,J)=FY(66,J)

3 CONTINUE
C
RETURN
END
MAIN PROGRAM
STRESS FIELD OF A LAYERED MEDIUM WITH A CAVITY, THE TOP
EDGE OF THE CAVITY IS AT THE INTERFACE

IMPLICIT REAL*8 (A-H,O-Z)

X & Y = COORDINATES IN THE PHYSICAL PLANE
A = MATRIX TO BE SOLVED
B = RIGHT HAND SIDE OF THE ALGEBRAIC EQUATIONS
U & V = DISPLACEMENTS IN X AND Y DIRECTION, RESPECTIVELY
S11,S12,S22 = STRESSES
TS,FXS,FYS = TEMPERATURE AND ITS GRADIENTS FROM TEMPERATURE FIELD

DIMENSION X(67,35),Y(67,35),A(649740),B(4420),TS(67,35),
AFXS(67,35),FYS(67,35),U(67,35),V(67,35),S11(67,35),
S22(67,35)
COMMON /Z1/ RMU,RMU2,RMUI,RMUC,RMUIC,RMU1,RMU2,CMUC1,CMUC2
COMMON /Z2/ RLI,RL2,RLI,RLC,RLIC,RLI1,RLI2,RLC1,RLC2
COMMON /Z3/ DN1,DN2,DN3,DI,DJ,RHC

LI1 & KJ1 = THE TOTAL NUMBER OF GRID POINTS IN X AND Y DIRECTION
LI1=67
KJ1=35
L1=LI1-2
L2=LI1-1
K1=KJ1-1

MBAND = HALF BANDWIDTH
MBAND=K1*2+6-1

NEQ = TOTAL NUMBER OF EQUATIONS TO BE SOLVED
NEQ=L1*K1*2

NTOT = TOTAL DIMENSION OF "A" VECTOR
NTOT=(2*MBAND+1)*NEQ
JJ=K1*2

M1 & M2 = X COORDINATES OF THE CAVITY CORNERS
M1=19
M2=31
MR1=M1+1
MR2=M2+1

M1 & M2 = Y COORDINATES OF THE CAVITY CORNERS
M1=14
M2=24
M111=M1-1
M121=M1+1
END
DATE
FILMED 7-88
DTIC