NASA Technical Memorandum 83070

Finite Element Formulation for Transient Heat Treat Problems

R. L. Mullen
Case Western Reserve University
Cleveland, Ohio

and

R. C. Hendricks
Lewis Research Center
Cleveland, Ohio

Prepared for the
Thermal Engineering Joint Conference
cosponsored by the American Society of Mechanical Engineers
and the Japan Society of Mechanical Engineers
Honolulu, Hawaii, March 20–24, 1983

NASA

FINITE ELEMENT FORMULATION FOR TRANSIENT HEAT TREAT PROBLEMS

R. L. Mullen
Case Western Reserve University
Cleveland, Ohio 44106

and

R. C. Hendricks
National Aeronautics and Space Administration
Lewis Research Center
Cleveland, Ohio 44135

E-1520

ABSTRACT

A formulation is presented that describes the macrotheromechanical behavior of materials subjected to rapid thermal or mechanical loading such as occurs in most heat treatments. The equations are developed for Lagrangian, Eulerian, and intermediary kinematic descriptions and are independent of the constitutive laws and the equation of state; they can be solved numerically for a specified material and boundary conditions. The coupled transport effects between dissipation and energy are included. The conventional linearized stability approach indicates the numerical procedure to be stable, with certain restrictions on the time step size.

NOMENCLATURE

A, B, D, G, Q, R, S	element matrices
b	body force
c	wave speed
C	heat capacity
C_1, C_2, C_3	arbitrary constants
C_{ijkl}	elastic constitutive tensor
E	total energy density
$\mathscr{E}$	internal energy density function
f	arbitrary function
H	Heaviside step function
H^0, H^1	Hilbert spaces
J	determinant of Jacobian matrix for the transformation from inertial to reference frame coordinate system
k, $\hat{k}_{ij}$	thermal conductivity (scalar and tensor)
L	Boolean connectivity matrix
n	outward normal unit vector to Ω
N	shape function
q	heat flux vector
r	heat generated per unit mass
t	time
T	absolute temperature
T_0	absolute temperature at zero strain
u	displacement
U	arbitrary function
U_g	reference frame displacement
w	relative displacement
x	spacial coordinate
α	thermal expansion coefficient
Γ	boundary of open set
γ	frequency
Δ	increment
ϵ_{ij}	linear strain tensor components
η	test function
κ	wave number
λ, μ	Lame elastic constants
ξ	natural coordinates
ρ	density
σ	Cauchy stress tensor
τ	relaxation time
Φ	shape function
ψ	natural coordinate
Ω	open set
∇	gradient

Subscripts:

n	grid location
~	vector
≈	second-order tensor

Superscripts:

•	time derivative
e	element quantity
j	time step

Einstein summation convention implied.

INTRODUCTION

The use of heat and stress to alter materials and material surfaces has been known for over 5000 years. Although many of the compositions, heat treating, and joining techniques have been lost, it is evident that the objective was to combine the proper material composition at a temperature and stress with heating and cooling rates to produce a more durable material. This is still the objective today; however, we are rapidly approaching some limitations in heat transfer rates and induced stresses. These processes are very important to our understanding of subsequent wear in gas path seals for turbine engines, as well as many other rapidly cooled surfaces.

Conventional Cooling

High heat transfer rates are experienced in boiling from a cylinder which passes through the stable regimes of film, transition, nucleation, and incipience boiling prior to passing to the conduction and convection regimes. Nukiyama (ref.1) appears to have first recorded this phenomenon, but it was undoubtedly well known to the heat-treating practitioners as a method of controlling material strength (eg. use of ice, salts, and oils). The peak nucleate flux for water is about 15.8×10^5 W/m^2 (5×10^5 Btu/hr-ft^2) at DNB (departure from nucleate boiling) under steady-state conditions. However, the rate of cooling (heating) associated with the Leidenfrost (incipience) temperature (which varies with bath subcooling, the material etc.) ranges from the metastable condition (ref. 2) to over 4.5×10^3 K/s, as measured for bubble growth in saturated water (ref. 3). Giarrantano (ref. 4) investigated transient boiling in fluid helium for heating rates from steady state to the order of 1×10^4 K/s. The peak nucleate fluxes increased an order of magnitude over the steady-state values.

If one increases the body force component (favorably) through flow augmentation devices (ref. 5) or by rotation (refs. 6,7) the heat flux can be increased by a factor of perhaps 20 (i.e., to 3×10^7 W/m^2 (1×10^7 Btu/hr-ft^2) under steady-state conditions).

The heat fluxes at the throat of a high-pressure rocket engine are 0.9×10^8 to 3×10^8 W/m^2 (0.3×10^8 to 1×10^8 Btu/hr-ft^2) and represent some of the highest

operational steady fluxes. As to the temperature rise time of the materials during the starting and shutdown transients, which last for several milliseconds, the temperature changes are usually less than $1x10^4$ K/s (nominally $3x10^3$ K/s).

Rapid Quench

In rapid quenching techniques and formation of metallic glasses, Davies (ref. 8) cites cooling rates which are very large. In the quenching literature the surface temperatures are used as boundary conditions (Dirichlet formulations) rather than the heat flux (Neumann formulations). Ice water, salt water, and oil quenching are commonly used in heat treating and forming of bulk materials. The rates are variable and depend on the mass, with fluxes and cooling rates both of the order of $1x10^6$ K/s. The rates for producing metallic glasses all appear to be larger than 100 K/s to effect vitrification, with rates greater than $1x10^4$ K/s generally considered practical.* Calculated values for the glass transition in metals lie between $3x10^4$ and $1x10^6$ K/s (ref. 8). These rates are usually associated with at least one boundary in continuous motion, such as in turbine engine blade/seal rubbing. Laser glazing and splat cooling associated with plasma spraying are considered to produce the highest rates, $1x10^7$ K/s and $1x10^8$ to $1x10^{10}$ K/s, respectively (ref. 8).

For splat quenching of 40Fe-40Ni-14P-6B, with $h = 2.5$ MW/m^2-K and $T_{melt} - T_{glass} = 600$ K (ref. 8), the average heat flux would be 1.5 GW/m^2 ($5x10^8$ Btu/hr-ft^2). Thus although the cooling rates are very high, the heat flux requirements appear to be similar to those known to rocket designers.

Mechanical Rubs

In seal rubs, grinding, and wear phenomena, the problem is further complicated by the simultaneous application of a high normal load along with the moving boundary condition. Such problems may be classified as the Blok type (ref. 9): Blok studied the motion of a finite-width block sliding over a semi-infinite half space. Extension include dry rub geometries (turbine blades, seals, bearings, and brushes (refs. 10-12), and third-body effects (e.g., lubricant due to melt or conventional lubricants) are discussed by Godet et al. (ref. 13) and Braun et al. (ref. 14).

The duration of the event is very short and more explosive in nature than either conventional cooling or rapid quenching; furthermore ablative losses can and do occur. Marscher (ref. 11) estimates the heat flux per unit of true contact area (including asperities) to be $4x10^3$ Btu/in^2-s or 6.5 GW/m^2 ($2x10^9$ Btu/hr-ft^2). Such high fluxes for even very short times are usually destructive because the stresses in the materials exceed the failure stress and surface cracking ensues.

Objectives

Although transient thermostress computations have been carried out for rocket engine channels and mechanical rubs, the analyses are based on steady- and pseudo-steady-state postulates. In this paper, we develop an explicit transient formulation of the coupled thermal and mechanical equations, including wave effects, which can be used to predict stresses and thermal profiles under conditions of very rapid cooling or heating as associated with seal rubs, the formation of metallic glasses, other equivalent heat treat processes and rocket engine channels. For this information, boundary constraints of either the Lagrangian or Eulerian type can be handled.

*Exceptions occur e.g., metallic glass spherules of 55-Au 22.5Pb-22.5Sb form at 10^2 to 10^3 K/s, ref. 32.

MODELING AND MOTIVATION

Consider, for example, problems with transient energy input and pressure loading of a fluid with deformable boundaries. The equations of motion for fluid dynamics (usually Eulerian in form) possess boundary conditions which are Lagrangian in form (usually associated with solid mechanics). The standard methodology is to decouple the equations and introduce steady- or quasi-steady-state techniques. In this section we develop the equations and criteria for predicting the coupled thermomechanical behavior under very rapid and more conventional transients.

The governing equation for the combined thermomechanical system is based on four conservation laws: conservation of mass, linear momentum, angular momentum, and energy. The form of the partial differential equations that represent these conservation laws depends on the coordinate system and the kinematic description used. In this derivation the governing equations are constructed by using an arbitrary moving reference system as defined by its displacement $\underset{\sim}{U}_g$, see figure 1.

$$\underset{\sim}{u} = \underset{\sim}{U}_g + \underset{\sim}{w}$$

When $\underset{\sim}{U}_g$ is zero, the description is the usual Eulerian formulation (stationary observer); when $\underset{\sim}{U}_g$ is the same as the material displacement $\underset{\sim}{u}$, the description reduces to the Lagrangian formulation (moving observer).

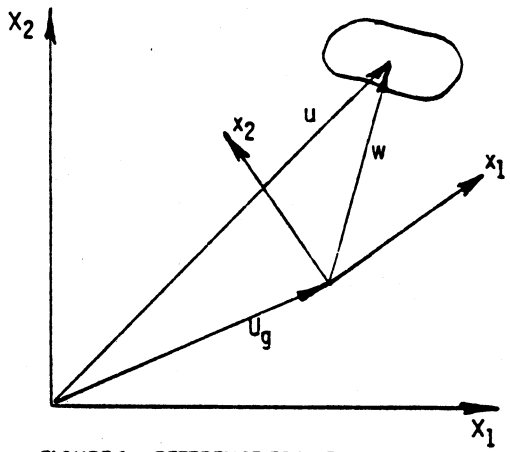

FIGURE 1. REFERENCE FRAME

To complete the formulation, three sets of equations are required in addition to the conservation principles: a constitutive set, an equation or set of equations of state, and a heat diffusion law or laws. However, to specify these equations requires a specific material and, since we wish to maintain generality, these equations will remain arbitrary.

The use of this general description will allow the convenient numerical solution of problems involving large displacements in part of the mesh such as in sliding contacts (ref 15) and production of high-strength, corrosion-resistant ribbon materials (ref. 16). Ribbons for transformer windings or pulverized for powder metallurgy and general ribbon materials of practical interest such as Fe, Ni, Co, Au, Al complexes are alloys which have predicted critical cooling rates for vitrification of the order of $3x10^4$ to $1x10^6$ K/s. The equations can be useful in problems involving large material flows such as in the analysis of continuous casting of steel (ref. 17). The formulation will also be useful in problems involving the

development of high-speed rubber products such as tires and crawler tracks where the speeds are lower but the applied loads are high.

GOVERNING EQUATIONS

Conservation of Mass

In this formulation the mass of any body is assumed to be fixed. The change of mass due to chemical reactions is ignored. The change of mass in any open region Ω is then given by the mass flux into the region. Expressing this statement in integral form yields

$$\frac{\partial}{\partial t}\int_{\Omega(t)} \rho \, d\Omega - \int_{\Gamma} \rho \dot{\underset{\sim}{w}} \cdot \underset{\sim}{n} \, d\Gamma = 0 \tag{1}$$

where ρ is the mass density, Γ is the boundary of the open region, and $\dot{\underset{\sim}{w}}$ is the velocity vector with Cartesian components $\dot{w}_j$ of the mass with respect to the region Ω.

The inertial velocity of the material $\dot{\underset{\sim}{u}}$ can be decomposed into two components: the velocity of the material with respect to the reference frame, and the velocity of the reference frame $\dot{\underset{\sim}{w}}$ with respect to the inertial frame $\dot{\underset{\sim}{U}}_g$ (fig. 1). The vector identity relating these three velocities is

$$\dot{\underset{\sim}{u}} = \dot{\underset{\sim}{U}}_g + \dot{\underset{\sim}{w}} \tag{2}$$

In most previous work using an Arbitrary Lagrangian-Eulerian description, Hirt, Noh, Donea, and Belystchko (refs. 18-21) used the grid velocity as the independent variable describing the reference frame. When the grid velocity is used, the Eulerian description can be obtained by setting the grid velocity to zero. The Lagrangian description, on the other hand, can only be obtained by setting the grid velocity to the material velocity, which is unknown apriori. The preference of grid velocity over relative velocity is due to the application of the previous researcher's formulations to fluid problems where the Eulerian description is preferred.

In the heat treatment problems the bulk material velocities are either known, as in the sliding-contact problem, or can be reasonably estimated, as in the continuous-casting process. The motion of the boundary of the material is not known apriori; therefore the description that most easily reduces to the Lagrangian description is used. Since equation (1) is true for an arbitrary boundary, by applying the divergence theorem and the Leibniz rule, the conservation law can be written in differential form as

$$\frac{\partial}{\partial t}(\rho J) + \underset{\sim}{\nabla} \cdot (\rho \dot{\underset{\sim}{w}}) J = 0 \tag{3}$$

where J is the determinate of the Jacobian matrix. By using the identity due to Euler

$$\underset{\sim}{\nabla} \cdot \dot{\underset{\sim}{U}}_g = \frac{\dot{J}}{J} \tag{4}$$

equation (3) can be rewritten in our final form as

$$\dot{\rho} + \rho \underset{\sim}{\nabla} \cdot \dot{\underset{\sim}{u}} + \underset{\sim}{\nabla}\rho \cdot \dot{\underset{\sim}{w}} = 0 \tag{5}$$

Conservation of Linear Momentum

The conservation of linear momentum in an arbitrary moving open region Ω with boundary Γ can be written in integral form as

$$\frac{\partial}{\partial t}\int_{\Omega(t)} \rho \ddot{\underset{\sim}{u}} \, d\Omega - \int_{\Omega(t)} \rho \underset{\sim}{b} \, d\Omega + \int_{\Gamma} (\rho \dot{\underset{\sim}{u}} \dot{\underset{\sim}{w}} \cdot \underset{\sim}{n} - \underset{\sim}{\sigma} \cdot \underset{\sim}{n}) \, d\Gamma = 0 \tag{6}$$

The first term is the change of momentum within the volume Ω, the second term is the contribution from the body force vector $\underset{\sim}{b}$, the third term is the momentum flux out of the region, and the fourth term is the momentum on the body from the boundary traction. By converting equation (6) to a differential form in a similar manner as used in the mass conservation equation, the following differential equation results:

$$\rho \ddot{\underset{\sim}{u}} - \rho \underset{\sim}{b} - \underset{\sim}{\nabla} \cdot \underset{\sim}{\sigma} + \rho(\dot{\underset{\sim}{w}} \cdot \underset{\sim}{\nabla})\dot{\underset{\sim}{u}} = 0 \tag{7}$$

Conservation of Angular Momentum

It can be easily shown that the conservation of angular momentum is satisfied only if the stress tensor $\underset{\approx}{\sigma}$ is symmetric (which is the usual case).

Conservation of Energy

The conservation of energy for a thermomechanical system with an arbitrary moving reference frame can be expressed in integral form as

$$\int_{\Gamma} (\underset{\sim}{\sigma} \cdot \underset{\sim}{n}) \cdot \dot{\underset{\sim}{u}} \, d\Gamma + \int_{\Omega(t)} \rho \underset{\sim}{b} \cdot \dot{\underset{\sim}{u}} \, d\Omega - \int_{\Gamma} \rho E \dot{\underset{\sim}{w}} \cdot \underset{\sim}{n} \, d\Gamma - \int_{\Gamma} \underset{\sim}{q} \cdot \underset{\sim}{n} \, d\Gamma + \int_{\Omega(t)} r\rho \, d\Omega = \frac{\partial}{\partial t}\int_{\Omega(t)} \rho E \, d\Omega \tag{8}$$

By splitting the energy density E into internal energy density $\mathscr{E}$ and kinetic parts and by using a similar procedure as in the derivation of the other conservation laws, a differential form of the conservation of energy can be written as

$$\underset{\sim}{\sigma} : \underset{\sim}{\varepsilon} - \rho \underset{\sim}{\nabla}\mathscr{E} \cdot \dot{\underset{\sim}{w}} - \underset{\sim}{\nabla} \cdot \underset{\sim}{q} + \rho r = \rho \dot{\mathscr{E}} \tag{9}$$

To complete the governing equations, a constitutive equation, an equation of state, and a heat diffusion law must be specified. For example, restrictions of the form of these equations can be rationally shown as done in the works of Carlson, Trusedell, Noll, Gurtin, and Eringen (refs. 22-26). However, complete specification of these relations requires experimental information on a particular material.

As an example, the constitutive relation for a linear thermoelastic solid is

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} - \alpha_{ij}(T - T_0) \tag{10}$$

and the equation of state is given by

$$\rho\mathscr{E} = \frac{1}{2}\varepsilon_{ij}\varepsilon_{ij} + \rho CT + T_0\alpha_{ij}\varepsilon_{ij} \tag{11}$$

When these relations are used with the classic Fourier law of heat diffusion

$$q_i = -k_{ij}\frac{\partial T}{\partial x_j} \tag{12}$$

and isotropy is assumed, the energy equation will yield the linear coupled heat conduction equations as given in Boley (ref. 27).

$$\rho C\dot{T} + (3\lambda + 2\mu)\alpha T_0 \dot{\epsilon}_{kk} = \frac{\partial}{\partial x_i}\left(k \frac{\partial T}{\partial x_i}\right) \tag{13}$$

where λ and μ are the Lame elastic constants.

However, in problems involving very rapid temperature changes and large heat fluxes, which characterize the heat-treating processes, the assumption of linear behavior often leads to erroneous predictions.

To develop useful numerical tool to investigate these problems, a formulation that is easily adapted to various nonlinear constitutive and state equations must be used. We therefore develop a finite element approximation to the field equations without assuming a form of the constitutive relations or a form of the equation of state. A general form of the heat diffusion equation is assumed as described in the following section.

Heat Diffusion Equation

The most valid first-order relation which exists between the heat flux vector and the temperature gradient is

$$q_i = -k \frac{\partial T}{\partial x_i} - \hat{k}_{ij} \frac{\partial T}{\partial x_j} \tag{14}$$

When this equation is used in a purely thermal problem with a fixed reference system, the energy equation becomes the parabolic heat conduction equation

$$\rho C\dot{T} = k\nabla^2 T \tag{15}$$

This equation, although adequate for slow processes, predicts an infinite propagation velocity for a finite heat flux. One method to resolve this error is the modification to equation (14) proposed by Maxwell and Grad (refs. 28, 29)

$$q_i = -k \frac{\partial T}{\partial x_i} - \hat{k}_{ij} \frac{\partial T}{\partial x_j} - \tau \frac{\partial q_i}{\partial t} \tag{16}$$

We use a modified form which is more convenient to incorporate into the finite element formulation:

$$q_i = -\left(k \frac{\partial T}{\partial x_i} + \hat{k}_{ij} \frac{\partial T}{\partial x_j}\right) - \tau\left(k \frac{\partial \dot{T}}{\partial x_i} + \hat{k}_{ij} \frac{\partial \dot{T}}{\partial x_j}\right) \tag{17}$$

This diffusion law in a purely thermal problem will yield an energy equation that is of the form of the telegraph equation which was studied by Weymann, Baumeister, and Hamill (refs. 30, 31).

Further heuristic generalization involving powers of the thermal gradients and multiple relaxation times can be made but are not considered in the proposed finite element formulation.

FINITE ELEMENT FORMULATION

Approximate solutions to the field equation will be developed by applying the finite element technique in space and a simple explicit integration method in time. The use of the explicit temporal integration method permits the transient solution to proceed without the need to solve simultaneous systems of nonlinear equations. The behavior of current techniques for solving systems of nonlinear equations depends on the properties of the equations to be solved. Since the equations for the state and constitutive relations are assumed to be arbitrary, the explicit method provides an effective formulation.

The limitation for explicit methods is that the time increment used must be small enough to keep the integration stable. In rapid heat-treating problems this restriction is not excessive. The stability of our finite element formulation is investigated in the section Analysis of the Discrete Equations.

By multiplying the differential forms of the conservation equations by a test function η and integrating over the domain of the problem, the following weak forms for the conservation principles results:

Conservation of Mass

$$\text{Find } \rho \epsilon H^0,\ u_i,\ w_i \in H^7 \ \forall\ \eta \in H^7 \text{ such that}$$

$$\int_\Omega \eta\left[\left(\dot{\rho} + \rho \frac{\partial \dot{u}_j}{\partial x_j} - \rho \frac{\partial \dot{w}_j}{\partial x_j}\right) - \frac{\partial \eta}{\partial x_j} \dot{w}_j\right] d\Omega + \int_\Gamma \rho \dot{w}_j\, \eta n_j\, d\Gamma = 0 \tag{18}$$

Conservation of Linear Momentum

$$\text{Find } u_i,\ w_i \in H^1,\ \rho,\ \sigma_{ij} \in H^0 \ \forall\ \eta \in H^1 \text{ such that}$$

$$\int_\Omega \left[\eta_i \rho \left(\ddot{u}_i - b_i + \frac{\partial \dot{u}_i}{\partial x_j} \dot{w}_j\right) + \frac{1}{2}\left(\frac{\partial \eta_i}{\partial x_j} + \frac{\partial \eta_j}{\partial x_i}\right)\sigma_{ij}\right] d\Omega + \int_\Gamma \eta_i \sigma_{ij} n_j\, d\Gamma = 0 \tag{19}$$

Conservation of Energy

$$\text{Find } \mathcal{E},\ T \in H^1,\ \rho,\ \sigma_{ij},\ \epsilon_{ij} \in H^0 \ \forall\ \eta \in H^1 \text{ such that}$$

$$\int_\Omega \left\{\eta \sigma_{ij} \dot{\epsilon}_{ij} - \rho\eta \frac{\partial}{\partial x_j} \dot{w}_j - \frac{\partial \eta}{\partial x_j}\left[k \frac{\partial T}{\partial x_j} + \hat{k}_{ij} \frac{\partial T}{\partial x_i} + \tau\left(k \frac{\partial \dot{T}}{\partial x_j} + \hat{k}_{ij} \frac{\partial \dot{T}}{\partial x_i}\right)\right] + \eta\rho r - \rho\eta \dot{\mathcal{E}}\right\} d\Omega = 0 \tag{20}$$

We will now develop a finite element approximation to the weak form of the conservation equations for two-dimensional problems. All functions will be approximated in space by assuming the form of the functions on each element to be given by

$$\underline{U}(\underline{x},t) = N_I(\underline{x})\underline{U}_I(t) \tag{21}$$

where the majuscule subscripts indicate the node number and N are the shape functions defining the type of element. For a four-node bilinear quadrilateral element, shown in figure 2, the shape functions used to approximate H^1 functions in natural coordinates are

$$N_1 = \frac{1}{4}(1 - \xi)(1 - \psi)$$

$$N_2 = \frac{1}{4}(1 + \xi)(1 - \psi)$$

$$N_3 = \frac{1}{4}(1 + \xi)(1 + \psi) \tag{22}$$

$$N_4 = \frac{1}{4}(1 - \xi)(1 + \psi)$$

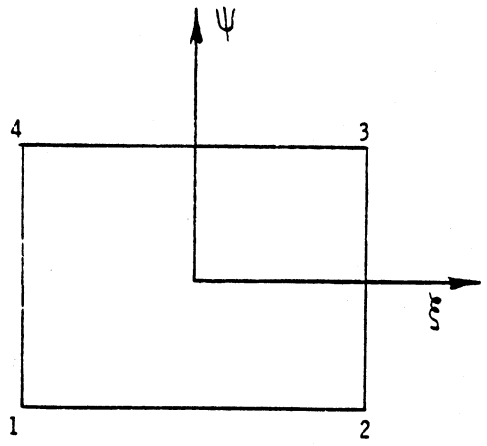

FIGURE 2. GENERIC ELEMENT

The shape functions used to approximate H^0 functions are

$$\begin{aligned}\phi_1 &= [1 - H(\xi)][1 - H(\psi)]\\ \phi_2 &= H(\xi)[1 - H(\psi)]\\ \phi_3 &= H(\xi)H(\psi)\\ \phi_4 &= [1 - H(\xi)]H(\psi)\end{aligned} \tag{23}$$

Using the shape functions in the weak form of the mass conservation equation results in the following semi-discrete system of equations:

$$B_{JI}\dot{\rho}_J + A_{IJ}\rho_J = 0 \tag{24}$$

where

$$B_{IJ} = \sum^{e} L^e_{KI} \int_{\Omega^e} \phi_K N_P \, d\Omega \, L^e_{PJ} \tag{25}$$

$$A_{IJ} = \sum^{e} L^e_{KI} \int_{\Omega^e} \left[N_K \frac{\partial N_M}{\partial x_q} (\dot{u}_{Mq} - \dot{w}_{Mq}) - \frac{\partial N_K}{\partial x_q} N_M \dot{w}_{Mq} \right] \phi_P \, d\Omega \, L^e_{PJ} \tag{26}$$

The finite element approximation to the momentum equation is obtained from the weak form in a similar manner.

$$G_{IJ}\ddot{u}_{Jk} = Q_{Ik} + R_{IJ}u_{Jk} + S_{Ik} \tag{27}$$

Here the matrices G, Q, R, and S are defined by

$$G_{IJ} = \sum^{e} L^e_{KI} \int_{\Omega^e} N_K N_P \rho_M \phi_M \, d\Omega \, L^e_{PJ} \tag{28}$$

$$Q_{Ij} = \sum^{e} L^e_{KI} \int_{\Omega^e} \phi_J \rho_J b_{Mj} N_M N_K \, d\Omega \tag{29}$$

$$R_{IJ} = \sum^{e} L^e_{KI} \int_{\Omega^e} -\phi_J \rho_J N_K N_P w_{Pm} N_{Sm} \, d\Omega \, L^e_{SJ} \tag{30}$$

$$S_{Jk} = \sum^{e} L^e_{IJ} \int_{\Omega^e} \frac{1}{2}\left(\frac{\partial N_{Ik}}{\partial x_i} + \frac{\partial N_{Ik}}{\partial x_j} \right) \sigma_{ij} \, d\Omega \tag{31}$$

The finite element approximation to the energy equation is

$$G_{IJ}\dot{\mathscr{E}}_J = D_I \tag{32}$$

where

$$D_I = \sum^{e} L^e_{IJ} \int_{\Omega^e} \left[N_J \phi_K \rho_K \left(r - \dot{w}_{Mj} N_M \frac{\partial N_S}{\partial x_j} \mathscr{E}_K \right) + N_J(\sigma_{ij}\dot{\varepsilon}_{ij}) - \frac{\partial N_J}{\partial x_i}\left(\hat{k}_{ij}^T S \frac{\partial N_S}{\partial x_j} \right) \right] d\Omega \tag{33}$$

All first-order time derivatives will be approximated by a forward difference operator

$$\dot{f}^i = \frac{f^{i+1} - f^i}{\Delta t} \tag{34}$$

and all second-order time derivatives will be approximated by a central difference operator.

$$\ddot{f}^i = (\Delta t)^{-2}(f^{i+1} - 2f^i + f^{i-1}) \tag{35}$$

When the temporal difference operators are applied simultaneously, the temporal integration scheme is always unstable. To mitigate the instability of the discrete system, a staggered approach to the temporal integration is used. The properties of the discrete equations are analyzed in the next section.

ANALYSIS OF THE DISCRETE EQUATIONS

The stability of the preceding discrete equations is investigated by examining several model equations.

The first model equation is the Lagrangian formulation for one-dimensional elastic solids. The difference equations for this system are

$$\begin{aligned}&\frac{\Delta x}{\Delta t}\left(\rho_{n-1}^{j+1} - \rho_{n-1}^{j} + 6\rho_n^{j+1} - 6\rho_n^j + \rho_{n+1}^{j+1} - \rho_n^j \right)\\ &+ \left(\dot{u}_n^j + \dot{u}_{n-1}^j \right)\rho_{n-1}^j + 3\left(\dot{u}_{n+1}^j - \dot{u}_{n-1}^j \right)\rho_n^j\\ &+ \left(\dot{u}_{n+1}^j - \dot{u}_n^j \right)\rho_{n+1}^j = 0\end{aligned} \tag{36}$$

$$\begin{aligned}&\frac{\Delta x}{\Delta t}\Big[2\left(\rho_{n-1}^j + \rho_n^j \right)\left(\dot{u}_{n-1}^{j+1} - \dot{u}_{n-1}^j \right)\\ &+ \left(\rho_{n-1}^j + 14\rho_n^j + \rho_{n+1}^j \right)\left(\dot{u}_n^{j+1} - \dot{u}_n^j \right)\\ &+ 2\left(\rho_n^j + \rho_{n+1}^j \right)\left(\dot{u}_{n+1}^{j+1} - \dot{u}_{n+1}^j \right)\Big] = 12\left(\sigma_{n-1}^j - \sigma_{n+1}^j \right)\end{aligned} \tag{37}$$

$$\frac{C}{2}\frac{\Delta x}{\Delta t}\Big[2\left(\rho_{n-1}^{j}+\rho_{n}^{j}\right)\left(T_{n-1}^{j+1}-T_{n-1}^{j}\right)$$

$$+\left(\rho_{n-1}^{j}+14\,\rho_{n}^{j}+\rho_{n+1}^{j}\right)\left(T_{n}^{j+1}-T_{n}^{j}\right)$$

$$+2\left(\rho_{n}^{j}+\rho_{n+1}^{j}\right)\left(T_{n+1}^{j+1}-T_{n+1}^{j}\right)\Big]$$

$$+\frac{\lambda\alpha}{4}\left(T_{n+1}^{j}+2T_{n}^{j}+T_{n-1}^{j}\right)\left(2\dot{u}_{n}^{j}-\dot{u}_{n+1}^{j}-\dot{u}_{n-1}^{j}\right)$$

$$+k\left(2T_{n}^{j}-T_{n-1}^{j}-T_{n+1}^{j}\right)=0 \qquad (38)$$

To study the stability of this system, it will be linearized by considering linear perturbations of ρ, u, and T.

$$\rho^{TOTAL}=\rho_{o}+\rho \qquad (39)$$

$$\dot{u}^{TOTAL}=\dot{u}_{o}+\dot{u} \qquad (40)$$

$$T^{TOTAL}=T_{o}+T \qquad (41)$$

where the last term in each expression is assumed to be small. The linearized difference equations are then

$$\frac{\Delta x}{\Delta t}\left(\rho_{n-1}^{j+1}-\rho_{n-1}^{j}+6\rho_{n}^{j+1}-6\rho_{n}^{j}+\rho_{n+1}^{j+1}-\rho_{n+1}^{j}\right)$$

$$+4\rho_{o}\left(\dot{u}_{n+1}^{j}-\dot{u}_{n-1}^{j}\right)=0 \qquad (42)$$

$$\frac{\Delta x}{\Delta t}\rho_{o}\left[\dot{u}_{n-1}^{j+1}-\dot{u}_{n-1}^{j}+4\left(\dot{u}_{n}^{j+1}-\dot{u}_{n}^{j}\right)+\dot{u}_{n+1}^{j+1}-\dot{u}_{n+1}^{j}\right]$$

$$-3c^{2}\left(\rho_{n+1}^{j}-\rho_{n-1}^{j}\right)=0 \qquad (43)$$

$$\frac{\Delta x}{\Delta t}\rho_{o}C\left[T_{n-1}^{j+1}-T_{n-1}^{j}+4\left(T_{n}^{j+1}-T_{n}^{j}\right)+T_{n+1}^{j+1}-T_{n+1}^{j}\right]$$

$$+k\left(2T_{n}^{j}-T_{n-1}^{j}-T_{n+1}^{j}\right)+\frac{\lambda\alpha}{4}T_{o}\left(2\dot{u}_{n}^{j}-\dot{u}_{n+1}^{j}-\dot{u}_{n-1}^{j}\right)$$

$$+\frac{\lambda\alpha}{4}\dot{u}_{o}\left(T_{n+1}^{j}+2T_{n}^{j}+T_{n-1}^{j}\right)=0 \qquad (44)$$

Exact solutions to the linear difference equations in the form

$$\rho_{n}^{j}=C_{1}\exp\left(i\Delta t\gamma j+\kappa n\Delta x\right) \qquad (45)$$

$$\dot{u}_{n}^{j}=C_{2}\exp\left(i\Delta t\gamma j+\kappa n\Delta x\right) \qquad (46)$$

$$T_{n}^{j}=C_{3}\exp\left(i\Delta t\gamma j+\kappa n\Delta x\right) \qquad (47)$$

can be found; for the difference equations to be stable, the modulus of

$$e^{i\Delta t\gamma},\quad i=\sqrt{-1} \qquad (48)$$

must be less than 1. Since this is not the case when the central-forward difference method is applied, a modified integration approach that is still explicit in form must be used.

One such approach is to advance one variable at a time. For example, advance the density by the standard forward difference operator; then, in the momentum equation, use the new values for the density to calculate the right side and solve for the linear displacement. The internal energy (temperature) can be advanced by using the new values for both the density and the displacements to compute the right-side vector.

The linearized difference equation for this temporal integration method when applied to the linear problem can be shown to be stable when

$$\Delta t<\left(\frac{\Delta x}{c}\right)\sqrt{2} \qquad (49)$$

$$\Delta t<\frac{\sqrt{3}}{2}\left(\frac{\rho C}{k}\right)(\Delta x)^{2}. \qquad (50)$$

The second model problem is that of linear thermoelasticity with a motion of the reference frame. By a similar analysis the conditions for a stable solution are

$$\Delta t<\left(\frac{\Delta x}{c}\right)\sqrt{2} \qquad (51)$$

$$\Delta t<\frac{\sqrt{3}}{2}\left(\frac{\rho C}{k}\right)(\Delta x)^{2} \qquad (52)$$

$$\Delta t<\frac{2\Delta x}{|\dot{\underline{w}}|} \qquad (53)$$

The last restriction can be eliminated by introducing upwinding. One way to accomplish this is to postmultiply all transport terms in the discrete equations by an amplification matrix (ref. 22).

SUMMARY

1. A formulation for transient heating which is independent of constitutive laws and the equation of state has been developed. The user selects a material, the appropriate constitutive law, and the equation of state; the numerical solution will then provide the thermomechanical effects for that material.

2. The formulation applies to systems which respond to very rapid thermomechanical loadings such as occur in gas path seal rubs and in forming vitrified products where the quenching rates are greater than 1×10^{4} K/s. It can also be applied to more conventional thermomechanical loadings but may not represent the most efficient technique.

3. This formulation includes transport effects such as can occur in sliding contacts (e.g., bearings, seals, continuous casting, ribbon production, rubber products, and some types of heat treating). The coupled conservation laws predict two transport terms. The conventional heat transport $|\dot{w}|\,dT/dx$ and a strain energy transport term which is not included in the conventional governing equations for heat transfer (ref. 9). Studies need to be carried out to verify the magnitude of these terms.

4. The stability analysis, although based on a linearized model, is effective because the estimate provides the maximum disturbance. Experience has shown systems with smaller perturbations to be stable. The time-step restrictions calculated from linear stabililty analysis can be used to estimate acceptable time steps in nonlinear problems. Experience indicates that from the maximum value of each coefficient (e.g., sound speed and thermal

diffusivity, etc.) the linear theory predicts reasonable values for the time increments in the nonlinear problem. These estimates can be used to judge the applicability of this formulation to a particular problem.

REFERENCES

1. Nukiyama, S., "Maximum and Minimum Values of Heat Transmitted from a Metal to Boiling Water under Atmospheric Pressure," Journal of the Japan Society of Mechanical Engineers, Vol. 37, No. 206, June 1934, pp. 367-374.

2. Baumeister, K. J., Hendricks, R. C. and Hamill, T. D., "Metastable Leidenfrost States," NASA TN D-3226, Apr. 1966, National Aeronautics and Space Administration, Cleveland, OH.

3. Hendricks, R. C. and Sharp, R. R., "Initiation of Cooling due to Bubble Growth on a Heating Surface," NASA TN D-2290, Apr. 1964, National Aeronautics and Space Administration, Cleveland, OH.

4. Giarrantano, P. J. and Frederick, N. V., "Transient Pool Boiling of Liquid Helium using a Temperature-Controlled Heater Surface," Advances in Cryogenic Engineering, Vol. 25, Plenum Press, New York, 1979, pp. 455-466.

5. Bergles, A. E., "Enhancement of Heat Transfer," International Heat Transfer Conference, 6th, Hemisphere Publishing Corp., Vol. 6, 1978, pp. 89-108.

6. Gray, V. H., Joslyn, A. W. and Marto, P. J., "Boiling Heat Transfer Coefficients, Interface Behavior, and Vapor Quality in Rotating Boiler Operating to 475 g's," NASA TN D-4136, Mar. 1968, National Aeronautics and Space Administration, Cleveland, OH.

7. Negrano, M. J. (Braun, M. J.), "Two-Phase Boiling Heat Transfer in Rotating Boiler Systems," Ph.D. Thesis, Carnegie Mellon University, 1967.

8. Davies, H. A., "Rapid Quenching Techniques and Formation of Metallic Glasses," Rapidly Quenched Metals III, Vol. 1, London Metals Society, London, 1978, pp. 1-21.

9. Blok, H., "Theoretical Study of Temperature Rise at Surface of Actual Contact under Oiliness Lubricating Conditions," General Discussions on Lubrication, Vol. 2, Institute of Mechanical Engineers, 1937, p. 222.

10. Bill, R. C. and Ludwig, L. P., "Wear of Seal Materials Used in Aircraft Propulsion Systems," Wear, Vol. 59, 1980, pp. 165-189.

11. Marscher, W. D., "Thermal Versus Mechanical Effects in High Speed Sliding," Wear, Vol. 79, 1982, pp. 129-143.

12. Dow, T. A., ed, Thermomechanical Effects in Wear, Elsevier Sequoia S.A., New York, 1982.

13. Godet, M., Play, D., and Berthe, D., "An Attempt to Provide a Unified Treatment of Tribology Through Load Carrying Capacity, Transport, and Continuum Mechanics," Journal of Lubrication Technology, Vol. 102, No. 2, Apr. 1980, pp. 153-164.

14. Hendricks, R. C., Braun, M. J., Arp, V., and Giarrantano, P. J., "The Dryout Region in Frictionally Heated Sliding Contacts," presented at the 7th International Heat Transfer Conference, Sept. 6-10, 1982, Munich, American Society of Mechanical Engineers.

15. Kennedy, F. E., Jr. and Karpe, S. A., "Thermocracking of a Mechanical Face Seal," Wear, Vol. 79, 1982, pp. 21-36.

16. Gray, H. R.: NASA Le RC, Private Communication.

17. Pehlke, R. D., ed. Continuous Cast of Steel, U. of Michigan, Engineering Summer Conferences, pp. 8002-88, 19-23 May, 1980.

18. Hirt, C. W., Amsden, A. A., and Cook, J. L., "An Arbitrary Lagrangian-Eulerian Computing Method for All Flow Speeds," Journal of Computational Physics, Vol. 14, Mar. 1974, pp. 227-253.

19. Noh, W. F., "CEL: A Time Dependent Two-Space Dimensional Coupled Eulerian Lagrange Code, "Methods in Computational Physics, Vol. 3, Academic Press, New York, 1964, pp. 117-180.

20. Donea, J., "Lagrangian and Eulerian Finite Element Techniques for Transient Fluid-Structure Interaction Problems," Transactions of the International Conference on Structural Mechanics in Reactor Technology (SMIRT), 4th, Vol. B, Committee of the European Communities, 1977.

21. Belytschko, T., Kennedy, J. M., and Schoeberle, D. F., "Quasi-Eulerian Finite Element Formulation for Fluid-Structure Interaction," ASME 78-PVP-60, June 1978, American Society of Mechanical Engineers.

22. Carlson, D. E., "Linear Thermoelasticity," Solid-State Mechanics 2, Vol. 6a/2, Springer-Verlag, Berlin, 1972, pp. 297-345.

23. Truesdell, C, A First Course in Rational Continuum Mechanics, Academic Press, New York, 1977.

24. Noll, W. and Truesdell, C., "Nonlinear Field Theories of Mechanics," Nonlinear Field Theories of Mechanics, Vol. III/3, Springer-Verlag, Berlin, 1965.

25. Gurtin, M. E., "The Linear Theory of Elasticity," Solid-State Mechanics 2, Vol. 6a/2, Springer-Verlag, Berlin, 1972, pp. 1-295.

26. Eringen, A. C., Mechanics of Continua, John Wiley, New York, 1967.

27. Boley, B. A. and Weiner J. H., Theory of Thermal Stresses, John Wiley, New York, 1960.

28. Maxwell, J. C., Philosophical Transactions of the Royal Society, Vol. 157, 1867, p. 49.

29. Grad, H., "Principles of the Kinetic Theory of Gases," Thermodynamics of Gases, Vol. 12, Springer-Verlag, Berlin, 1958, pp. 205-294.

30. Weymann, H. D., "Finite Speed of Propagation in Heat Conduction, Diffusion, and Viscous Shear Motion," American Journal of Physics, Vol. 35, No. 6, June 1967, pp. 488-496.

31. Baumeister, K. J. and Hamill, T. D., "Hyperbolic Heat-Conduction Equation - A Solution for the Semi-Infinite Body Problem," ASME 69-HT-1, 1969, American Society of Mechanical Engineers.

32. Lee, M. C., Kendall, J. M., and Johnson, W. L., "Spheres of the Metallic Glasses $Au_{55}Pb_{22.5}Sb_{22.5}$ and Their Surface Characteristics," Applied Physcis Letters, Vol. 40, No. 5, Mar. 1982, pp. 382-384.

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
NASA TM-83070		

4. Title and Subtitle	5. Report Date
FINITE ELEMENT FORMULATION FOR TRANSIENT HEAT TREAT PROBLEMS	6. Performing Organization Code 505-33-52
7. Author(s) R. L. Mullen and R. C. Hendricks	8. Performing Organization Report No. E-1520
9. Performing Organization Name and Address National Aeronautics and Space Administration Lewis Research Center Cleveland, Ohio 44135	10. Work Unit No.
	11. Contract or Grant No.
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, D. C. 20546	13. Type of Report and Period Covered Technical Memorandum
	14. Sponsoring Agency Code

15. Supplementary Notes R. L. Mullen, Case Western Reserve University, Dept. of Civil Engineering, Cleveland, Ohio 44106; R. C. Hendricks, NASA Lewis Research Center. Prepared for the Thermal Engineering Joint Conference cosponsored by the American Society of Mechanical Engineers and the Japan Society of Mechanical Engineers, Honolulu, Hawaii, March 20-24, 1983.

16. Abstract

A formulation is presented that describes the macrotheromechanical behavior of materials subjected to rapid thermal or mechanical loading such as occurs in most heat treatments. The equations are developed for Lagrangian, Eulerian, and intermediary kinematic descriptions and are independent of the constitutive laws and the equation of state; they can be solved numerically for a specified material and boundary conditions. The coupled transport effects between dissipation and energy are included. The conventional linearized stability approach indicates the numerical procedure to be stable, with certain restriction on the time step size.

17. Key Words (Suggested by Author(s))	18. Distribution Statement
Heat transfer; Heat treat; Transient; Thermomechanical; Hyperbolic; Finite element Finite element method	Unclassified - unlimited STAR Category 34

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of Pages	22. Price*
Unclassified	Unclassified		

* For sale by the National Technical Information Service, Springfield, Virginia 22161