

THE UNIVERSITY OF CALGARY

CONTINUUM THERMODYNAMICS FORMULATION AND NUMERICAL SIMULATION
OF THE PROPAGATION OF COUPLED THERMOMECHANICAL WAVES IN
INELASTIC SOLIDS

by

IREWOLE RAPHAEL ORISAMOLU

A THESIS

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DEPARTMENT OF MECHANICAL ENGINEERING

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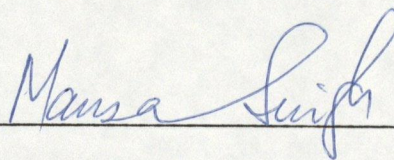
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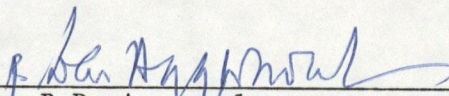
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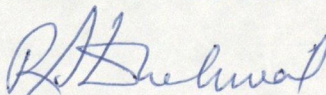
Dr. M.C. Singh, Supervisor
Department of Mechanical Engineering



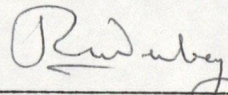
Dr. M. Epstein
Department of Mechanical Engineering



Dr. B.D. Aggarwala
Department of Mathematics & Statistics



Dr. R.S. Dhaliwal
Department of Mathematics & Statistics



Dr. R.N. Dubey, External Examiner
Department of Mechanical Engineering
University of Waterloo

September 22, 1988

ABSTRACT

Dynamic inelastic constitutive equations that take the dissipative nature of inelastic deformation processes into consideration are developed. This is accomplished by employing the theory of irreversible thermodynamics based on internal state variables. The thermodynamic state variables consist of two internal state variables (the strain hardening parameter and the thermoinelastic strain), the total strain, the temperature, and the temperature gradient. An explicit representation for the Helmholtz free energy functional is proposed, leading to explicit expressions for the stress and entropy functionals. The temperature-dependent thermoinelastic material properties that appear in the expression for the free energy are determined by a novel concatenation of the results of thermodynamics, materials science and mechanics experiments, and mathematical analysis. These state equations in conjunction with the evolution laws for the internal state variables and the modified Fourier law of heat conduction give a complete characterization of the thermomechanical material behavior.

The nonlinear material model so developed is non-isothermal, non-adiabatic, and applicable over a wide range of temperatures. Furthermore, it allows for the coupling of thermoelastic and thermoinelastic variables and automatically gives the dissipative part of the stress thereby eliminating the need for a separate dissipation potential.

The constitutive equations, in conjunction with the fundamental balance laws of continuum mechanics, are applied to the study of the

propagation of coupled thermomechanical waves in inelastic solids. Two computational algorithms: one based on the numerical method of characteristics and the other based on the MacCormack finite difference scheme, are developed for quantitative studies of the problem. The results of the numerical simulations illustrate the coupled nature of the thermal and mechanical fields in consistency with the physical process modelled. It is shown that neglecting the stored energy of cold work in the analysis of plastically deforming bodies leads to an appreciable overestimation of the temperature rise in the body. It is also shown that the law of conservation of energy is capable of predicting temperature rises without resorting to *ab initio* quantitative guesses concerning the interconversion of mechanical work into heat energy.

To my parents
EBUNOLUWA and ABIODUN
for their love and care
and
for initiating the process of my education

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NOMENCLATURE

Roman Letters

<u>Symbol</u>	<u>Meaning</u>
A_{ijkl}	Elastic Constant Tensor
A_1	Thermoelastic material function
A_{11}	Thermoelastic material constant
A_2	Thermoinelastic material property
A_3	Thermoinelastic material property
B_1	Thermoelastic material property
B_{11}	Reference value of B_1
B_{12}	Thermoelastic material constant defining variation of B_1 with temperature
B_2	Thermoinelastic material property
B_3	Thermoinelastic material property
B_4	Thermoinelastic material property (Hardening Modulus)
B_5	Thermoinelastic material property (Plastic Modulus)
B_6	Thermoinelastic material property
B_{4R}	Reference value of B_4
B_{5R}	Reference value of B_5
C	Right Cauchy-Green Strain tensor
C_{av2}	Second-order artificial viscosity constant
C_{av3}	Third-order artificial viscosity constant
C_{av4}	Fourth-order artificial viscosity constant
C_D	Specific heat capacity at a constant state of

<u>Symbol</u>	<u>Meaning</u>
	deformation
C^E	Thermoelastic deformation measure
$\tilde{C}^P$	Thermoinelastic deformation measure
$\sim$	
C_v	CFL number
C_1	Reference value of C_D
C_2	Thermal property defining variation of C_D with temperature
C_3^+	Characteristic curve with the positive slope V_3
C_3^-	Characteristic curve with the negative slope $-V_3$
C_5^+	Characteristic curve with the positive slope V_5
C_5^-	Characteristic curve with the negative slope $-V_5$
D_0	Inelastic material constant
D_1	Thermoelastic material function
D_2	Temperature-dependent elastic compliance
D_3	Thermoelastic/Thermoinelastic material function
D_4	Thermoelastic/Thermoinelastic material function
D_5	Analytical function of the thermodynamic state variables
D_6	Thermoelastic/Thermoinelastic material function
e	Internal energy per unit volume
e_{IRR}	Irrecoverable portion of e
e_R	Recoverable portion of e
E	Thermoelastic strain
$\tilde{E}$	Thermoelastic strain tensor

<u>Symbol</u>	<u>Meaning</u>
f	Body force per unit volume
F	Deformation gradient
F_2	Inelastic constitutive function describing the evolution of the strain hardening parameter
g	Temperature gradient
G_1	Inelastic constitutive function describing the evolution of the plastic strain
G_2	Analytical function
G_3	Analytical function
G_4	Analytical function
G_5	Analytical function
G_6	Analytical function
G_7	Analytical function
G_8	Analytical function
G_9	Analytical function
H	Unit step function
H_1	Analytical function
H_2	Analytical function
H_3	Analytical function
H_4	Analytical function
I_j	Constitutive invariant
j	Spatial label of a grid point
J_1	Analytical function
J_2	Analytical function
J_3	Analytical function
J_4	Analytical function

<u>Symbol</u>	<u>Meaning</u>
k	Coefficient of thermal conductivity
K	Experimentally determined constant of proportionality between the stored energy of cold work and the flow stress
K_A	Inelastic material property
$l^{(i)}$	The i th left eigenvector
m	Inelastic material constant
M	Analytic function
n	Time Label for a grid point; Inelastic material constant defining strain rate sensitivity
P	Plastic, thermoinelastic, or flow strain
q	Heat flux
q_2	Second-order artificial viscosity
q_4	Fourth-order artificial viscosity
Q_i	Numerical function
R	Reference configuration; analytical function
R_T	Terminated ramp function
S_P	Pulsive sine function
S_3	Point of intersection of the characteristic curve C_3^+ and the horizontal
S_4	Point of intersection of the characteristic curve C_3^- and the horizontal
S_5	Point of intersection of the characteristic curve C_5^+ and the horizontal
S_6	Point of intersection of the characteristic curve C_5^- and the horizontal

<u>Symbol</u>	<u>Meaning</u>
t	time
T	Absolute temperature
T_R	Reference absolute temperature
u	displacement
$\underline{u}_P$	Vector denoting a subset of the primary dependent variables at point P
$\underline{U}$	Vector denoting the totality of the primary dependent variables
$\underline{U}_A$	Vector denoting the value of $\underline{U}$ at point A
$\underline{U}_B$	Vector denoting the value of $\underline{U}$ at point B
$\underline{U}_C$	Vector denoting the value of $\underline{U}$ at point C
$\underline{U}_P$	Vector denoting the value of $\underline{U}$ at an interior grid point P
$\underline{U}_M$	Vector denoting the value of $\underline{U}$ at a boundary grid point M
$\underline{U}_t$	Partial derivative of $\underline{U}$ with respect to t
$\underline{U}_X$	Partial derivative of $\underline{U}$ with respect to X
v	Particle velocity
V_3	Larger characteristic speed
V_5	Smaller characteristic speed
V_G	Velocity of lagging shock wave
V_L	Velocity of leading shock wave
V_M	Velocity of purely mechanical shock wave
V_T	Velocity of purely thermal shock wave
W_i	Numerical function
W_P	Plastic work

<u>Symbol</u>	<u>Meaning</u>
X	Lagrangian position of a particle
X_{DF}	Nondimensionalization factor for X
Y	Thermoelastic material property ($\lambda + 2\mu$)
Y_1	Reference value of Y
Y_2	Constant defining the temperature dependence of Y
Z	Strain hardening parameter
Z_A	Saturation value of Z
Z^D	Internal state variable describing directional hardening
Z^I	Internal state variable describing isotropic hardening
Z_o, Z_R	Reference value of Z

Greek Letters

α	Coefficient of thermal expansion; ratio of Δt to Δx
α_1, α_R	Reference value of α
α_2	Constant defining the temperature dependence of α
α_A	Inelastic material constant
β	Thermal property: $(3\lambda + 2\mu)\alpha$
β_R	Reference value of β
γ	Heat generation per unit volume
Γ	Set of internal state variables
Δt	Time increment

<u>Symbol</u>	<u>Meaning</u>
ΔX	Spatial increment
ϵ	Total strain
ϵ_R	Reference value of ϵ
η	Entropy per unit volume
η_0	Constant defining the reference value of η
η_{IRR}	Negative of the partial derivative of ψ_{IRR} with respect to θ
θ	Differential temperature
λ	First Lamé constant
λ_i	The i th eigenvalue of matrix <u>A</u>
λ_R	Reference value of λ
Λ	Set of observable thermomechanical variables
i_A	Numerical function
μ	Second Lamé constant
μ_R	Reference value of μ
ν	Poisson's ratio
Π	Set of constitutive response functionals
ρ	Mass density
σ	Stress
σ^C	Quasiconservative part of the stress
σ^D	Dissipative part of the stress
τ_0	Thermal relaxation time
ϕ	Thermal constitutive function
$\tilde{\phi}_L$	Constitutive functional
$\tilde{\phi}_R$	Constitutive functional
ψ	Free energy per unit volume

<u>Symbol</u>	<u>Meaning</u>
ψ^E	Thermoelastic portion of ψ
ψ^I	Thermoinelastic portion of ψ
ψ_{IRR}	Irrecoverable portion of ψ
ψ_R	Recoverable portion of ψ
ψ_o	Constant defining the reference value of ψ
ω	Ratio of energy irrecoverably stored to the total plastic work
Ω	Set of thermodynamic constitutive state variables

ABBREVIATIONS

CFL	Courant-Friedrichs-Lewy
ISV	Internal state variable
SIAR	Semi-infinite aluminum rod
SICOR	Semi-infinite copper rod

CHAPTER 1

INTRODUCTION

1.1 Significance of Wave Phenomena

The fascinating subject of wave propagation is concerned with the study of the mechanism by which a suddenly applied, localized disturbance in a medium is transmitted to other parts of the medium. Familiar manifestations of the phenomenon of wave motion include the transmission of sound in air, the spreading of ripples on a pool of water, the transmission of seismic tremors in the earth, or the transmission of radio waves [1.1]. These examples show that wave phenomena could occur in gaseous, liquid, and solid media and free space. Although these media are diversified, a feature common to all is the transfer of energy so that the physical quantities of interest are necessarily associated with energy propagation [1.2].

Studies of wave propagation arise in virtually every branch of the applied sciences, and it is not surprising that practical applications are as diverse as to include ultrasound in medicine, ultrasonic flaw detection in opaque materials, nondestructive testing, oil reservoir exploration, earthquake monitoring and analysis of ground motion arising from seismic activities, and the characterization of the dynamic response of materials subjected to impacts, explosions and collisions such as we have in the defense and aerospace industries.

In analyzing the response of solids when loading rates are comparable with the transit times of the waves, wave propagation must be considered. This requirement is dictated by the high level of sophistication at which technology is being utilized nowadays which

demands accurate predictions and assessments of the performance of engineering structures. In particular, the desire for optimum utilization of engineering materials in dynamic situations is of paramount importance in a world with continuously diminishing natural resources.

The science of wave motion in elastic solids is very well developed because the theory of elasticity is very well understood. Several monographs [1.1, 1.3] have dealt with this subject. It is well known, however, that under severe loads, metals or metallic alloys may suffer local permanent deformation thus exhibiting plastic or inelastic behavior. Since in many practical situations the loadings are actually severe enough to cause this permanent deformation, the study of wave propagation in inelastic media is of significance and has attracted a lot of research workers as will be seen in the next section. In spite of this fact, the subject of inelastic waves cannot be said to be fully understood today because of the complex nature of the phenomenon of plastic flow.

1.2 Developments in Plastic Wave Theories

The stages involved in quantitatively analyzing wave motion generally consist of the following:

- (a) development of an appropriate mathematical model to represent the physical problem,
- (b) formulation of constitutive equations which are capable of adequately describing the dynamic behavior of the medium of interest,
- (c) solution of the resulting system of partial differential equations,

- (d) interpretation of the results obtained in (c),
- (e) experimental validation of the predicted results.

The development of an appropriate mathematical model is effected through an application of the modern theory of continuum mechanics. This involves a kinematic description of the motion and deformation behavior of the solid considered as a continuum and a systematic application of the fundamental balance laws of mass, momenta, energy, and the second law of thermodynamics. The desire to understand the details of the complex internal structure of plastically deforming solids brings to focus the demand of materials science, while the generation of mechanically induced thermal fields makes thermodynamic considerations a necessity. The solution of the resulting system of partial differential equations is of course enhanced by developments in analytical tools and numerical analysis which immediately reminds us of the role of computer hardware and software. Finally, experimental validations must rely on improvements in instrumentation. In practical terms, therefore, progress in inelastic wave studies relies on developments in the various branches mentioned above as illustrated in Figure 1.1 below.

The study of the propagation of longitudinal plastic or elastoplastic waves in rods has been the subject of extensive experimental and theoretical investigations in the past four decades. The subject was initiated during the second world war when, almost simultaneously, von Karman [1.4] in U.S.A., Taylor [1.5] in Great Britian and Rakhmatulin [1.6] in U.S.S.R. carried out their pioneering works in this field. In these works the partial differential equations governing the motion of the wave were derived under the assumption of a

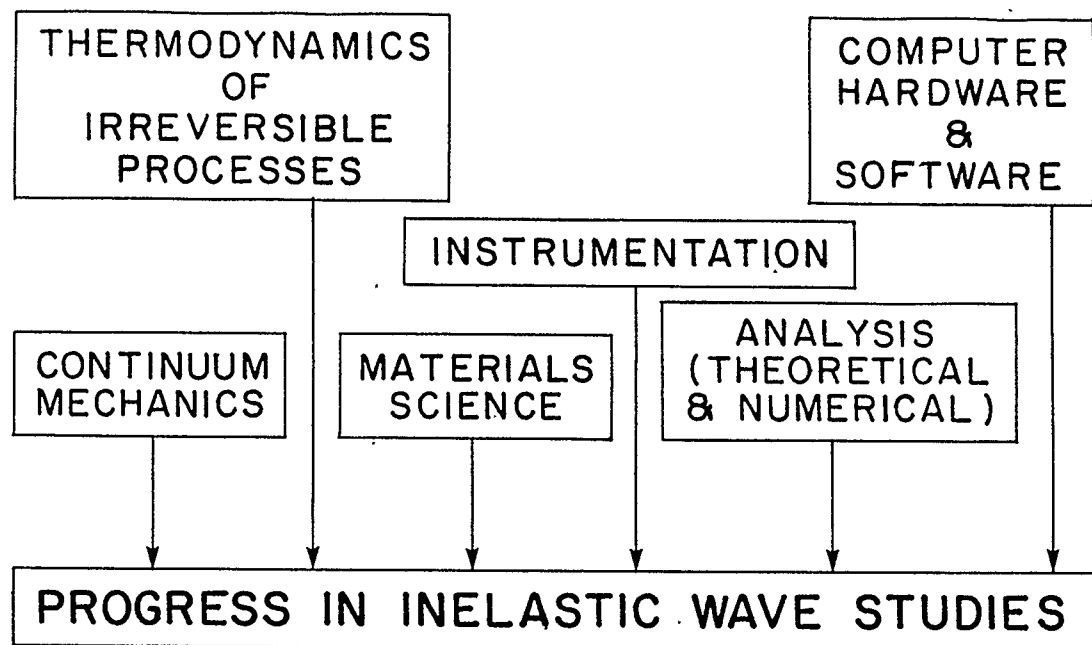


Figure 1.1 Illustration of the interdisciplinary nature of plastic wave propagation studies.

constitutive relationship that is independent of the strain rate; an assumption that implied that the stress-strain relation was the one obtained in a conventional quasistatic tensile test. This approach is referred to as the Rate-Independent (RI) theory and was also used by White and Griffis [1.7]. Experiments performed to verify the RI theory of these workers show clearly that the theory was not capable of describing certain aspects of wave propagation phenomena and that dynamic stress-strain relations were different from their static counterpart. Clifton [1.8] suggested that from a microphysical point of view, rate independence cannot be a possibly exact characterization of the behavior of real metals because the accumulation of plastic strain through the movement of dislocations cannot occur instantaneously.

The second classical plastic wave theory is the Rate-Dependent theory (RD) of Malvern [1.9] in which the stress is assumed to be a function, not only of the instantaneous strain, but also of the instantaneous strain rate. While the RD theory was able to remedy some of the deficiencies of the RI theory, it was unable to predict all the details of inelastic wave propagation. This fact, coupled with the relative mathematical simplicity of the RI theory for certain boundary value problems fueled a major controversy [1.9, 1.10, 1.11] over the necessity of including strain-rate effects in constitutive models for studying impacts in rods or bars.

Various applications and developments of the two approaches have appeared in well-known monographs [1.9, 1.10, 1.11]. We will not give a detailed review of works in plastic waves here because excellent review articles of earlier works have been published [1.12, 1.13, 1.14, 1.15, 1.16]. Also, recent updates have been provided by Nicholas [1.17] and by Clifton [1.18]. More recently, Clifton [1.19] presented a comprehensive review of plastic wave experiments, starting with the earliest experiments of Bell [1.20] on the propagation of incremental waves in prestressed bars and the pioneering work of Kolsky [1.21] concerning the plastic response of metals at high strain rates.

Like any problem of continuum mechanics, the complete formulation of a wave propagation model requires constitutive equations which realistically describe the material behavior under the particular loading conditions being considered. It is obvious then that analyses of inelastic wave propagation phenomena hinge on a thorough knowledge of the dynamic constitutive behavior of the materials concerned.

Ironically, however, it is these constitutive relations that are being sought in such studies. This dilemma makes it difficult to interpret experimental data obtained under conditions of high rates of loading where wave propagation phenomena must be considered, and explains why theoretical studies and experimentation are so closely intertwined. With this background, it is easy to see that any analysis of a problem is only as good as the constitutive relations employed in the study. This shows that constitutive relations have roles that are more important than the conventional in the formulation of wave propagation problems. It is therefore not surprising that controversies surrounding the classical theories are centered on the nature of the constitutive laws.

Expectedly, developments in plastic wave theories have depended on developments in the constitutive theories of plasticity.

The history of plasticity as a science may be traced to 1864 when Tresca published his results on punching and extrusion experiments and formulated his celebrated yield criterion [1.22]. These results were later employed by Saint-Venant and Levy to lay some of the foundations of the classical theory of plasticity. Important contributions that were made (after a long period of time following the papers of Tresca, Saint-Venant, and Levy) by von Mises, Hencky, Prandtl, Reuss, and others were reviewed in the classical treatises by Hill [1.23] and Prager [1.24].

The vast majority of constitutive equations in plasticity are empirically based. These include the plastic stress-strain relations proposed by St. Venant and the general three-dimensional equations

relating the increments of total strain to the stress deviations given by Levy and later independently by von Mises. So also are the Prandtl-Reuss equations which are generalizations of the Levy-Mises equations to include both elastic and plastic components of strain. Thus, it may be said that classical constitutive equations of plasticity are products of conjectures and inductive thoughts, growing as they did from attempts to model observed behavior of metals and metallic alloys under loading histories severe enough to cause permanent deformation.

Despite the numerous works and research efforts that have been directed to plasticity studies over the decades, it has still not been possible to bring together all the mathematical theories under a generally acceptable umbrella. Indeed, the question as to what the definition of 'plasticity' is can still be considered open even today. Only recently, Drucker [1.25] reported escalations of a flurry of excitement about the meaning of the word 'plastic' at a workshop organized by Professor E.H. Lee at Stanford University in 1981. This shows that a lot of work still remains to be done in this important field of applied mechanics.

This apparent backwardness of the subject of plasticity is due to the complex nature of the phenomenon of plastic deformation. The key ingredients responsible for the complex nature include irreversibilities or dissipation, time dependence, path dependence, hardening, and large ductility. The incorporation of these important items in the development of a general form of plastic constitutive equations is very difficult, to say the least. Indeed, Drucker [1.26] suggests that a general form for plasticity is no form at all! It should also be noted that the features mentioned above serve to distinguish the behavior of

an elastic-plastic continuum from that of a nonlinear elastic continuum.

Nevertheless, important advances have been made in generalizing the theory of plasticity. Most of these advances are the results of applications of the deductive methods of modern continuum mechanics in which the framework for theories of nonlinear material behavior is derived in a semi-axiomatic but systematic way from a set of fundamental laws of physics. In such applications, the need for the theory to be consistent with continuum thermodynamics and the classical plasticity theories is evidently brought to the limelight. So also is the requirement for consistency with observations from everyday experience and the results of experiments. A few examples concerning the application of thermodynamics to plasticity are given in Chapter 2.

The generation of thermal fields during inelastic deformation processes is the rule rather than the exception in practical situations. Early experimental evidence concerning this phenomenon of deformation-induced heating was reported by Farren and Taylor [1.27]. Subsequently, a lot of work has been directed towards the understanding and quantification of not only this phenomenon, but the twin phenomenon of heat-induced deformation. A review of experimental and analytical investigations concerning heat generation and their effects in plastic deformation processes can be found in a recent thesis by Kim [1.28]. These works have emphasized not only the need to include temperature in the development of inelastic constitutive equations but the importance of allowing for the interaction of mechanical and thermal fields. This interaction dictates that a realistic constitutive model be able to describe the coupled thermomechanical behavior of inelastic solids - a requirement that increases the degree of complexity of an already

difficult situation. Accordingly, a number of works on developments of thermoplasticity and thermoviscoplasticity models abound in the literature.

In addition to thermal effects, the works of materials scientists have shown that a full understanding of the mechanism of plastic flow must depend on knowledge of activities occurring at the microscopic level during deformation. While such microscopic mechanisms include twinning, void growth, grain boundary sliding and phase transformations, the most important of them all is the generation, motion and interaction of dislocations [1.29]. The theory of dislocations in connection with plastic flow is discussed in the excellent monograph by Gilman [1.30]. Drucker [1.31] was one of the first to attempt a continuum theory of plasticity on the microscale. Interesting applications of mechanics on the microscale to developments in plasticity include the works of Rice [1.32], Aifantis [1.29] and the references contained therein.

All the various aspects of plastic deformation described thus far have received attention of researchers in this vast area, thereby updating and enriching available knowledge on the theory of plasticity and its applications. The brief exposition given here further explains the complexities and intricacies involved in inelastic constitutive modelling. The diverse nature of the branches of knowledge involved as evidenced by the description given above and illustrated by Figure 1.1 is, in the view of the author, a major factor that has been detrimental to progress in this field. This is because collaboration of efforts of researchers in the different fields and coordination of research activities, developments and findings in the several branches have not

been feasible. Works in the different areas are scattered in different specialized publications and researchers tend to remain within the artificial boundaries of their own carved-out domains thus making the cross-breeding of information and ideas very difficult.

Since progress in plastic wave studies depends directly on progress in plasticity theories, it is to be expected that the same impediment alluded to in the preceding paragraph would hinder advances in dynamic plasticity too. This is especially so as 'dynamic effects', in itself is a further complication. We will now give a brief description of how the study of plastic wave propagation has been hampered (or enhanced) by impediments (or developments) in plasticity.

For a basis of discussion, we recall the basic equations governing the propagation of uniaxial waves in inelastic solids by the RD theory:

$$\text{equation of motion,} \quad \frac{\partial \sigma}{\partial X} = \rho \frac{\partial v}{\partial t}, \quad (1.1)$$

$$\text{compatibility equation,} \quad \frac{\partial \epsilon}{\partial t} = \frac{\partial v}{\partial X}, \quad (1.2)$$

$$\text{constitutive equation,} \quad \frac{\partial \epsilon}{\partial t} = f(\sigma, \epsilon) \frac{\partial \sigma}{\partial t} + g(\sigma, \epsilon), \quad (1.3)$$

where σ is the nominal stress, ϵ is the strain, v is the particle velocity, X is the position of the material particle, and t is the time. Equation (1.1) is obtained from an application of the law of balance of linear momentum, equation (1.2) ensures the kinematic compatibility of the definitions of the strain and the velocity which are derivatives of the displacement field, u . The strain and the velocity are respectively defined as:

$$\epsilon = \frac{\partial u}{\partial X}, \quad (1.4)$$

$$v = \frac{\partial u}{\partial t} . \quad (1.5)$$

Equation (1.3) is a rate-dependent type of constitutive equation in which, for a given material, the functions f and g are prescribed.

We note that in the above system of equations there are three unknowns: σ , v and ϵ , and three equations. Mathematically, therefore, the system of equations seems to completely represent the mechanical behavior of the system during wave propagation. However, on a close examination, one finds that out of the four fundamental balance laws of continuum mechanics only one, that of balance of linear momentum, has been used to derive the equation of motion (1.1). In the case of solids, the density of the body may be assumed to remain constant for small displacement gradients, and so the law of conservation of mass is identically satisfied. If the assumption of symmetry of the stress tensor is accepted at the outset, then the law of balance of angular momentum is identically satisfied even in a general three-dimensional state of stress. If thermal effects are neglected, thus restricting considerations to isothermal plasticity, the second law of thermodynamics is also identically satisfied. The implications of this will be discussed later on in the thesis. The law of conservation of energy, however, leads, in a uniaxial wave motion, to the equation

$$\frac{\partial e}{\partial t} = \sigma \frac{\partial v}{\partial X} , \quad (1.6)$$

where e is the internal energy per unit volume. The satisfaction of equation (1.6) is not obvious; nor is its role in the study of plastic waves since the system of equations (1.1 - 1.3) appear to be sufficient.

It is easy to show that in the case of a conservative system (which is associated with a reversible process), for example an elastic rod with a constitutive equation of the form

$$\sigma = f(\epsilon), \quad (1.7)$$

where f is any function of ϵ (linear or nonlinear), the equation of conservation of energy leads to the compatibility equation (1.2). This is because the internal energy is nothing but the strain energy which is the work of deformation. Thus, in the case of a reversible process of deformation (which occurs only for an elastic material undergoing a purely mechanical process), the compatibility equation may be taken to represent the equation of conservation of energy since they are identical. In other words, the equation of conservation of energy may be considered to be identically satisfied. Thus, for elastic materials the system of equations (1.1), (1.2) and (1.3) is complete - physically and mathematically - in isothermal situations and may be solved for the three unknowns.

For the inelastic case that is the subject of consideration in this thesis, however, the situation is quite different. It is common knowledge in the applied mechanics community that inelastic deformation is inevitably accompanied by energy dissipation or irreversibilities. Apart from the thermal fields generated due to conversion of mechanical work to heat energy, there is also the phenomenon of 'stored energy of cold work' in which part of the inelastic work due to externally applied mechanical loads is irrecoverably stored within the deforming body. Under this condition, the elastic strain energy is clearly not the same as the internal energy. Therefore, for nonconservative systems, the law of conservation of energy cannot lead to the compatibility equation

and as such it is not an identity. Thus, for inelastic deformation processes, the law of conservation of energy has a unique role to play and must enter the formulation independently. This requirement immediately necessitates a knowledge of the explicit form of representation for the internal energy density, e . The explicit representation of the internal energy functional is, in itself, a constitutive equation for the material and is not known *a priori*. In addition, the entropy production and temperature rise that are associated with irreversible deformations must be accounted for by the second law of thermodynamics.

These observations clearly show the inadequacy of the above formulation, particularly the form of the constitutive equation (1.3) which, unfortunately, is still employed for inelastic wave propagation studies. They also explain why the model is unable to explain all the pertinent details of dynamic plasticity.

The temporal and spatial temperature variations in a body produce thermal, dilatational deformation and changes in the constitutive properties which will either generate or influence wave propagation [1.15]. Only a few quantitative studies of inelastic wave propagation incorporating the presence of temperature fields through dissipation have been reported in the literature. Francis and Lindholm [1.33] were one of the first to explore the influence of temperature on the propagation of elastoplastic waves. They considered a stationary temperature profile and assumed the material to be bilinear with temperature-dependent mechanical properties but did not account for strain-rate effects. Further work by Francis [1.34] improved on this by the introduction of a more rational but still conventional viscoplastic

constitutive equation. The work of Raniecki [1.35] considered the effect of dynamical thermal expansion on the propagation of plane elastic-plastic stress waves. Other early investigations include the works of Nowacki which were extensively referenced and discussed in his text [1.10]. Studies dealing with thermal effects in inelastic bodies using the theory of propagating singular surfaces are also numerous, see for example, references [1.36] and [1.37].

Despite all these works, there is as yet no generally acceptable procedure for systematically incorporating temperature fields or their effects in inelastic wave studies because the theory of plasticity itself has not been generalized enough to give direction and guidance. There are several ways through which thermal effects have been accounted for. In the majority of cases, *ad hoc* procedures concerning the balance of work and energy are resorted to thereby pre-empting the law of conservation of energy. Date [1.38], for example, accounted for temperature rises during plastic wave propagation by assuming that the plastic mechanical work is wholly and adiabatically converted into heat energy. Many other workers assume a fixed ratio for the portion of the plastic work that is converted into heat energy. Such are the assumptions in references [1.39] and [1.40], for example. Although these studies recognize the non-isothermal nature of the deformation processes involved, the efforts fall short of the complete physical representation. While it is true that the process of plastic deformation is accompanied by a conversion of plastic work into heat energy, it is not true that all of the plastic work is converted, it is not true that the conversion process is adiabatic in all cases, nor is it true that a fixed ratio of the plastic work is converted. This is

because there is ample experimental evidence that some of the plastic work is stored in the material. Early experiments in this regard were reported by Taylor and Quinney [1.41] while comprehensive reviews of experimental and theoretical developments have been given by Titchener and Bever [1.42] and Bever et al [1.43]. A very recent theoretical investigation by Aravas et al [1.44] further attests to the importance of this stored energy of cold work phenomenon. All these investigations indicate that the assumptions discussed above are, in general, not founded on the actual behavior of inelastic solids.

To the author's knowledge, only the work of Bodner and Aboudi [1.45] has come close to recognizing the stored energy of cold work in the analysis of stress wave propagation in inelastic solids. Their investigation made use of a micromechanically based constitutive equation that accounts for isotropic work-hardening. However, the applications reported were restricted to isothermal cases. It should be mentioned in passing that other applications of micromechanically based theories have appeared, notably the studies of Clifton and Markenscoff [1.46] and Markenscoff and Clifton [1.47]. These studies are qualitative, however, perhaps not needing a quantification of the stored energy.

In summary, it may safely be said that the study of plastic wave propagation has not benefited enough from advances in the understanding of the microscopic phenomena of plastic flow.

1.3 Thesis Objectives

In our discussions so far, we have shown that a realistic description of plasticity should, in general, include thermal effects

even in the presence of only mechanical loads. This together with the fact that in many practical applications there also exist the presence of thermal loads show the importance of being able to characterize the thermomechanical behavior of inelastic solids. Such practical situations are encountered in aerospace engineering, internal combustion engines, hot gas turbines, nuclear reactors, nuclear blast environments, or experimental techniques like pulsed lasers and electron beam accelerators.

The main objectives of this thesis are as follows. First is the systematic development of dynamic constitutive relations that are suitable for studying the propagation of coupled thermomechanical waves in inelastic media when the transient disturbances are due to mechanical loads alone, thermal loads alone, or a combination of mechanical and thermal loads. Of particular interest is the ability to incorporate the essential features of dissipation and its implications and its effects such as heat generation, heat flow, thermomechanical coupling, hardening, and irrecoverable energy storage. The constitutive equations are then used to formulate a new form of the initial-boundary-value-problem describing wave propagation in inelastic solids in which the role of the law of conservation of energy is appropriately brought into focus and emphasized. The second major objective is the design and implementation of appropriate computational algorithms that may be used to numerically simulate the propagation of coupled thermomechanical shock and acceleration waves in inelastic solids under a variety of loading environments. The approaches through which these broad objectives are accomplished are described in what follows.

1.4 Organization of the Dissertation

The thesis is organized into seven chapters. In Chapter 2, a continuum thermodynamic development of constitutive equations using the theory of internal state variables (ISVs) is given. It includes a brief introduction of the application of thermodynamics to inelastic constitutive modelling and a review of available models based on the approach. This is followed by a discussion of the choice of the internal state variables. The formalism of thermodynamics is then employed to determine the nature of and the restrictions on the constitutive response functionals.

In Chapter 3, an explicit expression for the Helmholtz free energy functional is proposed, leading to explicit expressions for the stress and entropy functionals in terms of the thermodynamic state variables. In particular, the temperature-dependent thermoelastic material properties involved are determined by a novel concatenation of the results of the thermodynamic development in Chapter 2, the results of materials science and mechanics experiments, and mathematical analysis. Typical material properties characterizing the inelastic thermomechanical behavior of copper and aluminum over a wide range of temperatures are presented. We also propose a generalization of the procedure for the characterization of the inelastic thermomechanical behavior of inelastic solids. Other constitutive response functionals required are also given.

Chapter 4 provides a kinematic description of the problem of inelastic wave propagation in a half space. The balance laws of continuum mechanics and the constitutive equations developed in Chapter 3 are combined to formulate the corresponding initial boundary value

problem. A mathematical analysis to investigate the nature of the system of partial differential equations is presented as the computational algorithms for solving the system depends on this knowledge.

Chapter 5 presents the development of two computational algorithms to numerically solve the equations derived in Chapter 4. The first algorithm is based on the numerical method of characteristics while the second utilizes the MacCormack finite difference scheme.

The results of computer implementations of the algorithms are presented in Chapter 6. Numerical simulations of the propagation of coupled thermomechanical waves in copper and aluminum under a variety of loading situations are presented.

Chapter 7 closes the thesis with concluding remarks about the constitutive equations developed in this work and the algorithms presented earlier on. Recommendations for future work are also presented.

CHAPTER 2

CONTINUUM THERMODYNAMIC DEVELOPMENT OF INELASTIC CONSTITUTIVE EQUATIONS

2.1 Preamble

The discussions given in the last chapter illustrate that dissipation could have important consequences in inelastic wave propagation. It is important, therefore, that any constitutive model that seeks to characterize the behavior of inelastic solids include the effects and implications of dissipation in its development. In phenomenological theories of the dynamical behavior of continua there are several ways of accounting for dissipative effects [2.1, 2.2]. The four commonest ways are:

- (i) introducing a viscous constitutive response functional which depends on the rates of the independent constitutive variables,
- (ii) assuming that the entire past history of the independent constitutive variables influences the constitutive response functionals in a manner compatible with the principle of fading memory introduced by Coleman [2.3],
- (iii) partitioning the material into heterogeneous substructures, for example, hard and soft regions via an approach referred to as mixture theory,
- (iv) postulating the existence of internal state variables (or hidden variables) which influence the constitutive response functionals and whose rates of change are governed by evolution equations in which the independent constitutive variables appear.

At this juncture, it is to be noted that the RD theory discussed in Chapter 1 is a special case of the first approach in which

the constitutive response functional is merely the stress and the independent constitutive variable is the strain. Examples of recent applications of approach (i) to the study of rate-type materials can be found in references [2.4] and [2.5].

Approach (ii) requires a knowledge of the explicit structure of memory functionals. This is obtained by a nonlinear multiple integral representation. In practice, only the first few of these hereditary integrals can be used because of the formidable task involved in the evaluation of the corresponding kernels [2.6]. The approach has been widely applied to viscoelasticity studies.

The third approach has been applied primarily to multi-phase media and has not attracted the attention of workers in inelastic constitutive modelling appreciably.

The fourth approach which involves the use of ISVs is currently gaining wide applicability. This is due to the recognition of the fact that the mechanism of plastic deformation is governed by microscopic processes which can be described on the average by macroscopic variables.

It should be mentioned that all the four approaches have the same objective. For example, Coleman and Gurtin [2.1] showed that thermodynamics based on internal state variables yields results very similar to those derived from thermodynamics based on fading memory as developed by Coleman and his co-workers - see, for example, reference [2.3]. Lubliner [2.7] showed that materials with ISVs in fact possess fading memory if the evolution equations for the ISVs satisfy certain

equilibrium stability conditions. He also demonstrated the equivalence of the rate-type approach and that of ISVs for viscoelastic materials.

Current research trends in mechanics, however, have focused on the development of constitutive equations on a micromechanical basis using ISVs to rationalize some of the phenomenological features of inelastic deformation. This is because these models can be easily correlated with the microstructural changes which are associated with the physical deformation mechanisms. For wave propagation phenomena in particular, microstructural features are becoming increasingly recognized as important to the stress-wave process because they are most pronounced in the regime of rapid changes and strong gradients.

Although the theory of internal state variables may be employed for constitutive modelling outside the realm of thermodynamics, it is generally believed that ISVs are of the greatest value when employed under the umbrella of a thermodynamic framework. This is not only because purely mechanical efforts in this direction have not been entirely successful but because, as noted by Ziegler and Wehrli [2.8], the pursuit of continuum mechanics leads sooner or later into thermodynamics. The latter is especially true for dissipative processes. Accordingly, in the present work the approach of thermodynamics with internal state variables is employed for the development of the required relations.

The history of thermodynamics as a subject is a long and controversial one especially as it concerns the study of irreversible processes. These controversies include the distinction between absolute and empirical temperature; the existence, definition, and measurability of entropy; and the mathematical representation and interpretation of

the second law of thermodynamics. All these issues are of concern in the characterization of nonequilibrium states. So also is the question of uniqueness in such characterizations. An exposition of the theory of thermodynamics of irreversible processes is given in the book by Lavenda [2.9].

The concept of internal variables was introduced into thermodynamics by Onsager [2.10, 2.11]. Early applications to continuum mechanics include the works of Eckart [2.12], Biot [2.13, 2.14], and Ziegler [2.15]. However, the article by Coleman and Gurtin [2.1] was about the first to firmly establish the idea of modelling the behavior of a wide class of materials using the theory of thermodynamics with internal state variables. This statement is without prejudice to the excellent works of Schapery [2.16], who earlier applied this theory to study thermomechanical, fracture and birefringent phenomena in viscoelastic media, and Valanis [2.17] who later but independently presented a unified theory of the thermomechanical behavior of viscoelastic materials.

The literature on the applications of the theory of thermodynamics with internal state variables to inelastic solids is too vast to be reviewed here. Only a few representative references will be cited.

Kratochvil and Dillon [2.18] utilized the Coleman-Gurtin-type thermodynamics for the study of an elastic-plastic substance in which quantities related to the dislocation motion and the dislocation arrangement in the material were considered as ISVs. They later extended this study to include rate sensitivity [2.19]. Perzyna and Wojno [2.20] formulated a thermodynamic theory of a rate sensitive

material within the same framework. Also, Perzyna [2.21] presented a thermodynamic theory of rheological materials in which he used one group of ISVs to describe memory effects and another group to describe internal structural changes. The works of Rice [2.22] and Lubliner [2.23] provided theoretical foundations for the idea of utilizing nonequilibrium thermodynamics based on ISVs for the development of inelastic constitutive models. Lehmann [2.24] connected the description of non-isothermal elastic-plastic deformations and the description of such phenomena by thermodynamic state equations.

More recent developments include the works of Ponter et al. [2.25], Cernocky and Kremp1 [2.26], Allen [2.27], Ghoneim and Matsuoka [2.28], Riff et al. [2.29], and Lehmann [2.30], to mention but a few.

Most of these and other available works do not account for all the dissipative effects of plastic deformation processes discussed in Chapter 1. Even in cases where such effects are considered, the constitutive equations are not readily applicable to the quantitative dynamic analysis of concrete initial-boundary-value-problems. Reasons for this include non-availability of material properties for a given material, non-validity in some ranges of temperatures, making assumptions about energy balance that may be inconsistent with the provisions of the first law of thermodynamics, or, most common of all, disregarding the stored energy of cold work phenomenon. These shortcomings are the main motivations for the desire to develop dynamic inelastic constitutive equations that will more realistically describe the physical phenomena encountered during deformation. In the next section, a discussion of the choice of the ISVs employed is discussed before the presentation of the thermodynamic formalism in Section 2.3.

2.2 Choice of Internal State Variables

In using internal state variables we are seeking to replace the dependence of response upon deformation history by a dependence upon what that history has produced. Thus, these ISVs must be capable of characterizing the microstructural state and changes in that state. In the case of plastic deformation, these variables must describe the arrangement of dislocations in the material. In theory, an infinite number of ISVs are required to describe this microscopic phenomena. Obviously, this is a requirement that is not feasible for physical and analytical reasons if the ISVs are to be useful in practically predicting material behavior. On the basis of the good reproducibility observed in many types of plastic experiments (despite the fact that it is impossible to prepare two specimens of the same material which have exactly the same microscopic dislocation arrangement), Kroner [2.31] concluded that not the whole infinite set of ISVs is necessary in constructing a reasonable theory of plasticity. It is doubtless not reasonable to ask for a theory of plasticity which is better than the experimental reproducibility. Thus, the usual procedure is to settle for a finite number of phenomenological macroscopic variables that are average properties of the detailed microscopic phenomena.

Here we employ two ISVs: the strain hardening parameter, Z , and the thermoelastic, flow, or plastic strain, P .

The strain hardening (or work hardening) parameter (Z) is a measure of the overall resistance to plastic deformation. There is available experimental evidence that the mechanism of strain hardening is largely due to the development of internal stresses [2.32]. Physically, therefore, Z may be regarded as an internal stress. Some

authors, for example Allen [2.33], refer to Z as a drag stress. Merzer and Bodner [2.34] also speculated that a possible physical interpretation of Z is the stored energy of cold work per unit volume. Although the process of cold working is accompanied by work hardening, that is an increase in resistance to further deformation, the stored energy of cold work is the change in internal energy arising from plastic deformation and as such it is unlikely that this quantity is synonymous with the strain hardening parameter. This is because phenomena other than hardening may also contribute to the stored energy of cold work. On a microphysical basis, Z is associated with dislocation arrangement. The units of Z are the same as the units of stress.

The plastic strain (P) is the deformation remaining after the material has been unloaded to the stress-free configuration. As such, it is usually referred to as the "permanent set". According to Kratochvil [2.35], the plastic strain describes a shape change of the material element after a loading process by sufficiently fast unloading. A microphenomenological definition of plastic strain is given by Bamman and Aifantis [2.36] as the strain induced by dislocation motion.

Some authors, for example Lehmann [2.24, 2.37], Anand [2.38], Hart [2.39], and Riff et al. [2.29] are of the opinion that the plastic strain (being a path-dependent variable) is not suitable for use as an ISV for plasticity studies. However, a large number of workers have used the plastic strain as an ISV. Notable are the works of Perzyna [2.20, 2.21], Kratochvil and Dillon [2.18, 2.19], Kratochvil [2.35], Green and Naghdi [2.40], Lubliner [2.41], and Kluitenberg [2.42].

The author is not in agreement with the arguments of those who

belong to the school of thought that considers the plastic strain to be inadmissible as an ISV. Since those that use the plastic strain as an ISV do not usually give reasons to justify its use, the controversial issue is elaborated upon in this thesis.

Lehmann [2.24, 2.37] is one of the major proponents of the point of view that the plastic strain is in general not suitable as an ISV. According to Lehmann, "Dislocations which have completely passed the crystal produce plastic strains but no changes of internal state". This statement is equivalent to Anand's statement [2.38] which says that the surroundings of atoms before and after plastic straining are "essentially undistinguishable". The validity of this statement depends, of course, on the definition of "internal state". The internal state during a process of plastic deformation should not be taken to be synonymous with the "state of hardening". In other words, there might be plastic phenomena other than hardening which contribute to the thermodynamic state of plastic deformation. During an actual motion of a dislocation through a crystal, energy must be conserved just as in any physical process. Any decrease in the energy of the external agents caused by energy dissipation occurring as a result of dislocation interactions and resistance to dislocation motion must be balanced by the corresponding increase in the internal energy of the medium. Also, a small but finite stress is required to cause the motion of dislocations through crystals (at least crystals with defects). Thus, one cannot expect the totality of the state of a crystal that has just experienced the passage of a dislocation to be the same as the state before the passage. What is needed, perhaps, is the capability of being able to detect that change.

There are also claims that: "Most different states of hardening can belong to the same plastic strains (at the same stresses and the same temperatures)". First, it is to be noted that this statement is based on the implied assumption that the state of hardening alone uniquely and completely defines the state of the material. It has been remarked in the preceding paragraph that there is no justification to presume that the state of hardening is all that is required to characterize the plastic deformation state of a body. Even if it were so, the question of whether enough hardening state variables have been employed to describe the state of hardening remains an open one. If more hardening variables were introduced, it might be possible to notice a change of state that went undetected with the insufficient number of state variables.

For a clearer insight into this discussion, consider the following logic. Suppose, for instance, there exists a thermodynamic representation of the form

$$\sigma = \sigma(\epsilon, \theta, Z, P), \quad (2.1)$$

for the stress functional. For a well-behaved function σ , equation (2.1) may be expressed as

$$Z = Z(\epsilon, \theta, \sigma, P). \quad (2.2)$$

According to the statement quoted in the last paragraph, it is possible to find a situation where there is a Z_1 given by

$$Z_1 = Z(\epsilon_1, \theta_1, \sigma_1, P_1), \quad (2.3a)$$

and there also exists a Z_2 , different from Z_1 , such that

$$Z_2 = Z(\epsilon_1, \theta_1, \sigma_1, P_1). \quad (2.3b)$$

Obviously, this situation is undesirable because it is intended that the state variables should uniquely define all the state functions - the

dependent constitutive variables (or the response functions). However, the problem might not be with the plastic strain. It might be that more internal state variables are needed to describe the state of hardening or the state in general. If new hardening state variables X and Y , for instance, are introduced, we have, instead of (2.1),

$$\sigma = \sigma^*(\epsilon, \theta, X, Y, Z, P). \quad (2.4)$$

Thus, if

$$\sigma_1 = \sigma^*(\epsilon_1, \theta_1, X_1, Y_1, Z_1, P_1), \quad (2.5a)$$

it is totally acceptable to have a situation where

$$\sigma_1 = \sigma^*(\epsilon_1, \theta_1, X_2, Y_2, Z_2, P_1), \quad (2.5b)$$

since each element of the set of hardening variables: $\{X_2, Y_2, Z_2\}$ may adjust itself in such a way that the set has the same effect in the function σ^* as the set $\{X_1, Y_1, Z_1\}$. In practice, for example, the additional hardening variables X and Y may model, among other things, cyclic hardening, or, for that matter, other hardening phenomena that may yet be beyond the realm of present understanding. Therefore, (2.5a) and (2.5b) do not suggest a lack of uniqueness.

Furthermore, the value σ_s of the stress at a given state S is not what describes the state of the deformation process. The values of the other response functions are also needed as will become evident in the next section. For example, corresponding to (2.5a) and (2.5b) above, it may turn out that the value of the free energy associated with the first state of hardening $\{X_1, Y_1, Z_1\}$:

$$\psi_1 = \psi^*(\epsilon_1, \theta_1, X_1, Y_1, Z_1, P_1) \quad (2.6a)$$

differs from the value of ψ corresponding to the second state of hardening $\{X_2, Y_2, Z_2\}$. In other words, there may exist a ψ_2 , different

from ψ_1 , such that

$$\psi_2 = \psi^*(\epsilon_1, \theta_1, X_2, Y_2, Z_2, P_1) \quad (2.6b)$$

Also, it is easy to see that there is no apparent lack of uniqueness if more state variables that describe plastic phenomena other than hardening are included.

There are also arguments that the plastic strain does not uniquely describe the state. As noted above, no single state variable is expected to uniquely describe the state; indeed such a situation is impossible for a dissipative material - not even for a thermoelastic process. Such a "luxury" of simplicity is the sole possession of elastic materials undergoing purely mechanical processes, in which case the strain, and the strain alone, uniquely characterizes the state. What is required by the property of uniqueness is the capability of being able to deduce unique values of the response functions from a given set of the state variables used for the process description.

We find it reasonable to include the plastic strain as a state variable because we believe it affects the inelastic portion of the internal energy. This view is supported by the experimentally [2.43] and analytically [2.44] observed dependence of the stored energy of cold work on the "extent of deformation" - the plastic strain or the total strain is usually taken as a measure of the extent of deformation.

Although P is a path-dependent variable, it should be realized that what is being modelled is the deformation process. Thus, what is of interest is the thermodynamic state of the deformation process and not the "internal state" of the material *per se*. Indeed the complete elimination of path dependence requires an infinite set of ISVs - a requirement whose impracticality has been discussed earlier on.

Lastly, it is known that dislocation motion (which induces plastic strain) causes the external shape of a body to change and so is associated with shape-memory effects, see, for instance, Kluitenberg [2.42]. Thus, the plastic strain may be useful in describing the part of the deformation history associated with the change in shape of the body.

2.3 Thermodynamic Formalism

With the introduction of the two ISVs in the last section, the independent constitutive variables may be written in two sets as follows:

$$(i) \quad \Lambda = \{\epsilon, T, g\}. \quad (2.7a)$$

$$(ii) \quad \Gamma = \{Z, P\}. \quad (2.7b)$$

In (i), ϵ is the total strain, T is the absolute temperature and g is the temperature gradient, that is,

$$g = \frac{\partial T}{\partial X}. \quad (2.8)$$

Set (i) is the set of observable thermomechanical variables which describe the thermomechanical configuration of the body. Set (ii) describes the method of preparation of the observed thermomechanical configuration. Whereas the set Λ is sufficient to completely characterize the state of a conservative (or reversible) deformation process, a combination of the two sets (Λ and Γ) is required for the description of the state of a nonconservative (or irreversible) deformation process.

Thus, the set of the independent constitutive variables is the union of the two sets Λ and Γ which we may denote by Ω :

$$\Omega = \Lambda \cup \Gamma = \{\epsilon, T, g, Z, P\}. \quad (2.9)$$

According to the constitutive axiom of causality [2.45], therefore, the dependent constitutive variables or the response functionals must be the set Π given by:

$$\Pi = \{\psi, \sigma, \eta, q\}, \quad (2.10)$$

where ψ is the Helmholtz free energy per unit volume, σ is the stress, η is the entropy per unit volume, and q is the heat flux considered positive when directed outward from the body. The Helmholtz free energy (which we find more convenient to use than the internal energy or any of its other Legendre transforms) is related to the internal energy, e , through the equation:

$$\psi = e - T\eta \quad (2.11)$$

With these variables, we consider the process of wave propagation in inelastic solids (or indeed any inelastic deformation process) as a thermodynamic process (TP) consisting of all the independent and the dependent constitutive variables, that is

$$\text{TP: } \{\Lambda, \Gamma, \Pi\}, \quad (2.12a)$$

or

$$\text{TP: } \{\Omega, \Pi\}. \quad (2.12b)$$

The constitutive response functionals, Π , are now assumed to depend on the independent constitutive variables, Ω , in the form:

$$\psi = \hat{\psi}(\epsilon, T, g, Z, P), \quad (2.13a)$$

$$\sigma = \hat{\sigma}(\epsilon, T, g, Z, P), \quad (2.13b)$$

$$\eta = \hat{\eta}(\epsilon, T, g, Z, P), \quad (2.13c)$$

$$q = \hat{q}(\epsilon, T, g, Z, P), \quad (2.13d)$$

$$\dot{Z} = \hat{F}(\epsilon, T, g, Z, P), \quad (2.13e)$$

$$\dot{P} = \hat{G}(\epsilon, T, g, Z, P), \quad (2.13f)$$

where overdots denote differentiation with respect to time. It is to be

noted that the quantities $\hat{\psi}$, $\hat{\sigma}$, $\hat{\eta}$, $\hat{q}$, $\hat{F}$ and $\hat{G}$ are referred to as functionals in the sense that they are functions of quantities that are themselves functions of other quantities. For example,

$$\psi = \hat{\psi}(\epsilon(X,t), T(X,t), g(X,t), Z(X,t), P(X,t)). \quad (2.14)$$

where X denotes position and t denotes time. Equations (2.13e) and (2.13f) describe the change of the internal state variables with time and are referred to as EVOLUTION EQUATIONS for the ISVs. Mathematically, the equations are required in complementing the balance laws of continuum mechanics and the 'usual' constitutive relations in the complete formulation of a well-posed, determinate initial-boundary-value-problem.

The representation (2.13) is assumed to be unique for the deformation process at any point in space and time during the process in the sense that the specification of the values of the independent constitutive variables uniquely specifies the values of the dependent constitutive variables.

The assumed constitutive relations satisfy the principle of equipresence and the principle of material objectivity [2.45].

It will now be required that the assumed relations be admissible - that is they must be consistent with the basic principles of continuum mechanics which implies consistency with the principles of conservation of mass, balance of linear momentum, balance of moment of momentum, conservation of energy, and the second law of thermodynamics.

For thermomechanical processes, the law of conservation of energy, otherwise referred to as the first law of thermodynamics, is given by:

$$\frac{\partial \psi}{\partial t} + \eta \frac{\partial T}{\partial t} + T \frac{\partial \eta}{\partial t} = \sigma \frac{\partial \epsilon}{\partial t} + \frac{\partial q}{\partial x} + \gamma, \quad (2.15)$$

where γ is the heat generation per unit volume. There is as yet no consensus on the mathematical representation of the Second Law but the Clausius-Duhem inequality is accepted as a valid statement in this development, namely:

$$T \frac{\partial \eta}{\partial t} \geq \gamma + \frac{\partial q}{\partial x} - \frac{q}{T} g. \quad (2.16)$$

The requirement of the axiom of admissibility will now be invoked. First, equation (2.15) is combined with the inequality (2.16) to obtain:

$$\dot{\psi} + \eta \dot{T} - \sigma \dot{\epsilon} - \frac{q}{T} g \leq 0. \quad (2.17)$$

Now, from equation (2.13a), if the response functionals are assumed to be sufficiently smooth, then

$$\dot{\psi} = \frac{\partial \hat{\psi}}{\partial \epsilon} \dot{\epsilon} + \frac{\partial \hat{\psi}}{\partial T} \dot{T} + \frac{\partial \hat{\psi}}{\partial g} \dot{g} + \frac{\partial \hat{\psi}}{\partial Z} \dot{Z} + \frac{\partial \hat{\psi}}{\partial P} \dot{P}. \quad (2.18)$$

Substituting equation (2.18) into (2.17) gives.

$$\left\{ \frac{\partial \hat{\psi}}{\partial \epsilon} - \sigma \right\} \dot{\epsilon} + \left\{ \frac{\partial \hat{\psi}}{\partial T} + \eta \right\} \dot{T} + \frac{\partial \hat{\psi}}{\partial g} \dot{g} + \frac{\partial \hat{\psi}}{\partial Z} \dot{Z} + \frac{\partial \hat{\psi}}{\partial P} \dot{P} - \frac{q}{T} g \leq 0. \quad (2.19)$$

Since the quantities $\dot{\epsilon}$, $\dot{T}$, and $\dot{g}$ can be varied independently for any thermodynamic process, the inequality (2.19) is linear in $\dot{\epsilon}$, $\dot{T}$, and $\dot{g}$. Hence it can be satisfied if and only if:

$$\sigma = \frac{\partial \hat{\psi}}{\partial \epsilon}, \quad (2.20a)$$

$$\eta = \frac{-\partial \hat{\psi}}{\partial T}, \quad (2.20b)$$

$$\frac{\partial \hat{\psi}}{\partial g} = 0, \quad (2.20c)$$

and

$$\frac{\partial \hat{\psi}}{\partial Z} \dot{Z} + \frac{\partial \hat{\psi}}{\partial P} \dot{P} - \frac{q}{T} g \leq 0. \quad (2.20d)$$

The relations (2.20a) - (2.20d) constitute the restrictions imposed on the constitutive assumptions by the first and second laws of thermodynamics. We find that the free energy functional is, as usual, a potential from which the stress and entropy functionals are to be derived. We also find that the free energy functional does not depend on the temperature gradient. The inequality (2.20d) is the reduced form of the Clausium-Duhem inequality and is the new form of the dissipation inequality.. It is not surprising to observe that the entropy production arises from strain hardening, plastic straining, and heat conduction which are the three sources of irreversibilities in our model.

Note that the inequality (2.20d) is not linear in $\dot{Z}$ and $\dot{P}$ and these quantities cannot be arbitrarily assigned due to the connection provided by the evolution equations (2.13e) and (2.13f). This implies that the rate of strain hardening depends on the rate of plastic straining. This thermodynamic deduction is consistent with the observed physical behavior of the process of plastic deformation. Therefore, $\partial \hat{\psi} / \partial Z$ and $\partial \hat{\psi} / \partial P$ do not vanish and so the free energy does depend on both Z and P . Again, dependence of ψ on Z and P have firm experimental foundations.

A reformulation of the constitutive relations based on the above thermodynamic deductions will be:

$$\psi = \hat{\psi}(\epsilon, T, Z, P), \quad (2.21a)$$

$$\sigma = \frac{\partial \hat{\psi}}{\partial \epsilon}, \quad (2.21b)$$

$$\eta = - \frac{\partial \hat{\psi}}{\partial T}, \quad (2.21c)$$

$$q = \hat{q}(\epsilon, T, g, Z, P), \quad (2.21d)$$

$$\dot{Z} = \hat{F}(\epsilon, T, g, Z, P), \quad (2.21e)$$

$$\dot{P} = \hat{G}(\epsilon, T, g, Z, P), \quad (2.21f)$$

$$\frac{\partial \hat{\psi}}{\partial Z} \dot{Z} + \frac{\partial \hat{\psi}}{\partial P} \dot{P} - \frac{q}{T} g \leq 0. \quad (2.21g)$$

For convenience, the temperature difference, θ , defined as

$$\theta = T - T_R, \quad (2.22)$$

is introduced, where T_R is the absolute temperature at a reference state, R. With this, the relations (2.21) may be expressed in the form

$$\psi = \tilde{\psi}(\epsilon, \theta, Z, P), \quad (2.23a)$$

$$\sigma = \frac{\partial \tilde{\psi}}{\partial \epsilon}, \quad (2.23b)$$

$$\eta = \frac{-\partial \tilde{\psi}}{\partial \theta}, \quad (2.23c)$$

$$q = \tilde{q}(\epsilon, \theta, g, Z, P), \quad (2.23d)$$

$$\dot{Z} = \tilde{F}(\epsilon, \theta, g, Z, P), \quad (2.23e)$$

$$\dot{P} = \tilde{G}(\epsilon, \theta, g, Z, P), \quad (2.23f)$$

$$\frac{\partial \tilde{\psi}}{\partial Z} \dot{Z} + \frac{\partial \tilde{\psi}}{\partial P} \dot{P} - \frac{q}{(\theta + T_R)} g \leq 0, \quad (2.23g)$$

$$\text{where } g = \frac{\partial \theta}{\partial X}. \quad (2.23h)$$

In the classical theory of irreversible thermodynamics, the quantities $\frac{\partial \tilde{\psi}}{\partial Z}$, $\frac{\partial \tilde{\psi}}{\partial P}$, and $(-\frac{g}{\theta + T_R})$ would be looked upon as thermodynamic forces or affinities while the conjugate set $\dot{Z}$, $\dot{P}$, and q would be the corresponding thermodynamic fluxes. One would then set up linear constitutive equations between any one of the forces and all of the fluxes and invoke Onsager's symmetry principle to reduce the number of constitutive coefficients. This procedure is, however, not applicable to plastic deformation because of its highly irreversible nature.

Thus, the restrictions expressed in (2.23) are the extent to which one can go via thermodynamic arguments concerning the nature of the constitutive equations. Unfortunately, however, the representation given by (2.23) is far from being complete because the constitutive response functionals involved are still unknown. Although such relations may be used, for example, in qualitative studies of wave propagation processes at the wave fronts using the theory of propagating singular surfaces [2.46], explicit relations for the constitutive response functionals involved are required for a detailed quantitative analysis of the wave propagation process in the entire domain of interest. Therefore, explicit representations of the response functionals involved in the relations (2.23) must be sought. This is the subject of consideration in the next chapter.

CHAPTER 3

CHARACTERIZATION OF THE CONSTITUTIVE RESPONSE FUNCTIONALS

3.1 Explicit Expressions for the Helmholtz

Free Energy, Stress, and Entropy Functionals

The Helmholtz free energy functional or, equivalently, any of its Legendre transforms, is the most important constitutive response functional in thermodynamics-based material modelling. This is because it usually serves as a thermodynamic potential from which two other response functionals, namely, the stress and the entropy, may be derived. The free energy thus has a very important role to play in the characterization of material behavior and indeed the formulation of any initial-boundary-value-problem of continuum mechanics that involves the law of conservation of energy.

It appears that the important role of the free energy has not been accorded due recognition by inelastic deformation studies (static, quasistatic, and dynamic) because of the following. Most studies in plasticity and viscoplasticity employ empirically conjectured or experimentally determined stress-strain relations which fall outside the umbrella of a general thermodynamic framework. In such situations, for isothermal cases, the law of conservation of energy is usually ignored (since the system of equations describing the boundary-value-problem appears to be mathematically complete), or assumed to be identically satisfied as in the theory of elasticity. Moreover, in certain cases, some *ad hoc* assumptions concerning the balance of work and energy are employed at the outset or 'afterthought' energy balance checks are made at the end of computations! The inclusion of temperature brings the law

of conservation of energy well into focus and furthermore, the recognition of the physical phenomenon of the stored inelastic energy gives a very distinctive and important role to the law of conservation of energy.

Thus, the application of the law of conservation of energy, equation (2.15), requires a knowledge of the free energy, ψ , and the entropy, η , which is especially significant for the highly irreversible process of plastic flow. It is clear, therefore, that if we intend to properly analyze an inelastic deformation process, the constitutive equations are not synonymous with stress-strain relations. Indeed, the results of the thermodynamic analysis in the preceding chapter show that, for thermodynamic consistency, the relations for σ and η cannot be arbitrarily assigned. The best way to guarantee this consistency is to find a suitable expression for the free energy which has the role of a 'parent' potential.

A lot of researchers in thermoelastic constitutive modelling via thermodynamics assume that the free energy functional is of the same form as its thermoelastic counterpart. This assumption is, however, not consistent with available experimental results which indicate that a portion of the plastic mechanical work is irrecoverably stored in the material during inelastic deformation. A large number of experiments in this connection were reviewed by Titchener and Bever [3.1] and Bever et al. [3.2].

Only a few workers have explicitly incorporated an inelastic portion in their expression for the free energy function of an inelastic material.

Kratochvil and Dillon [3.3] proposed the following form for an

elastic-plastic material:

$$\psi = \mu(\epsilon^e)^2 + \nu_1 |\alpha^{(1)}| + \nu_2 \alpha^{(2)} - CT(\ln T - 1), \quad (3.1)$$

where ϵ^e is the elastic strain, T is the absolute temperature, $\alpha^{(1)}$ is an ISV representing the dislocation density, and $\alpha^{(2)}$ is the other ISV designating the density of more complicated dislocation arrangements known as tangelings. The quantities μ , ν_1 , ν_2 , and C are material constants assumed to be positive. The same workers [3.4] also proposed a similar functional representation for the free energy of an elastic-viscoplastic material, namely:

$$\psi = \frac{1}{2} \mu_o \sigma^2 + \nu \alpha - kT \left(\ln \frac{T}{T_R} - 1 \right), \quad (3.2)$$

where σ is the stress, T is the absolute temperature, and α (which is a scalar parameter that characterizes the defect arrangement) is the number of dislocations. Again, μ_o , ν , and k are assumed to be positive material constants. It can easily be seen from equations (3.1) and (3.2) that the expressions are linear in the ISVs and do not include a thermal expansion term. Furthermore, numerical values of the material constants involved were not given for any material.

Kim and Oden [3.5] proposed a temperature-independent expression in terms of the plastic work:

$$\psi = \frac{1}{2} [\lambda (\text{tr } \underline{\underline{E}})^2 + 2\mu \text{tr}(\underline{\underline{E}}^2)] - Z_1 W_p - \frac{1}{m} (Z_1 - Z_o) \exp(-mW_p). \quad (3.3)$$

In this expression, $\underline{\underline{E}}$ is the elastic strain tensor, W_p is the plastic work and it is the single internal state variable introduced to characterize isotropic hardening of the material. The quantities λ and μ are the well-known Lamé constants of classical elasticity. There is a hardness variable, Z , which is conjugate to the internal state variable,

W_p , and related to it through the equation:

$$Z = -\frac{\partial \psi}{\partial W_p} = Z_1 + (Z_0 - Z_1) \exp(-mW_p), \quad (3.4)$$

where Z_0 , Z_1 , and m are given material constants. Obviously the expression (3.3) is restricted to isothermal applications, with the attendant implications discussed in Chapter 1.

The free energy expression utilized by Besdo [3.6] is of the form:

$$\begin{aligned} \psi = & \frac{G}{4} \{ \tilde{C} \cdot \tilde{C} \cdot [\hat{B} \cdot \hat{C} \cdot \hat{B}] - 2\tilde{C} \cdot \tilde{B} + 3 + \frac{\nu}{1-2\nu} [\tilde{C} \cdot \tilde{B} - 3]^2 \} + \\ & + \sum_{\alpha, \beta}^{\alpha\beta} K^{\alpha} U \cdot [\hat{B} \cdot \hat{U} \cdot \hat{B}] + A[\theta - \theta_0] [\tilde{C} \cdot \tilde{B} - 3] + \psi_0(\theta). \end{aligned} \quad (3.5)$$

This includes thermoelasticity and purely thermal effects. However, the inelastic term, namely, $\sum_{\alpha, \beta}^{\alpha\beta} K^{\alpha} U \cdot [\hat{B} \cdot \hat{U} \cdot \hat{B}]$, is temperature-independent and no numerical values of the 'inelastic' material parameters $^{\alpha\beta}K$ were given for any material.

Benallal and Marquis [3.7] had an expression of the form:

$$\psi = \frac{1}{2} A_{ijkl} \epsilon_{ij}^e \epsilon_{kl}^e + \frac{1}{2} c_{ij} \epsilon_{ij}^e + Q[P + \frac{1}{\gamma} e^{-\gamma P}], \quad (3.6)$$

in which the first term represents the elastic strain energy, the second term is the energy density related to the kinematic hardening, and the last term is the energy density associated with isotropic hardening. This expression is restricted to isothermal applications. The anisothermal elasto-viscoplastic model of Benallal and Cheikh [3.8] is given by:

$$\psi = m(T) + \tilde{M}(T) : \tilde{\epsilon}^e + \frac{1}{2} \tilde{C}(T) : \tilde{\epsilon}^e : \tilde{\epsilon}^e + h_1(\alpha) + H(T, p), \quad (3.7a)$$

where

$$h_1(\alpha) = \frac{2}{3} C \cdot a \alpha : \alpha , \quad (3.7b)$$

and

$$H(T,p) = [a_1(1-\exp(-a_2T)) + a_3] \cdot [p + \frac{1}{\gamma} \exp(-\gamma p)], \quad (3.7c)$$

where the tensor α and the scalar p are the ISVs used to describe kinematic and isotropic hardening, respectively. The procedure for identifying the inelastic material properties was described and typical material constants for INCONEL 718 super-alloy were given.

A feature common to all the above expressions is the neglect of the coupling terms between (thermo)elastic and (thermo)inelastic deformation variables. The implication of this is the assumption that the stress-strain (or stress-strain-temperature) relations are the same as for (thermo)elastic materials which is inconsistent with the idea of a dissipative part of the stress. We are hence motivated in this study to seek to remedy this and the other shortcomings highlighted above. It is also of interest to give a firm physical basis for the determination of the material properties encountered.

First, a reference equilibrium state R is defined as:

$$R = \{\epsilon = \epsilon_R, Z = Z_R, P = P_R; \theta\}. \quad (3.8)$$

The function ψ is now to be expressed as a Taylor series expansion in terms of its thermodynamic arguments: ϵ , θ , Z , and P about this reference state of deformation. It is preferred, for physical reasons that will become clearer shortly, that the function ψ be expanded in terms of ϵ , Z , and P while keeping θ as a parameter that may appear as coefficients of the expansion terms. Of course, this mode of expansion is equivalent to the expansion of ψ in terms of all its arguments ϵ , θ , Z , and P . Thus, ψ is taken to be of the form:

$$\begin{aligned}\psi = \phi(\theta) + \bar{A}_1(\theta)\epsilon + \bar{B}_1(\theta)\epsilon^2 + \bar{A}_2(\theta)Z + \bar{A}_3(\theta)P + \bar{B}_2(\theta)Z^2 \\ + \bar{B}_3(\theta)P^2 + \bar{B}_4(\theta)\epsilon Z + \bar{B}_5(\theta)\epsilon P + \bar{B}_6(\theta)ZP.\end{aligned}\quad (3.9)$$

The quantities $\bar{A}_1(\theta)$, $\bar{B}_1(\theta)$, $\bar{A}_2(\theta)$, $\bar{A}_3(\theta)$, $\bar{B}_2(\theta)$, $\bar{B}_3(\theta)$, $\bar{B}_4(\theta)$, $\bar{B}_5(\theta)$, and $\bar{B}_6(\theta)$ are now identified as temperature-dependent material properties. Note that this nonlinear, non-isothermal representation of the free energy functional reduces to the free energy expression for thermoelastic materials in the absence of plastic deformation, allows for thermal expansion and purely thermal effects, incorporates the effect of strain hardening and permanent deformation, and includes a coupling of thermal, elastic and inelastic deformation variables. All these attributes are in conformity with the reality of the physical phenomena being modelled.

The additive decomposition of the total strain (ϵ) into its thermoelastic (E) and thermoinelastic (P) parts in the form:

$$\epsilon = E + P, \quad (3.10)$$

is now introduced. This decomposition is generally valid for infinitesimal deformations. With this, equation (3.9) takes the new form:

$$\begin{aligned}\psi = \phi(\theta) + A_1(\theta)E + B_1(\theta)E^2 + A_2(\theta)Z + A_3(\theta)P + B_2(\theta)Z^2 \\ + B_3(\theta)P^2 + B_4(\theta)EZ + B_5(\theta)EP + B_6(\theta)ZP.\end{aligned}\quad (3.11)$$

This expression for ψ may now be partitioned into its two constituent parts:

$$\psi = \psi^E + \psi^I, \quad (3.12a)$$

where

$$\psi^E = \phi(\theta) + A_1(\theta)E + B_1(\theta)E^2, \quad (3.12b)$$

and

$$\begin{aligned}\psi^I = & A_2(\theta)Z + A_3(\theta)P + B_2(\theta)Z^2 + B_3(\theta)P^2 + B_4(\theta)EZ + B_5(\theta)EP \\ & + B_6(\theta)ZP.\end{aligned}\quad (3.12c)$$

The quantity ψ^E is the thermoelastic portion of the free energy functional while ψ^I is the thermoinelastic portion. Now, ψ^E is either known from the classical theory of thermoelasticity, or can be found from a knowledge of the specific heat capacity at a constant state of deformation (C_D) and the thermoelastic stress-strain-temperature relation. However, ψ^I is unknown because the thermoinelastic material properties $A_2(\theta)$, $A_3(\theta)$, $B_2(\theta)$, $B_3(\theta)$, $B_4(\theta)$, $B_5(\theta)$, and $B_6(\theta)$ in (3.12c) are yet unknown.

With the decomposition (3.10), the results of Chapter 2 may be more conveniently expressed in terms of the thermoelastic strain rather than the total strain in the form:

$$\psi = \psi(E, \theta, Z, P), \quad (3.13a)$$

$$\sigma = \frac{\partial \psi}{\partial E}, \quad (3.13b)$$

$$\eta = -\frac{\partial \psi}{\partial \theta}, \quad (3.13c)$$

$$q = q(E, \theta, g, Z, P), \quad (3.13d)$$

$$\dot{Z} = F(E, \theta, g, Z, P), \quad (3.13e)$$

$$\dot{P} = G(E, \theta, g, Z, P), \quad (3.13f)$$

$$\frac{\partial \psi}{\partial Z} \dot{Z} + \frac{\partial \psi}{\partial P} \dot{P} - \frac{q}{(\theta + T_R)} g \leq 0. \quad (3.13g)$$

With the explicit expression for ψ given in equation (3.11), it is now possible to determine explicit expressions for the stress and

entropy functionals. From equations (3.13b) and (3.11), it follows that the stress is given by:

$$\sigma = A_1(\theta) + 2B_1(\theta)E + B_4(\theta)Z + B_5(\theta)P. \quad (3.14)$$

It can be seen that the stress has two parts: thermoelastic and thermoinelastic, or, alternatively, quasiconservative and dissipative. Thus,

$$\sigma = \sigma^C + \sigma^D, \quad (3.15a)$$

where

$$\sigma^C = A_1(\theta) + 2B_1(\theta)E, \quad (3.15b)$$

is the quasiconservative stress, and

$$\sigma^D = B_4(\theta)Z + B_5(\theta)P, \quad (3.15c)$$

is the dissipative stress. Thus, from our representation of ψ , it has been possible to explicitly determine the dissipative stress without the need of postulating a separate dissipation (or plastic) potential function, as in the case of Ziegler and Wehrli [3.9], for example. The portion σ^D ensures that the stress relation for thermoinelastic deformation differs from its thermoelastic counterpart.

Similarly, applying the result (3.13c) to the representation (3.11) yields the explicit expression for the entropy functional in the form:

$$\begin{aligned} \eta = - [\phi'(\theta) + A_1'(\theta)E + B_1'(\theta)E^2 + A_2'(\theta)Z + A_3'(\theta)P + B_2'(\theta)Z^2 \\ + B_3'(\theta)P^2 + B_4'(\theta)EZ + B_5'(\theta)EP + B_6'(\theta)ZP]. \end{aligned} \quad (3.16)$$

Again, it is seen that the entropy consists of contributions from thermoelastic (η^E) and thermoinelastic (η^I) deformations, that is,

$$\eta = \eta^E + \eta^I, \quad (3.17a)$$

where

$$\eta^E = -[\phi'(\theta) + A_1'(\theta)E + B_1'(\theta)E^2], \quad (3.17b)$$

and

$$\begin{aligned} \eta^I = & -[A_2'(\theta)Z + A_3'(\theta)P + B_2'(\theta)Z^2 + B_3'(\theta)P^2 + B_4'(\theta)EZ \\ & + B_5'(\theta)EP + B_6'(\theta)ZP]. \end{aligned} \quad (3.17c)$$

It is easy to see that the expression (3.17b) represents the usual entropy production in thermoelasticity while (3.17c) is considered to be the entropy due to irreversibility of plastic deformation. It may now be appreciated that the neglect of η^I is tantamount to assuming that the process of plastic deformation is reversible!

One of the important attributes of the theory of thermodynamics with internal state variables is the ability to characterize nonequilibrium states using thermodynamic state variables even if those states are considered to be constrained equilibrium states. The beauty of the above expressions for ψ , σ , η lies in the fact that those quantities can be uniquely computed whenever the values of E , θ , Z , and P are given at a particular point provided the material properties are known. Thus, the explicit relations are constitutive state equations in the same sense that is used in the kinetic theory of gases, for instance. It should be emphasized that the desire to be able to simply express constitutive response functionals in terms of some independent constitutive variables as is done for non-dissipative materials is the main motivation behind research efforts directed towards the application of internal state variables to dissipative processes.

3.2 Determination of the Thermoelastic Material Properties

The most challenging endeavor in constitutive modelling is the determination of the associated material properties especially if they are physically motivated. The methodology by which the thermoelastic material properties appearing in the expression for ψ in the preceding section are determined is now presented.

Materials scientists define the stored (or latent) energy of cold work as the portion of the plastic work that is irrecoverably stored in the material during deformation thereby raising its internal energy. Micromechanically, it is associated with the energy of residual stresses in the material due to crystal defects. In addition to the formal experimental evidence first provided by Taylor and Quinney [3.10], Titchener and Bever [3.1] and Bever et al. [3.2] carried out excellent comprehensive reviews of experiments that have been performed to determine the stored energy of cold work, E_s . Most of the experiments reported for various metals and metallic alloys [3.1, 3.2] indicated that the stored energy is proportional to the square of the flow stress, or, equivalently, that the rate of change of the stored energy with respect to the total expended energy is proportional to the rate of change of the stress with the strain in the plastic region. Since E_s represents the irrecoverable portion of the internal energy (which is designated e_{IRR} here), the experimental findings may be mathematically expressed as

$$e_{IRR} = K\sigma^2, \quad (3.18)$$

where K is the experimentally determined constant of proportionality. If an allowance is made for a small portion of the elastic energy to be irrecoverably stored, then

$$e_{IRR} = e_{IRR}^E + e_{IRR}^I, \quad (3.19)$$

where e_{IRR}^E is a small portion of the elastic strain energy, e^E , and e_{IRR}^I is the irrecoverable portion of the inelastic stored energy.

From the relation between ψ and e , namely:

$$\psi = e - (\theta + T_R)\eta, \quad (3.20)$$

it follows that ψ can be similarly split as:

$$\psi = \psi_R^E + \psi_{IRR}^E + \psi_R^I + \psi_{IRR}^I, \quad (3.21)$$

where the quantities are defined as follows:

$$\begin{aligned} \psi_R^E &= \text{recoverable portion of the} \\ &\quad \text{thermoelastic free energy,} \end{aligned} \quad (3.22a)$$

$$\begin{aligned} \psi_{IRR}^E &= \text{irrecoverable portion of the} \\ &\quad \text{thermoelastic free energy,} \end{aligned} \quad (3.22b)$$

$$\begin{aligned} \psi_R^I &= \text{recoverable portion of the} \\ &\quad \text{thermoinelastic free energy,} \end{aligned} \quad (3.22c)$$

$$\begin{aligned} \psi_{IRR}^I &= \text{irrecoverable portion of the} \\ &\quad \text{thermoinelastic free energy.} \end{aligned} \quad (3.22d)$$

It is known that no portion of the thermoinelastic free energy is recoverable, therefore,

$$\psi_R^I = 0, \quad (3.23a)$$

and so

$$\psi^I = \psi_{IRR}^I. \quad (3.23b)$$

Hence,

$$\psi = \psi_R^E + \psi_{IRR}^E + \psi_{IRR}^I. \quad (3.24)$$

Also, in practice, the amount of elastic energy stored is very small compared to either the total elastic energy or the total inelastic energy. Thus,

$$\frac{\psi_{IRR}^E}{\psi_R^E} < < 1, \quad (3.25a)$$

and

$$\frac{\psi_{IRR}^E}{\psi_{IRR}^I} < < 1. \quad (3.25b)$$

If the irrecoverable portion of ψ is denoted ψ_{IRR} , then, from (3.23b) and (3.24), it follows that

$$\psi_{IRR} = \psi_{IRR}^E + \psi_{IRR}^I. \quad (3.26)$$

Thus, in terms of the development here, the experimental findings expressed in equation (3.18) becomes

$$\psi_{IRR} + (\theta + T_R)\eta_{IRR} = K\sigma^2, \quad (3.27)$$

where

$$\eta_{IRR} = - \frac{\partial \psi_{IRR}}{\partial \theta}. \quad (3.28)$$

Because ψ is a function of $\{E, \theta, Z, P\}$, ψ_{IRR} is also a function of $\{E, \theta, Z, P\}$, and so is η_{IRR} . Therefore, the expression on the left hand side of equation (3.27) is a functional $\tilde{\Phi}_L$, say, of $\{E, \theta, Z, P\}$. Similarly, since $\sigma = \sigma(E, \theta, Z, P)$ as can be seen from equation (3.14), the right hand side of equation (3.27) is also a functional $\tilde{\Phi}_R$, say, of $\{E, \theta, Z, P\}$. Equation (3.27) may therefore be expressed as:

$$\tilde{\Phi}_L(E, \theta, Z, P) = \tilde{\Phi}_R(E, \theta, Z, P). \quad (3.29)$$

Since all the constitutive response functionals are assumed to be smooth functions of their thermodynamic arguments, the functions $\tilde{\Phi}_L$ and $\tilde{\Phi}_R$ must also be smooth functions of those arguments. Smoothness of the functionals $\tilde{\Phi}_L$ and $\tilde{\Phi}_R$ leads to the ordinary differential equations:

$$A_2 - (\theta + T_R)A_2' = 2KA_1B_4, \quad (3.30a)$$

$$A_3 - (\theta + T_R)A_3' = 2KA_1B_5, \quad (3.30b)$$

$$B_2 - (\theta + T_R)B_2' = KB_4^2, \quad (3.30c)$$

$$B_3 - (\theta + T_R)B_3' = KB_5^2, \quad (3.30d)$$

$$B_4 - (\theta + T_R)B_4' = 4KB_1B_4, \quad (3.30e)$$

$$B_5 - (\theta + T_R)B_5' = 4KB_1B_5, \quad (3.30f)$$

$$B_6 - (\theta + T_R)B_6' = 2KB_4B_5, \quad (3.30g)$$

where a prime denotes differentiation with respect to the differential temperature, θ . Equations (3.30) are obtained by differentiating $\tilde{\Phi}_L$ and $\tilde{\Phi}_R$ with respect to their arguments as many times as necessary in equation (3.29).

The solution of equations (3.30) requires a knowledge of the appropriate auxiliary conditions. These auxiliary conditions are indeed material constants at say the reference temperature T_R , and they must be found from experiments.

First, the possibility of determining these auxiliary conditions (or the material properties themselves) from experiments that are specifically designed for that purpose will be considered.

Recall that the explicit representation for the stress is:

$$\sigma = A_1(\theta) + 2B_1(\theta)E + B_4(\theta)Z + B_5(\theta)P. \quad (3.31)$$

It is easy to obtain from (3.31):

$$B_4(\theta) = \frac{\partial \sigma}{\partial Z}, \quad (3.32)$$

$$B_5(\theta) = \frac{\partial \sigma}{\partial P}, \quad (3.33)$$

$$2B_1(\theta) = \frac{\partial \sigma}{\partial E}. \quad (3.34)$$

In the sense that the quantity $2B_1(\theta)$ is the modulus of elasticity

(assuming elastic incompressibility), $B_4(\theta)$ may be regarded as a "HARDENING MODULUS", while $B_5(\theta)$ may be called a "PLASTIC MODULUS".

Thus, it seems that $B_4(\theta)$ may be found from experiments performed to see how the stress (σ) varies with the strain hardening parameter (Z) at constant strain (that is, constant E and P). Such experiments performed isothermally but at different temperatures would give $B_4(\theta)$ as shown in Figure 3.1. Similarly, $B_5(\theta)$ may be experimentally obtained by varying the stress and the plastic strain at constant E and Z for varying temperatures. This kind of experiment should provide data that would enable one to plot graphs like those shown in Figure 3.2. The hypothetical experiments just described have limited (if any) feasibility. It is difficult to physically measure the strain hardening parameter; there is currently no available means of quantifying the resistance to further plastic deformation. Also, there is no experimental procedure by which the plastic strain could be directly measured (without unloading) while keeping the elastic strain and the strain hardening parameter constant.

From the expression for the free energy functional, equation (3.11), it is observed that

$$\frac{\partial \psi}{\partial Z} = A_2(\theta) + 2B_2(\theta)Z + B_4(\theta)E + B_6(\theta)P, \quad (3.35)$$

$$\frac{\partial \psi}{\partial P} = A_3(\theta) + 2B_3(\theta)P + B_5(\theta)E + B_6(\theta)Z, \quad (3.36)$$

$$\frac{\partial}{\partial Z} \left(\frac{\partial \psi}{\partial Z} \right) = 2B_2(\theta), \quad (3.37)$$

$$\frac{\partial}{\partial P} \left(\frac{\partial \psi}{\partial P} \right) = 2B_3(\theta), \quad (3.38)$$

$$\frac{\partial}{\partial Z} \left(\frac{\partial \psi}{\partial P} \right) = B_6(\theta). \quad (3.39)$$

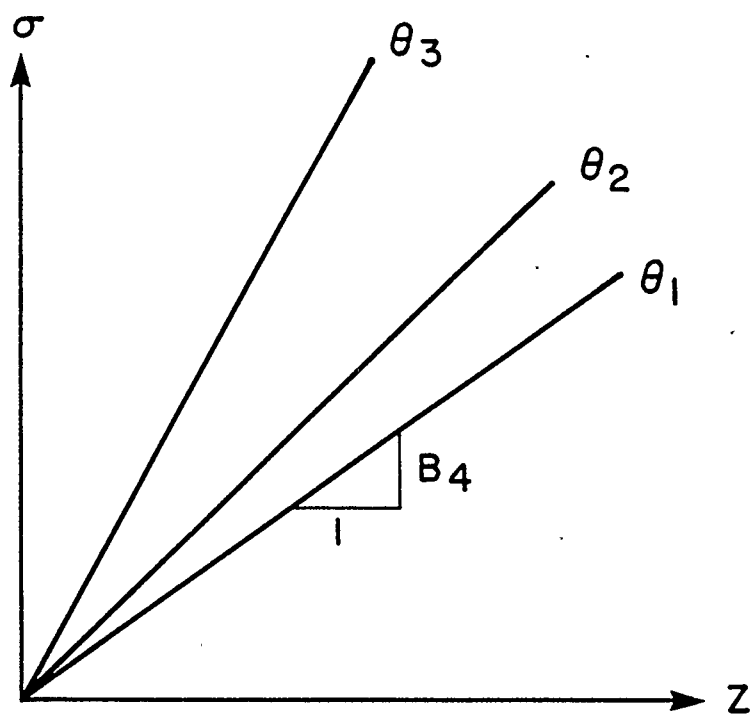


Figure 3.1 Hypothetical isothermal stress-hardening curves for various temperatures.

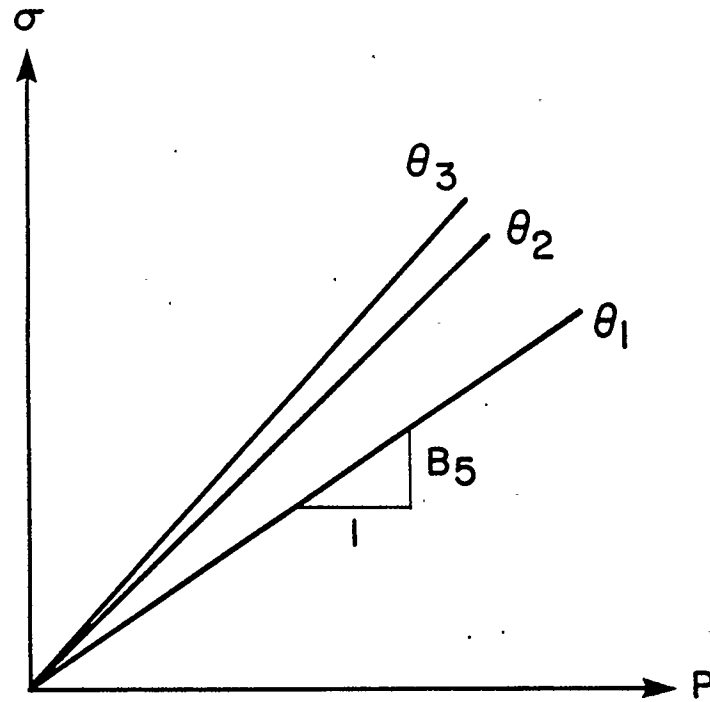


Figure 3.2 Hypothetical isothermal stress-plastic strain curves for various temperatures.

The quantities $A_2(\theta)$ and $A_3(\theta)$ may be looked upon as the values of $\partial\psi/\partial Z$ and $\partial\psi/\partial P$ respectively, at the reference state of deformation where $E = 0$, $Z = Z_R = Z_0$, and $P = 0$. However the physical meanings of $\partial\psi/\partial Z$ and $\partial\psi/\partial P$ are not known. One is therefore not in a position to think of hypothetical experimental programs by which $A_2(\theta)$, $A_3(\theta)$, $B_2(\theta)$, $B_3(\theta)$, and $B_6(\theta)$, or even their values at a given temperature, could be determined. There is no choice then other than seeking alternate procedures by which the auxiliary conditions can be determined.

Consider equation (3.30e) which is recalled here for easy reference:

$$B_4 - (\theta + T_R)B_4' = 4KB_1B_4. \quad (3.40a)$$

Let the value of $B_4(\theta)$ at the reference temperature, T_R , be B_{4R} , that is,

$$B_4(\theta) \Big|_{\theta=0} = B_{4R}. \quad (3.40b)$$

Then the solution of equations (3.40) is given by

$$B_4(\theta) = B_{4R} \left(1 + \frac{\theta}{T_R}\right)^{1-\lambda_1-\lambda_2 T_R} \exp(\lambda_2 \theta), \quad (3.41)$$

where

$$\lambda_1 = 4KB_{11}, \quad (3.42a)$$

and

$$\lambda_2 = 4KB_{12}, \quad (3.42b)$$

in which the thermoelastic material property $B_1(\theta)$ is defined as

$$B_1(\theta) = B_{11} - B_{12}\theta, \quad (3.43)$$

B_{11} and B_{12} being material constants to be precisely defined later.

Also, the solution of equation (3.30f) for B_5 is:

$$B_5(\theta) = B_{5R} \left(1 + \frac{\theta}{T_R}\right)^{1-\lambda_1-\lambda_2 T_R} \exp(\lambda_2 \theta), \quad (3.44)$$

where

$$B_5(\theta) \Big|_{\theta=0} = B_{5R}. \quad (3.45)$$

The constants B_{4R} and B_{5R} are determined from the usual experimentally determined isothermal stress-strain curves as

$$B_{4R} = -\left[\frac{(3\lambda_R + 2\mu_R)\alpha_R}{Z_0}\right] \cdot [1 - \exp(\lambda_2) \left(1 + \frac{1}{T_R}\right)^{1-\lambda_1-\lambda_2 T_R}]^{-1}, \quad (3.46)$$

where, λ_R and μ_R are the values of Lamé constants at the reference temperature, α_R is the coefficient of thermal expansion at the reference temperature, and Z_0 is the reference value of the strain hardening parameter given by Bodner and Partom [3.11] and by Bodner et al. [3.12]. The value of B_{5R} is determined as

$$B_{5R} = \frac{Y_R E_T}{Y_R - E_T}, \quad (3.47)$$

where Y_R is the value of the Young's modulus at the reference temperature and E_T is the slope of the plastic region of the stress-strain curve (otherwise referred to as the tangent modulus) at the reference temperature. The detailed determination of B_{4R} and B_{5R} is given in the Appendix. The other equations cannot be precisely solved since the appropriate auxiliary conditions are not available as explained above. Thus, the other material properties are determined by assuming that the entropy contribution to the free energy function is negligibly small. This assumption is quite valid for moderate temperature applications [3.1, 3.2].

In summary, the solutions of the equations (3.30) are determined as:

$$B_4(\theta) = B_{4R} \left(1 + \frac{\theta}{T_R}\right)^{1-\lambda_1-\lambda_2 T_R} \exp(\lambda_2 \theta), \quad (3.48a)$$

$$B_5(\theta) = B_{5R} \left(1 + \frac{\theta}{T_R}\right)^{1-\lambda_1-\lambda_2 T_R} \exp(\lambda_2 \theta), \quad (3.48b)$$

$$A_2(\theta) = 2KA_1(\theta)B_4(\theta), \quad (3.48c)$$

$$A_3(\theta) = 2KA_1(\theta)B_5(\theta), \quad (3.48d)$$

$$B_2(\theta) = KB_4^2(\theta), \quad (3.48e)$$

$$B_3(\theta) = KB_5^2(\theta), \quad (3.48f)$$

$$B_6(\theta) = 2KB_4(\theta)B_5(\theta). \quad (3.48g)$$

Thus, since K is known, all the thermoinelastic material properties are now known and hence the thermoinelastic portion of the free energy functional is explicitly known.

Typical parameters for copper and aluminum are given in Table 3.1 below.

As remarked earlier on, most studies disregard ψ^I on the basis that it is small compared to ψ . This is generally not true, however. Chrysochoos [3.13] performed experiments to measure the stored energy during plastic deformation processes using the traditional microcalorimetric techniques and a more modern approach based on infra-red thermography. For the three metals considered in his experiments, he observed that the fraction of the stored energy could reach 50% to 60%. More recently, Aravas et al. [3.14] reported

Table 3.1 Thermoelastic material constants that characterize the stored energy of cold work phenomenon in copper and aluminum

Material Parameter	Copper	Aluminum
$K(\text{m}^2\text{N}^{-1})$	6.12 E -11	2.39 E -10
λ_1	24.75	48.89
$\lambda_2(\text{K}^{-1})$	4.43 E -03	2.30 E -03
B_{4R}	-2.88	-1.25
$B_{5R}(\text{Nm}^{-2})$	2.18 E 09	1.24 E 09
$A_{11}(\text{Nm}^{-2})$	8.93 E 07	3.14 E 07

theoretical studies which show that the fraction of stored energy could be of the order measured by Chrysochoos or even higher.

A lot of workers usually assume that only 10% of the plastic mechanical work is stored in the material while the remainder is converted into heat energy. It was on this basis, for example, that Klopp et al. [3.15] carried out the necessary thermomechanical analysis required to interpret their high-strain-rate plastic wave experimental data. Riff and Simitzes [3.16] also made the same assumption in a recent work concerning thermoviscoplastic analysis. From the works reviewed by Bever and his associates, and more evidently the works of Chrysochoos [3.13] and Aravas et al. [3.14], it is clear that this assumption is, in general, not in harmony with the physical material behavior. Factors ranging from 10% to 90% have been suggested in the literature [3.17, 3.18]. Reference [3.18] comments on this state of uncertainty. Indeed, based on observations that some workers (for example, Date [3.19]) assume all the plastic mechanical work to be

adiabatically converted into heat energy while others assume plastic deformation to be isothermal, it may be concluded that this factor practically ranges from 0% to 100%! The situation is, therefore, even more serious than apparent.

This is why the author believes that the ability to quantify the thermoinelastic portion of the free energy is significant, especially as it has been achieved on a physical basis in this thesis. This is because the need to try to guess *a priori* the relative magnitudes of ψ^I to ψ is eliminated. Furthermore, in a systematic application of the principle of conservation of energy, the question of how much of the inelastic mechanical work is converted into heat energy takes care of itself. We like to emphasize that the principle of conservation of energy is applicable to inelastic deformation processes even though they are highly irreversible. From the formulation presented, it is easy to see that the fraction of the stored energy is indeed a variable that depends on the thermodynamic state of the deformation process. If this fraction is denoted by ω , then

$$\omega = \frac{e_{IRR}}{W_P} = \frac{\psi_{IRR} + (\theta + T_R)\eta_{IRR}}{W_P}, \quad (3.49a)$$

or

$$\omega = \frac{\psi^I - (\theta + T_R) \frac{\partial \psi^I}{\partial \theta}}{W_P}, \quad (3.49b)$$

where W_P is the plastic work defined as:

$$W_P = \int_0^P \sigma(E, \theta, Z, P) dP. \quad (3.49c)$$

From the above, it is clearly seen that

$$\omega = \tilde{\omega}(E, \theta, Z, P). \quad (3.49d)$$

For a material whose stress-strain-temperature relation in the thermoelastic range is of the form

$$\sigma = A_{11} + [\lambda(\theta) + 2\mu(\theta)]E - [3\lambda(\theta) + 2\mu(\theta)]\alpha(\theta)\theta, \quad (3.50)$$

where A_{11} is the reference stress, $\alpha(\theta)$ is the coefficient of thermal expansion, and whose specific heat capacity at a constant state of deformation, C_D , is of the form

$$C_D = C_1 + C_2\theta, \quad (3.51)$$

it can be shown that the thermoelastic free energy functional is given by

$$\begin{aligned} \psi^E = \psi_R = \psi_0 - \eta_0\theta + A_{11}E + \frac{1}{2}(\lambda + 2\mu)E^2 - (3\lambda + 2\mu)\alpha E\theta \\ + \rho(C_2T_R - C_1)(\theta + T_R)\ln(1 + \frac{\theta}{T_R}) - \rho(C_2T_R - C_1)\theta - \frac{1}{2}\rho C_2\theta^2, \end{aligned} \quad (3.52)$$

where ψ_0 and η_0 are the reference values of the free energy and the entropy respectively. Comparing this relation with the expression for ψ^E (equation (3.12b)), it follows that:

$$\begin{aligned} \phi(\theta) = \psi_0 - \eta_0\theta + \rho(C_2T_R - C_1)(\theta + T_R)\ln(1 + \frac{\theta}{T_R}) \\ - \rho(C_2T_R - C_1)\theta - \frac{1}{2}\rho C_2\theta^2, \end{aligned} \quad (3.53a)$$

$$A_1(\theta) = A_{11} - [3\lambda(\theta) + 2\mu(\theta)]\alpha(\theta)\theta, \quad (3.53b)$$

$$B_1(\theta) = \frac{1}{2}[\lambda(\theta) + 2\mu(\theta)]. \quad (3.53c)$$

With these, the full nonlinear expression for the free energy functional is completely and explicitly defined. So also are the expressions for the stress and the entropy functionals.

It should be pointed out that the expression for ψ^E , equation (3.52), makes no assumptions concerning smallness of the incremental temperature (θ) and as such is valid over a very wide range of temperatures. It may be noted in passing that (3.52) reduces to the classical free energy expression of linear thermoelasticity if the smallness assumption for θ is invoked, and the specific heat capacity is assumed to be temperature-independent.

3.3 Other Constitutive Response Functionals

Three other constitutive response functionals remain to be characterized in the model, namely:

$$q = \tilde{q}(E, \theta, g, Z, P), \quad (3.54)$$

$$\dot{Z} = \tilde{F}(E, \theta, g, Z, P), \quad (3.55)$$

$$\dot{P} = \tilde{G}(E, \theta, g, Z, P). \quad (3.56)$$

A systematic way of finding explicit representations for the functionals $\tilde{q}$, $\tilde{F}$, and $\tilde{G}$ would be to adopt the same procedure that was employed for the free energy functional above. This would again call for a barrage of experiments to determine the resulting material properties or, worse still, it might even be impossible to think of appropriate experiments in some cases. Fortunately, however, it is possible to utilize available experimentally substantiated relations insofar as such relations do not conflict with the constitutive model developed in this work.

The relation (3.54) is concerned about the nature of the heat flow law. Since it is generally agreed that heat flow is not influenced by the process of plastic deformation (or, for that matter, any kind of deformation), it is assumed that the heat conduction is governed by the

modified form of the Fourier law of heat conduction. This modified law, usually referred to as the Maxwell-Cattaneo relation, is of the form:

$$q + \tau_0 \frac{\partial q}{\partial t} = k \frac{\partial \theta}{\partial X}, \quad (3.57)$$

where k is the coefficient of thermal conductivity and τ_0 is the so-called THERMAL RELAXATION TIME incorporated to allow second-sound effects. This heat flow law has been used for thermoelastic wave propagation studies by Lord and Shulman [3.20], Achenbach [3.21], Norwood and Warren [3.22], Sherief and Dhaliwal [3.23], and many others.

For the evolution functions ($\hat{F}$ and $\hat{G}$) it is assumed that the temperature gradient (g) is of no practical significance. Many kinds of evolution equations for hardening and plastic strain have been proposed in the literature. The usual procedure for their determination is to curve-fit empirical relations using experimental results. The Bodner-Partom model [3.11, 3.12] has been very widely applied to the analysis of inelastic deformation processes and is the one adopted in this work. The expressions are given by:

$$\dot{Z} = m(Z_A - Z)\sigma\dot{P} - K_A Z_A \left(\frac{Z - Z_0}{Z_A} \right)^{\alpha_A}, \quad (3.58)$$

$$\dot{P} = \frac{2D_0}{\sqrt{3}} \operatorname{sgn}(\sigma) \exp\left[-\left(\frac{n+1}{2n}\right)\left(\frac{Z}{\sigma}\right)^{2n}\right], \quad (3.59)$$

where Z_A , Z_0 , K_A , D_0 , α_A , m , and n are known material constants. Note that $\dot{Z}$ and $\dot{P}$ are functions of $\{E, \theta, Z, P\}$ through their dependence on the stress, σ , which is a function of the same set of arguments. In equation (3.58), Z_A is the limiting (saturation) value of Z , and m is the hardening rate. The negative of the first term is the "dynamic

recovery" while the second term corresponds to thermal or "static" recovery of hardening. The inclusion of thermal recovery of hardening is important at high temperatures and enables response characteristics such as secondary creep to be properly predicted. The parameter n in equation (3.59) controls strain rate sensitivity and also influences the overall level of the flow stress.

It should be noted that no yield criterion is involved in the development presented in this work. It is assumed that both thermoelastic and thermoinelastic deformations are present at any state of the thermodynamic process. This eliminates the need to specify loading and unloading conditions so that the same equations may be directly applied for all loading and unloading histories. Thus, this development may be considered to belong to the class of the endochronic theories of plasticity.

3.4 A Proposal for Generalization of the Procedure for the Explicit Characterization of the Free Energy, Stress, and Entropy Functionals

It is reasonable to expect that the experimental finding:

$$e_{IRR} = K\sigma^2 \quad (3.60)$$

is not valid for every metal. However, it will be desirable to be able to apply such a systematic procedure as applied above to the explicit characterization of the inelastic thermomechanical behavior of metals and metallic alloys even under multidimensional stress states. In particular, the systematic determination of the inelastic portion of the free energy functional is very vital.

For the most general case, let the thermodynamic state

variables be made up of the set

$$\text{TSV} = \{\underline{\tilde{C}}^E, T, \underline{g}, \underline{Z}^I, \underline{Z}^D, \underline{C}^P\}. \quad (3.61)$$

In (3.61), $\underline{\tilde{C}}$ is a measure of the total deformation; for example, it may be the right Cauchy-Green strain tensor defined as

$$\underline{\tilde{C}} = \underline{\tilde{F}}^T \underline{\tilde{F}}, \quad (3.62)$$

where $\underline{\tilde{F}}$ is the deformation gradient, and it is assumed that this total deformation measure can be suitably decomposed into thermoelastic ($\underline{\tilde{C}}^E$) and thermoinelastic parts ($\underline{C}^P$). The quantities $\underline{Z}^I$ and $\underline{Z}^D$ represent, respectively, the isotropic hardening and the directional (that is anisotropic or kinematic) hardening. Thus, the set $\{\underline{\tilde{C}}^E, T, \underline{g}\}$ represents the external variables while the set $\{\underline{Z}^I, \underline{Z}^D, \underline{C}^P\}$ represent the internal state variables.

Application of the thermodynamic formalism to constitutive modelling as shown in Chapter 2 leads to the following:

$$\psi = \tilde{\psi}(\underline{\tilde{C}}^E, \theta, \underline{Z}^I, \underline{Z}^D, \underline{C}^P), \quad (3.62a)$$

$$\underline{\sigma} = \frac{\partial \tilde{\psi}}{\partial \underline{\tilde{C}}^E}, \quad (3.62b)$$

$$\eta = - \frac{\partial \tilde{\psi}}{\partial \theta}, \quad (3.62c)$$

$$\underline{q} = \tilde{q}(\underline{\tilde{C}}^E, \theta, \underline{g}, \underline{Z}^I, \underline{Z}^D, \underline{C}^P), \quad (3.62d)$$

$$\dot{\underline{Z}}^I = \tilde{F}_I(\underline{\tilde{C}}^E, \theta, \underline{g}, \underline{Z}^I, \underline{Z}^D, \underline{C}^P), \quad (3.62e)$$

$$\dot{\underline{Z}}^D = \tilde{F}_D(\underline{\tilde{C}}^E, \theta, \underline{g}, \underline{Z}^I, \underline{Z}^D, \underline{C}^P), \quad (3.62f)$$

$$\frac{\partial \tilde{\psi}}{\partial \underline{Z}^I} \dot{\underline{Z}}^I + \frac{\partial \tilde{\psi}}{\partial \underline{Z}^D} \dot{\underline{Z}}^D + \frac{\partial \tilde{\psi}}{\partial \underline{C}^P} \dot{\underline{C}}^P - \frac{1}{(\theta + T_R)} \underline{q} \cdot \underline{g} \leq 0, \quad (3.62g)$$

where

$$\underline{g} = \nabla \theta, \quad (3.62h)$$

and

$$\theta = T - T_R. \quad (3.62i)$$

Now, the free energy ψ is given by

$$\psi = \tilde{\psi}(C^E, \theta, Z^I, Z^D, C^P). \quad (3.63)$$

Let there be N invariants: $I_1, I_2, I_3, \dots, I_N$, associated with the set of thermodynamic state variables

$$S_\psi = \{C^E, \theta, Z^I, Z^D, C^P\}. \quad (3.64)$$

Then in a manner similar to the presentation in Section 3.2, a polynomial representation of the free energy functional may be written as:

$$\psi = \phi_G(\theta) + f_1(\theta)I_1 + f_2(\theta)I_2 + f_3(\theta)I_3 + \dots + f_N(\theta)I_N. \quad (3.65)$$

Out of the N invariants, let there be M invariants associated with purely thermoelastic deformation variables, so that

$$I_j = \tilde{I}_j(C^E, \theta), \quad j = 1, 2, 3, \dots, M. \quad (3.66)$$

Then equation (3.65) may be expressed as

$$\begin{aligned} \psi = & \phi_G(\theta) + f_1(\theta)I_1 + f_2(\theta)I_2 + \dots + f_M(\theta)I_M \\ & + f_{M+1}(\theta)I_{M+1} + f_{M+2}(\theta)I_{M+2} + \dots + f_N(\theta)I_N. \end{aligned} \quad (3.67)$$

Thus, the expression for ψ may again be partitioned into thermoelastic (or recoverable) and thermoinelastic (or irrecoverable) portions in the form

$$\psi = \psi^E + \psi^I, \quad (3.68a)$$

where

$$\psi^E = \phi_G(\theta) + f_1(\theta)I_1 + f_2(\theta)I_2 + \dots + f_M(\theta)I_M, \quad (3.68b)$$

$$\psi^I = f_{M+1}(\theta)I_{M+1} + f_{M+2}(\theta)I_{M+2} + \dots + f_N(\theta)I_N. \quad (3.68c)$$

The quantity ψ^E can always be readily determined from a knowledge of the thermoelastic stress-strain-temperature relation (linear or nonlinear) and the temperature dependence of the specific

heat at constant state of deformation. Thus, the function $\phi_G(\theta)$ and the material properties $f_1(\theta)$, $f_2(\theta)$, ..., $f_N(\theta)$ in equation (3.68b) can be determined. The quantity ψ^I represents the irrecoverable portion of the free energy function. The stored energy of cold work, e_{IRR} , which can be measured directly is related to ψ^I through the expression

$$e_{IRR} = \psi^I - (\theta + T_R) \frac{\partial \psi^I}{\partial \theta}. \quad (3.69)$$

Since ψ^I is a function of the invariants I_{M+1} , I_{M+2} , ..., I_N , it follows that the right hand side of equation (3.69) is a function of the same arguments. Similarly, e_{IRR} must depend on those arguments. Thus, equation (3.69) may be expressed as

$$\phi_L^*(I_{M+1}, I_{M+2}, \dots, I_N) = \phi_R^*(I_{M+1}, I_{M+2}, \dots, I_N), \quad (3.70)$$

where

$$e_{IRR} = \phi_L^*(I_{M+1}, I_{M+2}, \dots, I_N), \quad (3.71a)$$

and

$$\psi^I - (\theta + T_R) \frac{\partial \psi^I}{\partial \theta} = \phi_R^*(I_{M+1}, I_{M+2}, \dots, I_N) \quad (3.71b)$$

The form of ϕ_R^* is explicitly known from the expression for ψ^I , equation (3.68c). Several experiments are now to be performed to measure the stored energy of cold work and determine the nature of the dependence of e_{IRR} on the measurable deformation variables and temperature. From this, the dependence of e_{IRR} on the invariants I_{M+1} , I_{M+2} , ..., I_N , or at least a subset of these invariants, can be expressed as a polynomial representation in the same form as the right hand side of equation (3.71b), and the material coefficients obtained in the polynomial curve-fitting process. With this, the left hand side of (3.70), that is ϕ_L^* , is now fully and explicitly known. On invoking the

smoothness properties of the functions ϕ_L^* and ϕ_R^* (as a consequence of the assumed smoothness of the constitutive response functionals involved), the unknown material properties $f_{M+1}(\theta)$, $f_{M+2}(\theta)$, ..., $f_N(\theta)$, are readily obtained. Hence, the free energy functional has been fully and explicitly characterized to incorporate the stored energy of cold work phenomenon. This leads to explicit expressions of the stress and entropy functionals on the application of the thermodynamic results (3.62b) and (3.62c).

For the heat flow law and the evolution equations for the internal state variables, the same treatment given in Section 3.3 is adequate.

CHAPTER 4

PROBLEM FORMULATION

4.1 Lagrangian Kinematic Description of the Problem

Consider the very long rod or bar whose geometry is shown in Figure 4.1 below.

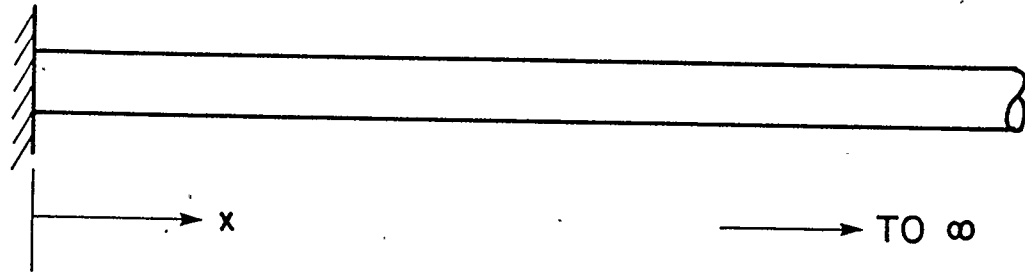


Figure 4.1 Schematic illustration of a semi-infinite rod

As shown above, x describes the position of a material particle at time t . The motion of a typical particle is described by

$$x = \chi(X, t), \quad (4.1)$$

where x specifies the present position. Thus, the displacement of the particle is given by

$$u = u(X, t), \quad (4.2)$$

If geometrically linear strains are assumed, then the strain (which measures the observed deformation) is given by

$$\epsilon = \frac{\partial u}{\partial X}. \quad (4.3)$$

The particle velocity, defined as the time rate of change of the displacement is

$$v = \frac{\partial u}{\partial t}. \quad (4.4)$$

If the displacement function is assumed to be well behaved,

then

$$\frac{\partial^2 u}{\partial X \partial t} = \frac{\partial}{\partial X} \left(\frac{\partial u}{\partial t} \right) = \frac{\partial}{\partial t} \left(\frac{\partial u}{\partial X} \right) , \quad (4.5a)$$

or

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial v}{\partial X} . \quad (4.5b)$$

Equation (4.5b) is the kinematic compatibility condition.

The formal derivation of the local forms of the fundamental balance laws may be found in any classical text of continuum mechanics (for example, the book by Eringen [4.1]) and as such is not repeated here.

The law of conservation of mass is identically satisfied if we assume infinitesimal deformation so that the density remains essentially constant throughout the deformation process.

The law of balance of linear momentum gives the equation of motion as:

$$\frac{\partial \sigma}{\partial X} = \rho \frac{\partial v}{\partial t} - f , \quad (4.6)$$

where f is the body force per unit volume.

The law of balance of moment of momentum is identically satisfied since symmetry of the stress tensor is automatically guaranteed with only one component of stress.

The principle of conservation of energy states that the time rate of change of the kinetic plus internal energy is equal to the sum of the rate of work of the external forces plus all other energies that enter or leave the body per unit time. It is to be emphasized once again that this principle is valid for every process including

dissipative ones. The local form for a general thermomechanical process was given as equation (2.15), namely:

$$\frac{\partial \psi}{\partial t} + \eta \frac{\partial T}{\partial t} + T \frac{\partial \eta}{\partial t} = \sigma \frac{\partial \varepsilon}{\partial t} + \frac{\partial q}{\partial X} + \gamma. \quad (4.7a)$$

With the developments in Chapter 2, this equation assumes the reduced form:

$$\frac{\partial \psi}{\partial Z} \dot{Z} + \frac{\partial \psi}{\partial P} \dot{P} + (\theta + T_R) \dot{\eta} = \frac{\partial q}{\partial X} + \gamma. \quad (4.7b)$$

The Clausius-Duhem inequality, which is the mathematical form of the Second Law adopted in this work, may be recalled as:

$$T \frac{\partial \eta}{\partial t} \geq \gamma + \frac{\partial q}{\partial X} - \frac{q}{T} g, \quad (4.8a)$$

while the reduced form gives the dissipation inequality:

$$\frac{\partial \psi}{\partial Z} \dot{Z} + \frac{\partial \psi}{\partial P} \dot{P} - \frac{q}{(\theta + T_R)} g \leq 0. \quad (4.8b)$$

4.2 Summary of Fundamental Equations

The equations governing the propagation of uniaxial coupled thermomechanical waves in inelastic solids will now be assembled. These equations consist of the fundamental balance laws just given and the constitutive equations developed in Chapter 2 and Chapter 3.

Thus, the system of fundamental equations required is given by the following:

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial v}{\partial X}, \quad (4.9a)$$

$$\varepsilon = E + P, \quad (4.9b)$$

$$\frac{\partial \sigma}{\partial X} = \rho \frac{\partial v}{\partial t} - f, \quad (4.9c)$$

$$\frac{\partial \psi}{\partial Z} \dot{Z} + \frac{\partial \psi}{\partial P} \dot{P} + (\theta + T_R) \dot{\eta} = \frac{\partial q}{\partial X} + \gamma, \quad (4.9d)$$

$$\begin{aligned} \psi = & \psi_0 - \eta_0 \theta + \rho(C_2 T_R - C_1)(\theta + T_R) \ln(1 + \frac{\theta}{T_R}) \\ & - \rho(C_2 T_R - C_1) \theta - \frac{1}{2} \rho C_2 \theta^2 + A_1(\theta)E + B_1(\theta)E^2 + A_2(\theta)Z + A_3(\theta)P \\ & + B_2(\theta)Z^2 + B_3(\theta)P^2 + B_4(\theta)EZ + B_5(\theta)EP + B_6(\theta)ZP, \end{aligned} \quad (4.9e)$$

$$\sigma = A_1(\theta) + 2B_1(\theta)E + B_4(\theta)Z + B_5(\theta)P, \quad (4.9f)$$

$$\begin{aligned} \eta = & -[\eta_0 - \rho(C_2 T_R - C_1) \ln(1 + \frac{\theta}{T_R}) + \rho C_2 \theta + A'_1(\theta)E \\ & + B'_1(\theta)E^2 + A'_2(\theta)Z + A'_3(\theta)P + B'_2(\theta)Z^2 + B'_3(\theta)P^2 + B'_4(\theta)EZ \\ & + B'_5(\theta)EP + B'_6(\theta)ZP], \end{aligned} \quad (4.9g)$$

$$q + \tau_0 \frac{\partial q}{\partial t} = k \frac{\partial \theta}{\partial X}, \quad (4.9h)$$

$$\dot{Z} = m(Z_A - Z)\sigma\dot{P} - K_A Z_A \left(\frac{Z - Z_0}{Z_A}\right)^{\alpha_A}, \quad (4.9i)$$

$$\dot{P} = \frac{2D_0}{\sqrt{3}} \operatorname{sgn}(\sigma) \exp\left[-\left(\frac{n+1}{2n}\right)\left(\frac{Z}{\sigma}\right)^{2n}\right]. \quad (4.9j)$$

Note that overdots in equations (4.9) denote partial differentiation with respect to time and the material functions $A_1(\theta)$, $B_1(\theta)$, $A_2(\theta)$, $A_3(\theta)$, $B_2(\theta)$, $B_3(\theta)$, $B_4(\theta)$, $B_5(\theta)$, and $B_6(\theta)$ have been explicitly defined in Chapter 3.

The above is a system of ten simultaneous algebraic and partial differential equations in the ten unknowns σ , v , ε , ψ , θ , η , q , Z , E , and P and so it forms a determinate system. Thus, in principle the system (4.9) can be solved for the unknowns if the auxiliary

conditions are appropriately prescribed. The boundary and initial conditions must be prescribed in such a way that the mathematical model is well-posed. This will ensure the uniqueness of the resultant wave motion.

Before we proceed further, it is desirable to reduce the system to one of partial differential equations alone.

From equation (4.9f), the thermoelastic strain is readily determined as

$$E = D_1(\theta) + D_2(\theta)\sigma + D_3(\theta)Z + D_4(\theta)P, \quad (4.10)$$

where

$$D_1(\theta) = -\frac{A_1(\theta)}{2B_1(\theta)}, \quad (4.11a)$$

$$D_2(\theta) = \frac{1}{2B_1(\theta)}, \quad (4.11b)$$

$$D_3(\theta) = -\frac{B_4(\theta)}{2B_1(\theta)}, \quad (4.11c)$$

$$D_4(\theta) = -\frac{B_5(\theta)}{2B_1(\theta)}, \quad (4.11d)$$

Thus,

$$E = \tilde{E}(\sigma, \theta, Z, P). \quad (4.12)$$

Since $\psi = \tilde{\psi}(E, \theta, Z, P)$, equation (4.10) may be used to eliminate E from equation (4.9e) so that

$$\psi = \psi^*(\sigma, \theta, Z, P). \quad (4.13)$$

Similarly, the entropy can be expressed as

$$\eta = \eta^*(\sigma, \theta, Z, P). \quad (4.14)$$

The total strain, ϵ , may also be eliminated since the application of

(4.10) to (4.9b) leads to

$$\epsilon = E + P = \tilde{\epsilon}(\sigma, \theta, Z, P). \quad (4.15)$$

Thus, with the above, the dependent variables E , ϵ , η , and ψ have been eliminated. There now remains a system of six partial differential equations in the six unknowns v , σ , θ , q , Z , and P which are as follows:

$$\rho \frac{\partial v}{\partial t} - \frac{\partial \sigma}{\partial X} = f, \quad (4.16a)$$

$$\begin{aligned} D_2(\theta) \frac{\partial \sigma}{\partial t} + D_5(\sigma, \theta, Z, P) \frac{\partial \theta}{\partial t} + D_3(\theta) \frac{\partial Z}{\partial t} \\ + D_6(\theta) \frac{\partial P}{\partial t} - \frac{\partial v}{\partial X} = 0, \end{aligned} \quad (4.16b)$$

$$\begin{aligned} J_1(\sigma, \theta, Z, P) \frac{\partial \sigma}{\partial t} + J_2(\sigma, \theta, Z, P) \frac{\partial \theta}{\partial t} \\ + J_3(\sigma, \theta, Z, P) \frac{\partial Z}{\partial t} + J_4(\sigma, \theta, Z, P) \frac{\partial P}{\partial t} - \frac{\partial q}{\partial X} = \gamma, \end{aligned} \quad (4.16c)$$

$$\tau_0 \frac{\partial q}{\partial t} - k \frac{\partial \theta}{\partial X} = -q, \quad (4.16d)$$

$$\frac{\partial Z}{\partial t} = -F_2(\sigma, Z), \quad (4.16e)$$

$$\frac{\partial P}{\partial t} = G_1(\sigma, Z). \quad (4.16f)$$

In the above,

$$J_1 = (\theta + T_R) D_2(\theta) \frac{\partial \eta}{\partial E}, \quad (4.17a)$$

$$J_2 = (\theta + T_R) \left\{ \frac{\partial \eta}{\partial E} [D'_1(\theta) + D'_2(\theta)\sigma + D'_3(\theta)Z + D'_4(\theta)P] + \frac{\partial \eta}{\partial \theta} \right\}, \quad (4.17b)$$

$$J_3 = (\theta + T_R) [D_3(\theta) \frac{\partial \eta}{\partial E} + \frac{\partial \eta}{\partial Z}] + \frac{\partial \psi}{\partial Z}, \quad (4.17c)$$

$$J_4 = (\theta + T_R) [D_4(\theta) \frac{\partial \eta}{\partial E} + \frac{\partial \eta}{\partial P}] + \frac{\partial \psi}{\partial P} - \sigma , \quad (4.17d)$$

$$D_5 = D_1'(\theta) + D_2'(\theta)\sigma + D_3'(\theta)Z + D_4'(\theta)P , \quad (4.17e)$$

$$D_6 = 1 + D_4(\theta) . \quad (4.17f)$$

In (4.17), the quantities $\partial \eta / \partial E$, $\partial \eta / \partial \theta$, $\partial \eta / \partial Z$, $\partial \eta / \partial P$, $\partial \psi / \partial Z$, and $\partial \psi / \partial P$ are expressed in terms of $\{\sigma, \theta, Z, P\}$. Of course, the functions F_2 and G_1 are given by

$$F_2 = m(Z_A - Z)\sigma - K_A Z_A \left(\frac{Z - Z_0}{Z_A} \right)^{\alpha_A} , \quad (4.18)$$

$$G_1 = \frac{2D_0}{\sqrt{3}} \operatorname{sgn}(\sigma) \exp \left[- \left(\frac{n+1}{2n} \right) \left(\frac{Z}{\sigma} \right)^{2n} \right] . \quad (4.19)$$

Examination of equations (4.16a)-(4.16f) reveals that the system is highly nonlinear and that the thermal and mechanical variables are fully coupled. The degree of complexity is especially appreciated on examination of the functions J_1 , J_2 , J_3 , and J_4 which in turn are dependent on the nonlinear temperature-dependent material properties given in the last chapter. Thus, it is quite evident that no closed-form or analytic solution can be found for the above system of equations. A numerical approach must be applied. However, the system must be analyzed to examine the nature of the partial differential equations so that appropriate numerical techniques can be applied.

4.3 Mathematical Analysis of the System of Equations

Equations (4.16) form a system of six simultaneous first-order

quasilinear partial differential equations in the six unknowns v , σ , θ , q , Z , P .

Let the vector $\underline{U}$ be defined as

$$\underline{U} = [v \quad \sigma \quad \theta \quad q \quad Z \quad P]^T, \quad (4.20)$$

where the superscript "T" denotes transpose. Then the above system may be expressed in the vector form

$$\underline{A}_0 \underline{U}_t + \underline{B}_0 \underline{U}_X = \underline{C}_0, \quad (4.21)$$

where:

$$\underline{U}_t = \frac{\partial \underline{U}}{\partial t} = [v_t \quad \sigma_t \quad \theta_t \quad q_t \quad Z_t \quad P_t]^T, \quad (4.22a)$$

$$\underline{U}_X = \frac{\partial \underline{U}}{\partial X} = [v_x \quad \sigma_x \quad \theta_x \quad q_x \quad Z_x \quad P_x]^T, \quad (4.22b)$$

$$\underline{A}_0 = \begin{bmatrix} \rho & 0 & 0 & 0 & 0 & 0 \\ 0 & D_2 & D_5 & 0 & D_3 & D_6 \\ 0 & J_1 & J_2 & 0 & J_3 & J_4 \\ 0 & 0 & 0 & \tau_0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad (4.22c)$$

$$\underline{B}_0 = \begin{bmatrix} 0 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -k & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad (4.22d)$$

and

$$\underline{C}_0 = [f \quad 0 \quad \gamma \quad -q \quad -F_2 \quad G_1]^T. \quad (4.22e)$$

Since the matrix $\underline{A}_0$ is non-singular with its determinant given by

$$\det \underline{A}_0 = \rho \tau_0 G_2, \quad (4.23a)$$

where

$$G_2 = D_2 J_2 - J_1 D_5, \quad (4.23b)$$

its inverse, $\underline{A}_0^{-1}$, may be computed as:

$$\underline{A}_0^{-1}(U) = \frac{1}{\rho \tau_0 G_2} \begin{bmatrix} \tau_0 G_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & \rho \tau_0 J_2 & -\rho \tau_0 D_5 & 0 & -\rho \tau_0 G_5 & \rho \tau_0 G_4 \\ 0 & -\rho \tau_0 J_1 & \rho \tau_0 D_2 & 0 & -\rho \tau_0 G_7 & \rho \tau_0 G_6 \\ 0 & 0 & 0 & \rho G_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & \rho \tau_0 G_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & \rho \tau_0 G_2 \end{bmatrix} \quad (4.23c)$$

On premultiplying equation (4.21) by $\underline{A}_0^{-1}$, we obtain the equation:

$$\frac{\partial \underline{U}}{\partial t} + \underline{A}(U) \frac{\partial \underline{U}}{\partial X} + \underline{B}(U) = 0, \quad (4.24)$$

where

$$\underline{A}(U) = \begin{bmatrix} 0 & \frac{1}{\rho} & 0 & 0 & 0 & 0 \\ -J_2 G_3 & 0 & 0 & D_5 G_3 & 0 & 0 \\ J_1 G_3 & 0 & 0 & -D_2 G_3 & 0 & 0 \\ 0 & 0 & -\frac{k}{\tau_0} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad (4.25a)$$

$$\underline{B}(U) = \left[-\frac{1}{\rho} f \quad -G_3 G_8 \quad -G_3 G_9 \quad \frac{q}{\tau_0} \quad F_2 \quad -G_1 \right]^T, \quad (4.25b)$$

and the functions $G_3, G_4, G_5, G_6, G_7, G_8$, and G_9 are defined as

$$G_3 = \frac{1}{G_2}, \quad (4.25c)$$

$$G_4 = D_5 J_4 - D_6 J_2, \quad (4.25d)$$

$$G_5 = J_2 D_3 - J_3 D_5, \quad (4.25e)$$

$$G_6 = D_6 J_1 - D_2 J_4, \quad (4.25f)$$

$$G_7 = D_2 J_3 - J_1 D_3, \quad (4.25g)$$

$$G_8 = G_1 G_4 + F_2 G_5 - \gamma D_5, \quad (4.25h)$$

$$G_9 = G_1 G_6 + F_2 G_7 + \gamma D_2. \quad (4.25i)$$

It is easy to see from these definitions that

$$G_i = G_i^*(\sigma, \theta, Z, P), \quad i = 2, 3, \dots, 9. \quad (4.26)$$

Equation (4.24) now represents the system of equations in a form that standard methods may be applied to its classification.

The characteristic equation corresponding to the system (4.24) is

$$\det (\underline{A} - \lambda \underline{I}) = 0, \quad (4.27)$$

in which the λ 's are the eigenvalues and $\underline{I}$ is the 6 x 6 identity matrix.

Now, the matrix $\underline{A} - \lambda \underline{I}$ is given by:

$$\underline{A} - \lambda \underline{I} = \begin{bmatrix} -\lambda & \frac{1}{\rho} & 0 & 0 & 0 & 0 \\ -J_2 G_3 & -\lambda & 0 & D_5 G_3 & 0 & 0 \\ J_1 G_3 & 0 & -\lambda & -D_2 G_3 & 0 & 0 \\ 0 & 0 & -k/\tau_0 & -\lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & -\lambda \end{bmatrix}, \quad (4.28)$$

Substituting equation (4.28) into equation (4.27) gives:

$$\lambda^2 \{ \lambda^2 [\lambda^2 - \frac{k}{\tau_0} D_2 G_3] - \frac{G_3}{\rho} [J_2 (\lambda^2 - \frac{k}{\tau_0} D_2 G_3) + \frac{k}{\tau_0} D_5 J_1 G_3] \} = 0. \quad (4.29)$$

Thus, the six eigenvalues λ_i , $i = 1, 2, \dots, 6$, are given by:

$$\lambda_1 = 0 , \quad (4.30a)$$

$$\lambda_2 = 0 , \quad (4.30b)$$

$$\lambda_3 = +\{M[1 + \sqrt{(1-R)}]\}^{\frac{1}{2}} , \quad (4.30c)$$

$$\lambda_4 = -\{M[1 + \sqrt{(1-R)}]\}^{\frac{1}{2}} , \quad (4.30d)$$

$$\lambda_5 = +\{M[1 - \sqrt{(1-R)}]\}^{\frac{1}{2}} , \quad (4.30e)$$

$$\lambda_6 = -\{M[1 - \sqrt{(1-R)}]\}^{\frac{1}{2}} , \quad (4.30f)$$

in which

$$M = M^*(\sigma, \theta, Z, P) = \frac{1}{2} G_3 \left(\frac{k}{\tau_0} D_2 + \frac{1}{\rho} J_2 \right) , \quad (4.31a)$$

and

$$R = R^*(\sigma, \theta, Z, P) = \frac{kG_3}{\rho \tau_0 M^2} . \quad (4.31b)$$

With (4.30) and (4.31), therefore, it is easy to see that the eigenvalues, in general, depend on U , that is,

$$\lambda_i = \lambda_i^*(\sigma, \theta, Z, P). \quad (4.32)$$

It can also be seen that there are two coincident eigenvalues: λ_1 and λ_2 . For the eigenvalues λ_3 , λ_4 , λ_5 , and λ_6 to be real, the following conditions must be simultaneously satisfied:

$$(i) \quad R(\sigma, \theta, Z, P) < 1 , \quad (4.33a)$$

$$(ii) \quad M(\sigma, \theta, Z, P) > 0 , \quad (4.33b)$$

If these conditions are satisfied then all the six eigenvalues

are real and so the system (4.24) is classified as hyperbolic. If any of the two conditions is not satisfied then four of the eigenvalues (λ_3 , λ_4 , λ_5 , and λ_6) are complex quantities and the system will be said to be ultra-hyperbolic [4.2]. Thus, the conditions (4.33a) and (4.33b) are the HYPERBOLICITY CONDITIONS. It is intuitively conjectured that these conditions are satisfied for the thermodynamic process of wave propagation in inelastic solids.

With this classification, the eigenvalues are the characteristic speeds which may not coincide with the velocities of propagation of the waves because of the nonlinear nature of the problem. Thus

$$\lambda_1 = 0 \quad (4.34a)$$

$$\lambda_2 = 0 \quad (4.34b)$$

$$\lambda_3 = V_3, \quad (4.34c)$$

$$\lambda_4 = -V_3, \quad (4.34d)$$

$$\lambda_5 = V_5, \quad (4.34e)$$

$$\lambda_6 = -V_5, \quad (4.34f)$$

in which V_3 and V_5 are the characteristic speeds in the positive X direction. Even though these speeds may not coincide with the shock wave speeds, they give indication of the presence of two waves which is consistent with the physics of the problem. They also give indication of the coupled nature since both V_3 and V_5 are functions of $\{\sigma, \theta, Z, P\}$ which consist of both thermal and mechanical deformation variables.

In the absence of second-sound effects, the thermal relaxation time assumes a zero value. It can be shown that, under this situation, on neglecting heat conduction, system (4.24) is still hyperbolic but with only one positive wave speed given by:

$$\lambda = \left\{ \frac{1}{\rho D_2(\theta)} \right\}^{\frac{1}{2}} . \quad (4.35)$$

This is the velocity of propagation of thermoelastic waves. This finding is consistent with experimental results of plastic wave experiments which indicate that plastic waves propagate at the elastic wave velocity [4.3]. A major attribute of the rate-dependent theory of plasticity is its capability of correctly predicting the plastic wave velocity. It is important, therefore, that the constitutive model developed in this work is able to correctly predict this physical behavior.

4.4 Jump Conditions at the Wavefronts

The system of partial differential equations (4.24) govern the wave propagation process everywhere in the bar except at the location of the points of discontinuity - that is the wavefronts. Conditions valid at the wavefronts must be determined separately.

Achenbach [4.4] defines the wavefront as the moving surface which separates the disturbed from the undisturbed part of the body. In other words, the wavefront is the surface which travels through the medium as time t varies continuously, and across which there may exist a discontinuity in the primary dependent variables. Computation of variables at wavefronts is based on the theory of propagating singular surfaces which is well treated in the books by Eringen and Suhubi [4.5] and Chen [4.6].

Consider a regular surface $S(t)$ moving in a material body B which divides this body into two subregions B^+ and B^- and forms a common boundary between them as shown in Figure 4.2 below. The unit normal N

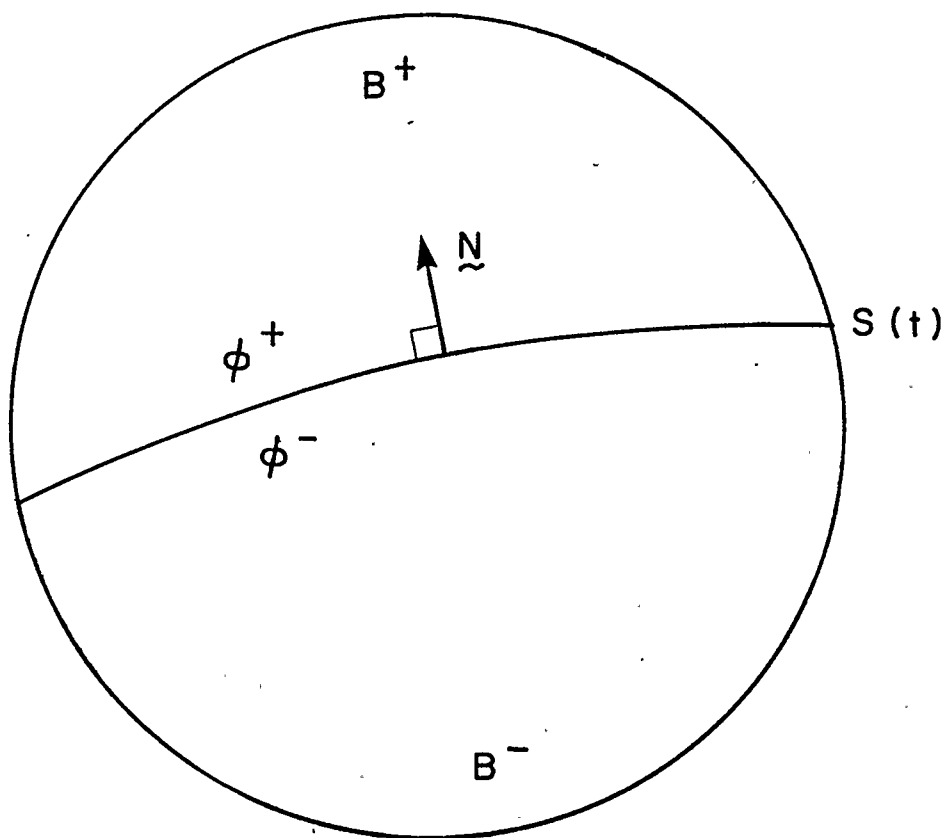


Figure 4.2 A body containing a moving surface of discontinuity.

of the surface is directed toward the region B^+ . Let $\phi(X,t)$ be a scalar-valued, vector-valued or tensor-valued function such that $\phi(X,t)$ is continuous within each of the regions B^+ and B^- , and let $\phi(X,t)$ have definite limits ϕ^+ and ϕ^- as X approaches a point on the surface $S(t)$ from paths entirely within the regions B^+ and B^- , respectively. The surface $S(t)$ is said to be singular with respect to $\phi(X,t)$ if and only

if

$$[\phi] \equiv \phi^- - \phi^+ \neq 0. \quad (4.36)$$

The quantity $[\phi]$ is referred to as the jump in ϕ across the singular surface $S(t)$. Further, the singular surface $S(t)$ is said to be a wave if its speed of propagation is non-vanishing.

There are jump conditions (usually referred to as the Rankine-Hugoniot conditions) corresponding to each of the ten equations given in equations (4.9a) - (4.9j). These equations are obtained in what follows.

For the partial differential equations, a theorem due to Kosinski [4.7] is applied. According to the theorem, for a partial differential equation of the form:

$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial X} F(U) + B(U) = 0, \quad (4.37)$$

the corresponding jump condition across a wavefront $X = S(t)$ is given by

$$V_w [U] = [F], \quad (4.38)$$

where V_w is the velocity of the moving wavefront.

In order to directly apply equation (4.38), the compatibility equation (4.9a), the momentum equation (4.9c), the energy equation (4.9d), the heat conduction equation (4.9h), and the evolution equations for Z and P equations (4.9i) and (4.9j) are expressed in the form:

$$\frac{\partial \varepsilon}{\partial t} - \frac{\partial v}{\partial X} = 0, \quad (4.39a)$$

$$\frac{\partial}{\partial t}(\rho v) - \frac{\partial \sigma}{\partial X} - f = 0, \quad (4.39b)$$

$$\frac{\partial}{\partial t} \left\{ \psi + (\theta + T_R) \eta + \frac{1}{2} \rho v^2 \right\} - \frac{\partial}{\partial X} (\sigma v + q) - (vf + \gamma) = 0, \quad (4.39c)$$

$$\frac{\partial}{\partial t}(\tau_0 q) - \frac{\partial}{\partial X}(k\theta) + q = 0 , \quad (4.39d)$$

$$\frac{\partial Z}{\partial t} + F_2 = 0 , \quad (4.39e)$$

$$\frac{\partial P}{\partial t} - G_1 = 0 . \quad (4.39f)$$

Applying Kosinski's theorem to (4.39) gives:

$$[v] = - V_w [\epsilon] , \quad (4.40a)$$

$$[\sigma] = - \rho V_w [v] , \quad (4.40b)$$

$$[\sigma v] + [q] = - V_w [\psi + (\theta + T_R)\eta + \frac{1}{2}\rho v^2] , \quad (4.40c)$$

$$[q] = - \frac{k}{\tau_0 V_w} [\theta] , \quad (4.40d)$$

$$[Z] = 0 , \quad (4.40e)$$

$$[P] = 0 . \quad (4.40f)$$

It is interesting to note that the jumps in the internal state variables Z and P vanish, which implies that Z and P are continuous across the wavefronts. This is usually the case for internal state variables whose evolution laws are of the rate form; similar results were obtained by Kosinski [4.7] and Bailey and Chen [4.8]. Yet, from physical considerations, it is expected that if a wave causes plastic deformation, a change of the plastic state of the body should be experienced immediately after the passage of the wave. The inclusion of a flux (or divergence) term to account for the spatial variation of an ISV will give non-vanishing values of the jumps of the ISVs thereby removing this anomaly. In this connection, it is noted that Aifantis [4.9, 4.10] has emphasized the importance of allowing the ISVs to be governed by what he referred to as "complete balance laws" in which both

the rate and divergence terms are included. The only problem with this approach is that these complete balance laws are not generally compatible with the Clausius-Duhem inequality and he proposed a generalization of the energy equation to include the work done by the gradients of thermodynamic variables or internal variables [4.10]. In the light of the seeming anomaly discussed above, it appears that the propositions of Aifantis deserve serious considerations by all researchers involved in the application of the theory of internal state variables to constitutive modelling.

For the four algebraic equations, the associated jump conditions are now determined. First, the assumption is made that since the evolution equations employed here give zero jumps in Z and P , the jumps in the thermoinelastic material properties are approximately zero. This is also true if the variations of these material properties are slowly varying functions of temperature. Thus, it is assumed that:

$$[A_2(\theta)] \cong 0, \quad (4.41a)$$

$$[A_3(\theta)] \cong 0, \quad (4.41b)$$

$$[B_2(\theta)] \cong 0, \quad (4.41c)$$

$$[B_3(\theta)] \cong 0, \quad (4.41d)$$

$$[B_4(\theta)] \cong 0, \quad (4.41e)$$

$$[B_5(\theta)] \cong 0, \quad (4.41f)$$

$$[B_6(\theta)] \cong 0. \quad (4.41g)$$

With these, the jump conditions associated with the algebraic relations (4.9b), (4.9e), (4.9f), and (4.9g) are given as:

$$[\varepsilon] = [E], \quad (4.42a)$$

$$[\psi] = -\eta_0[\theta] + \rho(C_2 T_R - C_1) \ln \left(\frac{T_R + \theta^-}{T_R + \theta^+} \right) \{[\theta] + \theta^+ + T_R\}$$

$$\begin{aligned}
& + \rho(C_2 T_R - C_1)[\theta] \left\{ \ln\left(1 + \frac{\theta^+}{T_R}\right) - 1 - \frac{C_2}{2(C_2 T_R - C_1)}[\theta] - \frac{C_2}{(C_2 T_R - C_1)}\theta^+ \right\} \\
& + [A_1(\theta)E] + [B_1(\theta)E^2] , \tag{4.42b}
\end{aligned}$$

$$[\sigma] = [A_1(\theta)] + 2[B_1(\theta)E] , \tag{4.42c}$$

$$[n] = \rho C_2[\theta] - \rho(C_2 T_R - C_1) \ln\left(\frac{T_R + \theta^-}{T_R + \theta^+}\right) - [A_1'(\theta)E] - [B_1'(\theta)E^2] . \tag{4.42d}$$

In equations (4.42), $[A_1(\theta)]$ and $[B_1(\theta)]$ are given by:

$$[A_1(\theta)] = -(3\lambda_R + 2\mu_R)\alpha_R[\theta] , \tag{4.43a}$$

$$[B_1(\theta)] = -B_{12}[\theta] , \tag{4.43b}$$

in which it has been assumed that the jumps in $\lambda(\theta)$, $\mu(\theta)$ and $\alpha(\theta)$ are negligible. These three thermoelastic properties have been defined already in Chapter 3.

It has been said earlier that the presence of two positive characteristic speeds suggest the existence of two wavefronts. Therefore, any discontinuity that exists will be split between the two wavefronts.

Let G denote the lagging wavefront and L the leading wavefront as shown in Figure (4.3) below.

The two wavefronts are propagating in the positive X direction with velocities V_G and V_L respectively. In Figure (4.3), region I is fully disturbed in the sense that both waves have passed through the region, region II is partially disturbed because only the leading wave has traversed the region, and region III is totally undisturbed since none

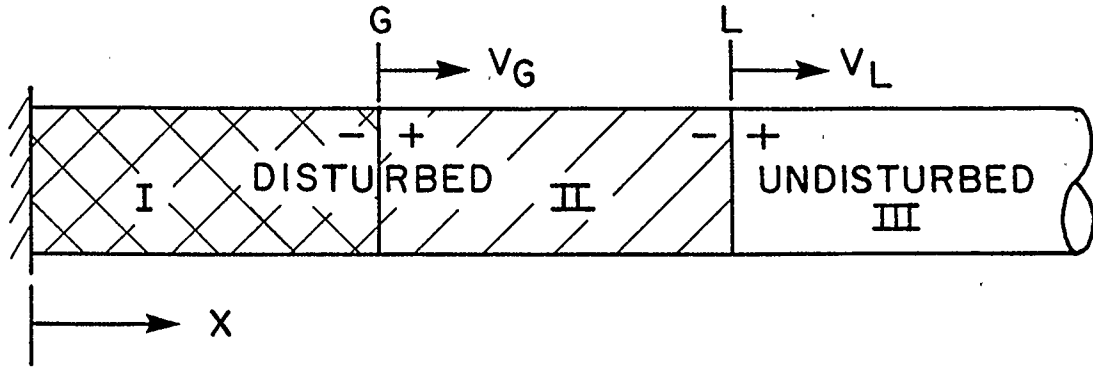


Figure 4.3 Illustration of the locations of the leading (L) and lagging (G) wavefronts in a bar.

of the waves has reached that region. In the (X,t) plane, therefore, the solution domain of interest is as shown in Figure (4.4).

The regions are identified as I, II, and III which correspond to the same regions in Figure (4.3).

First, the following notations are introduced.

- (i) f^{G-} denotes the value of a quantity f evaluated at a point immediately behind the lagging wavefront,
- (ii) f^{G+} denotes the value of a quantity f evaluated at a point immediately ahead of the lagging wavefront.

Similarly f^{L-} denotes the value of f immediately behind L and f^{L+} is the value immediately ahead of L .

Also,

$$[f]_G \equiv f^{G-} - f^{G+}, \quad (4.44a)$$

$$[f]_L \equiv f^{L-} - f^{L+}. \quad (4.44b)$$

Since for the investigations of interest in this thesis the body is assumed to be initially undisturbed, $f^{L+} = 0$, and so practically,

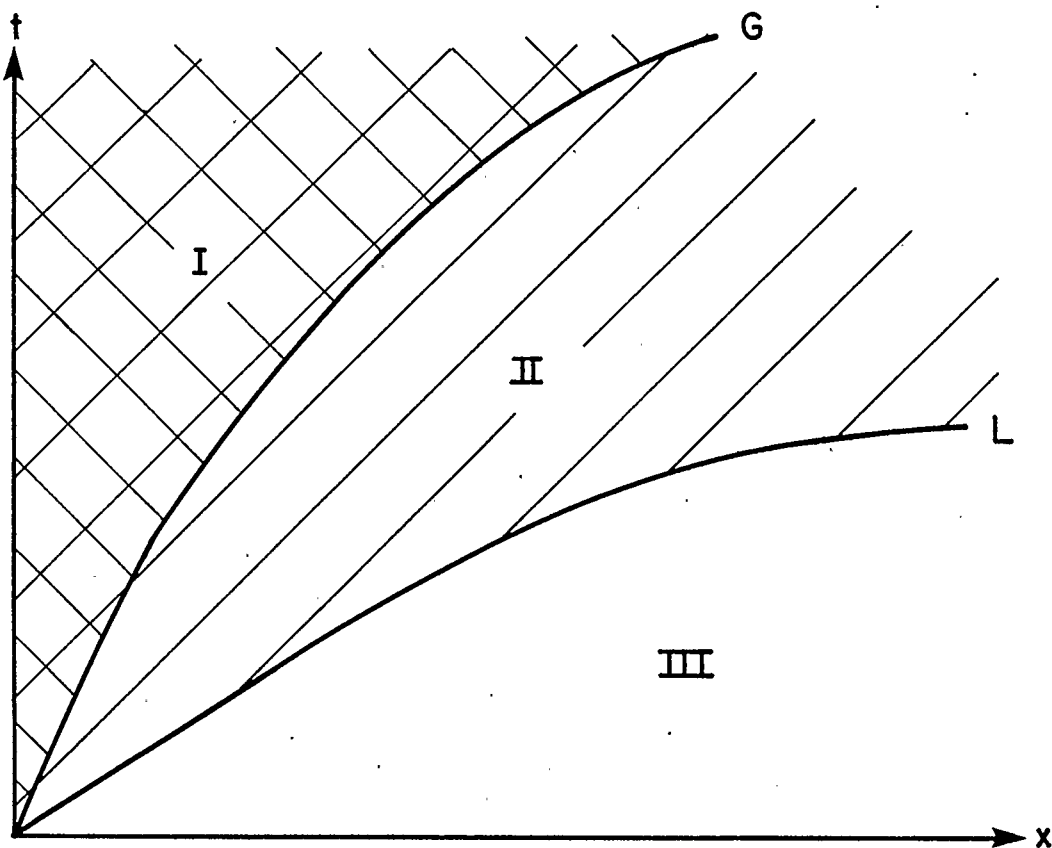


Figure 4.4 Illustration of the locations of the leading (L) and lagging (G) wavefronts in the x - t space.

$$[f]_L = f^{L-} . \quad (4.44c)$$

Also needed is a formula for evaluating the jumps of sums (or products) in terms of the jump of each of the summands (or factors). The following relations are useful in simplifying the jump relations (4.40) and (4.42) above.

$$[f + g] = [f] + [g] , \quad (4.45a)$$

$$[fg] = f^-[g] + [f]g^+ , \quad (4.45b)$$

$$[fg] = [f][g] + f^+[g] + g^+[f] . \quad (4.45c)$$

The proofs of these relations are easily obtained by invoking the definition of the jump in a quantity given earlier, equation (4.36).

On using the definitions (4.44) and the relations (4.45) in the jump relations, the following system of equations are obtained:

$$[\sigma] = [\sigma]_L + [\sigma]_G , \quad (4.46a)$$

$$[\theta] = [\theta]_L + [\theta]_G , \quad (4.46b)$$

$$[v] = [v]_L + [v]_G , \quad (4.46c)$$

$$[q] = [q]_L + [q]_G , \quad (4.46d)$$

$$[E] = [E]_L + [E]_G , \quad (4.46e)$$

$$[\psi] = [\psi]_L + [\psi]_G , \quad (4.46f)$$

$$[n] = [n]_L + [n]_G , \quad (4.46g)$$

$$[\sigma]_L = - \rho v_L [v]_L , \quad (4.46h)$$

$$[\sigma]_G = - \rho v_G [v]_G , \quad (4.46i)$$

$$[v]_L = - v_L [E]_L , \quad (4.46j)$$

$$[v]_G = -v_G[E]_G, \quad (4.46k)$$

$$[\sigma]_L[v]_L + [q]_L = -v_L[\psi]_L - \tau_R v_L[n]_L - v_L[\theta]_L[n]_L - \frac{1}{2}\rho v_L([v]_L)^2, \quad (4.46l)$$

$$\begin{aligned} & [\sigma]_G[v]_G + [\sigma]_L[v]_G + [v]_L[\sigma]_G + [q]_G = \\ & -v_G[\psi]_G - \tau_R v_G[n]_G - v_G[\theta]_G[n]_G - v_G[\theta]_L[n]_G \\ & - v_G[n]_L[\theta]_G - \frac{1}{2}\rho v_G([v]_G)^2 - \rho v_G[v]_L[v]_G, \end{aligned} \quad (4.46m)$$

$$[\theta]_L = -\tau_1 v_L[q]_L, \quad (4.46n)$$

$$[\theta]_G = -\tau_1 v_G[q]_G, \quad (4.46o)$$

$$[\psi]_L = -c_X([\theta]_L)^2 - \beta_R[\theta]_L[e]_L + \frac{1}{2}y_1([E]_L)^2, \quad (4.46p)$$

$$[\psi]_G = -c_X([\theta]_G)^2 - 2c_X[\theta]_L[\theta]_G - \beta_R[\theta]_G[E]_G$$

$$- \beta_R[\theta]_L[E]_G - \beta_R[\theta]_G[E]_L, \quad (4.46q)$$

$$[\sigma]_L = -\beta_R[\theta]_L + y_1[E]_L, \quad (4.46r)$$

$$[\sigma]_G = -\beta_R[\theta]_G + y_1[E]_G, \quad (4.46s)$$

$$[n]_L = c_y[\theta]_L + \beta_R[E]_L + \frac{1}{2}y_2([E]_L)^2, \quad (4.46t)$$

$$[n]_G = c_y[\theta]_G + \beta_R[E]_G + y_2[E]_L[E]_G + \frac{1}{2}y_2([E]_G)^2. \quad (4.46u)$$

In equations (4.46), the material constants involved are defined thus:

$$\tau_1 = \frac{\tau_0}{k} \quad (4.47a)$$

$$C_X = \frac{\rho C_1}{2T_R} \quad (4.47b)$$

$$C_Y = \frac{\rho C_1}{T_R} \quad (4.47c)$$

$$\beta_R = (3\lambda_R + 2\mu_R)\alpha_R, \quad (4.47d)$$

$$Y_1 = 2B_{11}, \quad (4.47e)$$

$$Y_2 = 2B_{12}. \quad (4.47f)$$

It is to be noted that the first seven equations in (4.46) are obtained by virtue of the fact that a physical discontinuity is split between the two wavefronts G and L.

The system of twenty-one simultaneous equations (4.46) contain the twenty-three unknowns:

$$[\sigma], [\sigma]_L, [\sigma]_G, [\theta], [\theta]_L, [\theta]_G,$$

$$[v], [v]_L, [v]_G, [q], [q]_L, [q]_G,$$

$$[\psi], [\psi]_L, [\psi]_G, [n], [n]_L, [n]_G,$$

$$[E], [E]_L, [E]_G, V_L, \text{ and } V_G.$$

Thus, in order for the system of algebraic equations to be solvable, two of these twenty-three quantities must be given. It is interesting that this immediately reminds one of the necessity to prescribe appropriate auxiliary conditions for the system. In this case, for example, $[\sigma]$ and $[\theta]$ could be known. This corresponds to prescribing the boundary conditions:

$$\sigma(0,t) = \sigma_0 f_\sigma(t) , \quad (4.48a)$$

$$\theta(0,t) = \theta_0 f_\theta(t) , \quad (4.48b)$$

which are time-dependent stress and temperature impacts that may be specified for the solution of the system of six simultaneous partial differential equations (4.24). Therefore, the jump analysis may also be used to determine the number of boundary conditions required to fully define a system of quasilinear hyperbolic equations.

4.5 Formal Statement of the Initial-Boundary-Value-Problem

The initial-boundary-value-problem to be solved may now be formally defined as follows:

Partial Differential Equations:

$$\frac{\partial v}{\partial t} - \frac{1}{\rho} \frac{\partial \sigma}{\partial X} - \frac{1}{\rho} f = 0 , \quad (4.49a)$$

$$\frac{\partial \sigma}{\partial t} - J_2(\sigma, \theta, Z, P) G_3(\sigma, \theta, Z, P) \frac{\partial v}{\partial X} + D_5(\sigma, \theta, Z, P) G_3(\sigma, \theta, Z, P) \frac{\partial q}{\partial X}$$

$$- G_3(\sigma, \theta, Z, P) G_8(\sigma, \theta, Z, P) = 0 , \quad (4.49b)$$

$$\frac{\partial \theta}{\partial t} + J_1(\sigma, \theta, Z, P) G_3(\sigma, \theta, Z, P) \frac{\partial v}{\partial X} - D_2(\theta) G_3(\sigma, \theta, Z, P) \frac{\partial q}{\partial X}$$

$$- G_3(\sigma, \theta, Z, P) G_9(\sigma, \theta, Z, P) = 0 , \quad (4.49c)$$

$$\frac{\partial q}{\partial t} - \frac{k}{\tau_0} \frac{\partial \theta}{\partial X} + \frac{q}{\tau_0} = 0 , \quad (4.49d)$$

$$\frac{\partial Z}{\partial t} + F_2(\sigma, Z) = 0 , \quad (4.49e)$$

$$\frac{\partial P}{\partial t} - G_1(\sigma, Z) = 0 . \quad (4.49f)$$

Initial Conditions:

$$\begin{aligned} v(X, 0) &= v_i(X) \\ \sigma(X, 0) &= \sigma_i(X) \\ \theta(X, 0) &= \theta_i(X) \\ q(X, 0) &= q_i(X) , \quad X > 0 , \\ Z(X, 0) &= Z_i(X) \\ P(X, 0) &= P_i(X) \end{aligned} \quad (4.50)$$

Boundary Conditions:

$$\begin{aligned} \text{Case (i):} \quad \sigma(0, t) &= \sigma_0(t) \\ \theta(0, t) &= \theta_0(t) , \quad t > 0 , \end{aligned} \quad (4.51a)$$

$$\begin{aligned} \text{Case (ii):} \quad v(0, t) &= v_0(t) \\ \theta(0, t) &= \theta_0(t) , \quad t > 0 , \end{aligned} \quad (4.51b)$$

Thus, the system of partial differential equations (4.49) is to be solved subject to the auxiliary conditions prescribed in equations (4.50) and (4.51). The solution will give the values of

$$\tilde{U}(X, t) = [v(X, t) \quad \sigma(X, t) \quad \theta(X, t) \quad q(X, t) \quad Z(X, t) \quad P(X, t)]^T. \quad (4.52)$$

The other four variables: E , ϵ , ψ , and η may now be computed from the algebraic relations given previously since

$$E(X, t) = \tilde{E}(\sigma(X, t), \theta(X, t), Z(X, t), P(X, t)) , \quad (4.53)$$

$$\epsilon(X, t) = E(X, t) + P(X, t) , \quad (4.54)$$

$$\psi = \tilde{\psi}(E(X,t), \theta(X,t), Z(X,t), P(X,t)) , \quad (4.55a)$$

or

$$\psi = \psi^*(\sigma(X,t), \theta(X,t), Z(X,t), P(X,t)) , \quad (4.55b)$$

$$\eta = \tilde{\eta}(E(X,t), \theta(X,t), Z(X,t), P(X,t)) , \quad (4.56a)$$

or

$$\eta = \eta^*(\sigma(X,t), \theta(X,t), Z(X,t), P(X,t)) . \quad (4.56b)$$

With these, all the ten dependent variables are now known at any location X and any time t .

The system of partial differential equations that govern the motion of the waves in smooth regions and the jump conditions which describe the relationships between discontinuities in the dependent variables have been fully defined. Both systems are highly nonlinear and coupled and can only be solved through numerical procedures.

CHAPTER 5

DEVELOPMENT OF COMPUTATIONAL ALGORITHMS

5.1 Introduction

The availability of modern advanced computers has made possible the solution of scientific and engineering problems of great complexity. This has, in turn, spurred a great deal of research in numerical analysis to effectively utilize the capabilities of present-day computers. In fact, developments are now reaching the stage where computing machines are being specifically designed for solving some particular problems.

Hyperbolic equations represent the most challenging class of partial differential equations (PDEs) to solve using standard numerical procedures. Whereas there are available many general-purpose computational algorithms for solving elliptic and parabolic PDEs the same cannot be said of hyperbolic equations. Yet such equations describe a variety of important physical phenomena such as neutron transport, wave mechanics, gas dynamics and vibrations. One of the important factors that makes the numerical solution of hyperbolic PDEs particularly difficult is the existence or development of strong discontinuities or shocks especially for nonlinear problems. It is known that in the case of nonlinear problems, shocks may develop even when the initial data are smooth.

The literature on the numerical solution of nonlinear hyperbolic PDEs is quite extensive. Standard procedures can be found in the texts by Ames [5.1], Mitchell and Griffiths [5.2], Leon and Lapidus [5.3], and Anderson et al. [5.4]. Most applications of available

numerical procedures have been in the area of fluid dynamics - especially gas dynamics. This is because equations which govern all unsteady flow and steady supersonic flow are hyperbolic in nature. The development of algorithms for numerically simulating these flows forms a very important branch of computational fluid dynamics (CFD) which is now a discipline in its own right. Applications in the area of solid mechanics, however, are comparatively very few since it is only in wave propagation and vibration problems that such equations arise.

The numerical methods that are used to analyze hyperbolic PDEs may be broadly classified into finite difference and finite element methods. Finite difference methods are discrete techniques in which the domain of interest is represented by a set of points or nodes and information between these points is commonly obtained using Taylor series expansions [5.3]. The finite element method employs piecewise continuous polynomials to interpolate between nodal points. Each of these techniques may lead to the phenomena of numerical dissipation and dispersion which create a lot of difficulties in formulating a numerical scheme. These problems have been well addressed (especially in the case of finite differences) for the so-called systems of hyperbolic conservation laws but a lot of work remains to be done for nonconservative systems such as the problem being considered in the present work.

There are considerable difficulties involved in the treatment of hyperbolic systems of PDEs by the finite element method especially in the presence of jump discontinuities. These difficulties require the development of new finite element techniques which differ from the standard ones to achieve satisfactory convergence properties. Efforts

in this direction are still very much in the developmental stage.

The application of the finite difference method may proceed via two main approaches. First, the system of PDEs may be directly discretized to obtain the appropriate difference equations which are then solved to obtain the values of the primary unknowns at the nodes. In the other approach, popularly referred to as the numerical method of characteristics, the system of equations is first transformed to a system of ordinary differential equations satisfied along the characteristic directions and finite differencing is subsequently applied. Furthermore, two different techniques are available when employing the method of characteristics. The first technique solves for the unknowns at grid points formed by the intersection of opposite families of characteristics. Whereas the grid of characteristics is useful in determining some physical features of the solution [5.5], extensive two-dimensional interpolation is required to obtain information along constant time lines, a given spatial position, or along a particle path [5.6]. Thus, this leads to programming difficulties. The second technique, usually referred to as the "constant-time technique" or "method of fixed time intervals" utilizes a computational mesh formed by lines of constant time and distance. However, the equations are still integrated along the characteristic directions and interpolation is employed to calculate the quantities of interest at the feet of the characteristic curves which do not coincide with a grid point. Although this latter technique introduces some additional errors due to interpolation, it has the advantage of being more orderly and manageable for efficient programming and high speed computations.

In this work, two separate computational algorithms are presented. The first is based on the application of the constant-time technique of the numerical method of characteristics while the other is based on the MacCormack finite difference scheme originally developed by MacCormack [5.7]. The latter has been widely applied to fluid dynamics problems but only a very few applications to problems in solid mechanics have been reported.

5.2 Application of the Numerical Method of Characteristics

The numerical method of characteristics is regarded as the natural technique for solving systems of hyperbolic equations and since the vast majority of wave propagation problems are hyperbolic in nature, the technique has been the most popular one applied to the numerical simulation of wave motions.

In this section, the numerical method of characteristics is applied for the development of a computational algorithm for solving the system of equations given in the preceding chapter. First, the differential equations satisfied along the characteristic directions are derived. These equations are then numerically integrated along the characteristic curves using the constant-time technique. Apart from the advantages given in the last section, this technique is considered more suitable in this work because of the highly nonlinear nature of the system of equations which gives rise to curvilinear characteristics.

It is to be recalled that the system of partial differential equations under consideration is given by:

$$\frac{\partial v}{\partial t} - \frac{1}{\rho} \frac{\partial \sigma}{\partial X} - \frac{1}{\rho} f = 0 , \quad (5.1a)$$

$$\frac{\partial \sigma}{\partial t} - J_2 G_3 \frac{\partial v}{\partial X} + D_5 G_3 \frac{\partial q}{\partial X} - G_3 G_8 = 0 , \quad (5.1b)$$

$$\frac{\partial \theta}{\partial t} + J_1 G_3 \frac{\partial v}{\partial X} - D_2 G_3 \frac{\partial q}{\partial X} - G_3 G_9 = 0 , \quad (5.1c)$$

$$\frac{\partial q}{\partial t} - \frac{k}{\tau_0} \frac{\partial \theta}{\partial X} + \frac{q}{\tau_0} = 0 , \quad (5.1d)$$

$$\frac{\partial Z}{\partial t} + F_2 = 0 , \quad (5.1e)$$

$$\frac{\partial P}{\partial t} - G_1 = 0 , \quad (5.1f)$$

where all the functions have been defined previously in Chapter 4. In the vector form, the equations are represented by:

$$\underline{U}_{\sim t} + \underline{A}(\underline{U}) \underline{U}_{\sim X} + \underline{B}(\underline{U}) = 0 , \quad (5.2)$$

where the vector $\underline{U}$, the matrix $\underline{A}$, and the vector $\underline{B}$ have also been defined in the preceding chapter.

From the eigenvalues of matrix $\underline{A}$ determined in the last chapter, it follows that the characteristic manifolds in the $\{X, t, \underline{U}\}$ hyperspace is given by the following:

$$\text{Corresponding to } \lambda_1: \frac{dX_1}{dt} = 0 , \quad (5.3a)$$

$$\text{Corresponding to } \lambda_2: \frac{dX_2}{dt} = 0 , \quad (5.3b)$$

$$\text{Corresponding to } \lambda_3: \frac{dX_3}{dt} = V_3(\underline{U}) , \quad (5.3c)$$

$$\text{Corresponding to } \lambda_4: \frac{dX_4}{dt} = V_4(\underline{U}) , \quad (5.3d)$$

$$\text{Corresponding to } \lambda_5: \frac{dX_5}{dt} = V_5(U) , \quad (5.3e)$$

$$\text{Corresponding to } \lambda_6: \frac{dX_6}{dt} = V_6(U) , \quad (5.3f)$$

where X_i , $i = 1, 2, \dots, 6$, are the characteristic curves.

Note that, as determined before,

$$V_4(\sigma, \theta, Z, P) = -V_3(\sigma, \theta, Z, P) , \quad (5.4a)$$

$$V_6(\sigma, \theta, Z, P) = -V_5(\sigma, \theta, Z, P) . \quad (5.4b)$$

Thus, two of the characteristic curves are straight lines (vertical in the X - t space) and the remaining four are curvilinear because the characteristic speeds V_3 and V_5 are nonlinear functions of the yet unknown solution vector, U .

For the equation (5.2), the left eigenvectors are found from the relation:

$$\ell^{(i)}(U) A(U) = \lambda^{(i)}(U) \ell^{(i)}(U) , \quad (5.5)$$

where $\ell^{(i)}(U)$ denotes the i^{th} left eigenvector which is also dependent on U . From equation (5.5), the following are found to be suitable left eigenvectors:

$$\ell^{(1)} = [0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0] , \quad (5.6a)$$

$$\ell^{(2)} = [0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1] , \quad (5.6b)$$

$$\tilde{\ell}^{(3)}(\tilde{U}) = \left\{ \begin{array}{c} 1 \\ -\frac{1}{\rho V_3} \\ \frac{\rho V_3^2 - J_2 G_3}{\rho V_3 J_1 G_3} \\ -\frac{\tau_0}{\rho k} \left(\frac{\rho V_3^2 - J_2 G_3}{J_1 G_3} \right) \\ 0 \\ 0 \end{array} \right\}^T, \quad (5.6c)$$

$$\tilde{\ell}^{(4)}(\tilde{U}) = \left\{ \begin{array}{c} 1 \\ \frac{1}{\rho V_3} \\ -\left(\frac{\rho V_3^2 - J_2 G_3}{\rho V_3 J_1 G_3} \right) \\ -\frac{\tau_0}{\rho k} \left(\frac{\rho V_3^2 - J_2 G_3}{J_1 G_3} \right) \\ 0 \\ 0 \end{array} \right\}^T, \quad (5.6d)$$

$$\tilde{\ell}^{(5)}(\tilde{U}) = \left\{ \begin{array}{c} 1 \\ -\frac{1}{\rho V_5} \\ \frac{\rho V_5^2 - J_2 G_3}{\rho V_5 J_1 G_3} \\ -\frac{\tau_0}{\rho k} \left(\frac{\rho V_5^2 - J_2 G_3}{J_1 G_3} \right) \\ 0 \\ 0 \end{array} \right\}^T, \quad (5.6e)$$

$$\tilde{\ell}^{(6)}(\tilde{U}) = \left\{ \begin{array}{c} 1 \\ \frac{1}{\rho V_5} \\ -(\frac{\rho V_5^2 - J_2 G_3}{\rho V_5 J_1 G_3}) \\ -\frac{\tau_0}{\rho k} (\frac{\rho V_5^2 - J_2 G_3}{J_1 G_3}) \\ 0 \\ 0 \end{array} \right\}^T, \quad (5.6f)$$

The equations satisfied along the characteristics are given by:

$$\tilde{\ell}^{(i)}(\tilde{U}) \frac{d\tilde{U}}{dt} + \tilde{\ell}^{(i)}(\tilde{U}) B(\tilde{U}) = 0, \quad i = 1, 2, \dots, 6. \quad (5.7)$$

Thus, the explicit form of equation (5.7) is as follows:

$$(i) \quad \frac{dZ}{dt} + F_2 = 0, \quad \text{along } \frac{dX}{dt} = 0. \quad (5.8a)$$

$$(ii) \quad \frac{dP}{dt} - G_1 = 0, \quad \text{along } \frac{dX}{dt} = 0. \quad (5.8b)$$

$$(iii) \quad \frac{dv}{dt} - \frac{1}{\rho V_3} \frac{d\sigma}{dt} + (\frac{\rho V_3^2 - J_2 G_3}{\rho V_3 J_1 G_3}) \frac{d\theta}{dt} - \frac{\tau_0}{\rho k} (\frac{\rho V_3^2 - J_2 G_3}{J_1 G_3}) \frac{dq}{dt} - \frac{1}{\rho} f \\ + \frac{1}{\rho V_3} G_3 G_8 - (\frac{\rho V_3^2 - J_2 G_3}{\rho V_3 J_1 G_3}) G_3 G_9 - \frac{1}{\rho k} (\frac{\rho V_3^2 - J_2 G_3}{J_1 G_3}) q = 0, \quad (5.8c)$$

$$\text{along } \frac{dX}{dt} = v_3.$$

$$(iv) \quad \frac{dv}{dt} + \frac{1}{\rho V_3} \frac{d\sigma}{dt} - (\frac{\rho V_3^2 - J_2 G_3}{\rho V_3 J_1 G_3}) \frac{d\theta}{dt} - \frac{\tau_0}{\rho k} (\frac{\rho V_3^2 - J_2 G_3}{J_1 G_3}) \frac{dq}{dt} - \frac{1}{\rho} f$$

$$-\frac{1}{\rho V_3} G_3 G_8 + \left(\frac{\rho V_3^2 - J_2 G_3}{\rho V_3 J_1 G_3} \right) G_3 G_9 - \frac{1}{\rho k} \left(\frac{\rho V_3^2 - J_2 G_3}{J_1 G_3} \right) q = 0, \quad (5.8d)$$

$$\text{along } \frac{dX}{dt} = -V_3.$$

$$\begin{aligned} (v) \quad & \frac{dv}{dt} - \frac{1}{\rho V_5} \frac{d\sigma}{dt} + \left(\frac{\rho V_5^2 - J_2 G_3}{\rho V_5 J_1 G_3} \right) \frac{d\theta}{dt} - \frac{\tau_0}{\rho k} \left(\frac{\rho V_5^2 - J_2 G_3}{J_1 G_3} \right) \frac{dq}{dt} - \frac{1}{\rho} f \\ & + \frac{1}{\rho V_5} G_3 G_8 - \left(\frac{\rho V_5^2 - J_2 G_3}{\rho V_5 J_1 G_3} \right) G_3 G_9 - \frac{1}{\rho k} \left(\frac{\rho V_5^2 - J_2 G_3}{J_1 G_3} \right) q = 0, \end{aligned} \quad (5.8e)$$

$$\text{along } \frac{dX}{dt} = V_5.$$

$$\begin{aligned} (vi) \quad & \frac{dv}{dt} + \frac{1}{\rho V_5} \frac{d\sigma}{dt} - \left(\frac{\rho V_5^2 - J_2 G_3}{\rho V_5 J_1 G_3} \right) \frac{d\theta}{dt} - \frac{\tau_0}{\rho k} \left(\frac{\rho V_5^2 - J_2 G_3}{J_1 G_3} \right) \frac{dq}{dt} - \frac{1}{\rho} f \\ & - \frac{1}{\rho V_5} G_3 G_8 + \left(\frac{\rho V_5^2 - J_2 G_3}{\rho V_5 J_1 G_3} \right) G_3 G_9 - \frac{1}{\rho k} \left(\frac{\rho V_5^2 - J_2 G_3}{J_1 G_3} \right) q = 0, \end{aligned} \quad (5.8f)$$

$$\text{along } \frac{dX}{dt} = -V_5.$$

These six equations are now to be numerically integrated along each of the six directions specified.

The solution grid in the X - t space is as shown in Figure 5.1. Starting with initial values of $\underline{U}$ at $A_0, A_1, A_2, A_3, A_4, \dots$, values of $\underline{U}$ at the next time step, that is, values of $\underline{U}$ at points $B_0, B_1, B_2, B_3, \dots$, and so on can be computed.

For example, starting from known values of $\underline{U}$ at A_0, A_1 and A_2 , we calculate the solution at point B_1 ; similarly we use the values of $\underline{U}$ at A_1, A_2, A_3 to calculate the value of $\underline{U}$ at B_2 , and continue this, say

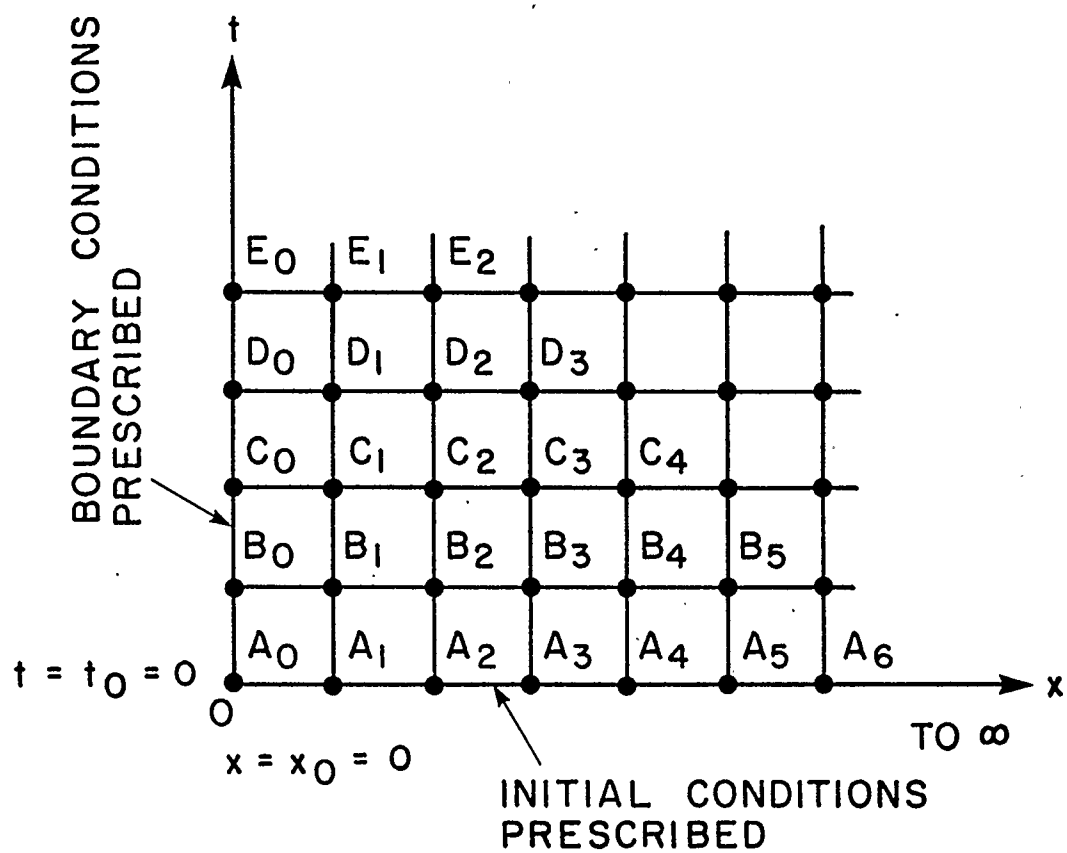


Figure 5.1 Solution grid in the $X-t$ plane.

until B_5 . Then we move on to the next time step and proceed in a similar fashion. The detailed description of this can be found in reference [5.5].

The grid points are classified as:

- (i) Interior Grid Points,
- (ii) Boundary Grid Points.

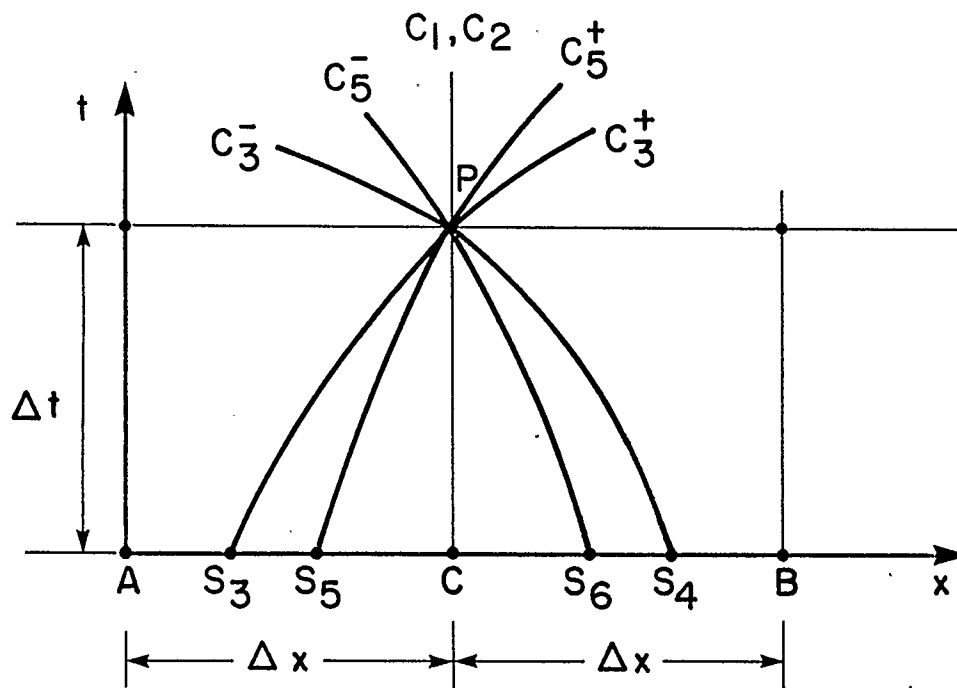
This is because the treatment given to a particular grid point depends on its type. Points (like B_1, B_2, C_1, D_3, E_2) which lie inside the domain of the solution are known as interior grid points. Points (like B_0, C_0, D_0, E_0) which lie on the boundary of the solution domain are boundary grid points.

In what follows, the finite difference schemes which correspond to each type of grid point are derived.

A second-order accurate scheme is used in order for the results to have a reasonable level of accuracy. This means that second-order approximations are used for the integrations and also quadratic interpolations are employed wherever interpolations are required.

5.2.1. Treatment of Interior Grid Points

A typical interior grid point, P , is shown in Figure 5.2. In Figure 5.2, S_3, S_5, S_6 , and S_4 are the feet of the characteristic curves C_3^+, C_5^+, C_5^- , and C_3^- , respectively. It is to be noted that the other characteristics are coincident and lie on the vertical line through point P . It should also be noted that $C_1, C_2, C_3^+, C_5^+, C_5^-$, and C_3^- are respectively associated with the eigenvalues $\lambda_1, \lambda_2, \lambda_3, \lambda_5, \lambda_6$, and λ_4 .



KNOWN :

$x_A, t_A, \underline{U}_A$

$x_C, t_C, \underline{U}_C$

$x_B, t_B, \underline{U}_B$

t_{S3}

t_{S5}

t_{S6}

t_{S4}

x_P, t_P

INTERMEDIATE UNKNOWN :

$x_{S3}, \underline{U}_{S3}$

$x_{S5}, \underline{U}_{S5}$

$x_{S6}, \underline{U}_{S6}$

$x_{S4}, \underline{U}_{S4}$

PRIMARY UNKNOWN :

$\underline{U}_P$

$$\underline{U} = [V \quad \sigma \quad \theta \quad q \quad Z \quad P]^T = \underline{U}(x, t)$$

Figure 5.2 Characteristic curves passing through a typical interior grid point, P.

The solution at point P is to be computed with the knowledge of the solutions at the points A, C, and B. In the procedure to be followed, the ordinary differential equations satisfied along the six characteristic curves will be numerically integrated along those curves. This will give six simultaneous equations for the unknowns at point P.

It is appropriate at this juncture to define the finite difference approximations of integrals. A first-order or linear approximation is defined by the relation:

$$\int_{x_0}^{x_1} f(x) dx = f(x_0)(x_1 - x_0) . \quad (5.9)$$

The second-order approximation is expressed by the trapezoidal rule formula as:

$$\int_{x_0}^{x_1} f(x) dx = \frac{1}{2}[f(x_0) + f(x_1)](x_1 - x_0) . \quad (5.10)$$

The X coordinates of the feet of the characteristic curves designated X_{S3} , X_{S5} , X_{S6} , and X_{S4} are determined by a second-order integration of the characteristic curves. The results obtained are:

$$X_{S3} = X_P - \frac{1}{2}(V_{3S3} + V_{3P})\Delta t , \quad (5.11a)$$

$$X_{S5} = X_P - \frac{1}{2}(V_{5S5} + V_{5P})\Delta t , \quad (5.11b)$$

$$X_{S6} = X_P + \frac{1}{2}(V_{5S6} + V_{5P})\Delta t , \quad (5.11c)$$

$$X_{S4} = X_P + \frac{1}{2}(V_{3S4} + V_{3P})\Delta t , \quad (5.11d)$$

where V_{iS_j} denotes the value of V_i at point S_j , and V_{iP} denotes the value of V_i at point P. Note that X_{S3} , X_{S5} , X_{S6} , and X_{S4} depend on the yet unknown values of the solution at point P. Furthermore, they also depend on the yet unknown quantities U_{S3} , U_{S5} , U_{S6} , and U_{S4} .

The next step, therefore, is to estimate the values of U_{S3} , U_{S5} , U_{S6} , and U_{S4} using quadratic interpolation with a knowledge of the values of U_A , U_C , U_B , X_A , X_C , X_B , and the estimates of X_{S3} , X_{S5} , X_{S6} , and X_{S4} given in equations (5.11). Thus, the following results are obtained:

$$\begin{aligned} U_{S3} = & U_C + \frac{1}{4}\alpha(U_A - U_B)(V_{3S3} + V_{3P}) \\ & + \frac{1}{8}\alpha^2(U_A + U_B - 2U_C)(V_{3S3} + V_{3P})^2, \end{aligned} \quad (5.12a)$$

$$\begin{aligned} U_{S5} = & U_C + \frac{1}{4}\alpha(U_A - U_B)(V_{5S5} + V_{5P}) \\ & + \frac{1}{8}\alpha^2(U_A + U_B - 2U_C)(V_{5S5} + V_{5P})^2, \end{aligned} \quad (5.12b)$$

$$\begin{aligned} U_{S6} = & U_C - \frac{1}{4}\alpha(U_A - U_B)(V_{5S6} + V_{5P}) \\ & + \frac{1}{8}\alpha^2(U_A + U_B - 2U_C)(V_{5S6} + V_{5P})^2, \end{aligned} \quad (5.12c)$$

$$U_{S4} = U_C - \frac{1}{4}\alpha(U_A - U_B)(V_{3S4} + V_{3P})$$

$$+ \frac{1}{8} \alpha^2 (\underline{U}_A + \underline{U}_B - 2\underline{U}_C) (\underline{V}_{3S4} + \underline{V}_{3P})^2, \quad (5.12d)$$

where

$$\alpha = \frac{\Delta t}{\Delta X}. \quad (5.12e)$$

Note, again, that the right hand sides of equations (5.12) depend on $\underline{U}_{S3}$, $\underline{U}_{S5}$, $\underline{U}_{S6}$, $\underline{U}_{S4}$, and $\underline{U}_P$ which are all yet unknown.

We now find second-order approximations to the integrals of the ordinary differential equations along the characteristic curves, that is, equations (5.8a - 5.8f). Because of the complex nature of equations (5.8a - 5.8f), their numerical integration involves lengthy algebraic manipulations and so the details are omitted here. The result is that six simultaneous algebraic equations which are nonlinear in the primary unknowns $\underline{U}_P = [\underline{v}_P \quad \underline{\sigma}_P \quad \underline{\theta}_P \quad \underline{q}_P \quad \underline{Z}_P \quad \underline{P}_P]^T$ are obtained. The equations also contain the unknowns $\underline{U}_{S3}$, $\underline{U}_{S5}$, $\underline{U}_{S6}$, and $\underline{U}_{S4}$. The nonlinear nature of the equations together with the presence of intermediate unknowns immediately suggest that an iterative procedure must be employed thereby giving the finite difference scheme an implicit character.

The iterative equations to be solved are therefore as follows:

$$\underline{Z}_P^{(k+1)} = \underline{Z}_C - \frac{1}{2} (\underline{F}_{2C} + \underline{F}_{2P}^{(k)}) \Delta t, \quad (5.13a)$$

$$\underline{P}_P^{(k+1)} = \underline{P}_C + \frac{1}{2} (\underline{G}_{1C} + \underline{G}_{1P}^{(k)}) \Delta t, \quad (5.13b)$$

$$({}^1Q_{S3}^{(k)} + Q_{1P}^{(k)}) \underline{v}_P^{(k+1)} - ({}^2Q_{S3}^{(k)} + Q_{2P}^{(k)}) \underline{\sigma}_P^{(k+1)} + ({}^3Q_{S3}^{(k)} + Q_{3P}^{(k)}) \underline{\theta}_P^{(k+1)}$$

$$\begin{aligned}
& - ({}^4Q_{S3}^{(k)} + Q_{4P}^{(k)})q_P^{(k+1)} = ({}^1Q_{S3}^{(k)} + Q_{1P}^{(k)})v_{S3}^{(k)} - ({}^2Q_{S3}^{(k)} + Q_{2P}^{(k)})\sigma_{S3}^{(k)} \\
& + ({}^3Q_{S3}^{(k)} + Q_{3P}^{(k)})\theta_{S3}^{(k)} - ({}^4Q_{S3}^{(k)} + Q_{4P}^{(k)})q_{S3}^{(k)} + \{ (Q_5^f)_{S3}^{(k)} + (Q_5^f)_P^{(k)} \\
& + (Q_8q)_{S3}^{(k)} + (Q_8q)_P^{(k)} + {}^7Q_{S3}^{(k)} + Q_{7P}^{(k)} - {}^6Q_{S3}^{(k)} - Q_{6P}^{(k)} \} \Delta t, \quad (5.13c)
\end{aligned}$$

$$\begin{aligned}
& ({}^1Q_{S4}^{(k)} + Q_{1P}^{(k)})v_P^{(k+1)} + ({}^2Q_{S4}^{(k)} + Q_{2P}^{(k)})\sigma_P^{(k+1)} - ({}^3Q_{S4}^{(k)} + Q_{3P}^{(k)})\theta_P^{(k+1)} \\
& - ({}^4Q_{S4}^{(k)} + Q_{4P}^{(k)})q_P^{(k+1)} = ({}^1Q_{S4}^{(k)} + Q_{1P}^{(k)})v_{S4}^{(k)} + ({}^2Q_{S4}^{(k)} + Q_{2P}^{(k)})\sigma_{S4}^{(k)} \\
& - ({}^3Q_{S4}^{(k)} + Q_{3P}^{(k)})\theta_{S4}^{(k)} - ({}^4Q_{S4}^{(k)} + Q_{4P}^{(k)})q_{S4}^{(k)} + \{ (Q_5^f)_{S4}^{(k)} + (Q_5^f)_P^{(k)} \\
& + (Q_8q)_{S4}^{(k)} + (Q_8q)_P^{(k)} + {}^6Q_{S4}^{(k)} + Q_{6P}^{(k)} - {}^7Q_{S4}^{(k)} - Q_{7P}^{(k)} \} \Delta t, \quad (5.13d)
\end{aligned}$$

$$\begin{aligned}
& ({}^1W_{S5}^{(k)} + W_{1P}^{(k)})v_P^{(k+1)} - ({}^2W_{S5}^{(k)} + W_{2P}^{(k)})\sigma_P^{(k+1)} + ({}^3W_{S5}^{(k)} + W_{3P}^{(k)})\theta_P^{(k+1)} \\
& - ({}^4W_{S5}^{(k)} + W_{4P}^{(k)})q_P^{(k+1)} = ({}^1W_{S5}^{(k)} + W_{1P}^{(k)})v_{S5}^{(k)} - ({}^2W_{S5}^{(k)} + W_{2P}^{(k)})\sigma_{S5}^{(k)} \\
& + ({}^3W_{S5}^{(k)} + W_{3P}^{(k)})\theta_{S5}^{(k)} - ({}^4W_{S5}^{(k)} + W_{4P}^{(k)})q_{S5}^{(k)} + \{ (W_5^f)_{S5}^{(k)} + (W_5^f)_P^{(k)} \\
& + (W_8q)_{S5}^{(k)} + (W_8q)_P^{(k)} + {}^7W_{S5}^{(k)} + W_{7P}^{(k)} - {}^6W_{S5}^{(k)} - W_{6P}^{(k)} \} \Delta t, \quad (5.13e)
\end{aligned}$$

$$({}^1W_{S6}^{(k)} + W_{1P}^{(k)})v_P^{(k+1)} + ({}^2W_{S6}^{(k)} + W_{2P}^{(k)})\sigma_P^{(k+1)} - ({}^3W_{S6}^{(k)} + W_{3P}^{(k)})\theta_P^{(k+1)}$$

$$\begin{aligned}
- ({}^4W_{S6}^{(k)} + W_{4P}^{(k)})q_P^{(k+1)} &= ({}^1W_{S6}^{(k)} + W_{1P}^{(k)})v_{S6}^{(k)} + ({}^2W_{S6}^{(k)} + W_{2P}^{(k)})\sigma_{S6}^{(k)} \\
- ({}^3W_{S6}^{(k)} + W_{3P}^{(k)})\theta_{S6}^{(k)} &- ({}^4W_{S6}^{(k)} + W_{4P}^{(k)})q_{S6}^{(k)} + \{ (W_{5f}^{(k)})_{S6} + (W_{5f}^{(k)})_P \\
+ (W_{8q}^{(k)})_{S6} + (W_{8q}^{(k)})_P &+ {}^6W_{S6}^{(k)} + W_{6P}^{(k)} - {}^7W_{S6}^{(k)} - W_{7P}^{(k)} \} \Delta t, \quad (5.13f)
\end{aligned}$$

Also, the intermediate unknowns are to be found from the following iterative equations:

$$\begin{aligned}
\tilde{U}_{S3}^{(k+1)} &= \tilde{U}_C + \frac{1}{4}\alpha (\tilde{U}_A - \tilde{U}_B) (v_{3S3}^{(k)} + v_{3P}^{(k)}) + \frac{1}{8}\alpha^2 (\tilde{U}_A + \tilde{U}_B - 2\tilde{U}_C) \\
&\quad (v_{3S3}^{(k)} + v_{3P}^{(k)})^2, \quad (5.14a)
\end{aligned}$$

$$\begin{aligned}
\tilde{U}_{S5}^{(k+1)} &= \tilde{U}_C + \frac{1}{4}\alpha (\tilde{U}_A - \tilde{U}_B) (v_{5S5}^{(k)} + v_{5P}^{(k)}) + \frac{1}{8}\alpha^2 (\tilde{U}_A + \tilde{U}_B - 2\tilde{U}_C) \\
&\quad (v_{5S5}^{(k)} + v_{5P}^{(k)})^2, \quad (5.14b)
\end{aligned}$$

$$\begin{aligned}
\tilde{U}_{S6}^{(k+1)} &= \tilde{U}_C - \frac{1}{4}\alpha (\tilde{U}_A - \tilde{U}_B) (v_{5S6}^{(k)} + v_{5P}^{(k)}) + \frac{1}{8}\alpha^2 (\tilde{U}_A + \tilde{U}_B - 2\tilde{U}_C) \\
&\quad (v_{5S6}^{(k)} + v_{5P}^{(k)})^2, \quad (5.14c)
\end{aligned}$$

$$\begin{aligned}
\tilde{U}_{S4}^{(k+1)} &= \tilde{U}_C - \frac{1}{4}\alpha (\tilde{U}_A - \tilde{U}_B) (v_{3S4}^{(k)} + v_{3P}^{(k)}) + \frac{1}{8}\alpha^2 (\tilde{U}_A + \tilde{U}_B - 2\tilde{U}_C) \\
&\quad (v_{3S4}^{(k)} + v_{3P}^{(k)})^2, \quad (5.14d)
\end{aligned}$$

$$(k = 0, 1, 2, \dots)$$

In these equations,

$$i_{Q_{Sj}}^{(k)} \equiv Q_i^{(k)}(U_{Sj}) , \quad (5.15a)$$

$$Q_{iP}^{(k)} \equiv Q_i^{(k)}(U_P) , \quad (5.15b)$$

$$i_{W_{Sj}}^{(k)} \equiv W_i^{(k)}(U_{Sj}) , \quad (5.15c)$$

$$W_{iP}^{(k)} \equiv W_i^{(k)}(U_P) , \quad (5.15d)$$

$$V_{iSj}^{(k)} = V_i^{(k)}(U_{Sj}) , \quad (5.15e)$$

$$V_{iP}^{(k)} = V_i^{(k)}(U_P) . \quad (5.15f)$$

Furthermore, the numerical functions Q_i and W_i are defined as:

$$Q_1(U) = \rho V_3 J_1 G_3 , \quad (5.16a)$$

$$Q_2(U) = J_1 G_3 , \quad (5.16b)$$

$$Q_3(U) = \rho V_3^2 - J_2 G_3 , \quad (5.16c)$$

$$Q_4(U) = \frac{\tau_0}{k} V_3 (\rho V_3^2 - J_2 G_3) , \quad (5.16d)$$

$$Q_5(U) = V_3 J_1 G_3 , \quad (5.16e)$$

$$Q_6(U) = G_3^2 G_8 J_1 , \quad (5.16f)$$

$$Q_7(U) = (\rho V_3^2 - J_2 G_3) G_3 G_9 , \quad (5.16g)$$

$$Q_8(U) = \frac{1}{k} (\rho V_3^2 - J_2 G_3) V_3 , \quad (5.16h)$$

$$W_1(U) = \rho V_5 J_1 G_3 , \quad (5.16i)$$

$$W_2(U) = J_1 G_3 , \quad (5.16j)$$

$$W_3(U) = \rho V_5^2 - J_2 G_3 , \quad (5.16k)$$

$$W_4(U) = \frac{\tau_0}{k} V_5 (\rho V_5^2 - J_2 G_3) , \quad (5.16l)$$

$$W_5(U) = V_5 J_1 G_3 , \quad (5.16m)$$

$$W_6(U) = G_3^2 G_8 J_1 , \quad (5.16n)$$

$$W_7(U) = (\rho V_5^2 - J_2 G_3) G_3 G_9 , \quad (5.16o)$$

$$W_8(U) = \frac{1}{k} (\rho V_5^2 - J_2 G_3) V_5 . \quad (5.16p)$$

Equations (5.13a) - (5.13f) constitute a system of algebraic equations to be solved for $v_P^{(k+1)}$, $\sigma_P^{(k+1)}$, $\theta_P^{(k+1)}$, $q_P^{(k+1)}$, $z_P^{(k+1)}$ and $P_P^{(k+1)}$ at each iteration level. It is to be noted that the system of six simultaneous algebraic equations are now linear in $v_P^{(k+1)}$, $\sigma_P^{(k+1)}$, $\theta_P^{(k+1)}$, $q_P^{(k+1)}$, $z_P^{(k+1)}$, and $P_P^{(k+1)}$ at each iteration step.

However, starting values of all the unknown quantities (both intermediate and primary) are required to begin the iterative process. In other words, values must be assigned to the quantities $U_{S3}^{(0)}$, $U_{S5}^{(0)}$, $U_{S6}^{(0)}$, $U_{S4}^{(0)}$, and $U_P^{(0)}$ in order to start the iterative process. In order for the iteration to have good convergence properties, these quantities cannot be arbitrarily assigned. A first-order-accurate procedure will be used to estimate the values of U_{S3} , U_{S5} , U_{S6} , U_{S4} , and U_P and these values will serve as the starting values for the above iterative procedure.

The major steps above are now repeated but this time first-order integrations and linear interpolations are employed to obtain:

$$z_P^{(0)} = z_C - F_{2C} \Delta t, \quad (5.17a)$$

$$P_P^{(0)} = P_C + G_{1C} \Delta t, \quad (5.17b)$$

$${}^1_{Q_{S3}} v_P^{(0)} - {}^2_{Q_{S3}} \sigma_P^{(0)} + {}^3_{Q_{S3}} \theta_P^{(0)} - {}^4_{Q_{S3}} q_P^{(0)} =$$

$$\Lambda_{S3}^1 + \Lambda_{S3}^2 \Delta t, \quad (5.17c)$$

$${}^1_{Q_{S4}} v_P^{(0)} + {}^2_{Q_{S4}} \sigma_P^{(0)} - {}^3_{Q_{S4}} \theta_P^{(0)} - {}^4_{Q_{S4}} q_P^{(0)} =$$

$$^3\Lambda_{S4} + ^4\Lambda_{S4}\Delta t , \quad (5.17d)$$

$$^1W_{S5}^{(0)} v_P^{(0)} - ^2W_{S5}^{(0)} \sigma_P^{(0)} + ^3W_{S5}^{(0)} \theta_P^{(0)} - ^4W_{S5}^{(0)} q_P^{(0)} =$$

$$^5\Lambda_{S5} + ^6\Lambda_{S5}\Delta t , \quad (5.17e)$$

$$^1W_{S6}^{(0)} v_P^{(0)} + ^2W_{S6}^{(0)} \sigma_P^{(0)} - ^3W_{S6}^{(0)} \theta_P^{(0)} - ^4W_{S6}^{(0)} q_P^{(0)} =$$

$$^7\Lambda_{S6} + ^8\Lambda_{S6}\Delta t . \quad (5.17f)$$

The quantities $^1\Lambda_{S3}$, $^2\Lambda_{S3}$, $^3\Lambda_{S4}$, $^4\Lambda_{S4}$, $^5\Lambda_{S5}$, $^6\Lambda_{S5}$, $^7\Lambda_{S6}$, and $^8\Lambda_{S6}$ are numerical functions defined as follows:

$$^1\Lambda_{S3} = ^1Q_{S3}^{(0)} v_{S3}^{(0)} - ^2Q_{S3}^{(0)} \sigma_{S3}^{(0)} + ^3Q_{S3}^{(0)} \theta_{S3}^{(0)} - ^4Q_{S3}^{(0)} q_{S3}^{(0)} , \quad (5.18a)$$

$$^2\Lambda_{S3} = ^7Q_{S3}^{(0)} + (Q_{5f})_{S3}^{(0)} + (Q_{8q})_{S3}^{(0)} - ^6Q_{S3}^{(0)} , \quad (5.18b)$$

$$^3\Lambda_{S4} = ^1Q_{S4}^{(0)} v_{S4}^{(0)} + ^2Q_{S4}^{(0)} \sigma_{S4}^{(0)} - ^3Q_{S4}^{(0)} \theta_{S4}^{(0)} - ^4Q_{S4}^{(0)} q_{S4}^{(0)} , \quad (5.18c)$$

$$^4\Lambda_{S4} = (Q_{5f})_{S4}^{(0)} + ^6Q_{S4}^{(0)} - ^7Q_{S4}^{(0)} + (Q_{8q})_{S4}^{(0)} , \quad (5.18d)$$

$$^5\Lambda_{S5} = ^1W_{S5}^{(0)} v_{S5}^{(0)} - ^2W_{S5}^{(0)} \sigma_{S5}^{(0)} + ^3W_{S5}^{(0)} \theta_{S5}^{(0)} - ^4W_{S5}^{(0)} q_{S5}^{(0)} , \quad (5.18e)$$

$$^6\Lambda_{S5} = ^7W_{S5}^{(0)} + (W_{5f})_{S5}^{(0)} + (W_{8q})_{S5}^{(0)} - ^6W_{S5}^{(0)} , \quad (5.18f)$$

$${}^7\Lambda_{S6} = {}^1W_{S6}^{(0)} v_{S6}^{(0)} + {}^2W_{S6}^{(0)} \sigma_{S6}^{(0)} - {}^3W_{S6}^{(0)} \theta_{S6}^{(0)} - {}^4W_{S6}^{(0)} q_{S6}^{(0)}, \quad (5.18g)$$

$${}^8\Lambda_{S6} = (W_{5f})_{S6}^{(0)} + {}^6W_{S6}^{(0)} - {}^7W_{S6}^{(0)} + (W_{8q})_{S6}^{(0)}. \quad (5.18h)$$

Again, it can be seen that equations (5.17) contain the intermediate unknowns $U_{S3}^{(0)}$, $U_{S5}^{(0)}$, $U_{S6}^{(0)}$, and $U_{S4}^{(0)}$ which are to be found from the relations:

$$U_{S3}^{(0)} = U_C(1 - \alpha V_{3C}) + \alpha U_A V_{3C}, \quad (5.19a)$$

$$U_{S5}^{(0)} = U_C(1 - \alpha V_{5C}) + \alpha U_A V_{5C}, \quad (5.19b)$$

$$U_{S6}^{(0)} = U_C(1 - \alpha V_{5C}) + \alpha U_B V_{5C}, \quad (5.19c)$$

$$U_{S4}^{(0)} = U_C(1 - \alpha V_{3C}) + \alpha U_B V_{3C}. \quad (5.19d)$$

Equations (5.17c) - (5.17f) may be put in the more compact form:

$$\underline{a}^{(0)} u_P^{(0)} = \underline{h}^{(0)}, \quad (5.20)$$

where the vector $u_P^{(0)}$ is defined as

$$u_P^{(0)} = \begin{Bmatrix} v_P^{(0)} \\ \sigma_P^{(0)} \\ \theta_P^{(0)} \\ q_P^{(0)} \end{Bmatrix}, \quad (5.21a)$$

the vector $\tilde{h}^{(0)}$ is defined as

$$\tilde{h}^{(0)} = \begin{Bmatrix} 1\Lambda_{S3} + 2\Lambda_{S3}\Delta t \\ 3\Lambda_{S4} + 4\Lambda_{S4}\Delta t \\ 5\Lambda_{S5} + 6\Lambda_{S5}\Delta t \\ 7\Lambda_{S6} + 8\Lambda_{S6}\Delta t \end{Bmatrix}, \quad (5.21b)$$

and the matrix $\underline{a}^{(0)}$ is defined as

$$\underline{a}^{(0)} = \begin{bmatrix} 1_{Q_{S3}}(0) & -2_{Q_{S3}}(0) & 3_{Q_{S3}}(0) & -4_{Q_{S3}}(0) \\ 1_{Q_{S4}}(0) & 2_{Q_{S4}}(0) & -3_{Q_{S4}}(0) & -4_{Q_{S4}}(0) \\ 1_{W_{S5}}(0) & -2_{W_{S5}}(0) & 3_{W_{S5}}(0) & -4_{W_{S5}}(0) \\ 1_{W_{S6}}(0) & 2_{W_{S6}}(0) & -3_{W_{S6}}(0) & -4_{W_{S6}}(0) \end{bmatrix}. \quad (5.21c)$$

It is also more convenient to put the simultaneous equations (5.13c) - (5.13f) in the compact form:

$$\underline{R}^{(k)} \underline{u}_P^{(k+1)} = \underline{b}^{(k)}, \quad (5.22)$$

where

$$\underline{u}_P^{(k+1)} = \begin{Bmatrix} v_P^{(k+1)} \\ \sigma_P^{(k+1)} \\ \theta_P^{(k+1)} \\ q_P^{(k+1)} \end{Bmatrix}. \quad (5.23)$$

It is easy to see from equations (5.13) that the four components of

vector $b^{(k)}$ are given by:

$$\begin{aligned}
 b_1^{(k)} = & ({}^1Q_{S3}^{(k)} + Q_{1P}^{(k)})v_{S3}^{(k)} - ({}^2Q_{S3}^{(k)} + Q_{2P}^{(k)})\sigma_{S3}^{(k)} \\
 & + ({}^3Q_{S3}^{(k)} + Q_{3P}^{(k)})\theta_{S3}^{(k)} - ({}^4Q_{S3}^{(k)} + Q_{4P}^{(k)})q_{S3}^{(k)} + \{ (Q_5^f)^{(k)}_{S3} \\
 & + (Q_5^f)_P^{(k)} + (Q_8q)_{S3}^{(k)} + (Q_8q)_P^{(k)} + {}^7Q_{S3}^{(k)} + Q_{7P}^{(k)} \\
 & - {}^6Q_{S3}^{(k)} - Q_{6P}^{(k)} \} \Delta t, \quad (5.24a)
 \end{aligned}$$

$$\begin{aligned}
 b_2^{(k)} = & ({}^1Q_{S4}^{(k)} + Q_{1P}^{(k)})v_{S4}^{(k)} + ({}^2Q_{S4}^{(k)} + Q_{2P}^{(k)})\sigma_{S4}^{(k)} - ({}^3Q_{S4}^{(k)} + Q_{3P}^{(k)})\theta_{S4}^{(k)} \\
 & - ({}^4Q_{S4}^{(k)} + Q_{4P}^{(k)})q_{S4}^{(k)} + \{ (Q_5^f)^{(k)}_{S4} + (Q_5^f)_P^{(k)} + Q_{8q}^{(k)}_{S4} + (Q_{8q})_P^{(k)} \\
 & + {}^6Q_{S4}^{(k)} + Q_{6P}^{(k)} - {}^7Q_{S4}^{(k)} - Q_{7P}^{(k)} \} \Delta t, \quad (5.24b)
 \end{aligned}$$

$$\begin{aligned}
 b_3^{(k)} = & ({}^1W_{S5}^{(k)} + W_{1P}^{(k)})v_{S5}^{(k)} - ({}^2W_{S5}^{(k)} + W_{2P}^{(k)})\sigma_{S5}^{(k)} + ({}^3W_{S5}^{(k)} + W_{3P}^{(k)})\theta_{S5}^{(k)} \\
 & - ({}^4W_{S5}^{(k)} + W_{4P}^{(k)})q_{S5}^{(k)} + \{ (W_5^f)^{(k)}_{S5} + (W_5^f)_P^{(k)} + (W_{8q})_{S5}^{(k)} + (W_{8q})_P^{(k)} \\
 & + {}^7W_{S5}^{(k)} + W_{7P}^{(k)} - {}^6W_{S5}^{(k)} - W_{6P}^{(k)} \} \Delta t, \quad (5.24c)
 \end{aligned}$$

$$\begin{aligned}
 b_4^{(k)} = & ({}^1W_{S6}^{(k)} + W_{1P}^{(k)})v_{S6}^{(k)} + ({}^2W_{S6}^{(k)} + W_{2P}^{(k)})\sigma_{S6}^{(k)} - ({}^3W_{S6}^{(k)} + W_{3P}^{(k)})\theta_{S6}^{(k)} \\
 & - ({}^4W_{S6}^{(k)} + W_{4P}^{(k)})q_{S6}^{(k)} + \{ (W_5^f)^{(k)}_{S6} + (W_5^f)_P^{(k)} + (W_{8q})_{S6}^{(k)} + (W_{8q})_P^{(k)}
 \end{aligned}$$

$$+ {}^6W_{S6}^{(k)} + W_{6P}^{(k)} - {}^7W_{S6}^{(k)} - W_{7P}^{(k)} \} \Delta t . \quad (5.24d)$$

The sixteen elements of matrix $\underline{R}^{(k)}$ may also be identified as:

$$\begin{aligned} R_{11}^{(k)} &= {}^1Q_{S3}^{(k)} + Q_{1P}^{(k)} , & R_{12}^{(k)} &= -({}^2Q_{S3}^{(k)} + Q_{2P}^{(k)}) , \\ R_{13}^{(k)} &= {}^3Q_{S3}^{(k)} + Q_{3P}^{(k)} , & R_{14}^{(k)} &= -({}^4Q_{S3}^{(k)} + Q_{4P}^{(k)}) , \\ R_{21}^{(k)} &= {}^1Q_{S4}^{(k)} + Q_{1P}^{(k)} , & R_{22}^{(k)} &= {}^2Q_{S4}^{(k)} + Q_{2P}^{(k)} , \\ R_{23}^{(k)} &= -({}^3Q_{S4}^{(k)} + Q_{3P}^{(k)}) , & R_{24}^{(k)} &= -({}^4Q_{S4}^{(k)} + Q_{4P}^{(k)}) , \\ R_{31}^{(k)} &= {}^1W_{S5}^{(k)} + W_{1P}^{(k)} , & R_{32}^{(k)} &= -({}^2W_{S5}^{(k)} + W_{2P}^{(k)}) , \\ R_{33}^{(k)} &= {}^3W_{S5}^{(k)} + W_{3P}^{(k)} , & R_{34}^{(k)} &= -({}^4W_{S5}^{(k)} + W_{4P}^{(k)}) , \\ R_{41}^{(k)} &= {}^1W_{S6}^{(k)} + W_{1P}^{(k)} , & R_{42}^{(k)} &= {}^2W_{S6}^{(k)} + W_{2P}^{(k)} , \\ R_{43}^{(k)} &= -({}^3W_{S6}^{(k)} + W_{3P}^{(k)}) , & R_{44}^{(k)} &= -({}^4W_{S6}^{(k)} + W_{4P}^{(k)}) . \end{aligned} \quad (5.25)$$

Thus, the procedure for solving for the primary unknowns $\underline{U}_P$ consists of the following main items:

- (i) Start iteration and set iteration counter to $k = 0$,
- (ii) Calculate the starting values of the intermediate unknowns $\underline{U}_{S3}^{(0)}$, $\underline{U}_{S5}^{(0)}$, $\underline{U}_{S6}^{(0)}$, and $\underline{U}_{S4}^{(0)}$ using the relations given in equations (5.19a)-(5.19d),

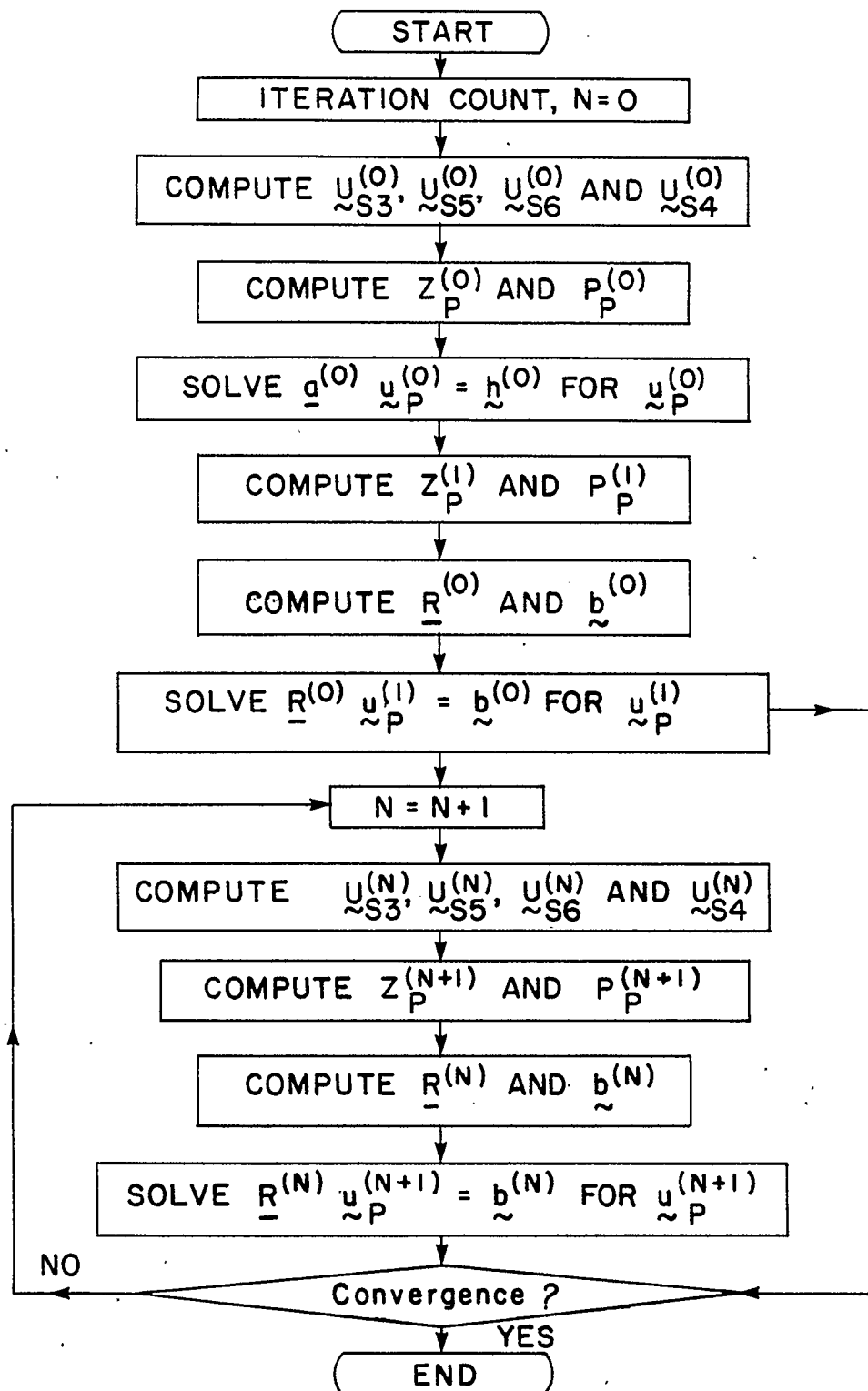


Figure 5.3 Simplified flow diagram of the procedure for computing the solution at interior grid points using the numerical method of characteristics.

- (iii) Compute $Z_P^{(0)}$ and $P_P^{(0)}$ using equations (5.17a) and (5.17b) respectively,
- (iv) Solve equation (5.20) for $u_P^{(0)}$,
- (v) Calculate the values of the intermediate unknowns $U_{S3}^{(k+1)}$, $U_{S5}^{(k+1)}$, $U_{S6}^{(k+1)}$, $U_{S4}^{(k+1)}$,
- (vi) Compute $Z_P^{(k+1)}$ and $P_P^{(k+1)}$ from equations (5.13a) and (5.13b) respectively,
- (vii) Solve equation (5.22) for $u_P^{(k+1)}$,
- (viii) Check convergence: stop iteration if convergence has been achieved or increment iteration counter (by one) and return to step (v).

Convergence is deemed to be achieved when

$$\max \frac{|U_P^{(k+1)} - U_P^{(k)}|}{|U_P^{(k)}|} < \text{TOL} , \quad (5.26)$$

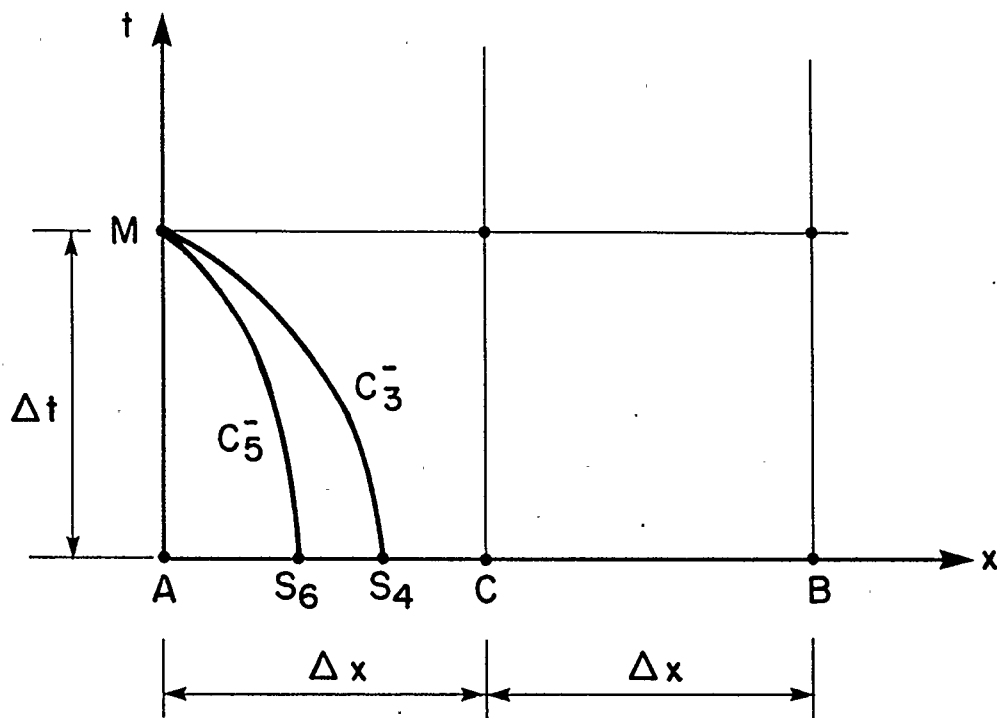
where TOL is a small number that defines the error tolerance.

A description of the skeletal procedure for solving for the unknowns at the interior grid points is given in the flow chart shown in Figure 5.3.

5.2.2 Treatment of Boundary Grid Points

Figure 5.4 shows a typical grid point, M, and the characteristic curves passing through it.

It will be recalled from Chapter 4 that two boundary conditions are required for the problem under consideration. In this thesis, two kinds of boundary conditions are considered. These are:



KNOWN:

$x_A, t_A, \underline{U}_A$

$x_C, t_C, \underline{U}_C$

$x_B, t_B, \underline{U}_B$

t_{S6}

t_{S4}

x_M, t_M

INTERMEDIATE UNKNOWN:

$x_{S6}, \underline{U}_{S6}$

$x_{S4}, \underline{U}_{S4}$

PRIMARY UNKNOWN:

$\underline{U}_M$

$$\underline{U} = \begin{bmatrix} V & \sigma & \theta & q & z & p \end{bmatrix}^T = \underline{U}(x, t)$$

Figure 5.4 Characteristic curves passing through a typical boundary grid point, M.

- (i) stress and temperature time-dependent input, that is, $\sigma(0,t)$ and $\theta(0,t)$ are prescribed for $t > 0$,
- (ii) velocity and temperature time-dependent input, that is, $v(0,t)$ and $\theta(0,t)$ are prescribed for $t > 0$.

Other physically reasonable combinations of boundary conditions (for example $\sigma(0,t)$ and $q(0,t)$ prescribed) may be considered following the same line of development presented below.

The procedure for computing the unknown solution at point M , that is U_M , is essentially the same as the procedure employed for the interior grid points.

In the case of the boundary grid points, there are only four characteristic equations (and not six) involved since there are only four characteristic curves through the point M that lie within the solution domain as shown in Figure 5.4. The positive characteristics C_3^+ and C_5^+ through point M lie outside the solution domain and hence the equations along those curves cannot be numerically integrated.

However, the four simultaneous equations that will be obtained from the numerical integrations along the characteristic curves AM , AM , S_6M and S_4M are sufficient to find the unknowns at point M . This is because two quantities have been prescribed along the boundary so that there are only four unknowns at point M .

We proceed as in the case of interior grid points to derive a second-order-accurate scheme for the iterative computations of the unknown solution at point M . The results are summarized below for the two types of boundary conditions.

Case (i): $\sigma(0,t)$ and $\theta(0,t)$ prescribed.

Starting values for the iterative process:

$$\underline{U}_{S6}^{(0)} = \underline{U}_A(1 - \alpha V_{5A}) + \alpha \underline{U}_C V_{5A} , \quad (5.27a)$$

$$\underline{U}_{S4}^{(0)} = \underline{U}_A(1 - \alpha V_{3A}) + \alpha \underline{U}_C V_{3A} , \quad (5.27b)$$

$$\underline{Z}_M^{(0)} = \underline{Z}_A - F_{2A} \Delta t , \quad (5.28a)$$

$$\underline{P}_M^{(0)} = \underline{P}_A + G_{1A} \Delta t , \quad (5.28b)$$

$$\begin{aligned} \underline{v}_M^{(0)} = & \Lambda_9^4 Q_{S4} \{ \Lambda_{S6}^7 + \Lambda_{S6}^8 \Delta t + {}^3W_{S6} \theta_M - {}^2W_{S6} \sigma_M \} \\ & - \Lambda_9^4 W_{S6} \{ \Lambda_{S4}^3 + \Lambda_{S4}^4 \Delta t + {}^3Q_{S4} \theta_M - {}^2Q_{S4} \sigma_M \} , \end{aligned} \quad (5.28c)$$

$$\begin{aligned} \underline{q}_M^{(0)} = & \Lambda_9^1 Q_{S4} \{ \Lambda_{S6}^7 + \Lambda_{S6}^8 \Delta t + {}^3W_{S6} \theta_M - {}^2W_{S6} \sigma_M \} \\ & - \Lambda_9^1 W_{S6} \{ \Lambda_{S4}^3 + \Lambda_{S4}^4 \Delta t + {}^3Q_{S4} \theta_M - {}^2Q_{S4} \sigma_M \} , \end{aligned} \quad (5.28d)$$

where

$$\Lambda_9 = \{ {}^1W_{S6}^4 Q_{S4} - {}^1Q_{S4}^4 W_{S6} \}^{-1} . \quad (5.29)$$

Iterative equations:

$$\underline{U}_{S6}^{(k+1)} = \underline{U}_C - \frac{1}{4}(\underline{U}_A - \underline{U}_B) \{ \alpha (V_{5S6}^{(k)} + V_{5M}^{(k)}) - 2 \} + \frac{1}{8}(\underline{U}_A + \underline{U}_B - 2\underline{U}_C)$$

$$\{\alpha(V_{5S6}^{(k)} + V_{5M}^{(k)}) - 2\}^2, \quad (5.30a)$$

$$U_{S4}^{(k+1)} = U_C - \frac{1}{4}(U_A - U_B)\{\alpha(V_{3S4}^{(k)} + V_{3M}^{(k)}) - 2\} + \frac{1}{8}(U_A + U_B - 2U_C)$$

$$\{\alpha(V_{3S4}^{(k)} + V_{3M}^{(k)}) - 2\}^2, \quad (5.30b)$$

$$(k = 0, 1, 2, \dots)$$

$$Z_M^{(k+1)} = Z_A - \frac{1}{2}(F_{2A} + F_{2M}^{(k)})\Delta t, \quad (5.31a)$$

$$P_M^{(k+1)} = P_A + \frac{1}{2}(G_{1A} + G_{1M}^{(k)})\Delta t, \quad (5.31b)$$

$$a_{\underline{g}}^{(k)} a_{\underline{r}_M}^{(k+1)} = a_{\underline{w}}^{(k)}, \quad (5.32)$$

where

$$a_{\underline{r}_M} = \begin{Bmatrix} v_M \\ q_M \end{Bmatrix}. \quad (5.33)$$

The two components of the vector $a_{\underline{w}}^{(k)}$ are:

$$\begin{aligned} a_{w_1}^{(k)} = & ({}^3Q_{S4}^{(k)} + Q_{3M}^{(k)})\theta_M - ({}^2Q_{S4}^{(k)} + Q_{2M}^{(k)})\sigma_M + ({}^1Q_{S4}^{(k)} + Q_{1M}^{(k)})v_{S4}^{(k)} \\ & + ({}^2Q_{S4}^{(k)} + Q_{2M}^{(k)})\sigma_{S4}^{(k)} - ({}^3Q_{S4}^{(k)} + Q_{3M}^{(k)})\theta_{S4}^{(k)} - ({}^4Q_{S4}^{(k)} + Q_{4M}^{(k)})q_{S4}^{(k)} \\ & + \{ (Q_{5f})_{S4}^{(k)} + (Q_{5f})_M^{(k)} + (Q_{8q})_{S4}^{(k)} + (Q_{8q})_M^{(k)} \} \end{aligned}$$

$$+ {}^6Q_{S4}^{(k)} + Q_{6M}^{(k)} - {}^7Q_{S4}^{(k)} - Q_{7M}^{(k)} \} \Delta t , \quad (5.34a)$$

$$\begin{aligned} a_{w_2}^{(k)} = & ({}^3W_{S6}^{(k)} + W_{3M}^{(k)}) \theta_M - ({}^2W_{S6}^{(k)} + W_{2M}^{(k)}) \sigma_M + ({}^1W_{S6}^{(k)} + W_{1M}^{(k)}) v_{S6}^{(k)} \\ & + ({}^2W_{S6}^{(k)} + W_{2M}^{(k)}) \sigma_{S6}^{(k)} - ({}^3W_{S6}^{(k)} + W_{3M}^{(k)}) \theta_{S6}^{(k)} - ({}^4W_{S6}^{(k)} + W_{4M}^{(k)}) q_{S6}^{(k)} \\ & + \{ (W_{5f})_{S6}^{(k)} + (W_{5f})_M^{(k)} + (W_{8q})_{S6}^{(k)} + (W_{8q})_M^{(k)} \\ & + {}^6W_{S6}^{(k)} + W_{6M}^{(k)} - {}^7W_{S6}^{(k)} - W_{7M}^{(k)} \} \Delta t , \end{aligned} \quad (5.34b)$$

while the elements of the 2x2 matrix $a_g^{(k)}$ are:

$$\begin{aligned} a_{g_{11}}^{(k)} &= {}^1Q_{S4}^{(k)} + Q_{1M}^{(k)} , & a_{g_{12}}^{(k)} &= - ({}^4Q_{S4}^{(k)} + Q_{4M}^{(k)}) , \\ a_{g_{21}}^{(k)} &= {}^1W_{S6}^{(k)} + W_{1M}^{(k)} , & a_{g_{22}}^{(k)} &= - ({}^4W_{S6}^{(k)} + W_{4M}^{(k)}) . \end{aligned} \quad (5.35)$$

A simplified flow diagram for computing the unknown solution for this case is shown in Figure 5.5.

Case (ii): $v(0,t)$ and $\theta(0,t)$ prescribed:

Starting values for the iterative process:

Values of $U_{S6}^{(0)}$, $U_{S4}^{(0)}$, $Z_M^{(0)}$, and $P_M^{(0)}$ are computed from the same equations given for case (i). However, the values of $\sigma_M^{(0)}$ and $q_M^{(0)}$ are given by:

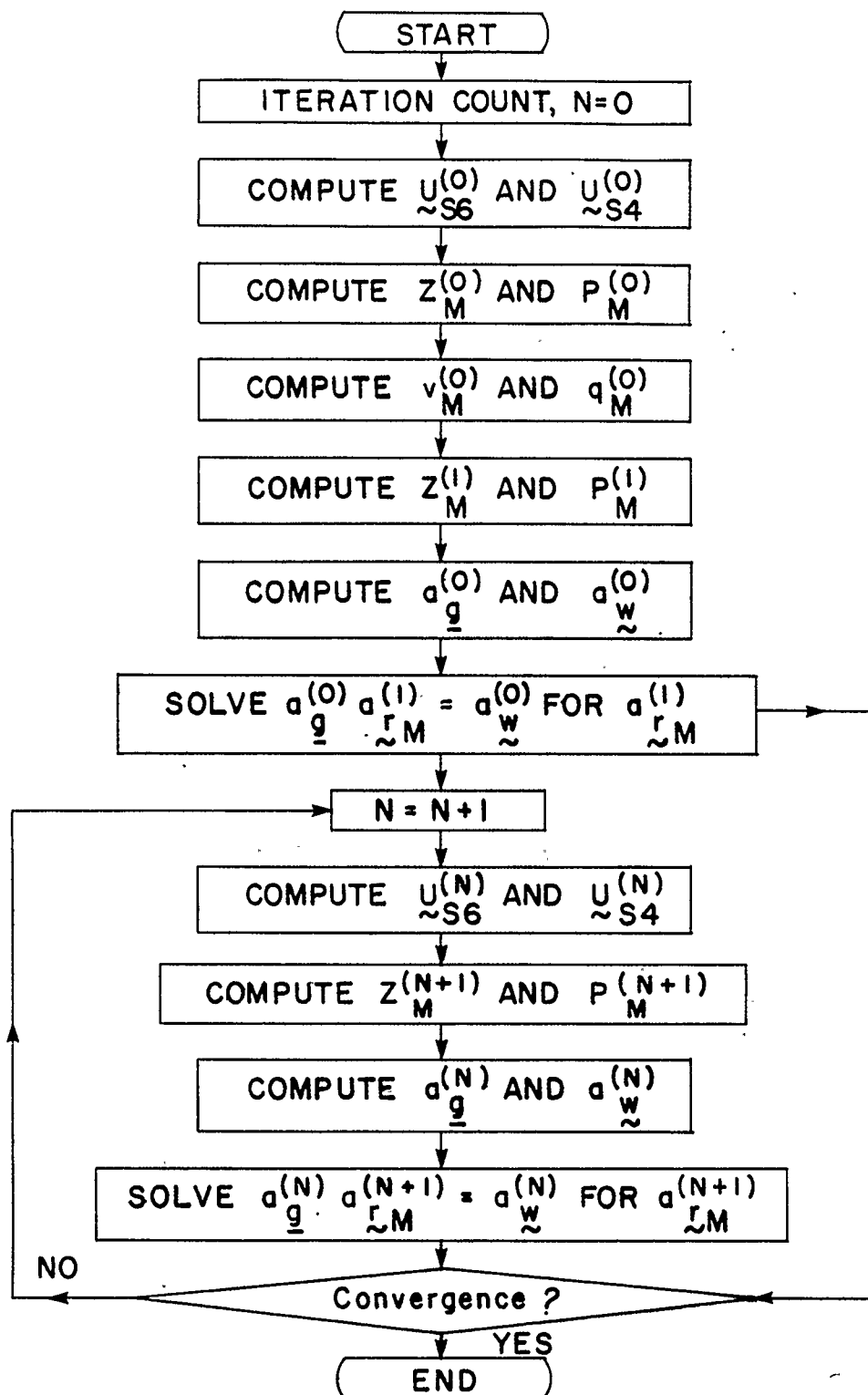


Figure 5.5 Simplified flow diagram of the procedure for computing the solution at boundary grid points using the numerical method of characteristics with $\sigma(0,t)$ and $\theta(0,t)$ prescribed.

$$\begin{aligned}\sigma_M^{(0)} &= \Lambda_T^4 Q_{S4} \{ {}^7\Lambda_{S6} + {}^8\Lambda_{S6} \Delta t + {}^3W_{S6} \theta_M - {}^1W_{S6} v_M \} \\ &\quad - \Lambda_T^4 W_{S6} \{ {}^3\Lambda_{S4} + {}^4\Lambda_{S4} \Delta t + {}^3Q_{S4} \theta_M - {}^1Q_{S4} v_M \} ,\end{aligned}\quad (5.36a)$$

$$\begin{aligned}q_M^{(0)} &= \Lambda_T^2 Q_{S4} \{ {}^7\Lambda_{S6} + {}^8\Lambda_{S6} \Delta t + {}^3W_{S6} \theta_M - {}^1W_{S6} v_M \} \\ &\quad - \Lambda_T^2 W_{S6} \{ {}^3\Lambda_{S4} + {}^4\Lambda_{S4} \Delta t + {}^3Q_{S4} \theta_M - {}^1Q_{S4} v_M \} ,\end{aligned}\quad (5.36b)$$

where

$$\Lambda_T = \{ {}^2W_{S6} {}^4Q_{S4} - {}^2Q_{S4} {}^4W_{S6} \}^{-1} . \quad (5.37)$$

Iterative equations:

Values of $U_{S6}^{(k+1)}$, $U_{S4}^{(k+1)}$, $Z_M^{(k+1)}$, and $P_M^{(k+1)}$ are computed from the same equations given for case (i). However the values of $\sigma_M^{(k+1)}$ and $q_M^{(k+1)}$ are determined from the equation:

$$\underline{b}_M(k) \quad \underline{b}_M^{(k+1)} = \underline{b}_W(k) , \quad (5.38)$$

where

$$\underline{b}_M^{(k+1)} = \begin{Bmatrix} \sigma_M^{(k+1)} \\ q_M^{(k+1)} \end{Bmatrix} . \quad (5.39)$$

The two components of vector $\underline{b}_W(k)$ are given by:

$$\begin{aligned}
b_{w_1}(k) &= ({}^3Q_{S4} + Q_{3M}^{(k)})\theta_M - ({}^1Q_{S4} + Q_{1M}^{(k)})v_M \\
&+ ({}^1Q_{S4} + Q_{1M}^{(k)})v_{S4}^{(k)} + ({}^2Q_{S4} + Q_{2M}^{(k)})\sigma_{S4}^{(k)} - ({}^3Q_{S4} + Q_{3M}^{(k)})\theta_{S4}^{(k)} \\
&- ({}^4Q_{S4} + Q_{4M}^{(k)})q_{S4}^{(k)} + \{ (Q_5^f)_{S4}^{(k)} + (Q_5^f)_M^{(k)} + (Q_8^q)_{S4}^{(k)} + (Q_8^q)_M^{(k)} \\
&\quad + {}^6Q_{S4} + Q_{6M} - {}^7Q_{S4} - Q_{7M} \} \Delta t , \tag{5.40a}
\end{aligned}$$

$$\begin{aligned}
b_{w_2}(k) &= ({}^3W_{S6} + W_{3M}^{(k)})\theta_M - ({}^1W_{S6} + W_{1M}^{(k)})v_M + ({}^1W_{S6} + W_{1M}^{(k)})v_{S6} \\
&+ ({}^2W_{S6} + W_{2M}^{(k)})\sigma_{S6}^{(k)} - ({}^3W_{S6} + W_{3M}^{(k)})\theta_{S6} - ({}^4W_{S6} + W_{4M}^{(k)})q_{S6}^{(k)} \\
&\quad + \{ (W_5^f)_{S6} + (W_5^f)_M + (W_8^q)_{S6} + (W_8^q)_M \\
&\quad + {}^6W_{S6} + W_{6M} - {}^7W_{S6} - W_{7M} \} \Delta t , \tag{5.40b}
\end{aligned}$$

while the elements of the 2x2 matrix $b_{\underline{g}}(k)$ are:

$$\begin{aligned}
b_{g_{11}}(k) &= {}^2Q_{S4} + Q_{2M}^{(k)} , & b_{g_{12}}(k) &= - ({}^4Q_{S4} + Q_{4M}^{(k)}) , \\
b_{g_{21}}(k) &= {}^2W_{S6} + W_{2M}^{(k)} , & b_{g_{22}}(k) &= - ({}^4W_{S6} + W_{4M}^{(k)}) . \tag{5.41}
\end{aligned}$$

The simplified flow diagram corresponding to case (ii) is given in Figure 5.6.

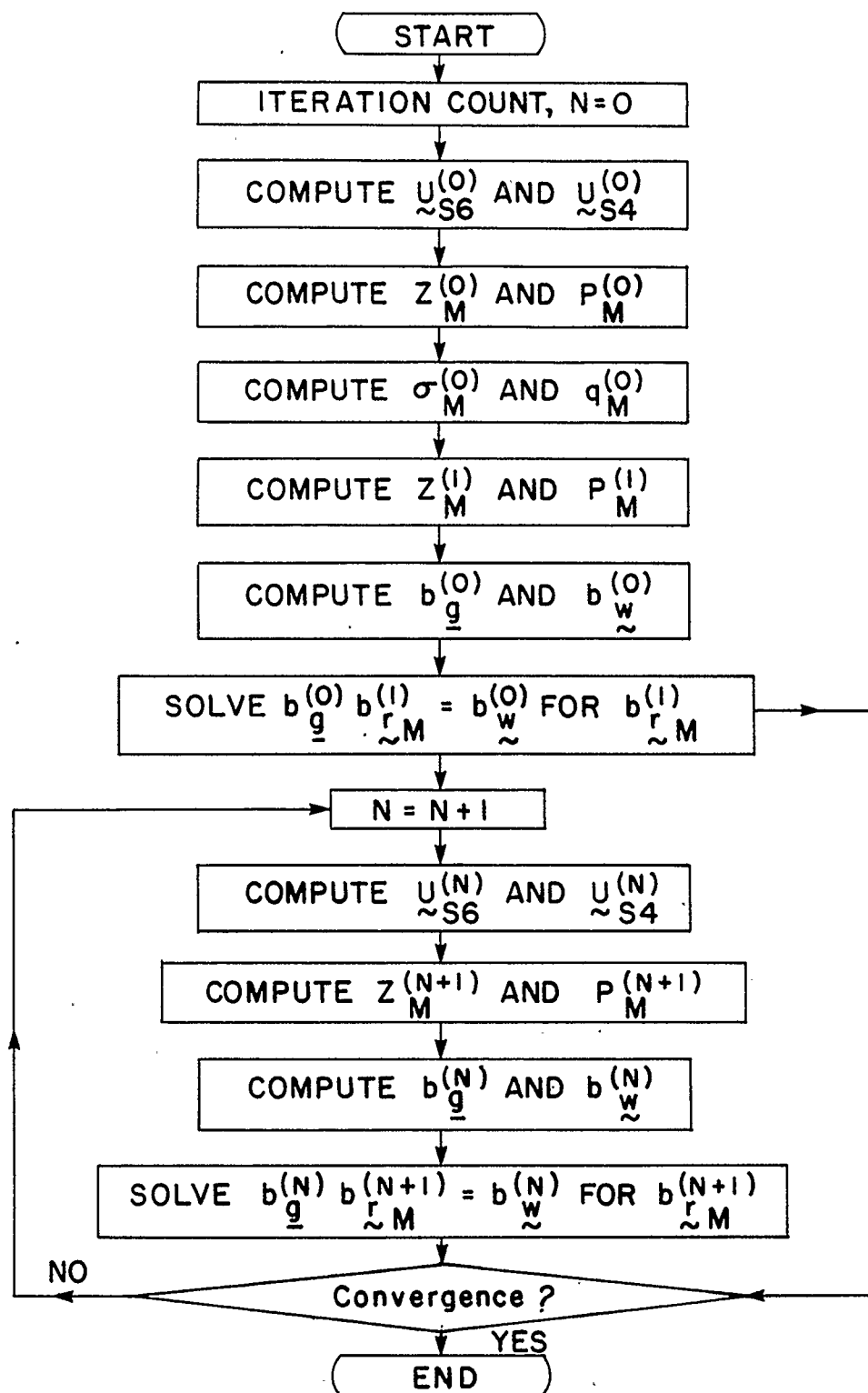


Figure 5.6 Simplified flow diagram of the procedure for computing the solution at boundary grid points using the numerical method of characteristics with $v(0,t)$ and $\theta(0,t)$ prescribed.

5.2.3 Remarks on the Properties of the Scheme

Finite difference approximations of partial differential equations are usually required to satisfy conditions of consistency, stability, and convergence. Consistency has to do with assurance that, as the finite difference mesh is refined, the truncation errors approach zero. This condition ensures that the scheme does in fact approximate the given problem rather than some other problem. Computational stability calls for the boundedness of all perturbations in a computed solution. Convergence requires the solution of the finite difference equations to approach the true solution of the partial differential equation as the mesh is refined. Stability and consistency of a scheme usually guarantee its convergence.

No rigorous analyses of the above properties are available for nonlinear problems. For schemes based on the method of characteristics however, it has been shown [5.8] that stability is assured when the domain of dependence of any point as given by the finite difference equation is not less than the exact domain of dependence of the differential equation. Mathematically, the requirement is expressed as

$$\max \left| \lambda^{(i)}(\underline{U}_P) \right| < \frac{\Delta X}{\Delta t} . \quad (5.42)$$

The condition (5.42) is commonly referred to as the CFL condition and the CFL number, C_v , is defined as

$$C_v = \max \left| \lambda^{(i)}(\underline{U}_P) \right| \frac{\Delta t}{\Delta X} . \quad (5.43)$$

Note that $\max \left| \lambda^{(i)}(\underline{U}_P) \right|$ denotes the numerically greatest eigenvalue of the matrix $\underline{A}(U)$ computed at point P.

5.3 Application of the MacCormack Finite Difference Scheme

5.3.1 Treatment of Interior Grid Points

The MacCormack finite difference scheme was originally developed by MacCormack [5.7] for the solution of the time-dependent compressible Navier-stokes equations and applied to calculate the axisymmetric flow field produced by hypervelocity impact. It was subsequently applied in a modified form for the solution of the interaction of a shock wave with a laminar boundary layer by the same author [5.9].

The vector form of the time-dependent Navier-stokes equations, in two dimensions, neglecting body forces and heat sources may be written as

$$\frac{\partial \underline{U}}{\partial t} + \frac{\partial \underline{F}}{\partial x} + \frac{\partial \underline{G}}{\partial y} = 0 , \quad (5.44)$$

where

$$\underline{U} = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{Bmatrix} , \quad (5.45a)$$

$$\underline{F} = \begin{Bmatrix} \rho u \\ \rho u^2 + \sigma_x \\ \rho uv + \tau_{xy} \\ (e + \sigma_x)u + \tau_{yx}v + k \frac{\partial T}{\partial x} \end{Bmatrix} , \quad (5.45b)$$

$$\tilde{G} = \left\{ \begin{array}{c} \rho v \\ \rho uv + \tau_{yx} \\ \rho v^2 + \sigma_y \\ (e + \sigma_y)v + \tau_{xy}u + k \frac{\partial T}{\partial y} \end{array} \right\}, \quad (5.45c)$$

$$\sigma_x = p - \lambda \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) - 2\mu \frac{\partial u}{\partial x}, \quad (5.45d)$$

$$\tau_{xy} = \tau_{yx} = -\mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right), \quad (5.45e)$$

$$\sigma_y = p - \lambda \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) - 2\mu \frac{\partial v}{\partial y}, \quad (5.45f)$$

where ρ is the density, u and v the x and y components of velocity, λ and μ are the viscosity coefficients, e is the total energy per unit volume, ϵ^* is the specific internal energy, k is the coefficient of heat conductivity, and T is the temperature. The pressure p is related to ϵ^* and ρ by the equation of state:

$$\epsilon^* = \frac{e}{\rho} - \frac{1}{2}(u^2 + v^2). \quad (5.46)$$

The two-step second-order accurate method devised by MacCormack to solve equation (5.44) is as follows:

$$\overline{U}_{i,j}^{n+1} = U_{i,j}^n - \frac{\Delta t}{\Delta x} (F_{i+1,j}^n - F_{i,j}^n) - \frac{\Delta t}{\Delta y} (G_{i,j+1}^n - G_{i,j}^n), \quad (5.47a)$$

$$U_{i,j}^{n+1} = \frac{1}{2} \{ U_{i,j}^n + \overline{U}_{i,j}^{n+1} - \frac{\Delta t}{\Delta x} (\overline{F}_{i,j}^{n+1} - \overline{F}_{i-1,j}^{n+1}) - \frac{\Delta t}{\Delta y} (\overline{G}_{i,j}^{n+1} - \overline{G}_{i,j-1}^{n+1}) \}, \quad (5.47b)$$

where

$$\tilde{F}_{i,j}^n \equiv F(U_{i,j}^n) , \quad (5.47c)$$

$$\tilde{G}_{i,j}^n \equiv G(U_{i,j}^n) . \quad (5.47d)$$

The subscripts in equations (5.47) refer to a spatial mesh of points (x_i, y_j) with spacing Δx and Δy , and the superscripts refer to times $t = n\Delta t$ where Δt is the time increment that the solution is advanced during each cycle of equations (5.47). Equation (5.47a) is referred to as the predictor step and equation (5.47b) is known as the corrector step. Whereas the predictor step uses forward differences to approximate the spatial derivatives, the corrector step employs backward differences.

Applications of the MacCormack scheme to problems in fluid dynamics are numerous while there has only been a few solid mechanics applications. The first concrete application in solids was by Hanagud and Abhyankar [5.10] who studied the finite deformation coupled torsional and longitudinal wave propagation problems in cylindrical rods made of neo-Hookean materials.

Despite its popularity in the solution of nonlinear systems of hyperbolic partial differential equations, the scheme has been predominantly applied to systems of the form:

$$\frac{\partial \underline{U}}{\partial t} + \underline{A}(\underline{U}) \frac{\partial \underline{U}}{\partial x} = 0 , \quad (5.48)$$

in which the so-called source terms are conspicuously absent. Lorimer

[5.11] and Haddow et al. [5.12] have presented a modified form of the MacCormack scheme suitable for the numerical solution of equations of the form:

$$\frac{\partial U}{\partial t} + \underline{A}(U) \frac{\partial U}{\partial X} + \underline{B}(U) = 0, \quad (5.49)$$

which is the type of problem being considered in this thesis. In those references the modifications were applied to the solution of elastodynamic problems for hyperelastic and viscoelastic solids.

The modifications given in references [5.11] and [5.12] are as follows. First, for the conservative form of systems of hyperbolic partial differential equations which are expressible as:

$$\frac{\partial U}{\partial t} + \frac{\partial Q(U)}{\partial X} + \underline{B}(U) = 0, \quad (5.50)$$

the modification is given as:

$$\overline{U_j^{n+1}} = U_j^n - \frac{\Delta t}{\Delta X} \{Q(\underline{U}_{j+1}^n) - Q(\underline{U}_j^n)\} - \Delta t \underline{B}(U_j^n) \quad (5.51a)$$

$$U_j^{n+1} = \frac{1}{2} \{ \overline{U_j^{n+1}} + U_j^n - \frac{\Delta t}{\Delta X} [Q(\overline{U_j^{n+1}}) - Q(\underline{U}_{j-1}^{n+1})] - \Delta t \underline{B}(\overline{U_j^{n+1}}) \}. \quad (5.51b)$$

In the above, equation (5.51a) is the predictor step while equation (5.51b) is the corrector step. This version of the MacCormack scheme is usually referred to as the forward backward (FB) scheme because the predictor step uses forward spatial differencing while the corrector step utilizes backward spatial differencing. For nonconservative systems of equations, that is, equations of the form (5.49), the

modified scheme is given by:

$$\overline{U_j^{n+1}} = U_j^n - \frac{\Delta t}{\Delta X} [A(U_j^n)] [U_{j+1}^n - U_j^n] - \Delta t B(U_j^n) , \quad (5.52a)$$

$$U_j^{n+1} = \frac{1}{2} \{ U_j^n + \overline{U_j^{n+1}} - \frac{\Delta t}{\Delta X} [A(\overline{U_j^{n+1}})] [\overline{U_j^{n+1}} - \overline{U_{j-1}^{n+1}}] - \Delta t B(\overline{U_j^{n+1}}) \} . \quad (5.52b)$$

Equation (5.52a) is the predictor step and equation (5.52b) is the corrector step. Note that in equations (5.51) and (5.52),

$$U_j^n \equiv U(j\Delta X, n\Delta t) . \quad (5.53)$$

The system of equations under study in the present work may be put into the semi-conservative form:

$$\frac{\partial \underline{U}^*}{\partial t} + \frac{\partial \underline{F}}{\partial x} + \underline{B}^* = 0 , \quad (5.54)$$

where

$$\underline{U}^* = \left\{ \begin{array}{c} \rho v \\ \epsilon \\ \psi + (\theta + T_R) \eta + \frac{1}{2} \rho v^2 \\ \tau_0 q \\ Z \\ P \end{array} \right\} , \quad (5.55a)$$

$$\tilde{F} = \begin{Bmatrix} -\sigma \\ -v \\ -(\sigma v + q) \\ -k\theta \\ 0 \\ 0 \end{Bmatrix}, \quad (5.55b)$$

and

$$\tilde{B}^* = \begin{Bmatrix} -f \\ 0 \\ -(vf + r) \\ q \\ F_2 \\ -G_1 \end{Bmatrix}, \quad (5.55c)$$

In equation (5.54), the dependent variables are the components of $\tilde{U}^*$. Although this equation is of a divergence form, it is not possible to express the vector function F as an explicit function of $\tilde{U}^*$. The same is also true of the vector function $\tilde{B}^*$. Thus, equation (5.54) is not strongly conservative and for the purposes of the discussion here is referred to as semi-conservative.

It is possible in principle to seek the application of the conservative version of the scheme to (5.54). In such a procedure, the primary dependent variables of physical interest, that is, $\tilde{U}$ (defined earlier) will have to be computed at each grid point from a knowledge of $\tilde{U}^*$. However, because of the highly nonlinear forms of the expressions for ψ and η , iterative processes must be applied. Since it is well known that good convergence properties of iterative procedures usually

depend on reasonable choices of initial values, which in this complex case is difficult to estimate, the procedure is infeasible. Therefore, in this study, the nonconservative version, equations (5.52) is directly applied.

A typical interior grid point is as shown in Figure 5.7.

A common practice in the numerical solution of hyperbolic partial differential equations is the addition of artificial viscosity. This practice, referred to as shock capturing, is aimed at the attenuation of the high frequency components of the numerical solution as the computation progresses. It was first applied by von Neumann and Richtmyer [5.13] for the numerical solution of hydrodynamic problems. Another type of an easy-to-use third-order artificial viscosity was proposed by Lapidus [5.15] in the form:

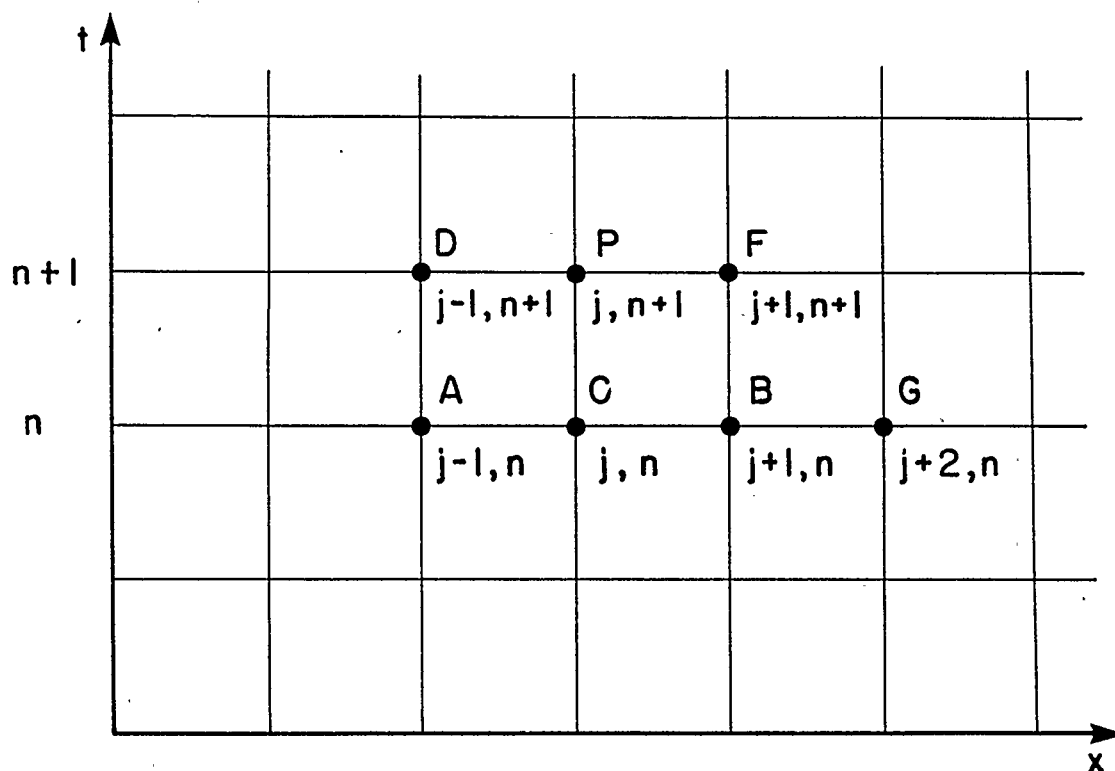
$$U_j^{*n+1} = U_j^{n+1} + \alpha C_{av3} \cdot \Delta' [1 \Delta' U_{j+1}^{n+1} - \Delta' U_{j+1}^{n+1}] , \quad (5.56a)$$

where the finite difference operator Δ' is defined as:

$$\Delta' U_j^n = U_j^n - U_{j-1}^n , \quad (5.56b)$$

and C_{av3} is an adjustable constant. In equations (5.56) U_j^{n+1} are the quantities calculated from the usual MacCormack scheme and U_j^{*n+1} are the new values obtained after the addition of artificial viscosity. Hanagud and Abhyankar [5.10] also recommended the addition of artificial viscosity terms of the forms:

$$q_2 = C_{av2} (U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) , \quad (5.57a)$$



KNOWN :

$$\tilde{U}_A = \tilde{U}_{j-1}^n$$

$$\tilde{U}_C = \tilde{U}_j^n$$

$$\tilde{U}_B = \tilde{U}_{j+1}^n$$

$$\tilde{U}_G = \tilde{U}_{j+2}^n$$

$$\tilde{U}_D = \tilde{U}_{j-1}^n$$

INTERMEDIATE UNKNOWN :

$$\tilde{U}_F = \tilde{U}_{j+1}^{n+1}$$

UNKNOWN :

$$\tilde{U}_P = \tilde{U}_j^{n+1}$$

Figure 5.7 Illustration of a typical interior grid point (P) in the MacCormack scheme.

for second order viscosity or

$$q_4 = C_{av4} (U_{j+2}^{n+1} - 4U_{j+1}^{n+1} + 6U_j^{n+1} - 4U_{j-1}^{n+1} + U_{j-2}^{n+1}) \quad (5.57b)$$

for a fourth order viscosity. The parameters C_{av2} and C_{av4} are also adjustable artificial viscosity constants.

The major attributes of artificial viscosity terms are the preservation of the high order of accuracy of the solution and removal of nonlinear instabilities which may appear in shock regions and near boundaries. The results of numerical experiments on the present problem show that the addition of artificial viscosity terms are unnecessary. This is not surprising because the physical process under study is dissipative in itself so that physical damping is already present.

It may be seen from the above that the MacCormack scheme (with or without artificial viscosity) is an explicit scheme and is very much simpler to apply than the method of characteristics presented in the last section.

5.3.2 Treatment of Boundary Grid Points

The procedure for determining the extraneous boundary conditions is described in what follows.

Gottlieb and Turkel [5.15] considered various types of boundary procedures for the MacCormack finite difference scheme. Their study recommended the reversal of the difference operator at a boundary so that either forward forward (FF) or backward backward (BB) differences are employed at boundary grid points. On a left boundary (corresponding to $X = 0$), it was recommended that FF differences be

utilized. Again, implementation of this recommendation was effected in references [5.11] and [5.12]. Thus, for a typical boundary point M shown in Figure 5.8, the modified schemes are given below.

For the conservative scheme:

$$\bar{u}_0^{n+1} = u_0^n - \frac{\Delta t}{\Delta x} [Q(u_1^n) - Q(u_0^n)] - \Delta t B(u_0^n) , \quad (5.58a)$$

$$u_0^{n+1} = \frac{1}{2} \{ \bar{u}_0^n + \bar{u}_0^{n+1} - \frac{\Delta t}{\Delta x} [Q(u_1^{n+1}) - Q(u_0^{n+1})] - \Delta t B(u_0^{n+1}) \} . \quad (5.58b)$$

For the nonconservative scheme:

$$\bar{u}_0^{n+1} = u_0^n - \frac{\Delta t}{\Delta x} [A(u_0^n)] [u_1^n - u_0^n] - \Delta t B(u_0^n) , \quad (5.59a)$$

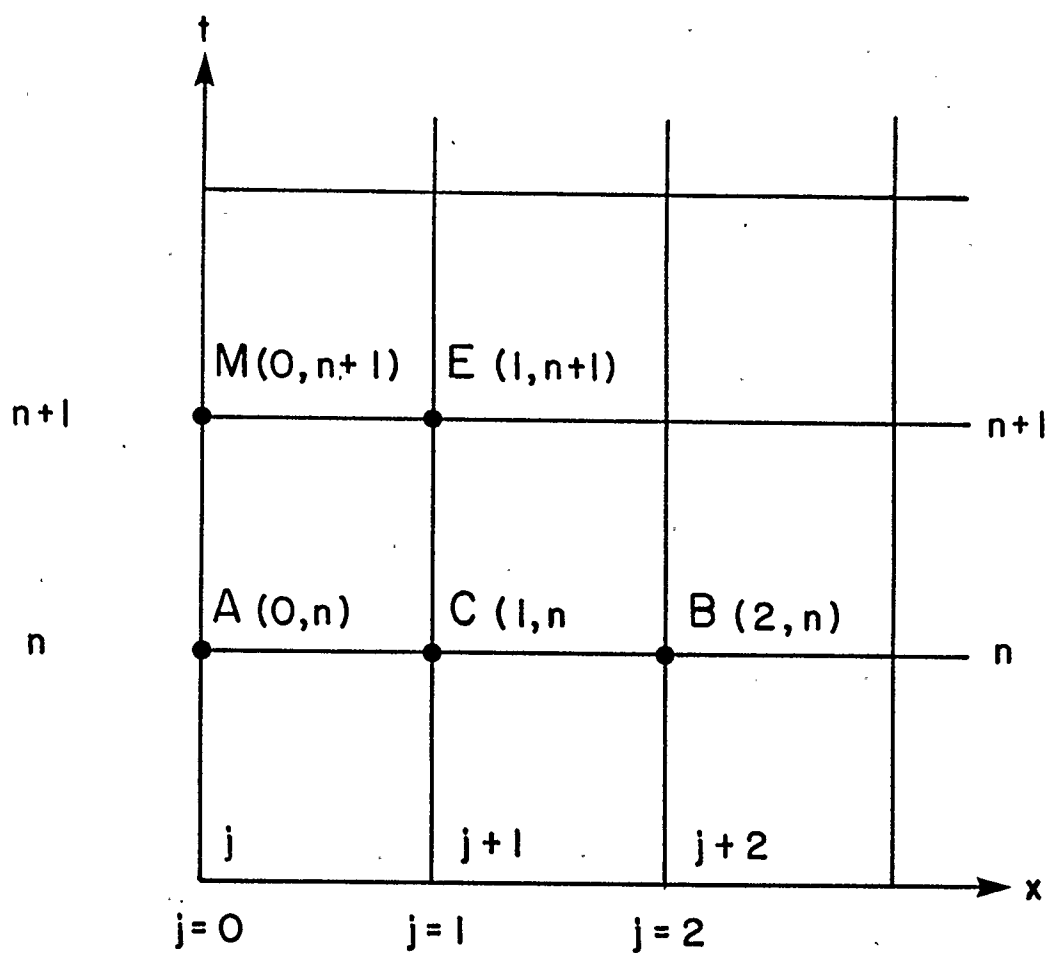
$$u_0^{n+1} = \frac{1}{2} \{ \bar{u}_0^n + \bar{u}_0^{n+1} - \frac{\Delta t}{\Delta x} [A(u_0^{n+1})] [u_1^{n+1} - u_0^{n+1}] - \Delta t B(u_0^{n+1}) \} . \quad (5.59b)$$

Of course, equations (5.59) are applied to the problem under study for reasons that have been discussed earlier.

Just as for most numerical schemes, no rigorous stability criteria of the present scheme have been established for nonlinear problems. However, it is known from linear stability analysis that the MacCormack finite difference scheme is stable if:

$$C_v \leq 1 . \quad (5.60)$$

In this computations, it was found that this is also a necessary condition for numerical stability.



KNOWN :

$$\tilde{U}_A = \tilde{U}_0^n$$

$$\tilde{U}_C = \tilde{U}_1^n$$

$$\tilde{U}_B = \tilde{U}_2^n$$

UNKNOWN :

$$\tilde{U}_M = \tilde{U}_0^{n+1}$$

INTERMEDIATE
UNKNOWN :

$$\tilde{U}_E = \tilde{U}_1^{n+1}$$

Figure 5.8 Illustration of a typical boundary grid point (M) in the MacCormack scheme.

CHAPTER 6

NUMERICAL SIMULATIONS

6.1 Introduction

The numerical simulations of the propagation of coupled thermomechanical waves in inelastic solids are presented in this chapter. Responses of initially quiescent semi-infinite aluminum and copper rods are considered under various kinds of time-dependent inputs.

Two computer programs corresponding to each of the computational algorithms presented in the last chapter are employed. The computer programs are coded in the FORTRAN 77 language and were implemented on the CDC Cyber 205 supercomputer for faster computations. The programs were written in a modular form for good computational efficiency and flexibility. Each of the programs has two major subroutines: one subroutine for computing solutions at boundary grid points and the other for interior grid points.

For the computer program based on the numerical method of characteristics, the subroutine for the boundary grid points is coded in line with the simplified flow diagram given in Figure 5.5 or Figure 5.6, depending on whether $\{\sigma(0,t), \theta(0,t)\}$ is prescribed or $\{v(0,t), \theta(0,t)\}$ is prescribed. The subroutine for the interior grid points is coded in line with the simplified flow diagram given in Figure 5.3.

For the computer program based on the MacCormack finite difference scheme, the interior point routine is coded in accordance with equations (5.52) while the boundary point routine is coded in accordance with equations (5.59).

The two main programs are essentially identical. The skeletal

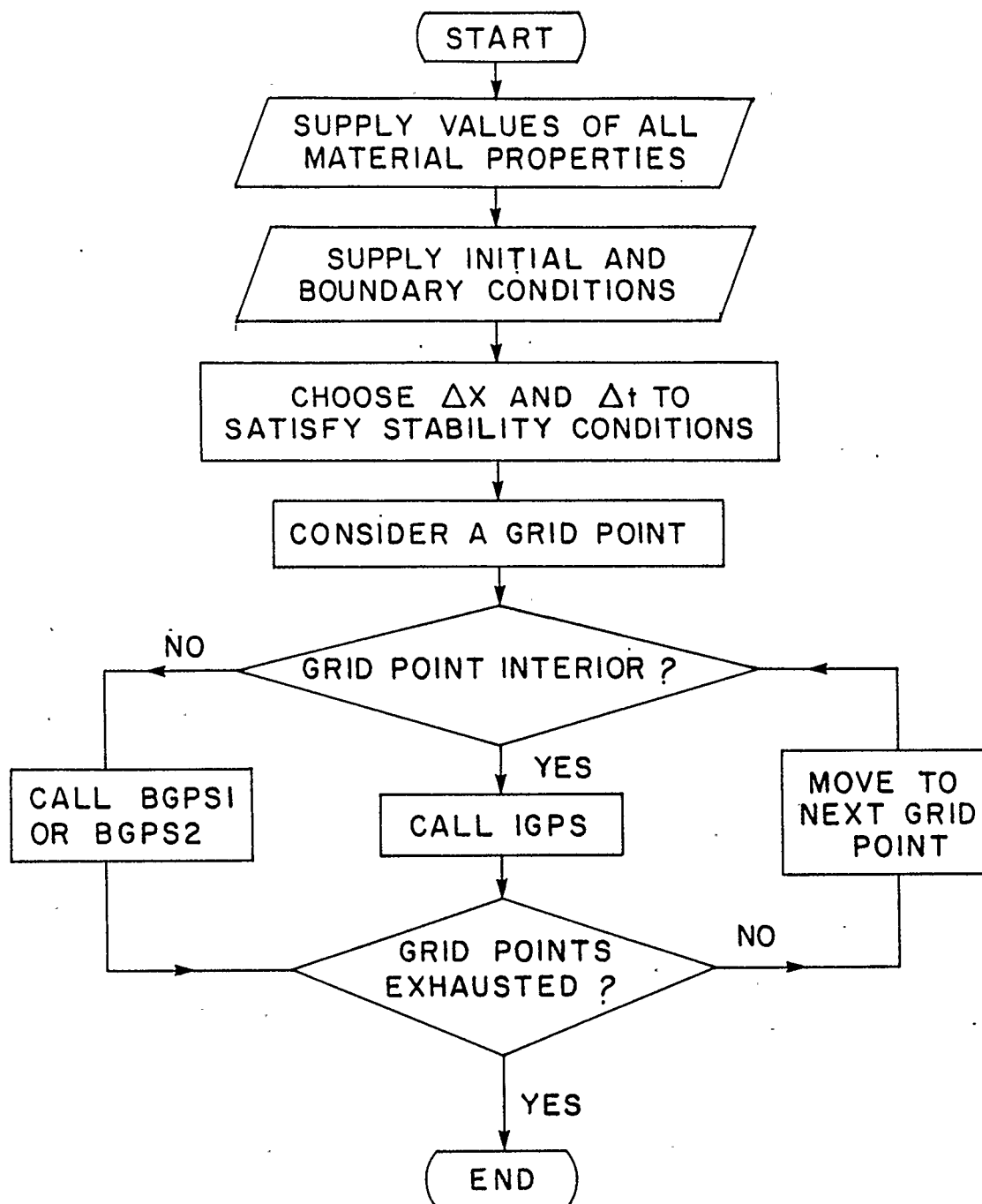


Figure 6.1 Simplified flow diagram of the main computer programs.

flow diagram for the main programs is as shown in Figure 6.1. The boundary point routines are referred to as BGPS1 for $\{\sigma(0,t), \theta(0,t)\}$ prescribed and BGPS2 for $\{v(0,t), \theta(0,t)\}$ prescribed while the interior point routines are referred to as IGPS. Although the main programs control the computations, most of the computations are carried out in the subroutines IGPS and BGPS1 or BGPS2.

6.2 Numerical Examples

Three kinds of time-dependent inputs applied to the ends of the rods are considered.

(i) Step input

The unit step function $H(t)$ is defined as

$$H(t) = \begin{cases} 0, & t < 0 \\ 1, & t > 0. \end{cases} \quad (6.1)$$

It describes a suddenly applied and maintained impact such as the following:

$$\text{Stress impact:} \quad \sigma(0,t) = \sigma_0 H(t) , \quad (6.2a)$$

$$\text{Velocity impact:} \quad v(0,t) = v_0 H(t) , \quad (6.2b)$$

$$\text{Temperature impact:} \quad \theta(0,t) = \theta_0 H(t) . \quad (6.2c)$$

This type of input corresponds to physical shock waves as the discontinuity in the boundary conditions propagate through the medium.

(ii) Pulsive sine input

The pulrive sine function is defined as

$$S_P(t) = \begin{cases} \sin \omega t , & t \leq \frac{\pi}{\omega} \\ 0 , & t > \frac{\pi}{\omega} \end{cases} , \quad (6.3)$$

where ω is a constant. Thus, pulrive-sine inputs in stress, velocity,

and temperature are of the form:

$$\sigma(0,t) = \sigma_0 S_P(t) , \quad (6.4a)$$

$$v(0,t) = v_0 S_P(t) , \quad (6.4b)$$

$$\theta(0,t) = \theta_0 S_P(t) . \quad (6.4c)$$

The pulsive-sine input propagates as an acceleration wave since it gives discontinuous derivatives of the dependent variables.

(iii) Terminated ramp input

The terminated ramp function is defined as

$$R_T(t) = \begin{cases} \frac{t}{t_0} & , \quad t \leq t_0 \\ 1 & , \quad t > t_0 \end{cases} , \quad (6.5)$$

where t_0 is a given time, chosen as π/ω in this work. Therefore, terminated ramp inputs for stress, velocity and, temperature are of the form:

$$\sigma(0,t) = \sigma_0 R_T(t) , \quad (6.6a)$$

$$v(0,t) = v_0 R_T(t) , \quad (6.6b)$$

$$\theta(0,t) = \theta_0 R_T(t) . \quad (6.6c)$$

Again, the terminated-ramp input propagates as an acceleration wave since it gives discontinuous derivatives of the dependent variables.

The material properties used in the numerical simulations are given in Tables 6.1 and 6.2. The inelastic material constants K_A , m , Z_A , Z_0 , n , and α_A pertain to the evolution equations for the Bodner-Partom model [6.1].

The numerical results are given in Figures 6.2a - 6.19e. For convenient graphical illustrations, the following dimensionalization scheme for the time and position have been employed. The nondimensional time, $\bar{t}$, is defined as

Table 6.1 Thermoelastic material constants for aluminum and copper.

Material Constant	Aluminum	Copper
$Y_1 \text{ (Nm}^{-2}\text{)}$	1.02 E 11	2.02 E 11
$Y_2 \text{ (Nm}^{-2}\text{K}^{-1}\text{)}$	4.81 E 06	3.62 E 07
$C_1 \text{ (J kg}^{-1}\text{K}^{-1}\text{)}$	900.42	382.67
$C_2 \text{ (J kg}^{-1}\text{K}^{-2}\text{)}$	0.46	0.10
ν	0.33	0.34
$\beta_R \text{ (Nm}^{-2}\text{K}^{-1}\text{)}$	4.72 E 06	6.94 E 06
$k \text{ (Wm}^{-1}\text{K}^{-1}\text{)}$	238.0	398.53
$\alpha_1 \text{ (K}^{-1}\text{)}$	2.32 E -05	1.68 E -05
$\alpha_2 \text{ (K}^{-2}\text{)}$	7.0 E -09	7.53 E -09
$\rho \text{ (kg m}^{-3}\text{)}$	2.70 E 03	8.94 E 03

$$\bar{t} = \left(\frac{Y_1}{\rho}\right) \frac{\rho C_1}{k} t, \quad (6.7a)$$

while the nondimensional distance, $\bar{X}$, is defined as

$$\bar{X} = X_{DF} \left(\frac{Y_1}{\rho}\right)^{\frac{1}{2}} \frac{\rho C_1}{k} X, \quad (6.7b)$$

where X_{DF} is a constant that varies from one plot to the other. For simplicity the 'bar' on $\bar{X}$ and $\bar{t}$ is omitted in the plots so that, henceforth, X and t refer to nondimensional position and nondimensional time respectively. For simplicity the semi-infinite aluminum rod is referred to as SIAR while the semi-infinite copper rod is called SICOR.

Table 6.2 Thermoelastic material constants for aluminum and copper.

Material Constant	Aluminum	Copper
$K \text{ (m}^2\text{N}^{-1}\text{)}$	2.39 E -10	6.12 E -11
K_A	0.0	0.0
λ_1	48.89	24.75
$\lambda_2 \text{ (K}^{-1}\text{)}$	2.30 E -03	4.43 E -03
B_{4R}	-1.25	-2.88
$B_{5R} \text{ (Nm}^{-2}\text{)}$	1.24 E 09	2.18 E 09
$m \text{ (m}^2\text{N}^{-1}\text{)}$	6.0 E -07	4.0 E -07
$Z_A \text{ (Nm}^{-2}\text{)}$	1.50 E 08	2.37 E 08
$Z_O \text{ (Nm}^{-2}\text{)}$	2.50 E 07	3.10 E 07
n	5.0	9.2
α_A	1.0	1.0
$A_{11} \text{ (Nm}^{-2}\text{)}$	3.14 E 07	8.93 E 07

The results presented in Figures 6.2a-6.19e cover the responses of semi-infinite aluminum and copper rods for all the three time-dependent inputs given above. The input and computation parameters are given in the titles of the figures. It should be noted that the values of the time step (Δt) and thermal relaxation time (τ_0) given in the figures are nondimensional quantities which are related to their corresponding dimensional values through equation (6.7a).

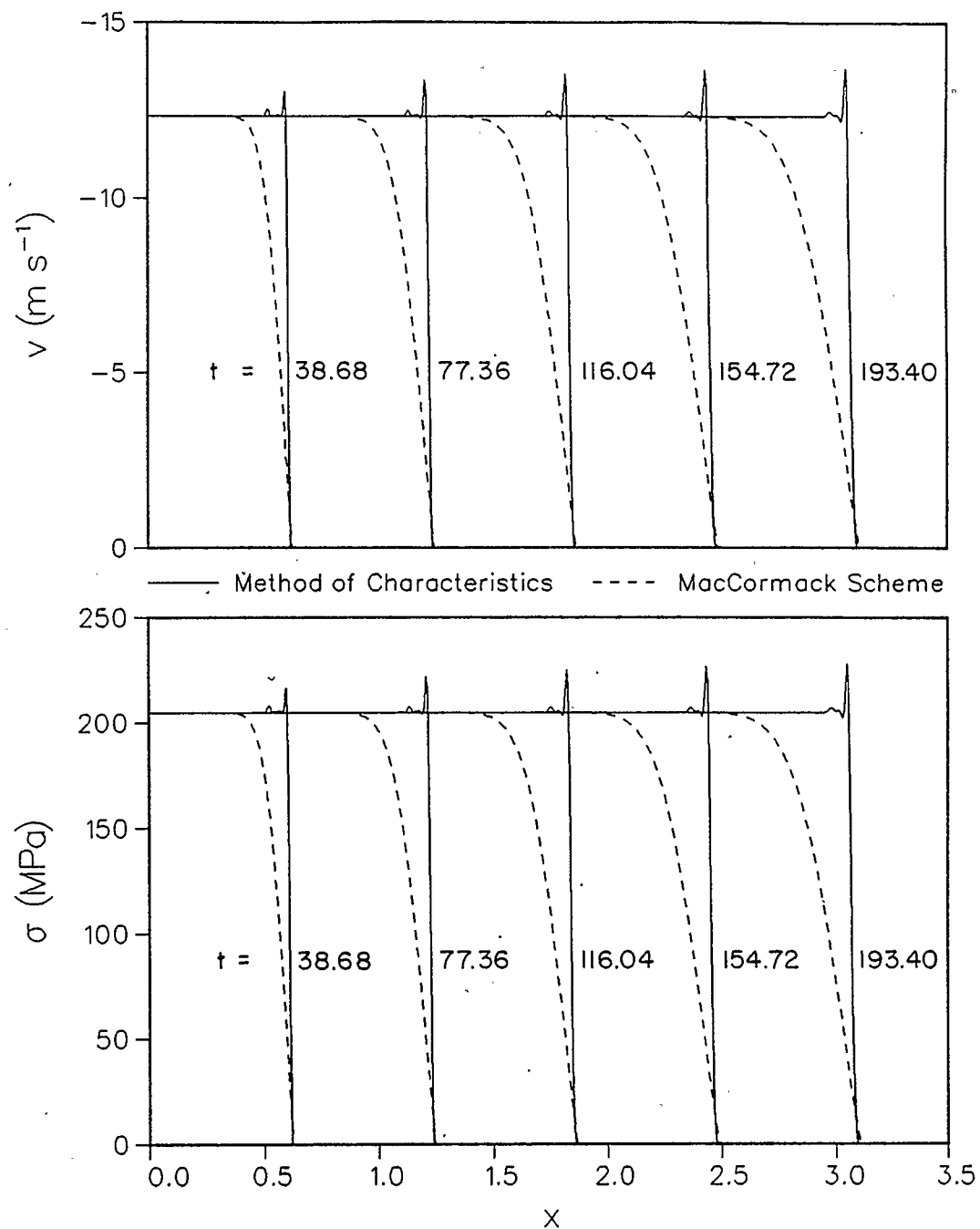


Figure 6.2a Velocity and stress response of SIAR to stress and temperature step inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.0158$, $\Delta t = 0.387$).

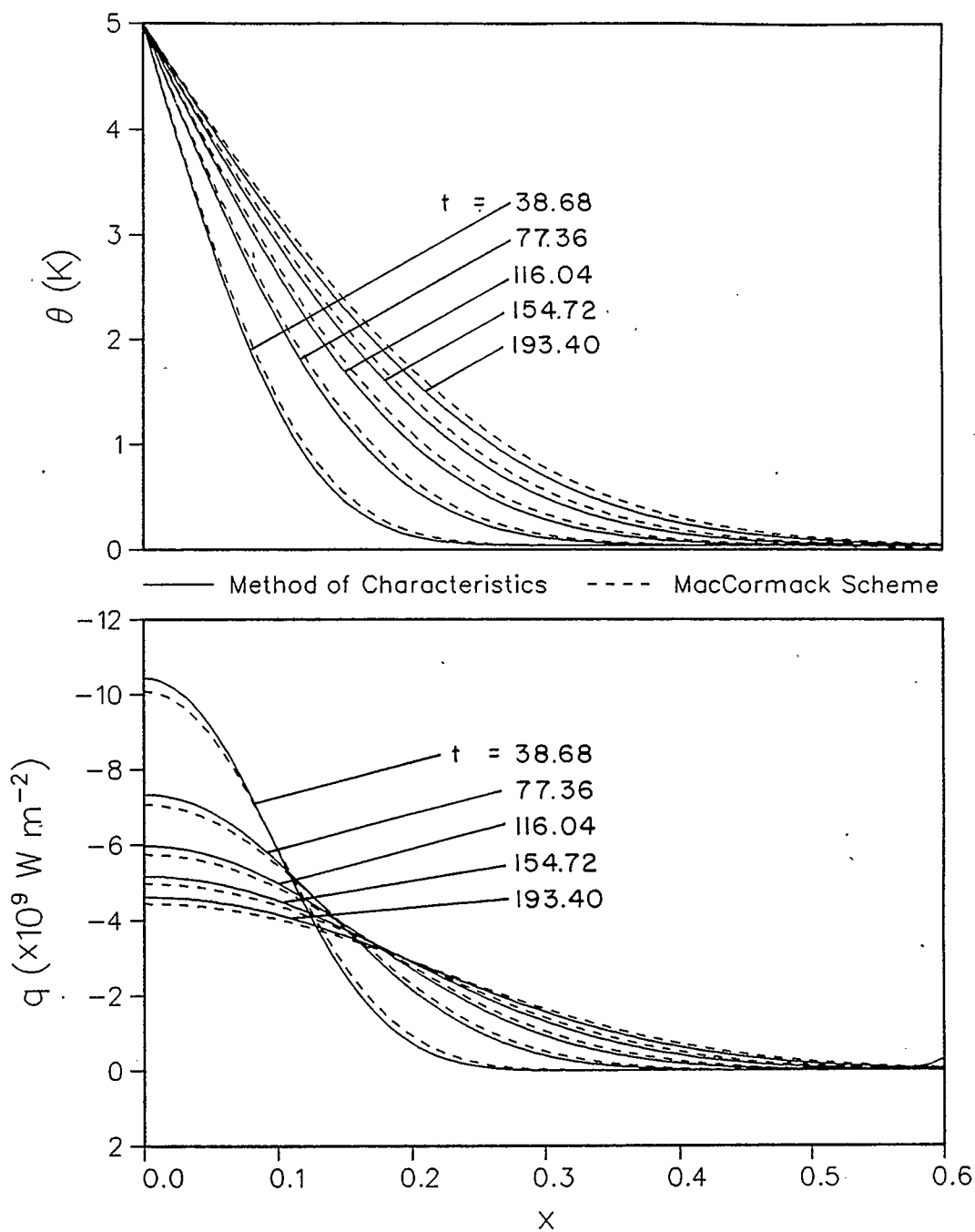


Figure 6.2b Temperature and heat flux response of SIAR to stress and temperature step inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $X_{DF} = 0.0158$, $\Delta t = 0.387$, $D_0 = 1.0 \text{ E } 03$).

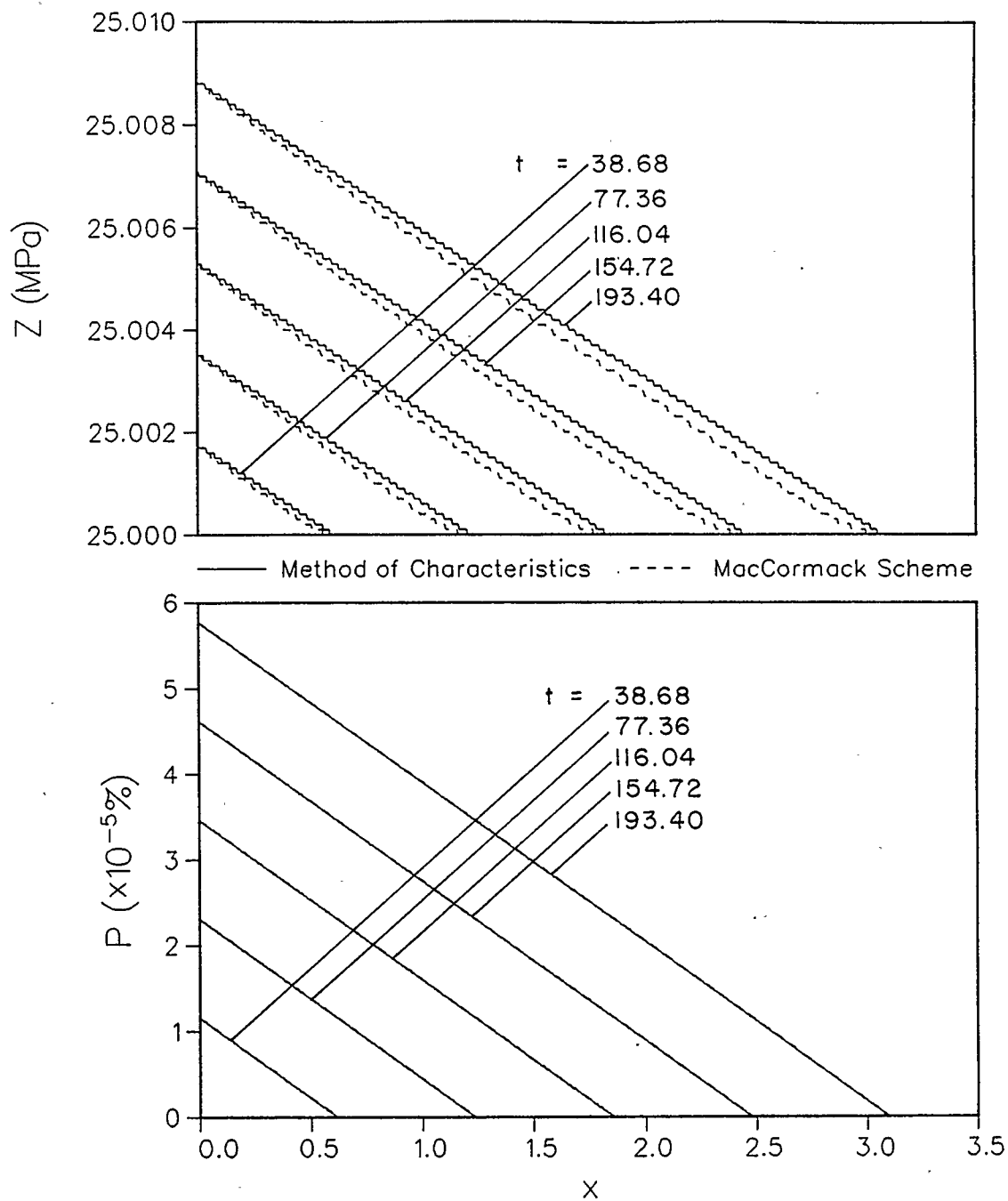


Figure 6.2c Strain hardening and plastic strain response of SIAR to stress and temperature step inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.0158$, $\Delta t = 0.387$).

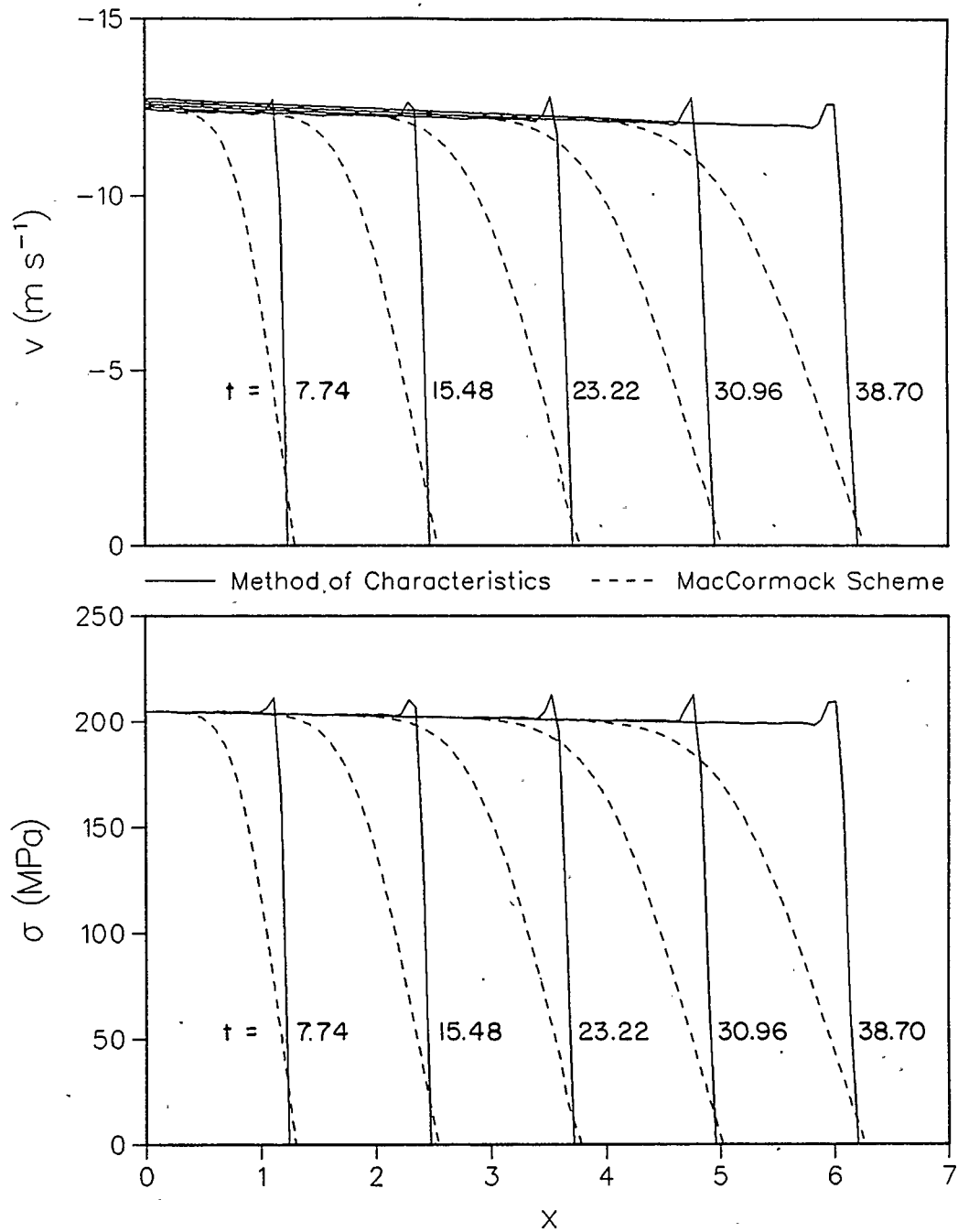


Figure 6.3a Velocity and stress response of SIAR to stress and temperature step inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $x_{DF} = 0.158$, $\Delta t = 0.0387$, $D_0 = 1.0 \times 10^6$).

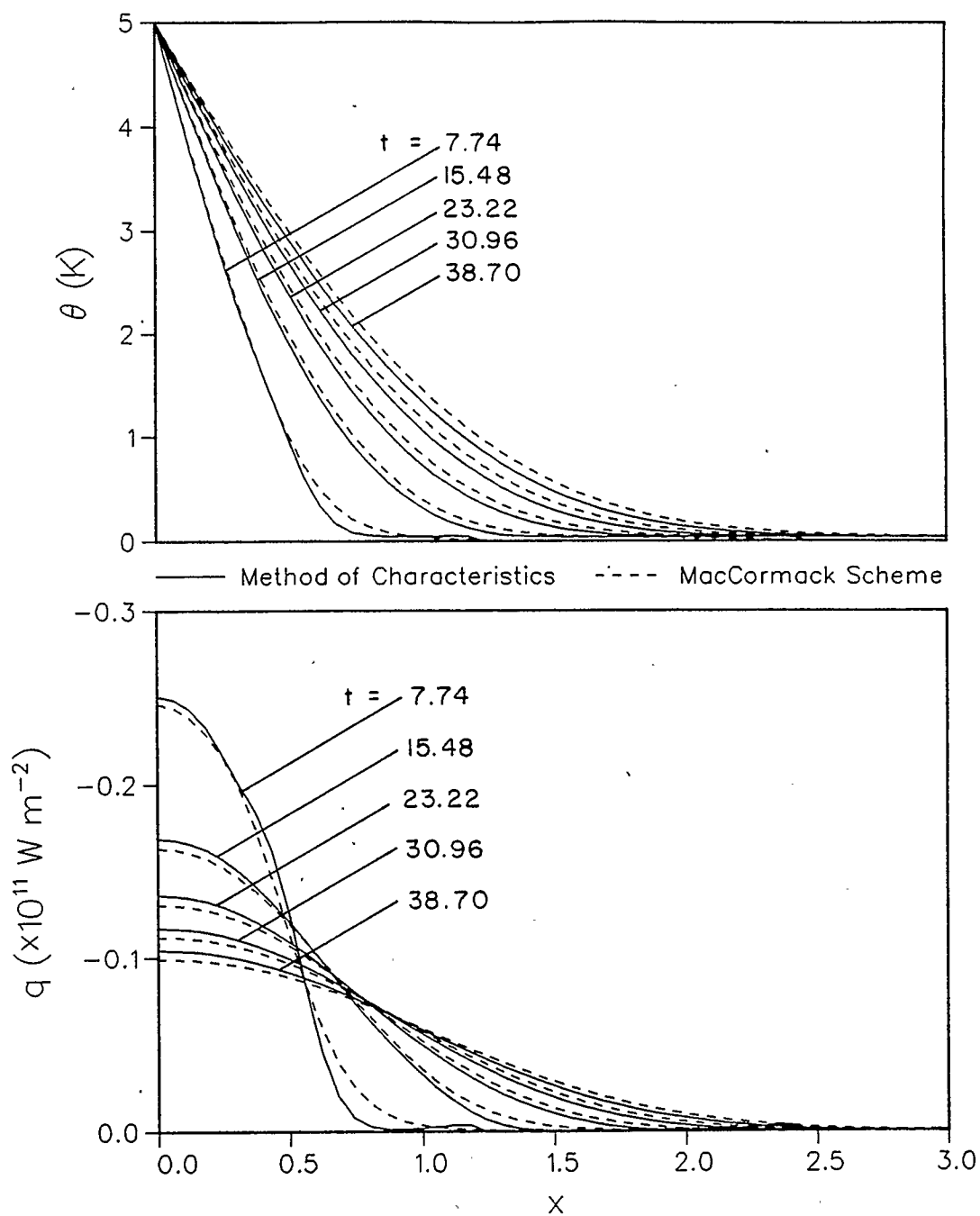


Figure 6.3b Temperature and heat flux response of SIAR to stress and temperature step inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 06$, $X_{DF} = 0.158$, $\Delta t = 0.0387$).

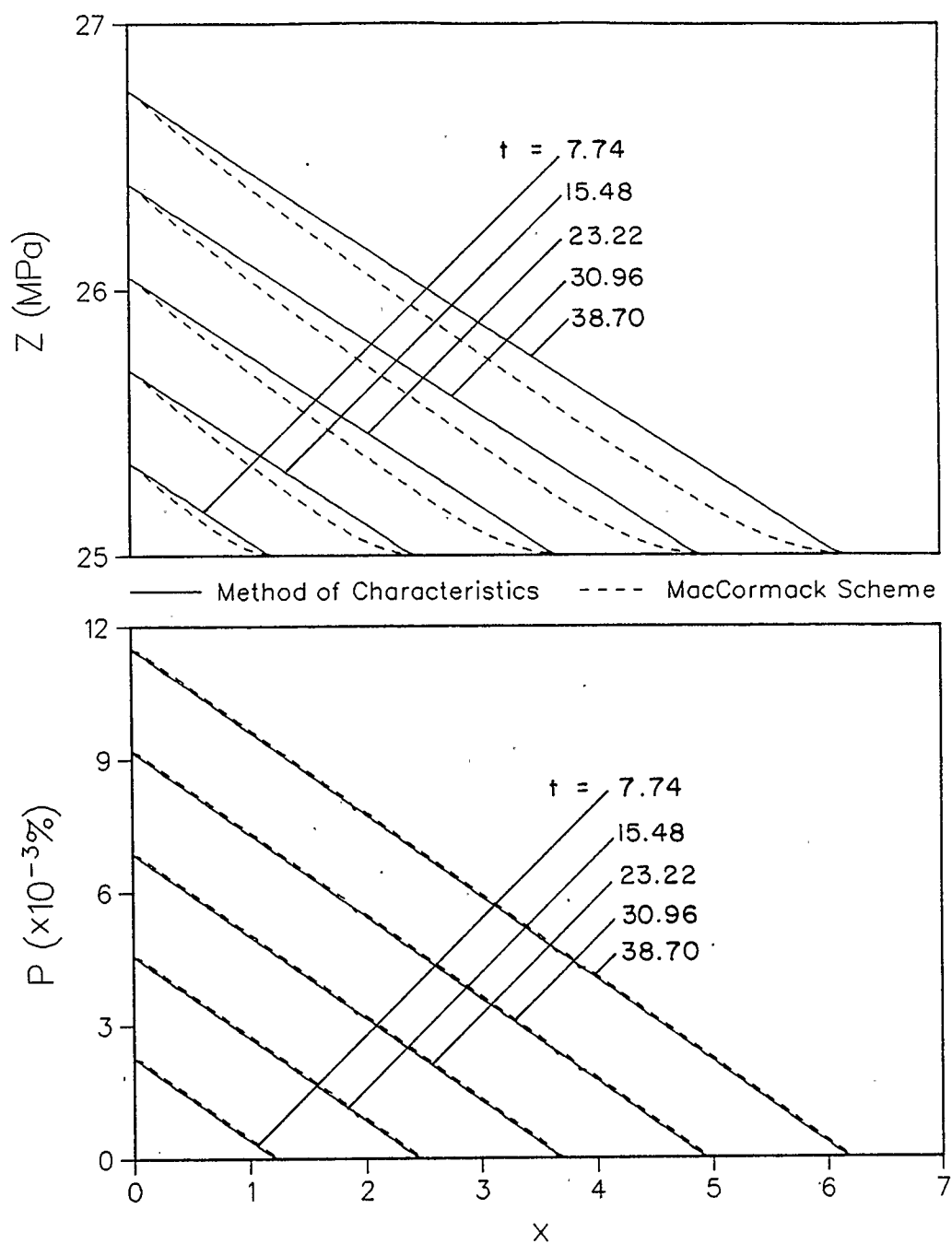


Figure 6.3c Strain hardening and plastic strain response of SIAR to stress and temperature step inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 06$, $X_{DF} = 0.158$, $\Delta t = 0.0387$).

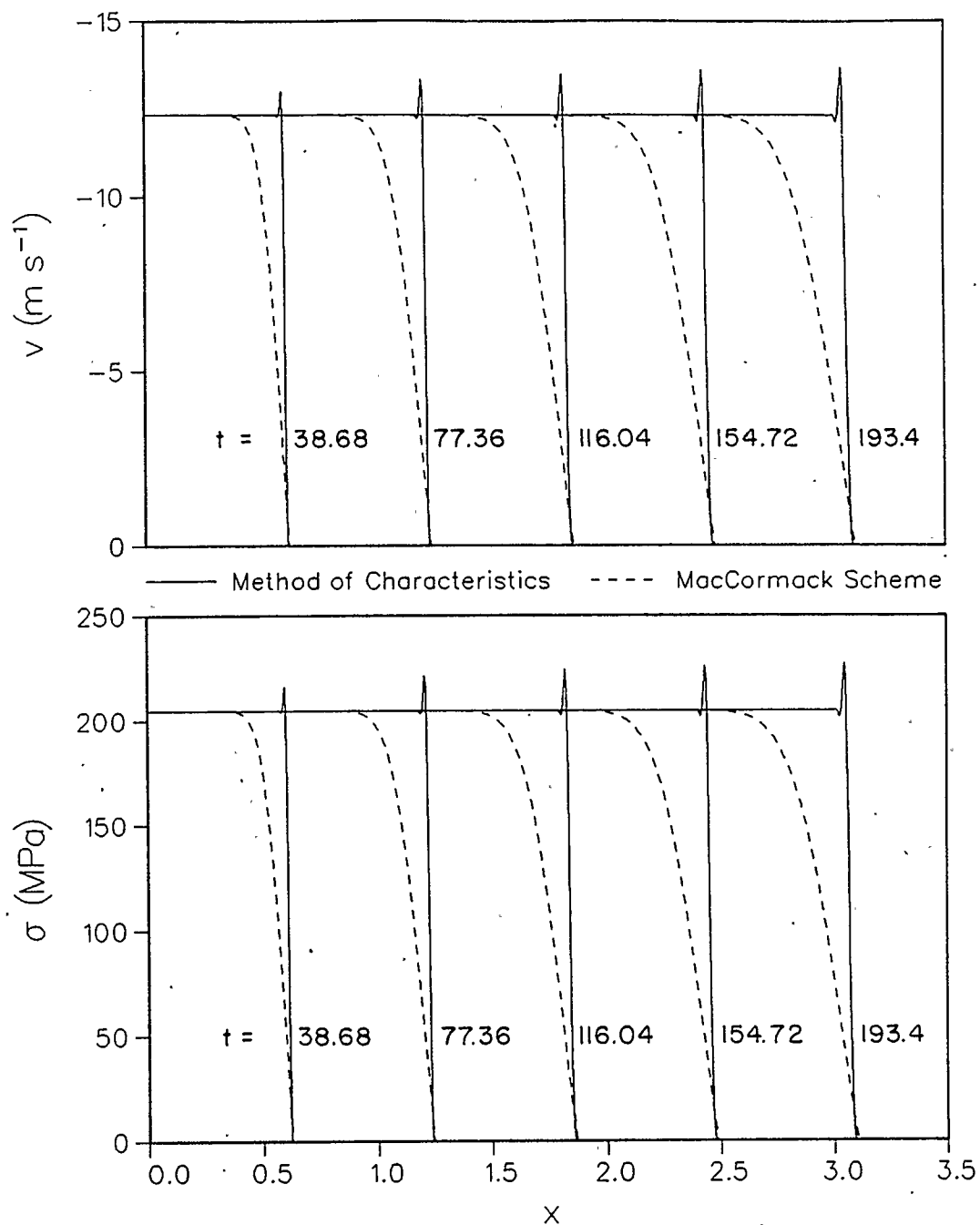


Figure 6.4a Velocity and stress response of SIAR to stress only step input ($\sigma_0 = 205$ MPa, $\theta_0 = 0$ K, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.0158$, $\Delta t = 0.387$).

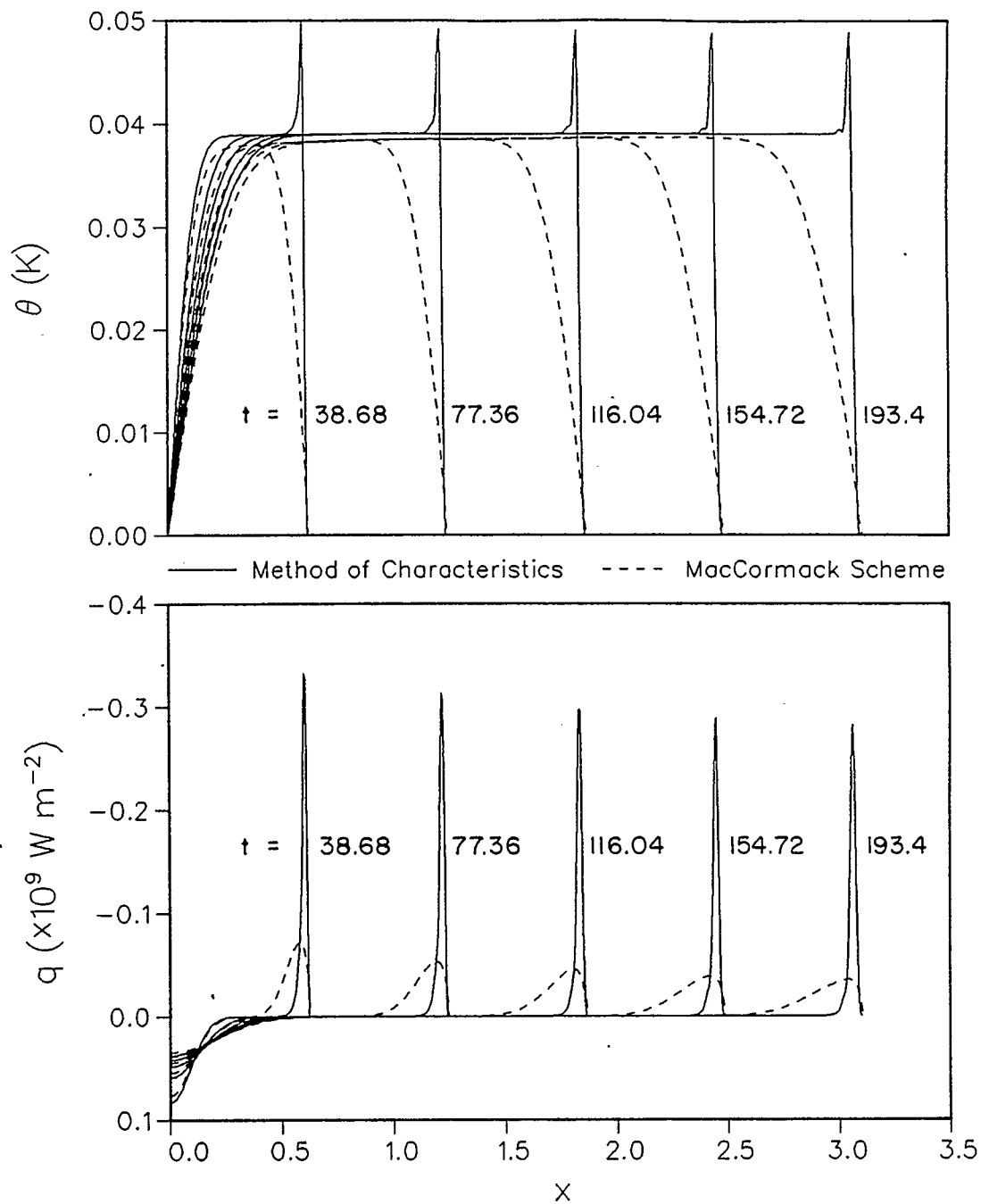


Figure 6.4b Temperature and heat flux response of SIAR to stress only step input ($\sigma_0 = 205$ MPa, $\theta_0 = 0$ K, $D_0 = 1.0$ E 03, $\Delta t = 0.387$, $X_{DF} = 0.0158$).

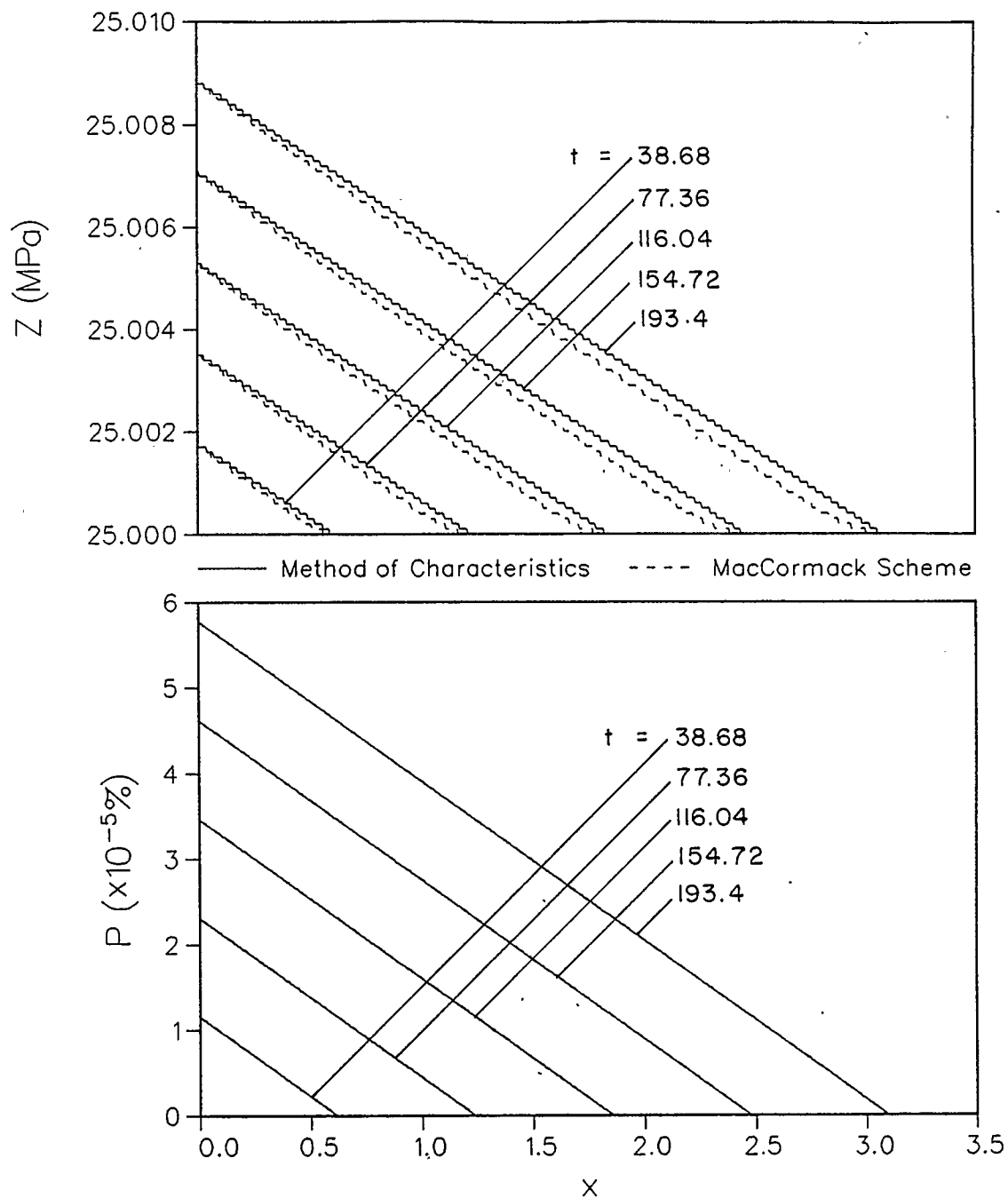


Figure 6.4c Strain hardening and plastic strain response of SIAR to stress only step input ($\sigma_0 = 205$ MPa, $\theta_0 = 0$ K, $X_{DF} = 0.0158$, $\Delta t = 0.387$, $D_0 = 1.0 \text{ E } 03$).

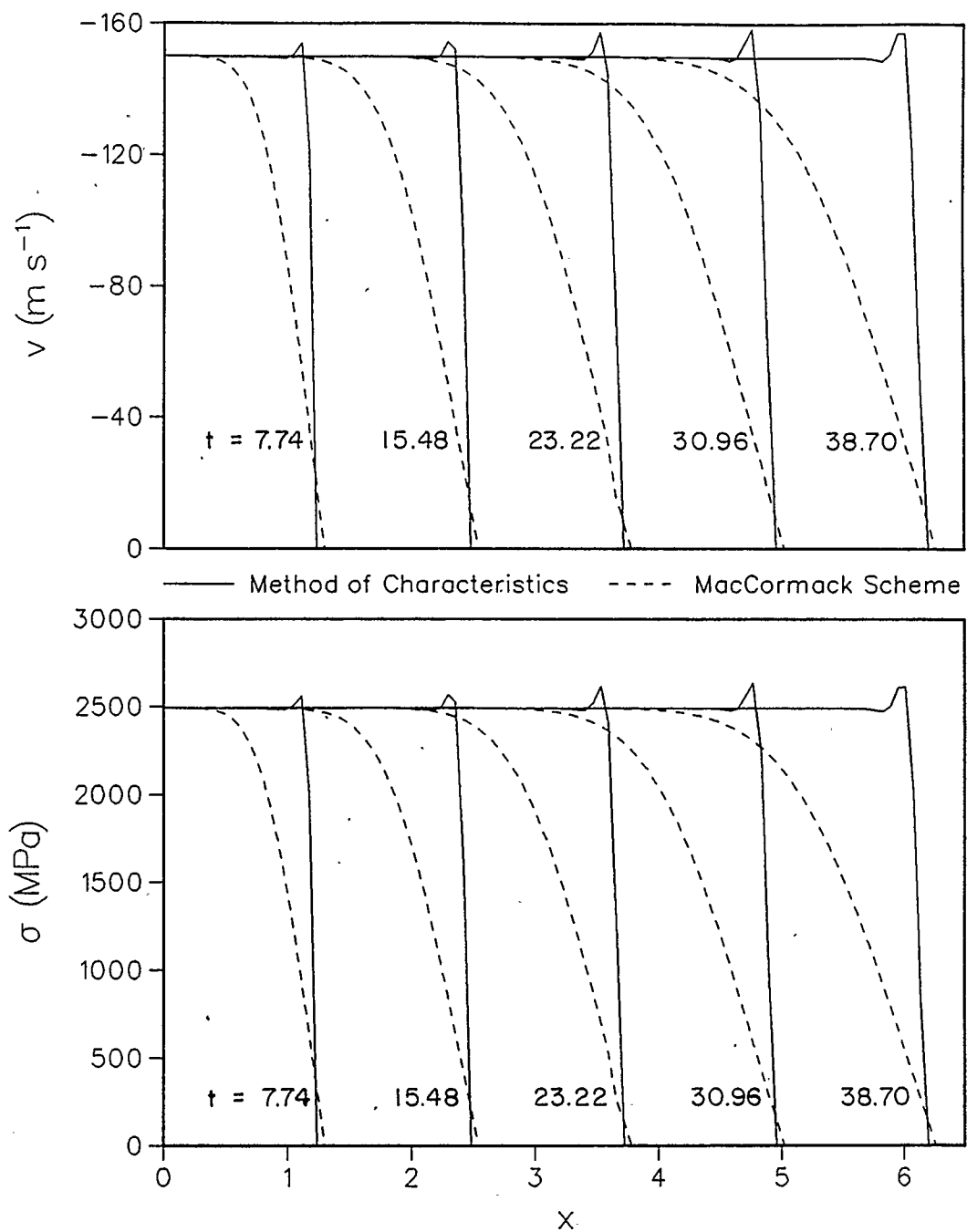


Figure 6.5a Velocity and stress response of SIAR to velocity and temperature step inputs ($v_0 = -150 \text{ ms}^{-1}$, $\theta_0 = 10 \text{ K}$, $D_0 = 1.0 \text{ E } 04$, $X_{DF} = 0.157$, $\Delta t = 0.387$).

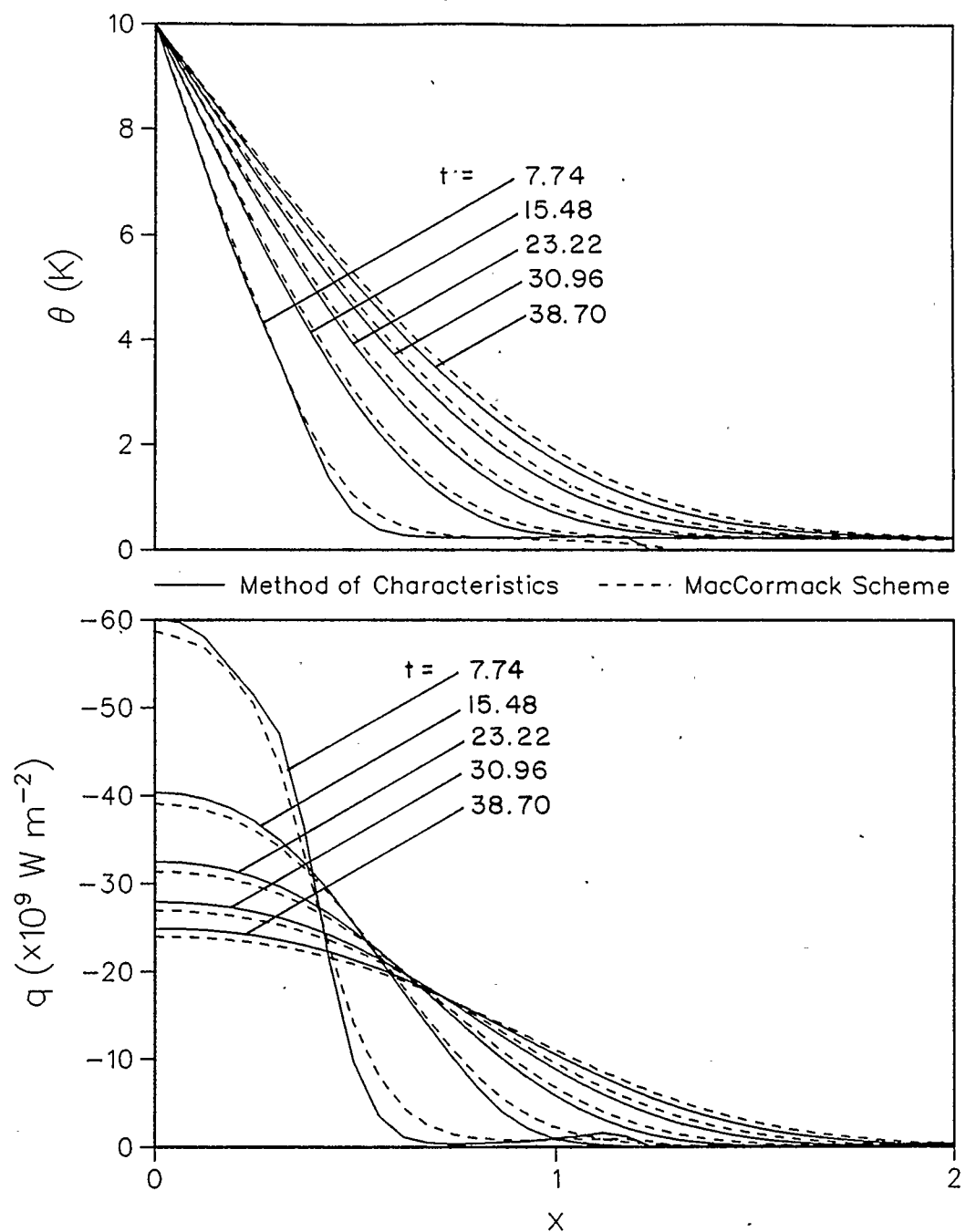


Figure 6.5b Temperature and heat flux response of SIAR to velocity and temperature step inputs ($v_0 = -150 \text{ ms}^{-1}$, $\theta_0 = 10 \text{ K}$, $D_0 = 1.0 \text{ E } 04$, $X_{DF} = 0.157$, $\Delta t = 0.387$).

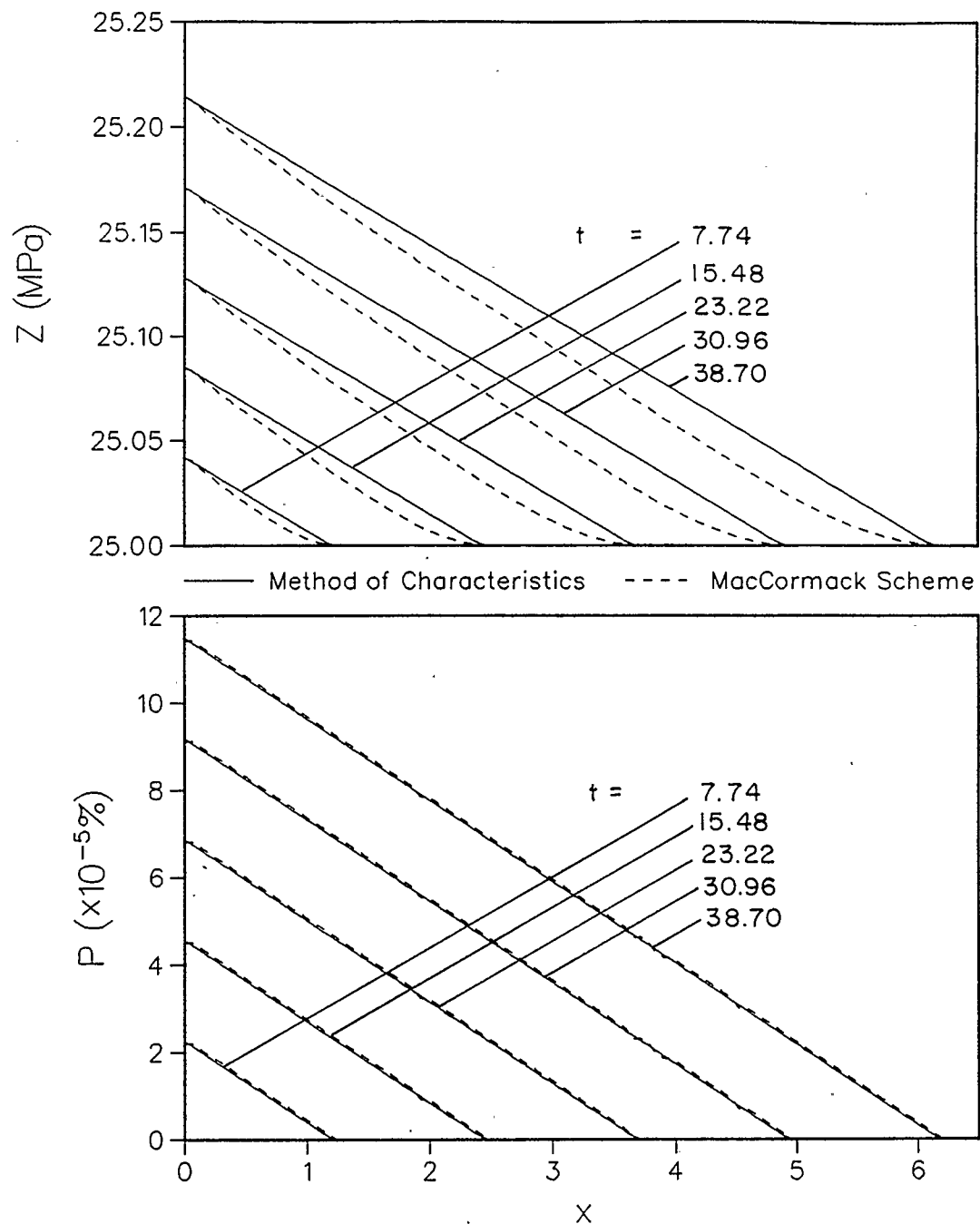


Figure 6.5c Strain hardening and plastic strain response of SIAR to velocity and temperature step inputs ($v_0 = -150 \text{ ms}^{-1}$, $\theta_0 = 10 \text{ K}$, $D_0 = 1.0 \text{ E } 04$, $X_{DF} = 0.157$, $\Delta t = 0.387$).

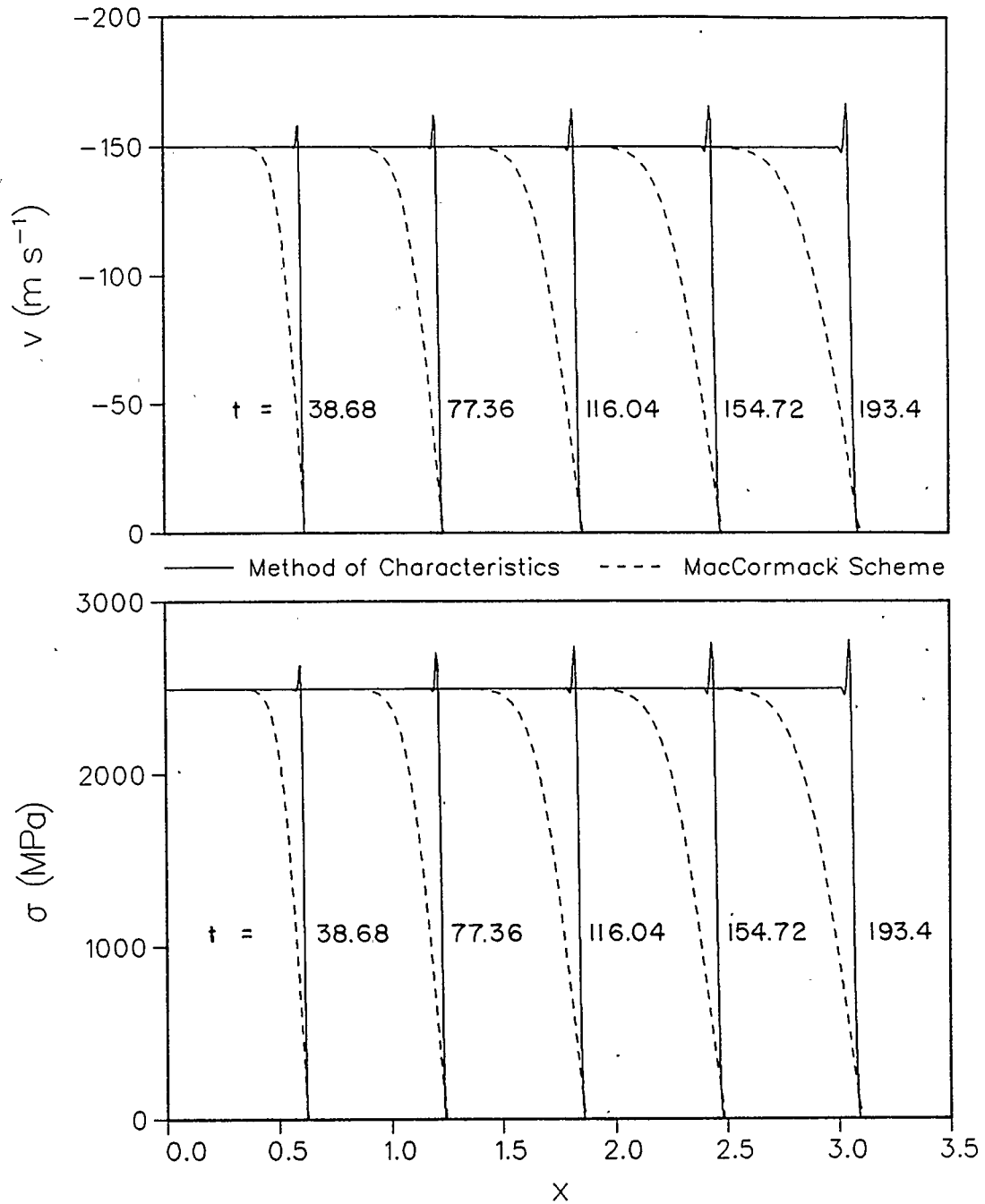


Figure 6.6a Velocity and stress response of SIAR to velocity only step input ($v_0 = -150 \text{ ms}^{-1}$, $\theta_0 = 0 \text{ K}$, $D_0 = 1.0 \text{ E } 03$, $\Delta t = 0.387$, $x_{DF} = 0.0158$).

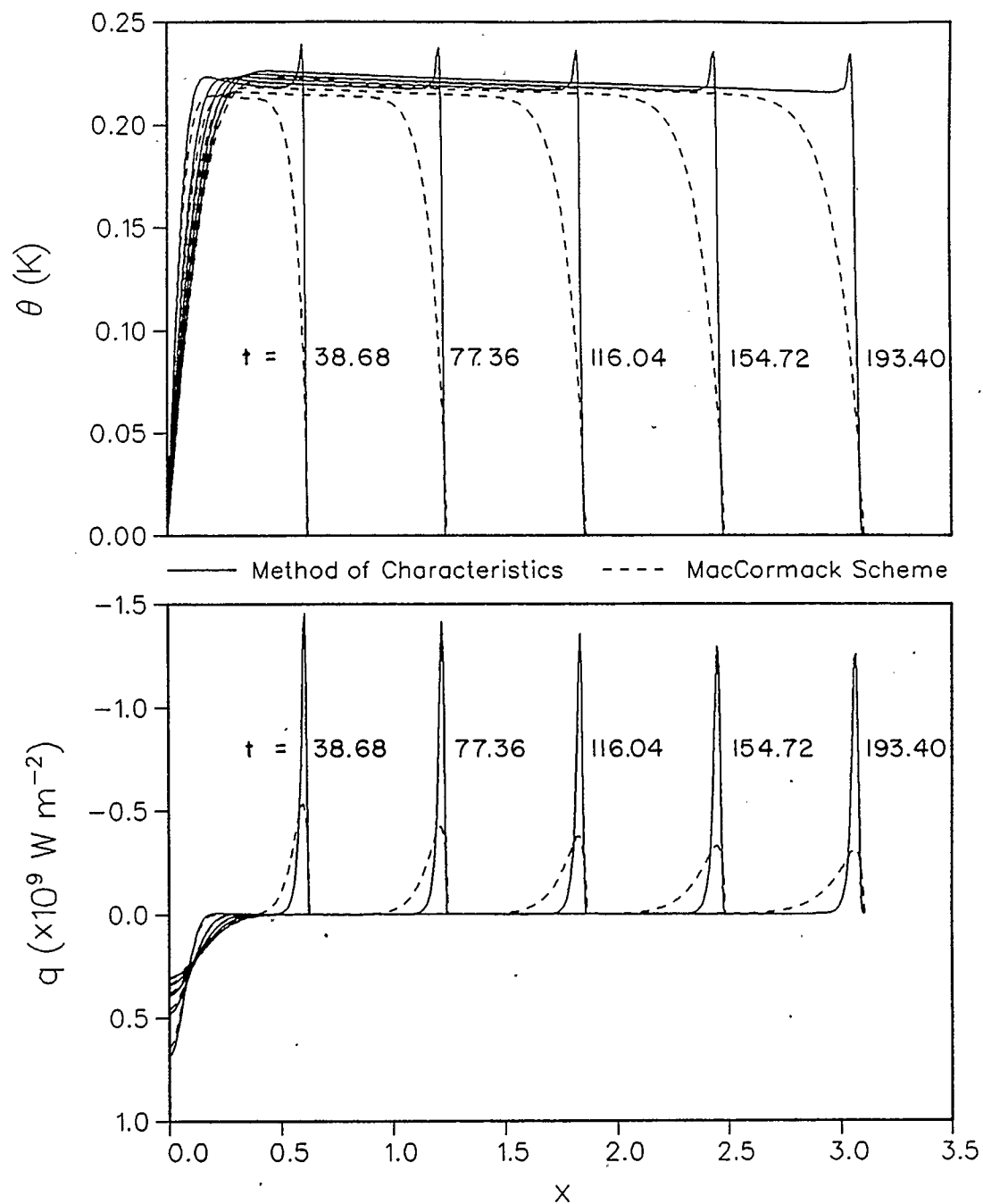


Figure 6.6b Temperature and heat flux response of SIAR to velocity only step input ($v_0 = -150 \text{ ms}^{-1}$, $\theta_0 = 0 \text{ K}$, $D_0 = 1.0 \text{ E } 03$, $\Delta t = 0.387$, $X_{DF} = 0.0158$).

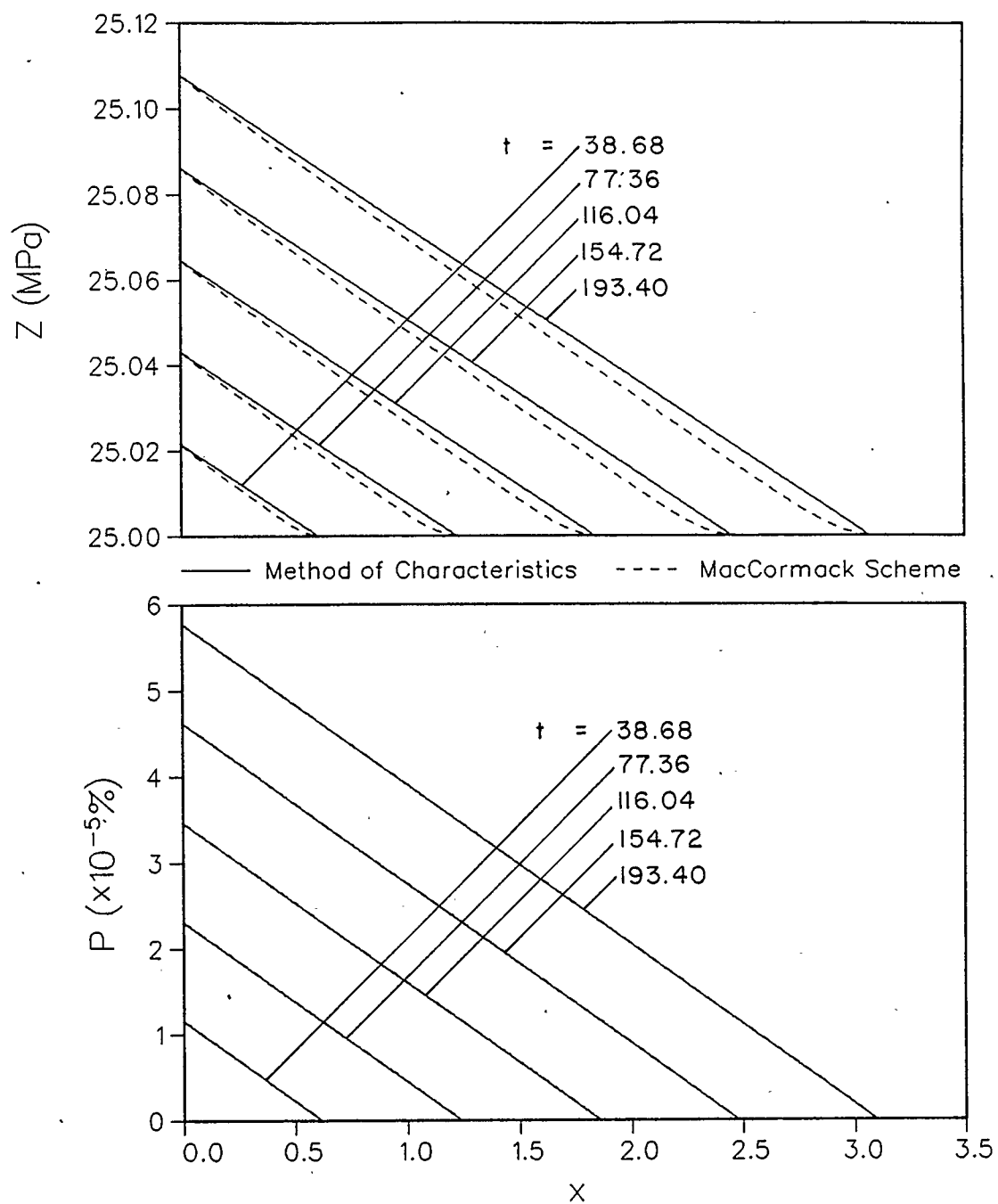


Figure 6.6c Strain hardening and plastic strain response of SIAR to velocity only step input ($v_0 = -150 \text{ ms}^{-1}$, $\theta_0 = 0 \text{ K}$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.0158$, $\Delta t = 0.387$).

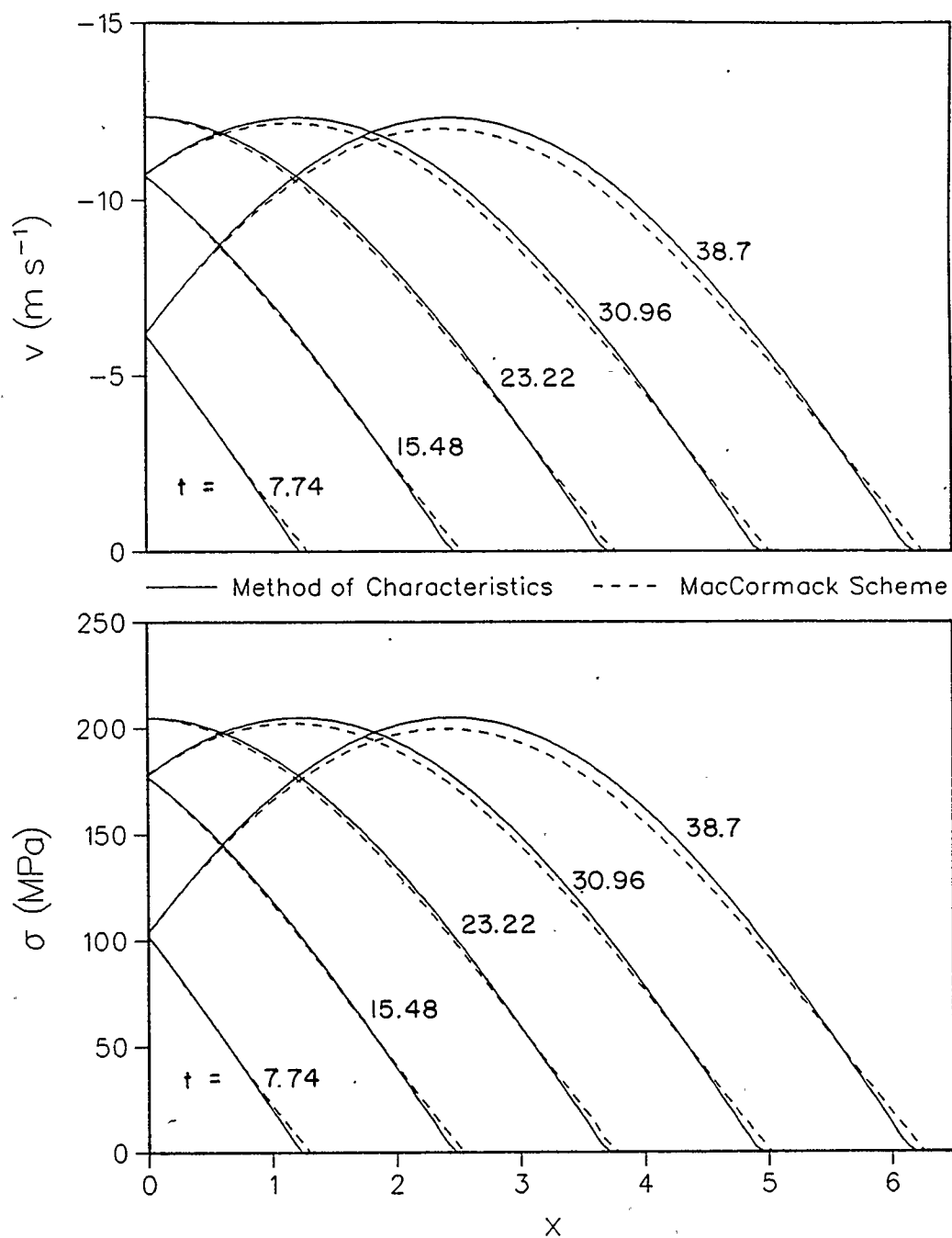


Figure 6.7a Velocity and stress response of SIAR to pulsive-sine stress and temperature inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.157$, $\Delta t = 0.387$, $\omega = 2.61 \text{ E } 10$).

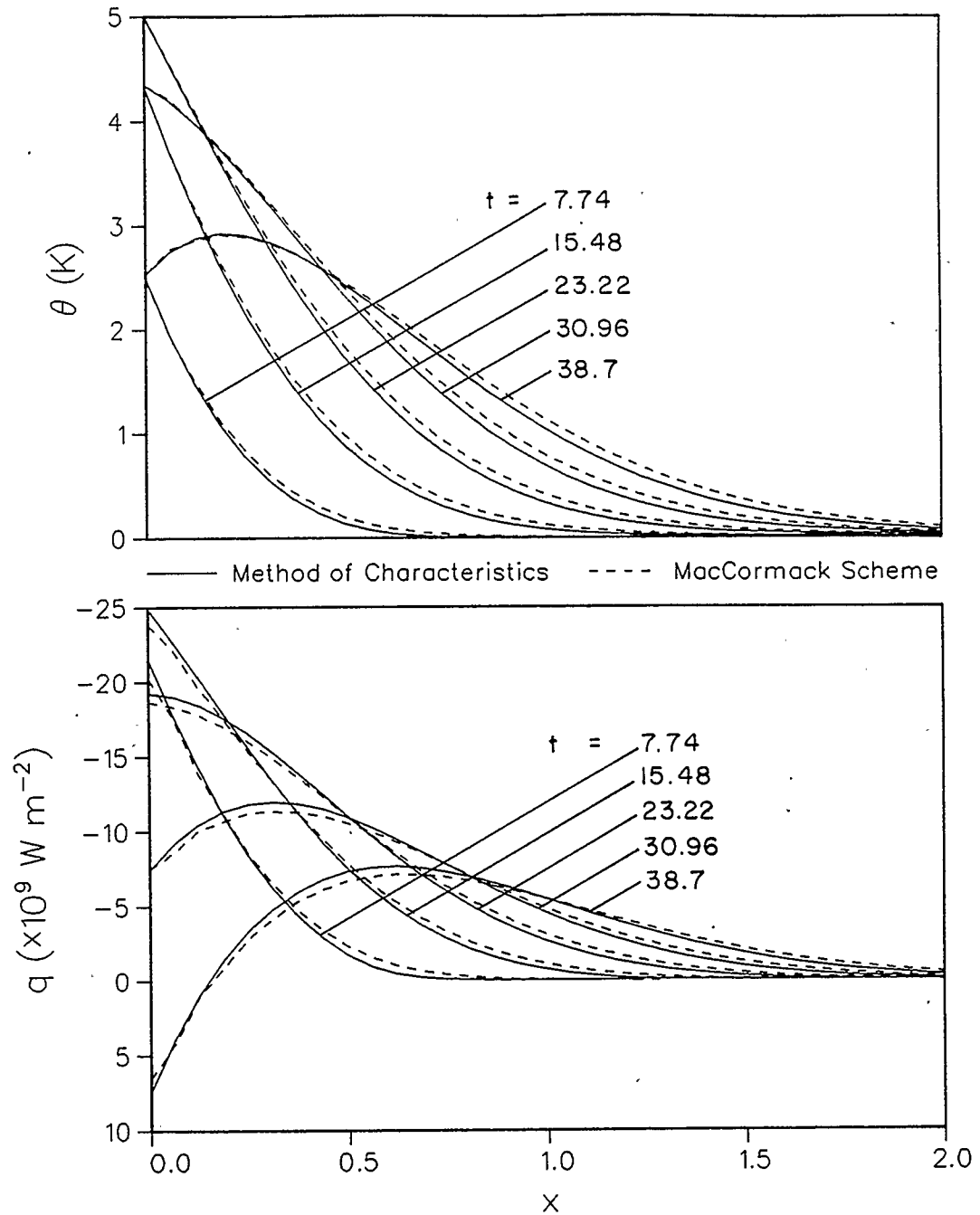


Figure 6.7b Temperature and heat flux response of SIAR to pulsed-sine stress and temperature inputs ($\sigma_0 = 205 \text{ MPa}$, $\theta_0 = 5 \text{ K}$, $\omega = 2.61 \text{ E } 10$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.157$, $\Delta t = 0.387$).

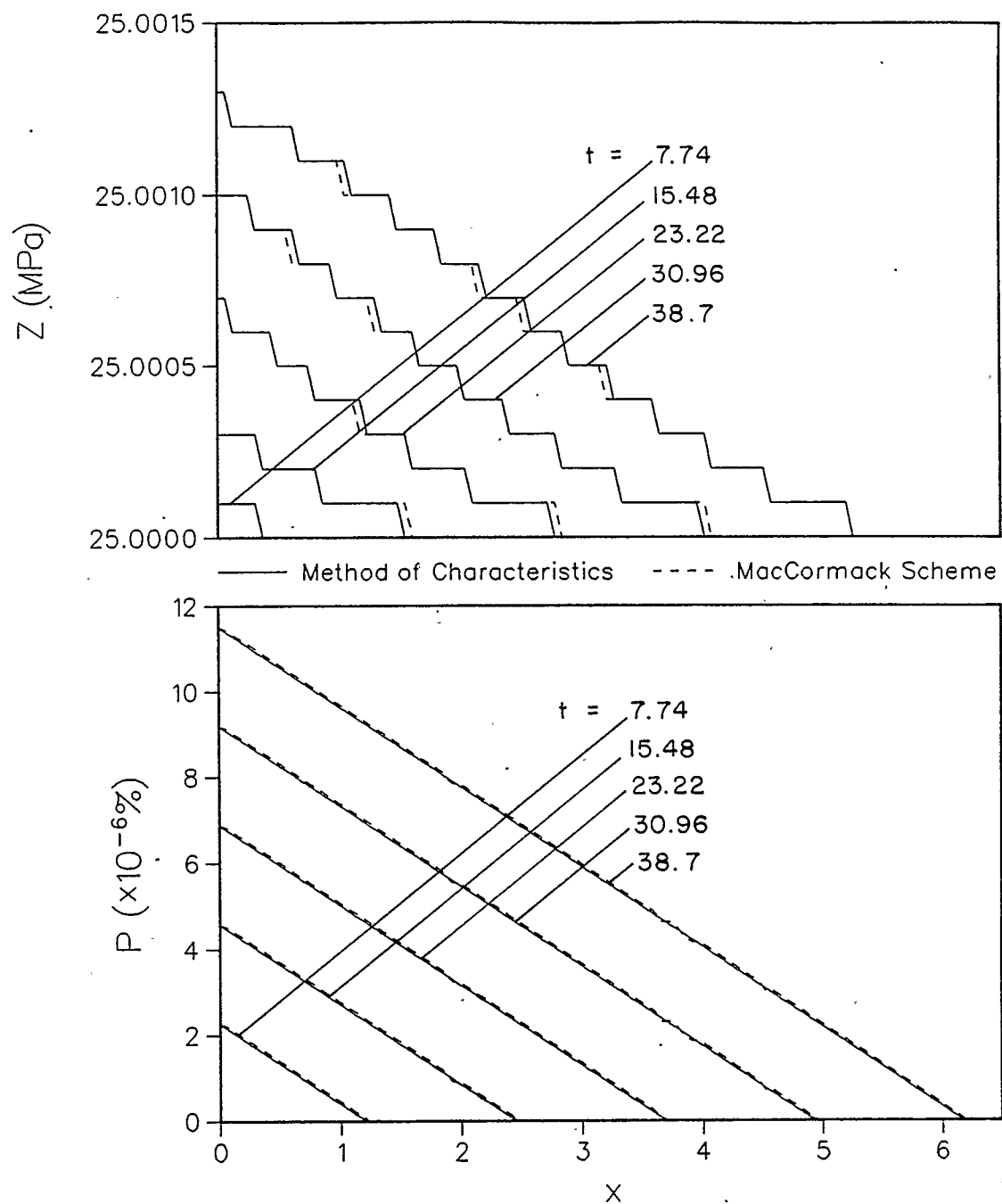


Figure 6.7c Strain hardening and plastic strain response of SIAR to pulsive-sine stress and temperature inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $\omega = 2.61 \text{ E } 10$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.157$, $\Delta t = 0.387$).

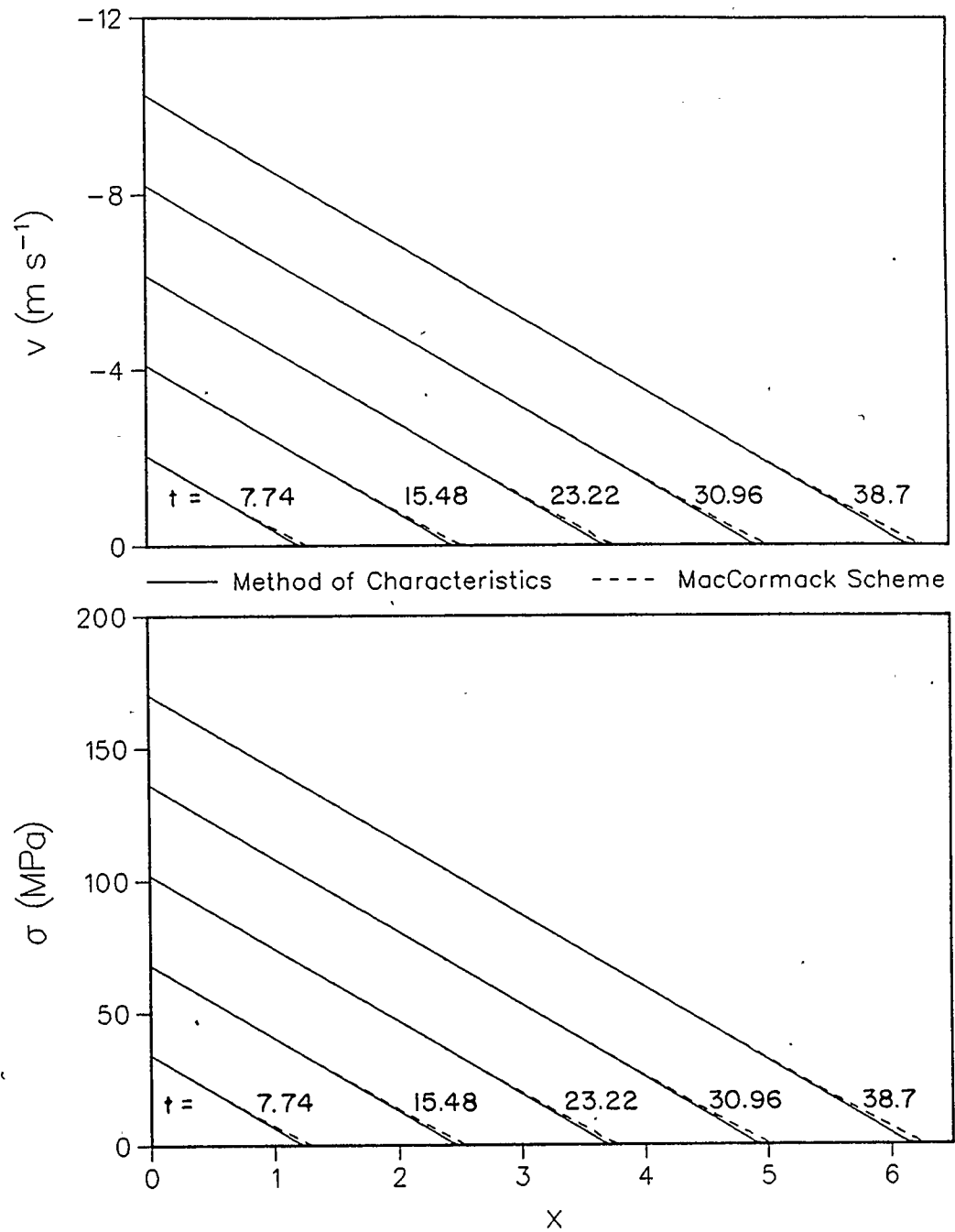


Figure 6.8a Velocity and stress response of SIAR to terminated-ramp stress and temperature inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $\omega = 2.61 \text{ E } 10$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.157$, $\Delta t = 0.387$).

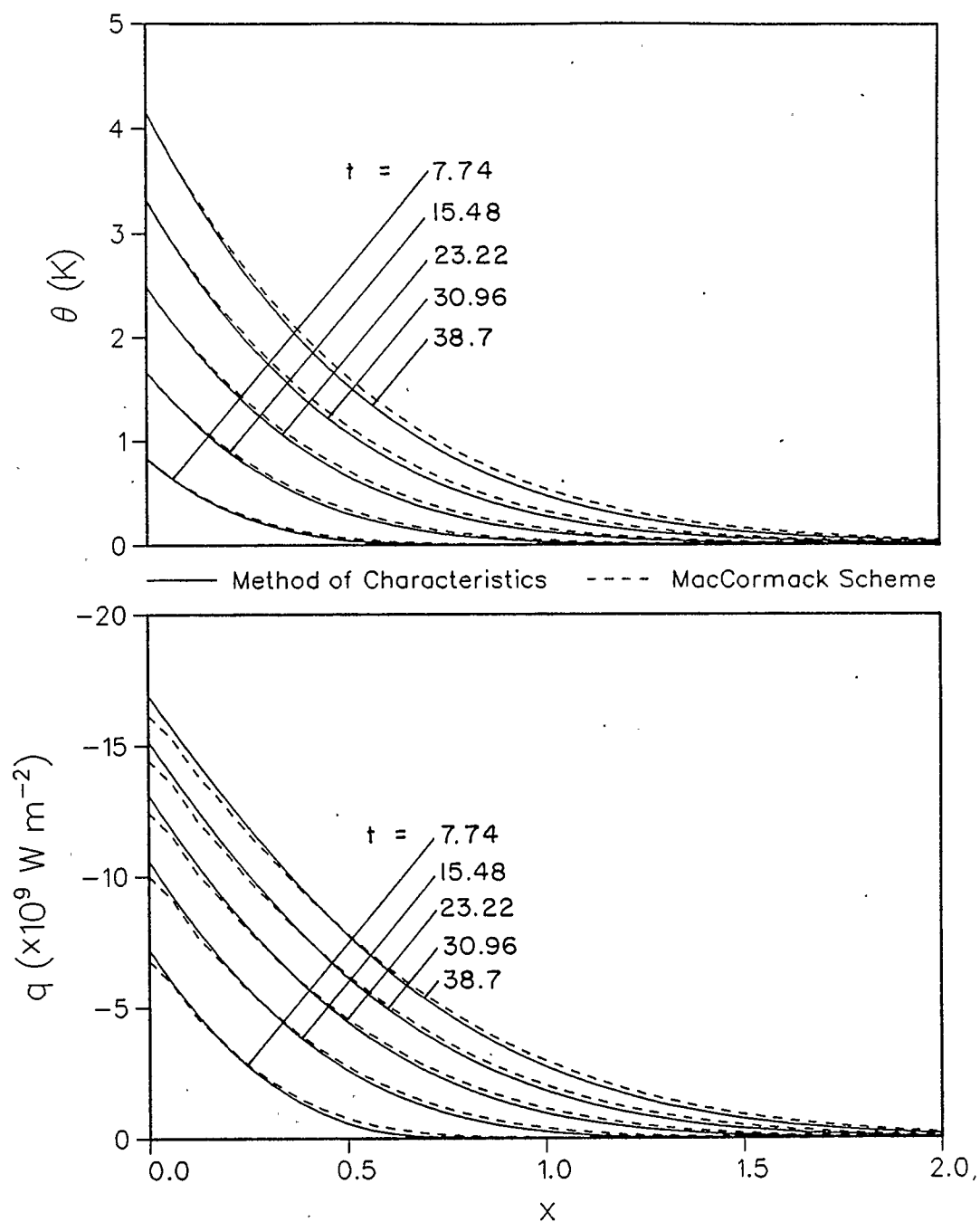


Figure 6.8b Temperature and heat flux response of SIAR to terminated-ramp stress and temperature inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $\omega = 2.61 \text{ E } 10$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.157$, $\Delta t = 0.387$).

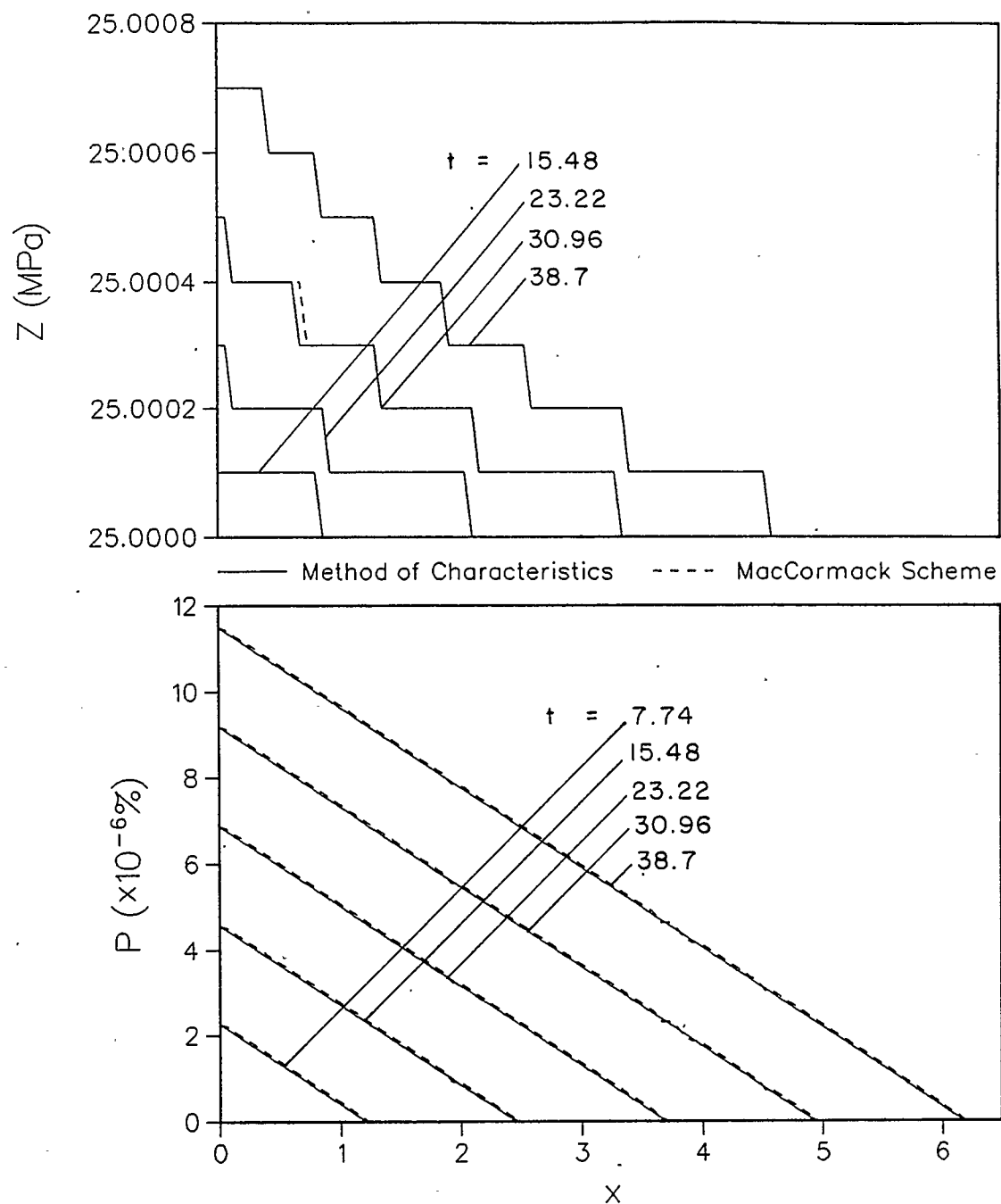


Figure 6.8c Strain hardening and plastic strain response of SIAR to terminated-ramp stress and temperature inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $\omega = 2.61 \text{ E } 10$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.157$, $\Delta t = 0.387$).

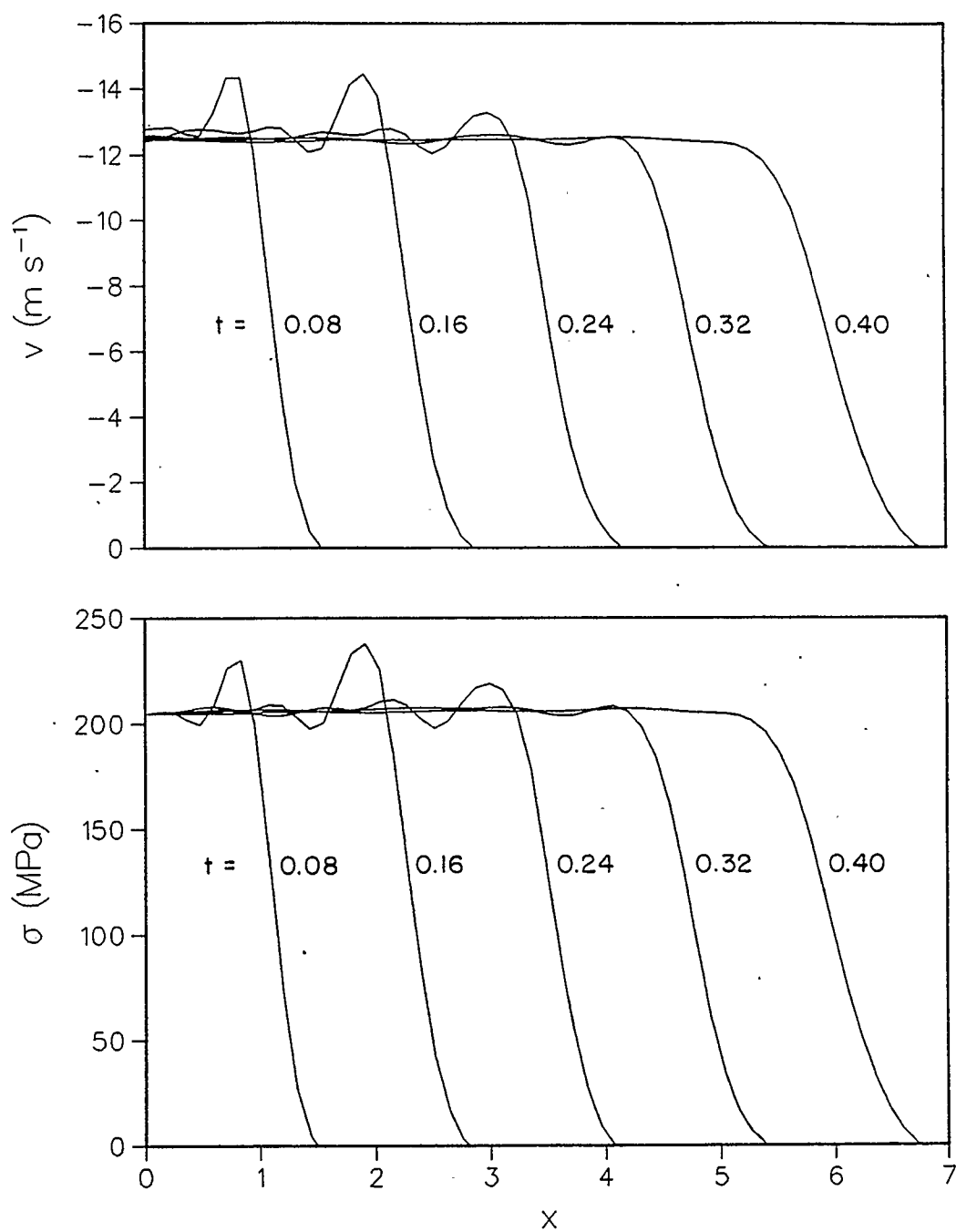


Figure 6.9a Velocity and stress response of SIAR to stress and temperature step inputs for a very high leading wave velocity ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $\bar{D}_0 = 1.0 \text{ E-}04$, $\tau_0 = 0.147$, $x_{DF} = 9.944$, $\Delta t = 0.00387$).

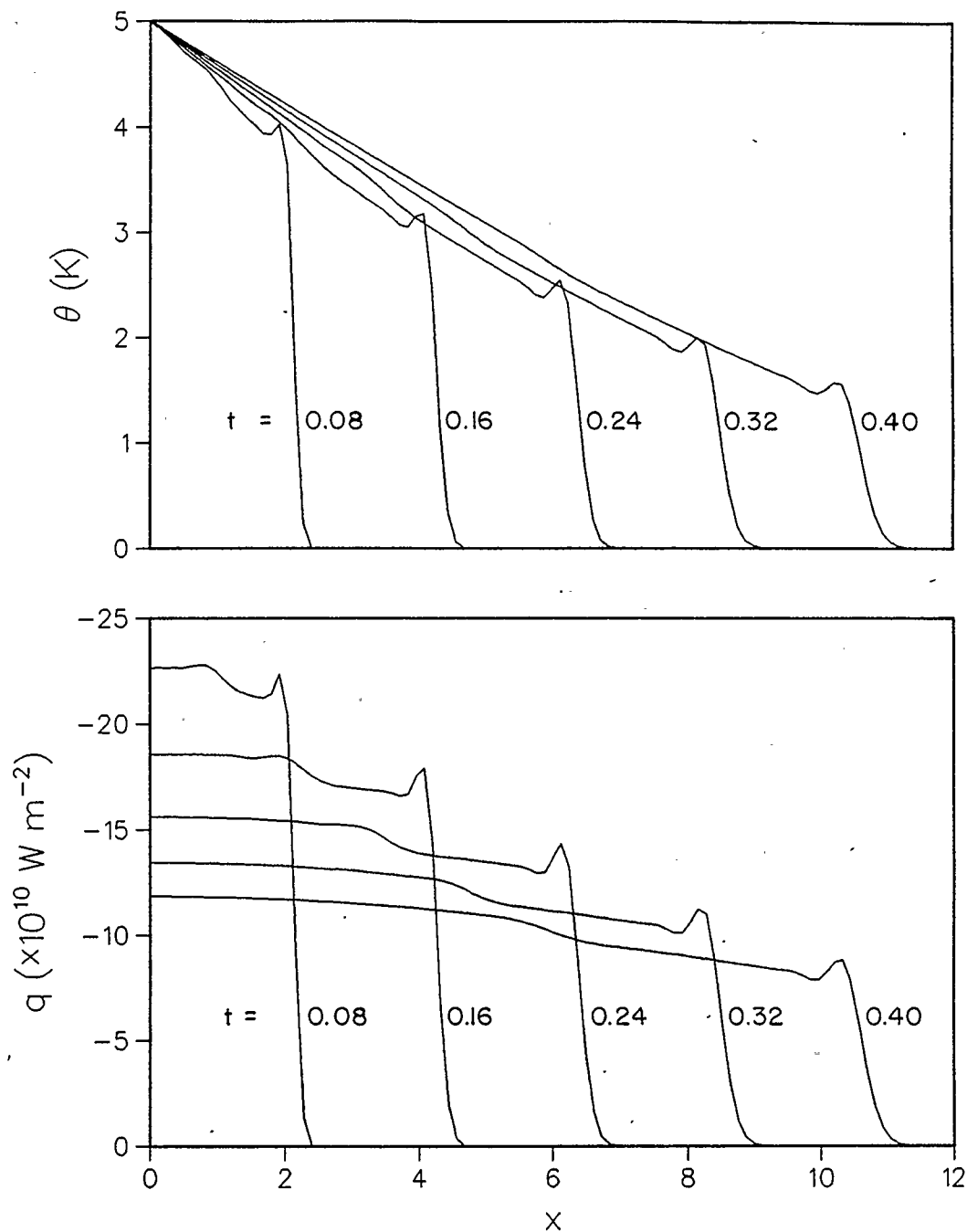


Figure 6.9b Temperature and heat flux response of SIAR to stress and temperature step inputs for a very high leading wave velocity ($\sigma_0 = 205 \text{ MPa}$, $\theta_0 = 5 \text{ K}$, $D_0 = 1.0 \text{ E } 04$, $\tau_0 = 0.147$, $\Delta t = 0.00387$, $X_{DF} = 9.944$).

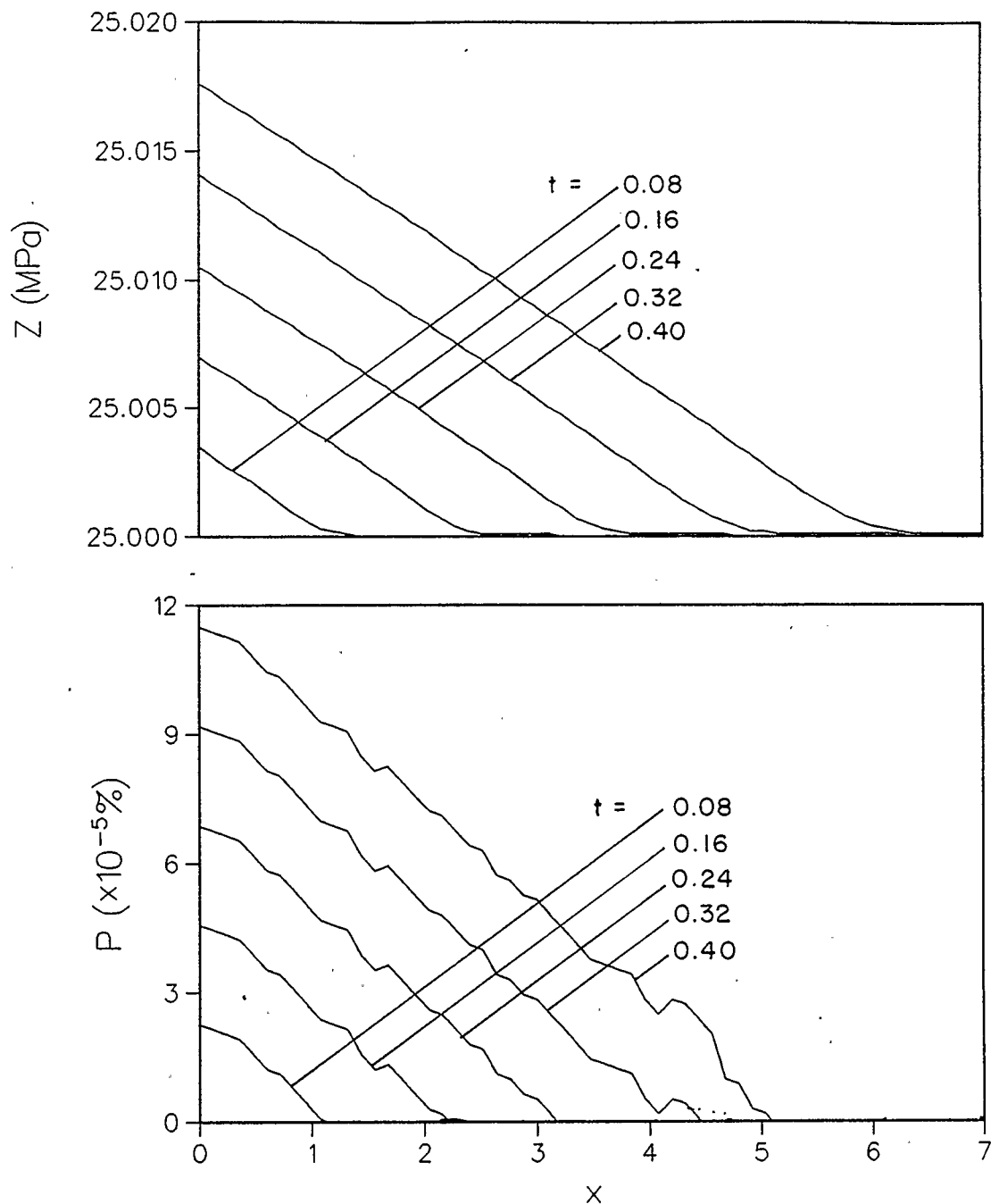


Figure 6.9c Strain hardening and plastic strain response of SIAR to stress and temperature step inputs for a very high leading wave velocity ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 04$, $\tau_0 = 0.147$, $X_{DF} = 9.944$, $\Delta t = 0.00387$).

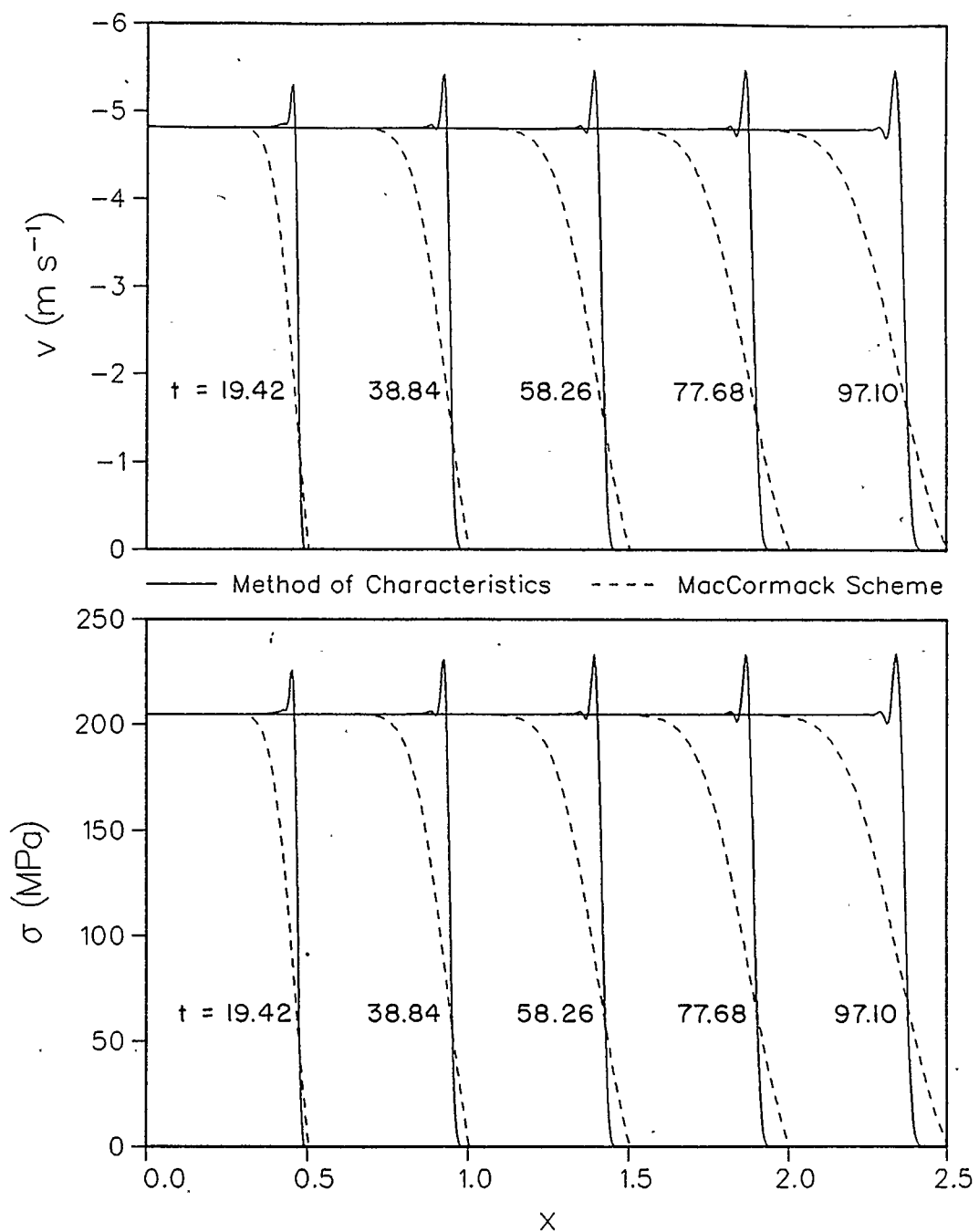


Figure 6.10a Velocity and stress response of SICOR to stress and temperature step inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.025$, $\Delta t = 0.1942$).

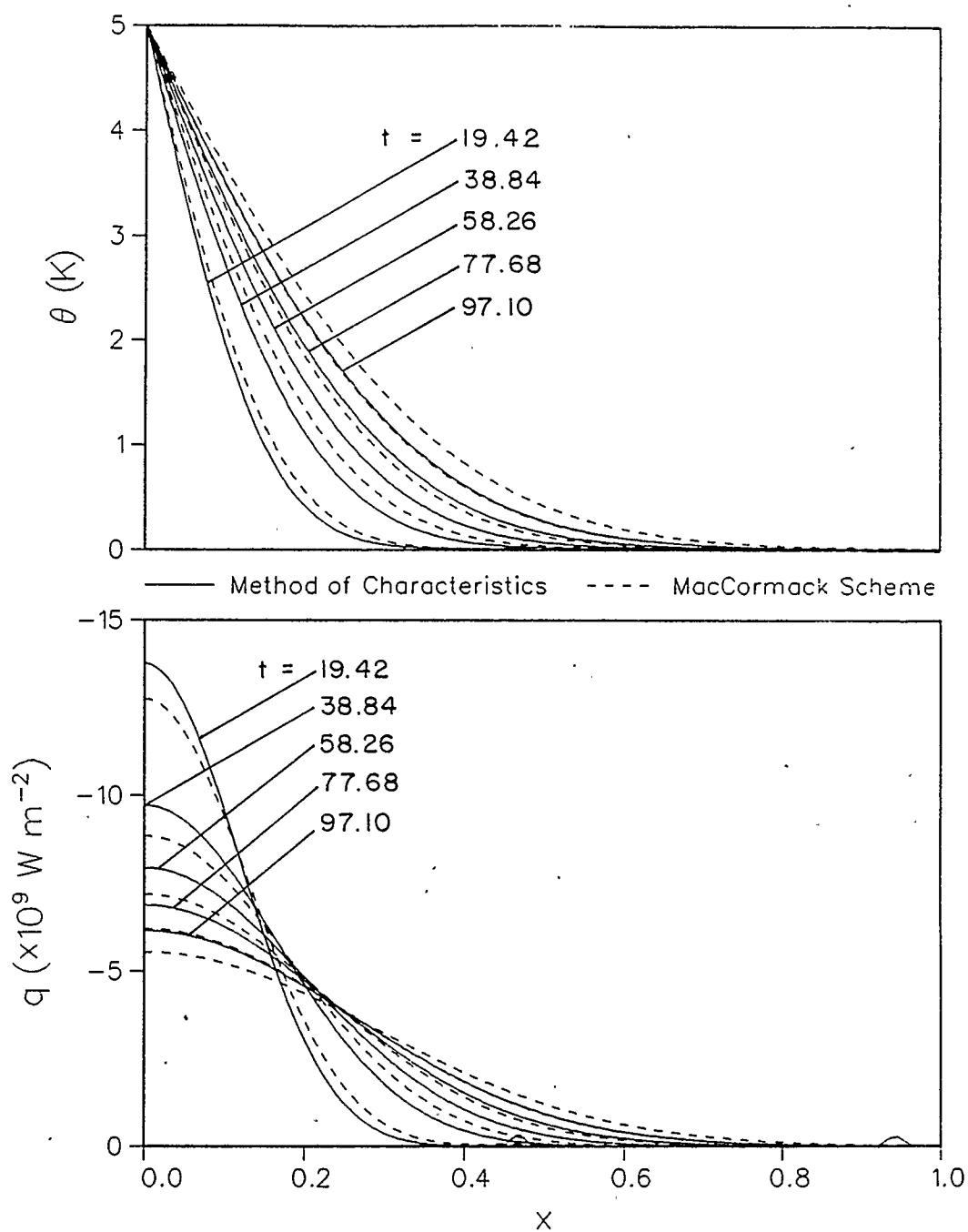


Figure 6.10b Temperature and heat flux response of SICORT to stress and temperature step inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $X_{DF} = 0.025$, $\Delta t = 0.1942$, $D_0 = 1.0 \text{ E}^{-03}$).

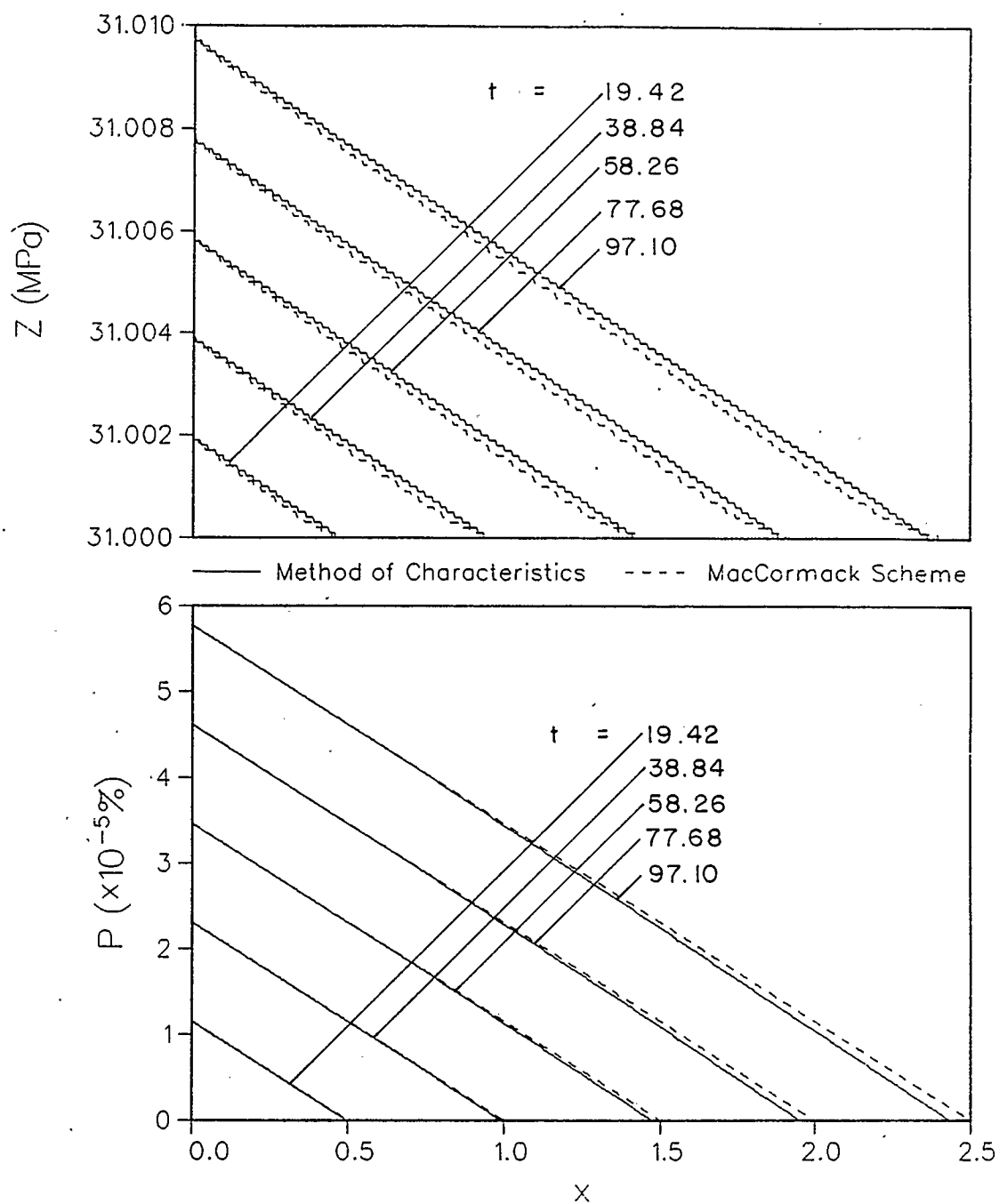


Figure 6.10c Strain hardening and plastic strain response of SICOR to stress and temperature step inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.025$, $\Delta t = 0.1942$).

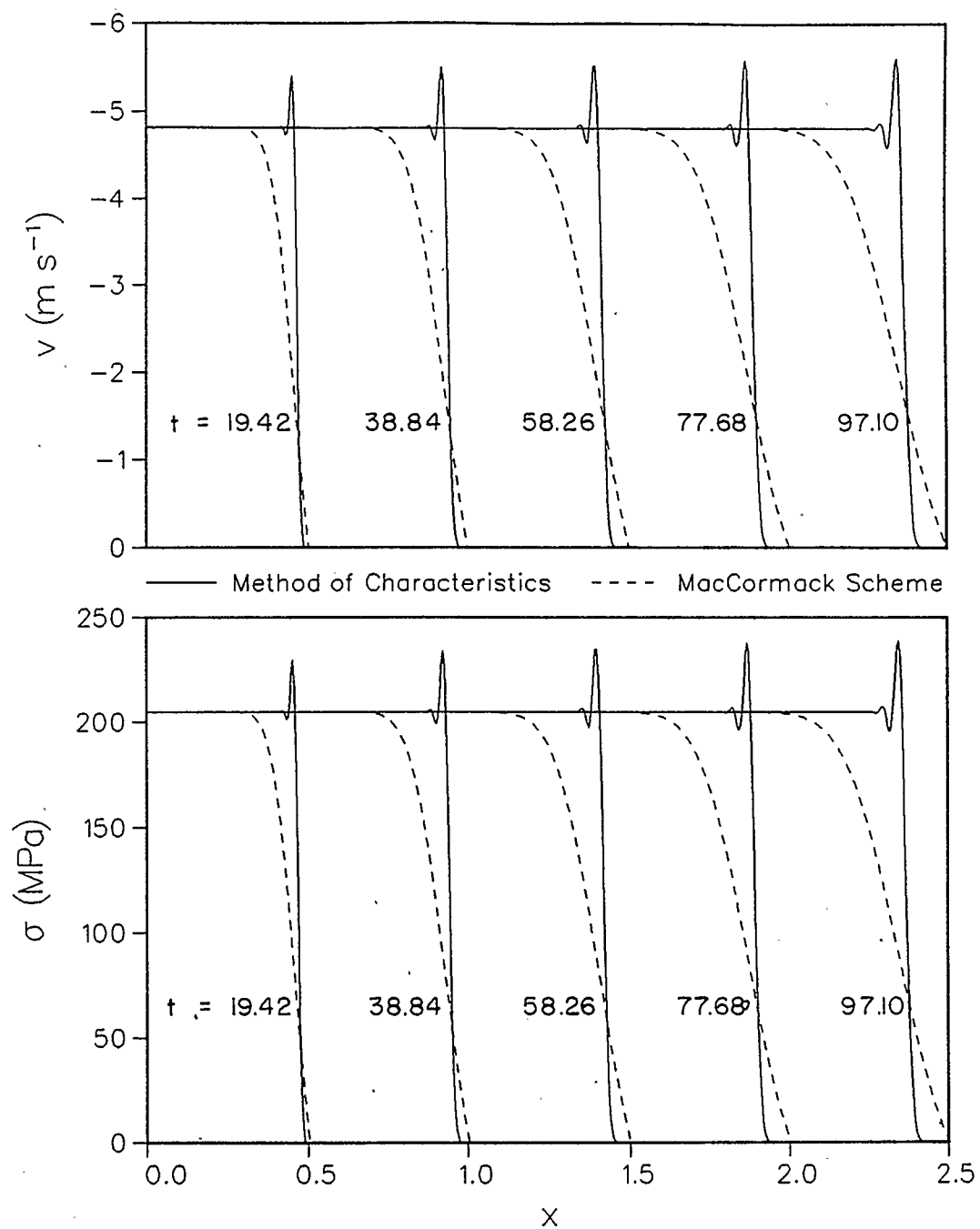


Figure 6.11a Velocity and stress response of SICOR to stress only step input ($\sigma_0 = 205$ MPa, $\theta_0 = 0$ K, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.025$, $\Delta t = 0.1942$).

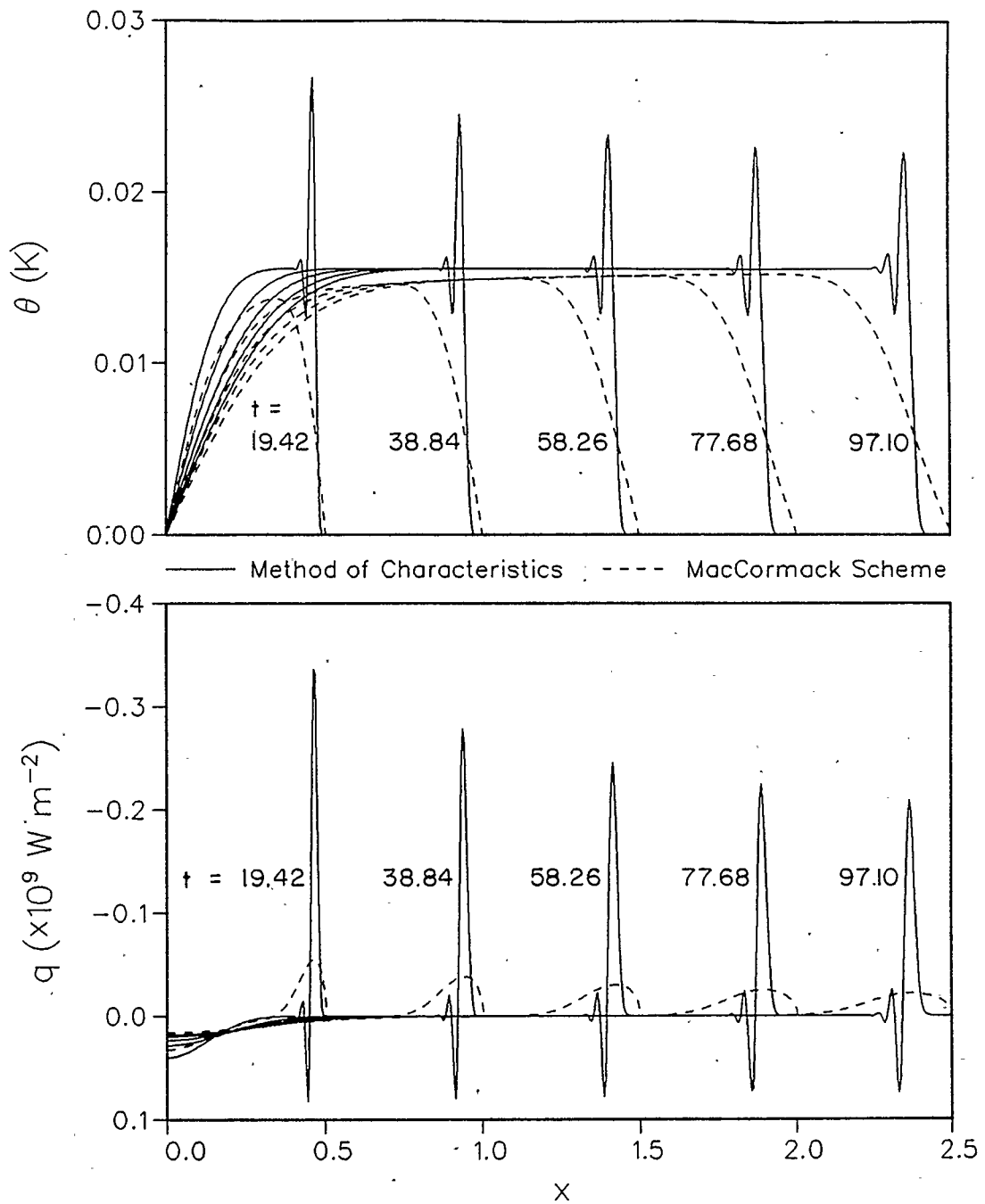


Figure 6.11b Temperature and heat flux response of SICOR to stress only step input ($\sigma_0 = 205 \text{ MPa}$, $\theta_0 = 0 \text{ K}$, $D_0 = 1.0 \text{ E } 03$, $\Delta t = 0.1942$, $x_{DF} = 0.025$).

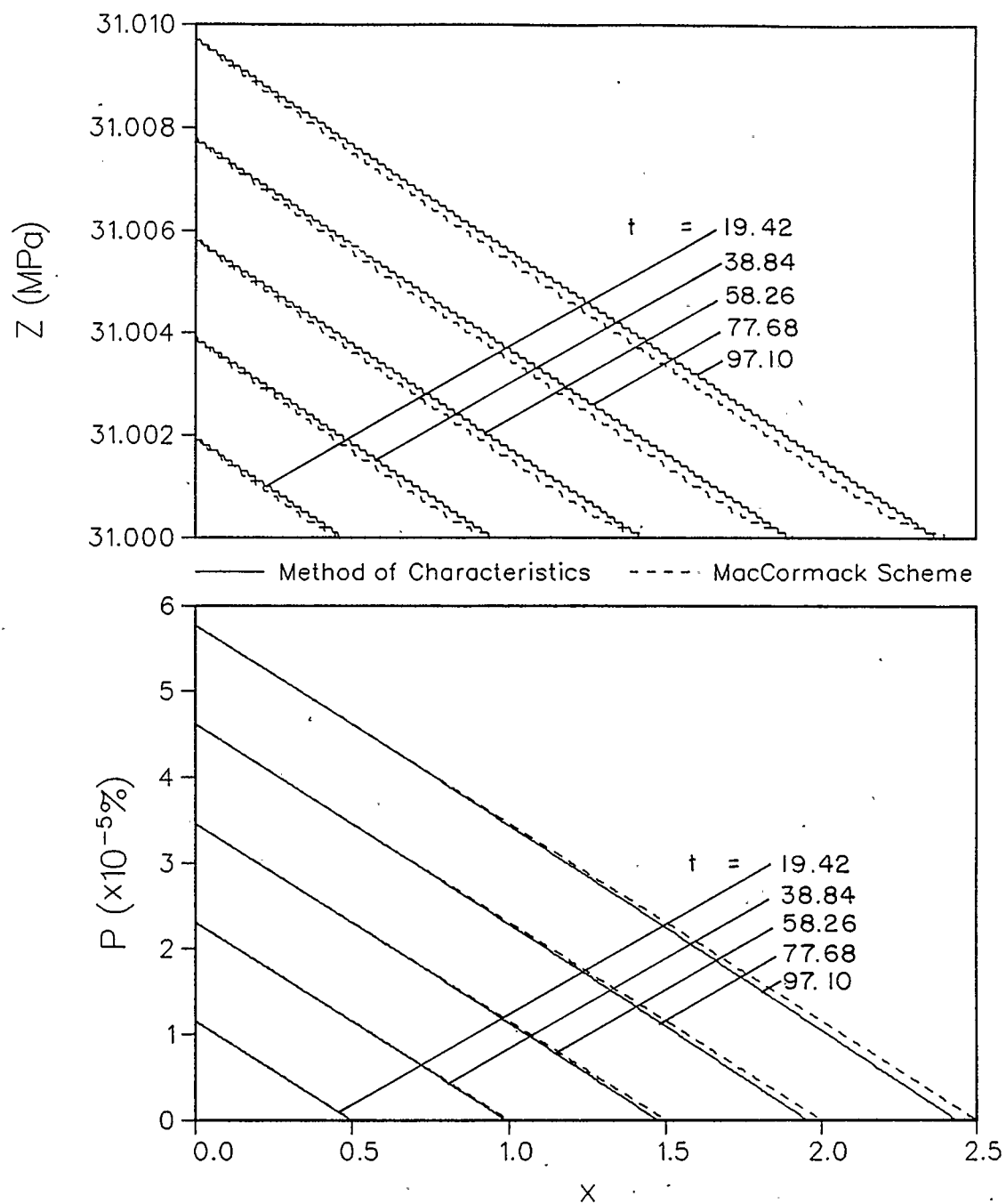


Figure 6.11c Strain hardening and plastic strain response of SICOR to stress only step input ($\sigma_0 = 205$ MPa, $\theta_0 = 0$ K, $X_{DF} = 0.025$, $\Delta t = 0.1942$, $D_0 = 1.0 \text{ E } 03$).

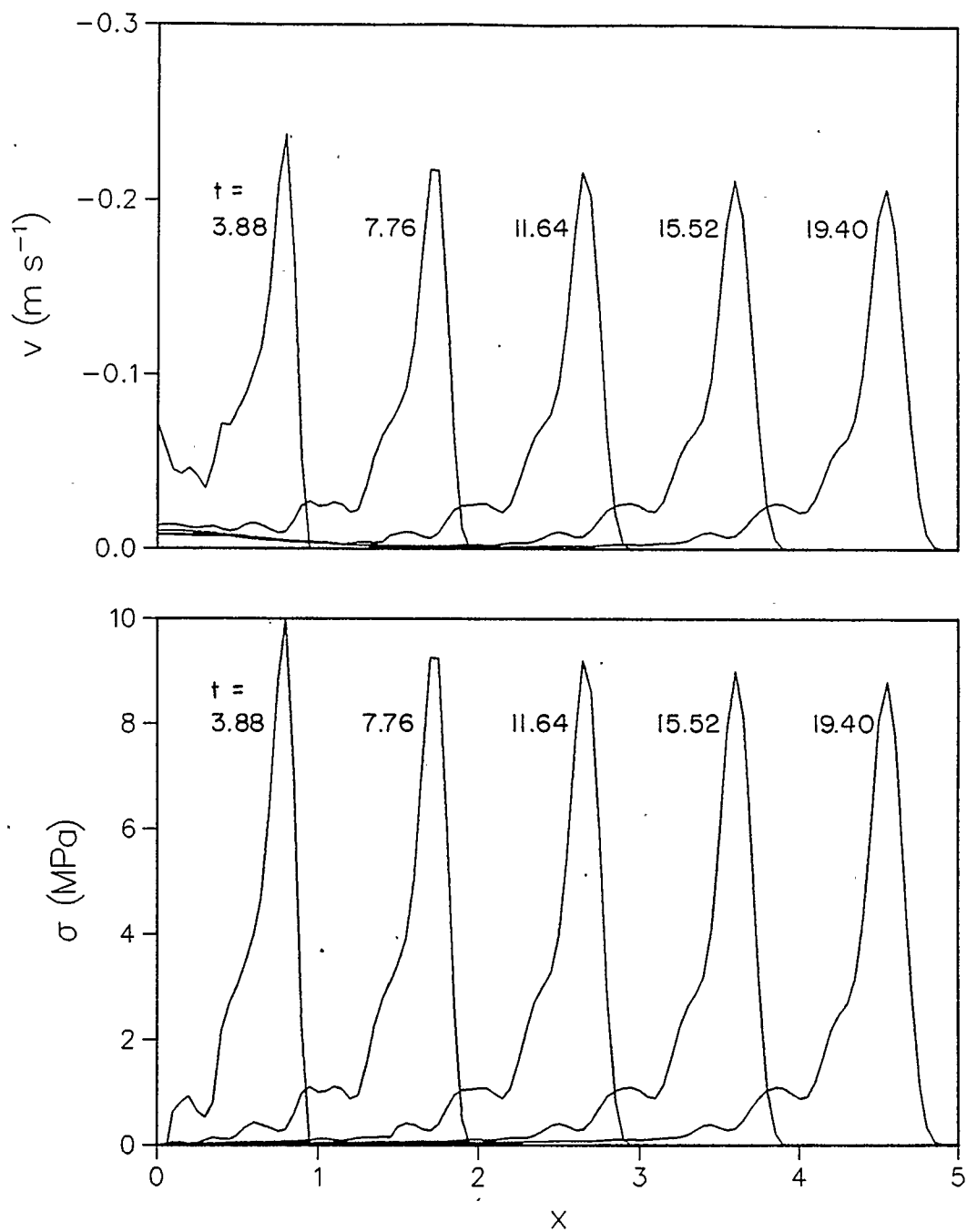


Figure 6.12a Velocity and stress response of SICOR to temperature only step input ($\sigma_0 = 0$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 03$, $\Delta t = 0.1942$, $x_{DF} = 0.230$).

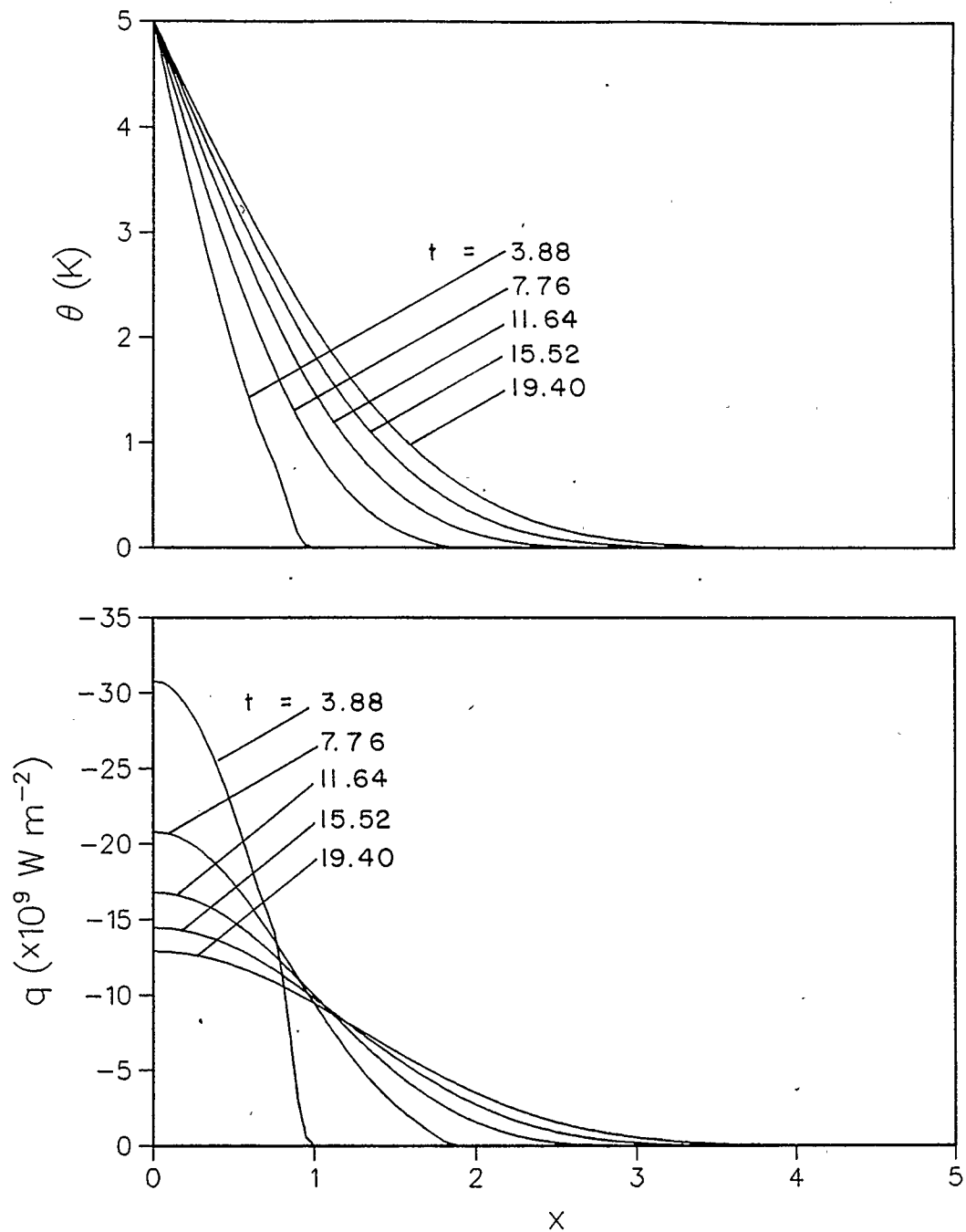


Figure 6.12b Temperature and heat flux response of SICOR to temperature only step input ($\sigma_0 = 0$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.230$, $\Delta t = 0.1942$).

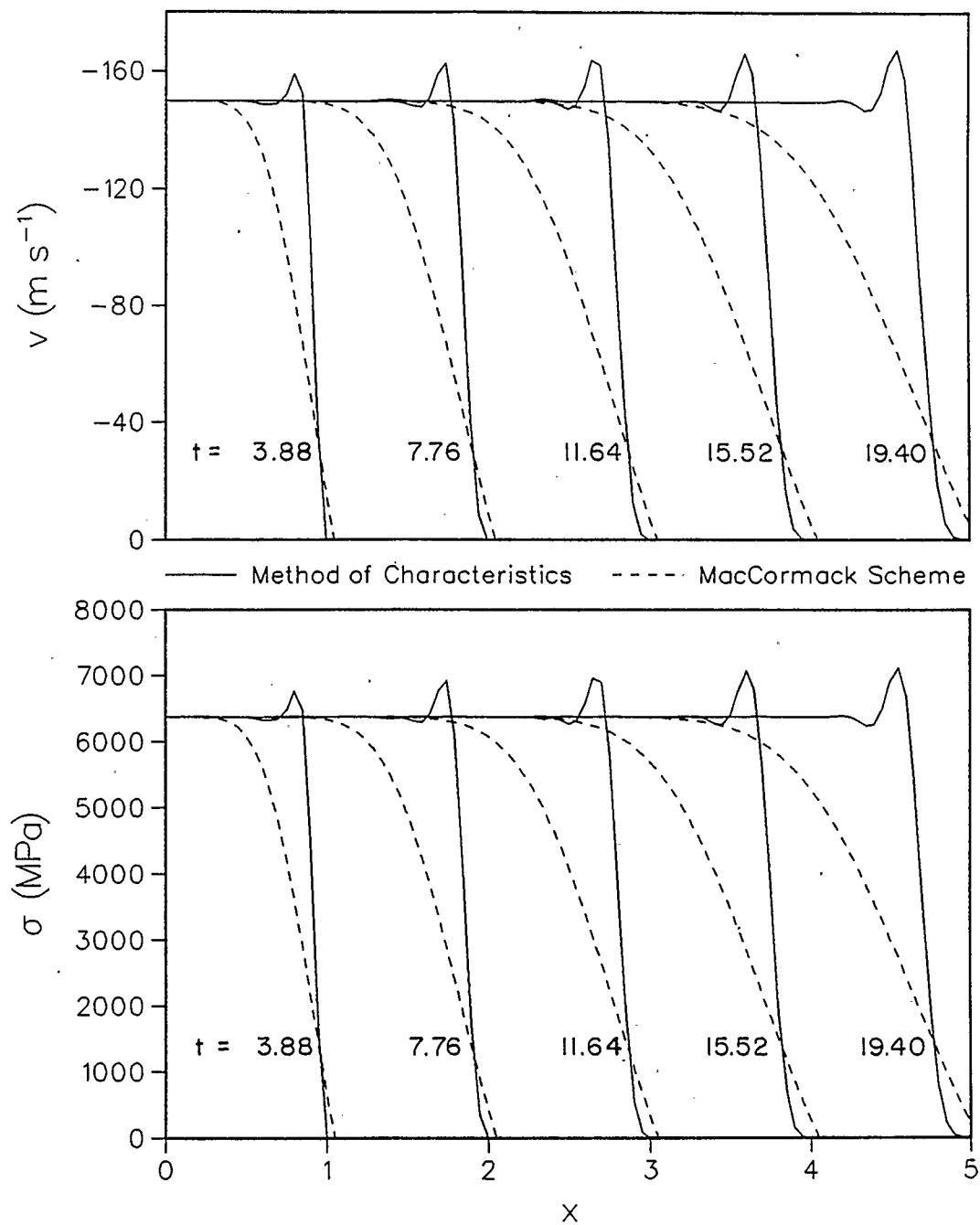


Figure 6.13a Velocity and stress response of SICOR to velocity and temperature step inputs ($v_0 = -150 \text{ ms}^{-1}$, $\theta_0 = 10 \text{ K}$, $D_0 = 1.0 \text{ E } 04$, $X_{DF} = 0.245$, $\Delta t = 0.1942$).

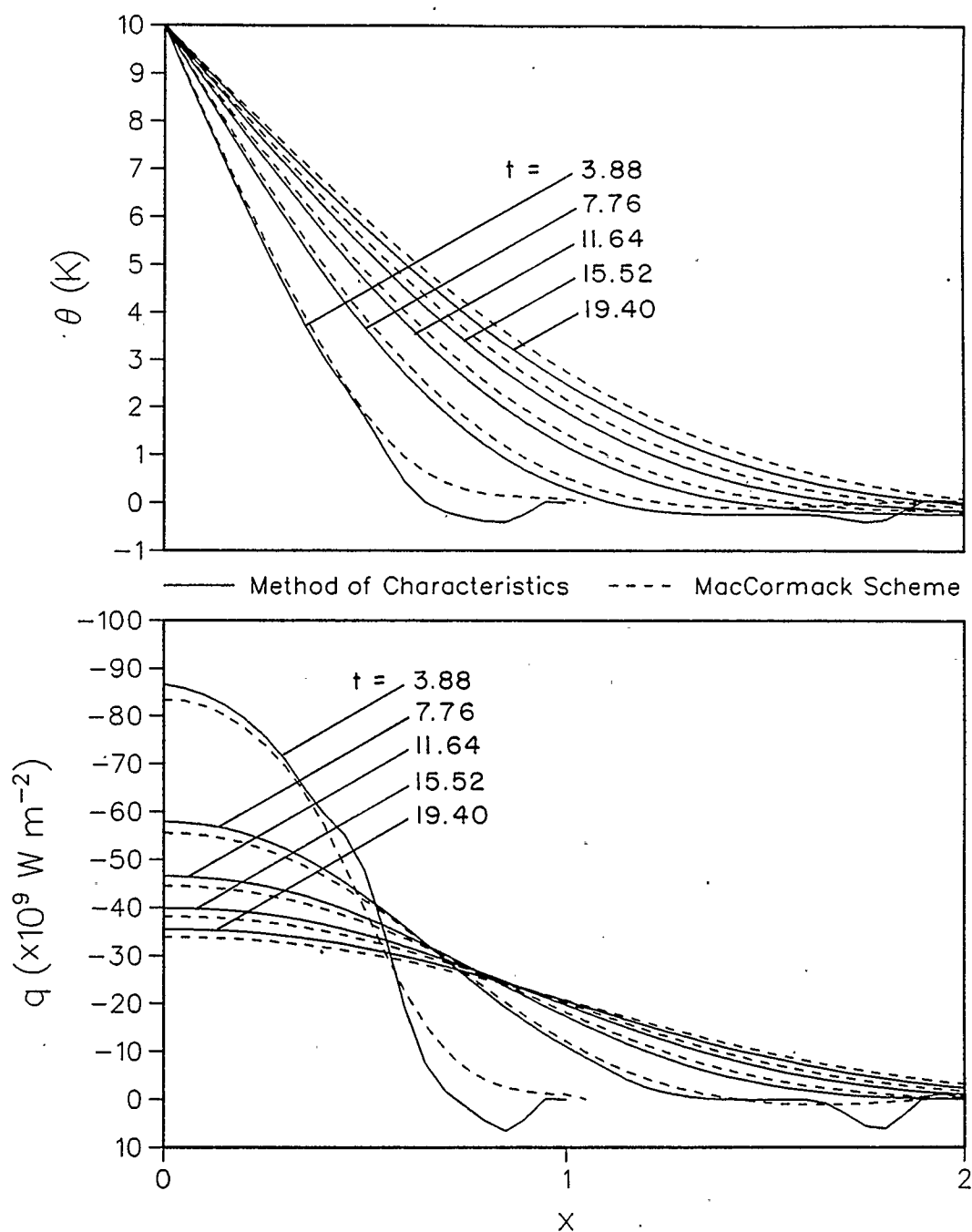


Figure 6.13b Temperature and heat flux response of SICOR to velocity and temperature step inputs ($v_0 = -150 \text{ ms}^{-1}$, $\theta_0 = 10 \text{ K}$, $D_0 = 1.0 \text{ E } 04$, $X_{DF} = 0.245$, $\Delta t = 0.1942$).

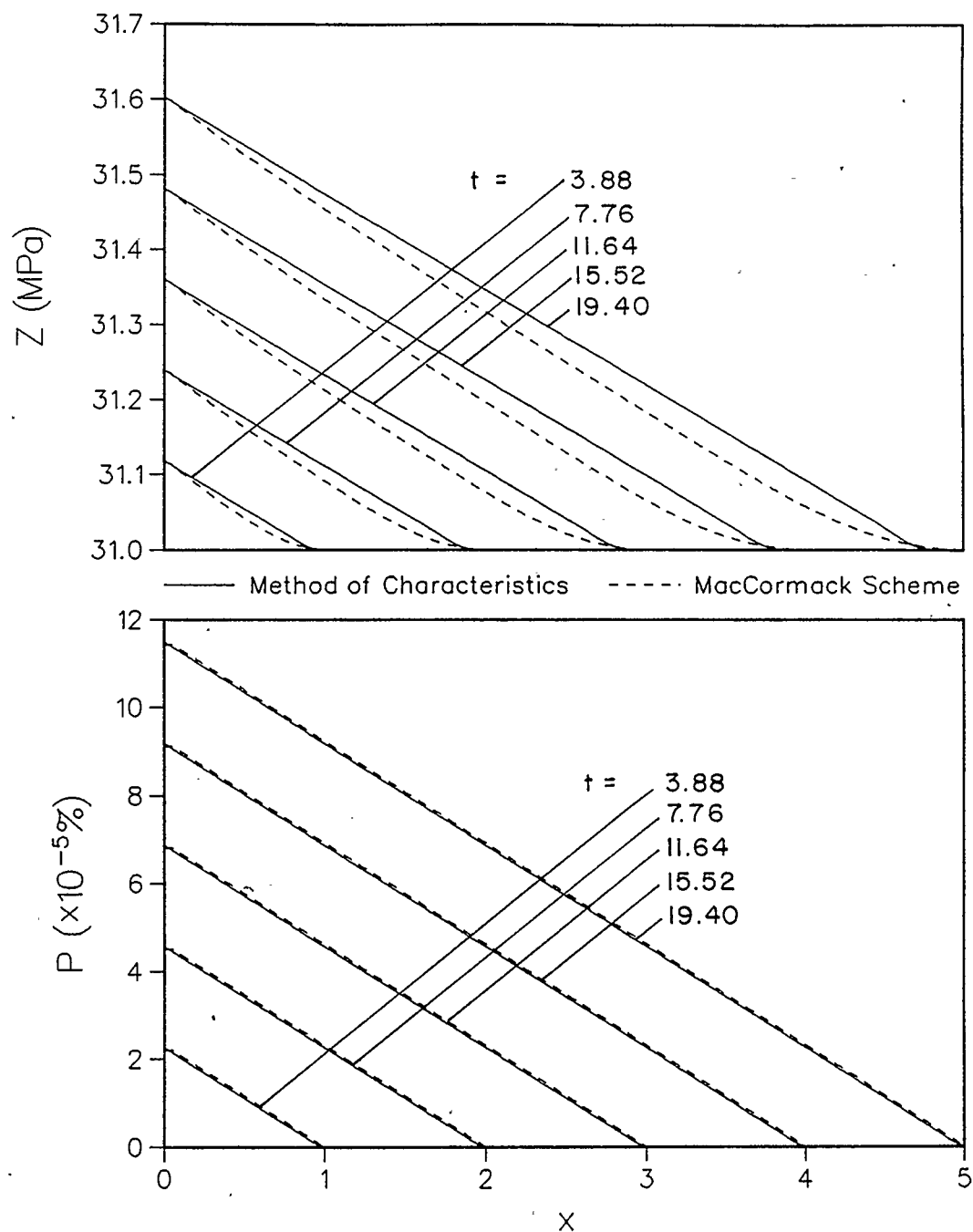


Figure 6.13c Strain hardening and plastic strain response of SICOR to velocity and temperature step inputs ($v_0 = -150 \text{ ms}^{-1}$, $D_0 = 1.0 \text{ E } 04$, $X_{DF} = 0.245$, $\Delta t = 0.1942$, $\theta_0 = 10 \text{ K}$).

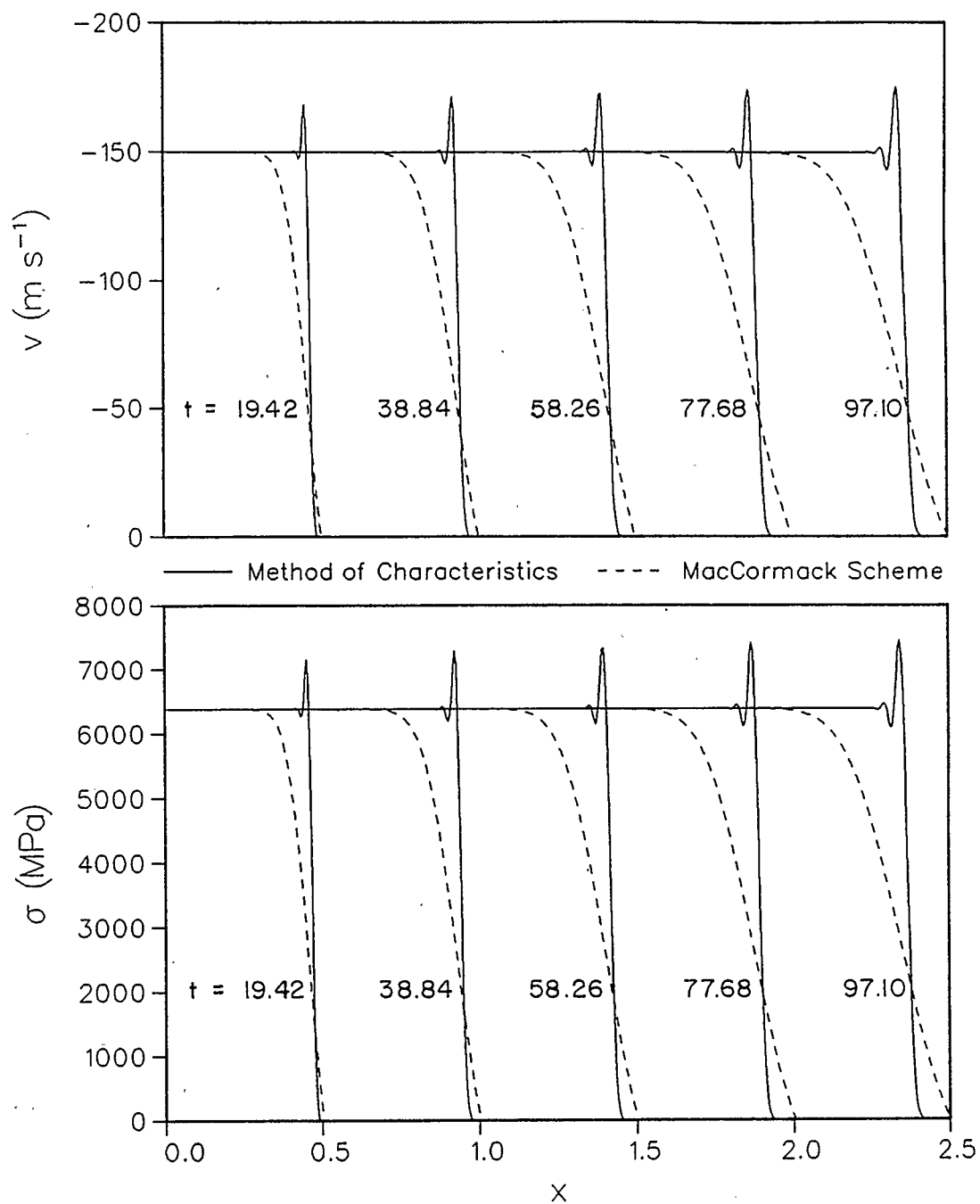


Figure 6.14a Velocity and stress response of SICOR to velocity only step input ($v_0 = -150 \text{ ms}^{-1}$, $\theta_0 = 0 \text{ K}$, $D_0 = 1.0 \text{ E } 03$, $\Delta t = 0.1942$, $X_{DF} = 0.025$).

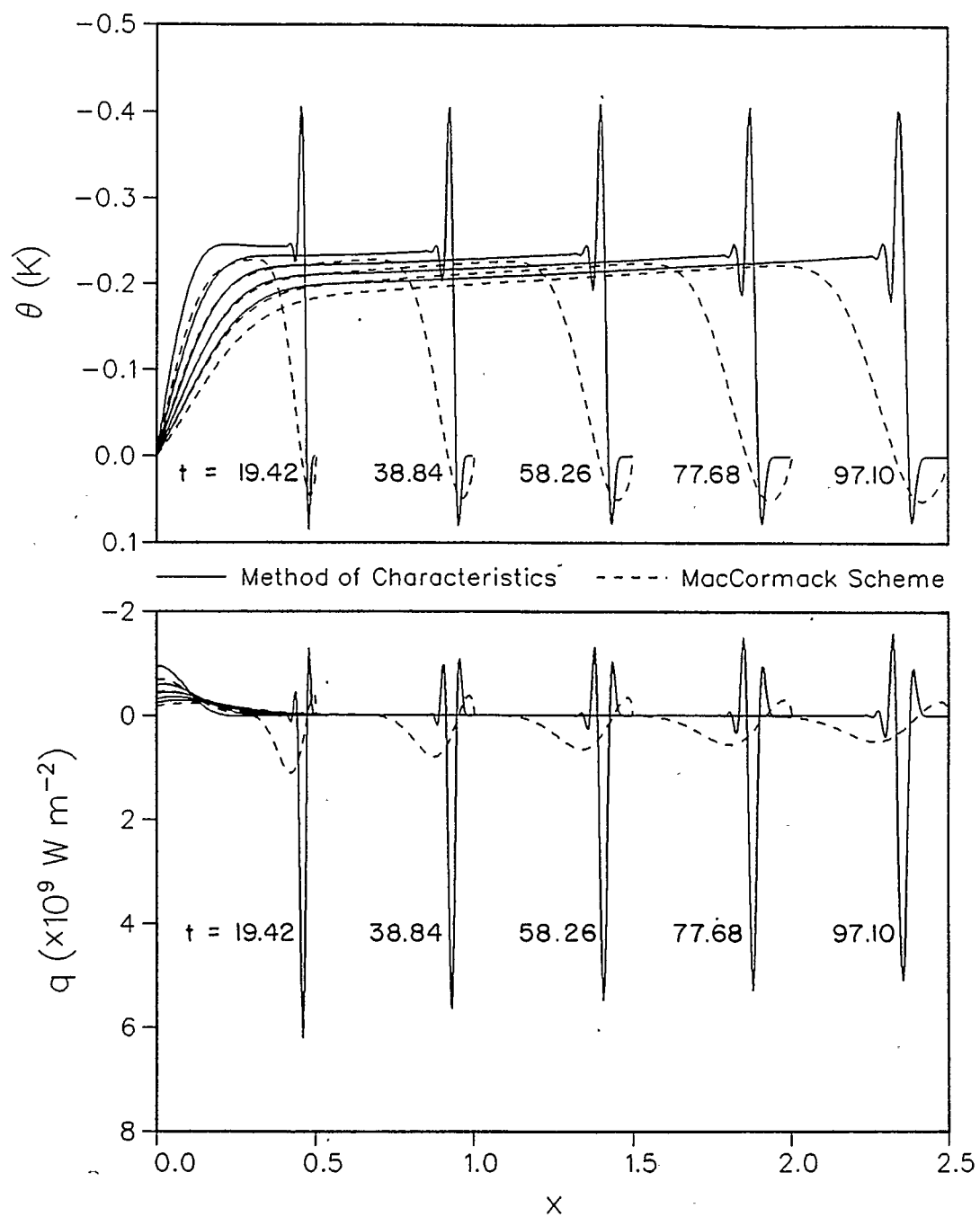


Figure 6.14b Temperature and heat flux response of SICOR to velocity only step input ($v_0 = -150 \text{ ms}^{-1}$, $\theta_0 = 0 \text{ K}$, $D_0 = 1.0 \text{ E } 03$, $\Delta t = 0.1942$, $x_{DF} = 0.025$).

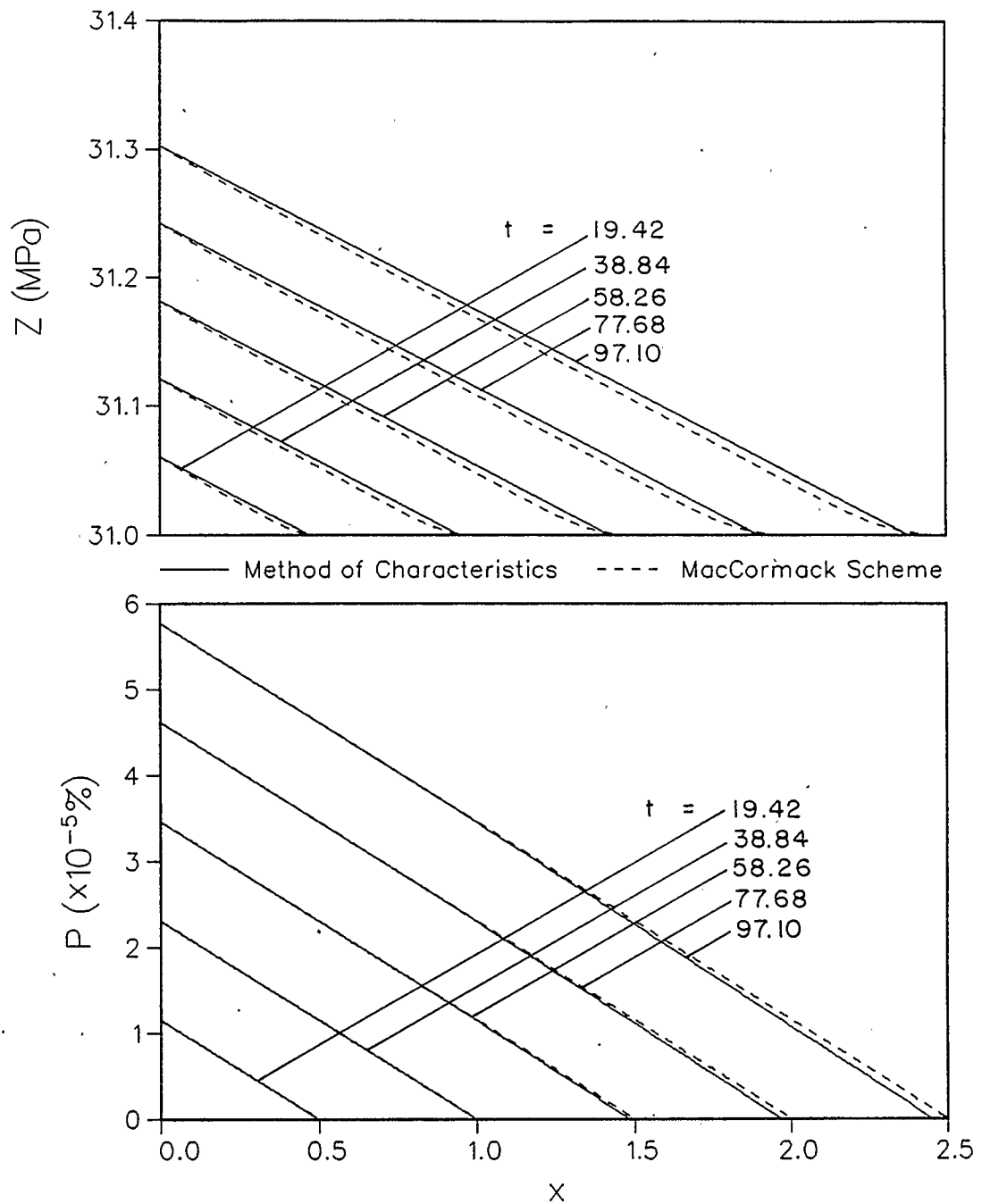


Figure 6.14c Strain hardening and plastic strain response of SICOR to velocity only step input ($v_0 = -150 \text{ ms}^{-1}$, $\theta_0 = 0 \text{ K}$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.025$, $\Delta t = 0.1942$).

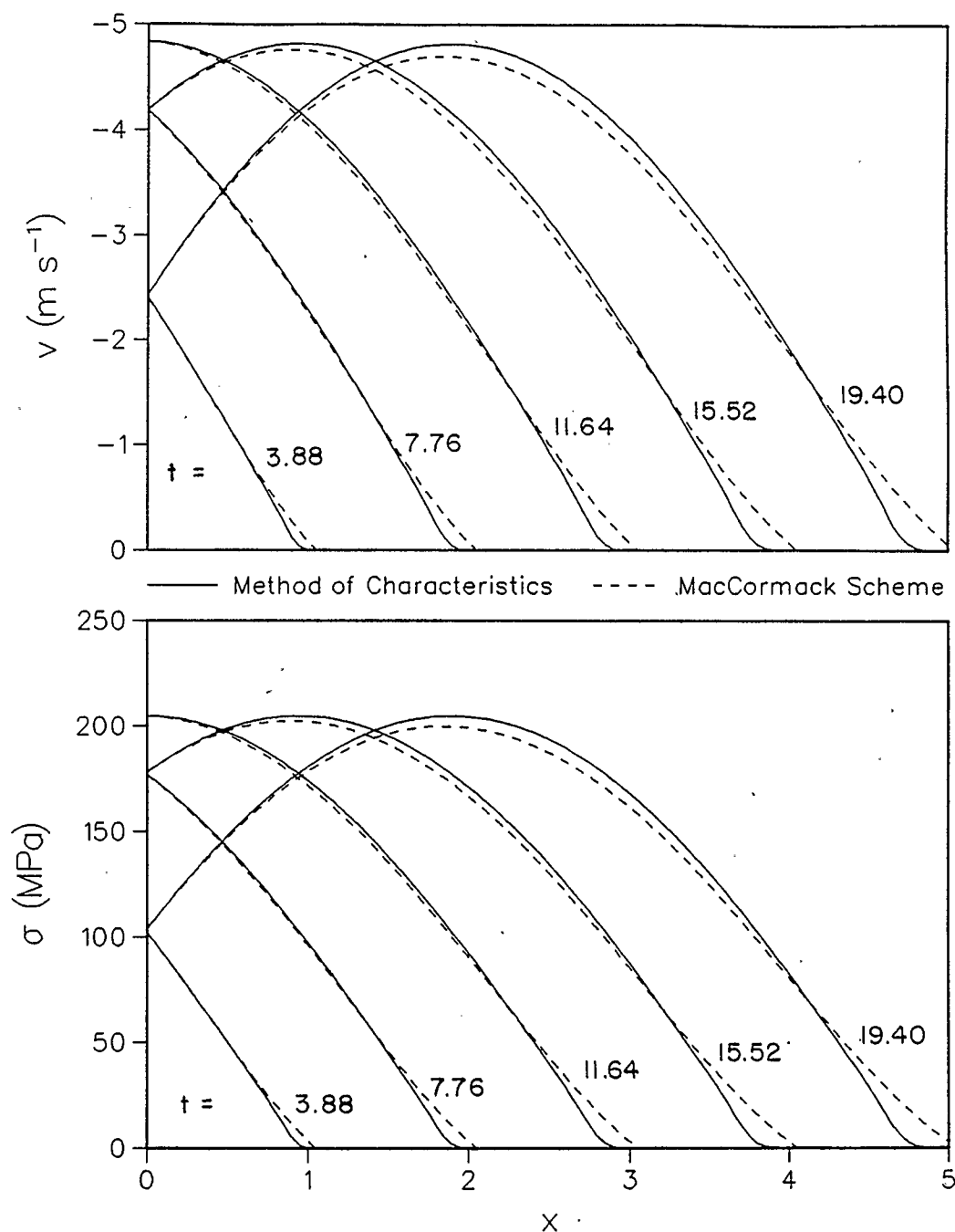


Figure 6.15a Velocity and stress response of SICOR to pulsive-sine stress and temperature inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.241$, $\Delta t = 0.1942$, $\omega = 2.61 \text{ E } 10$).

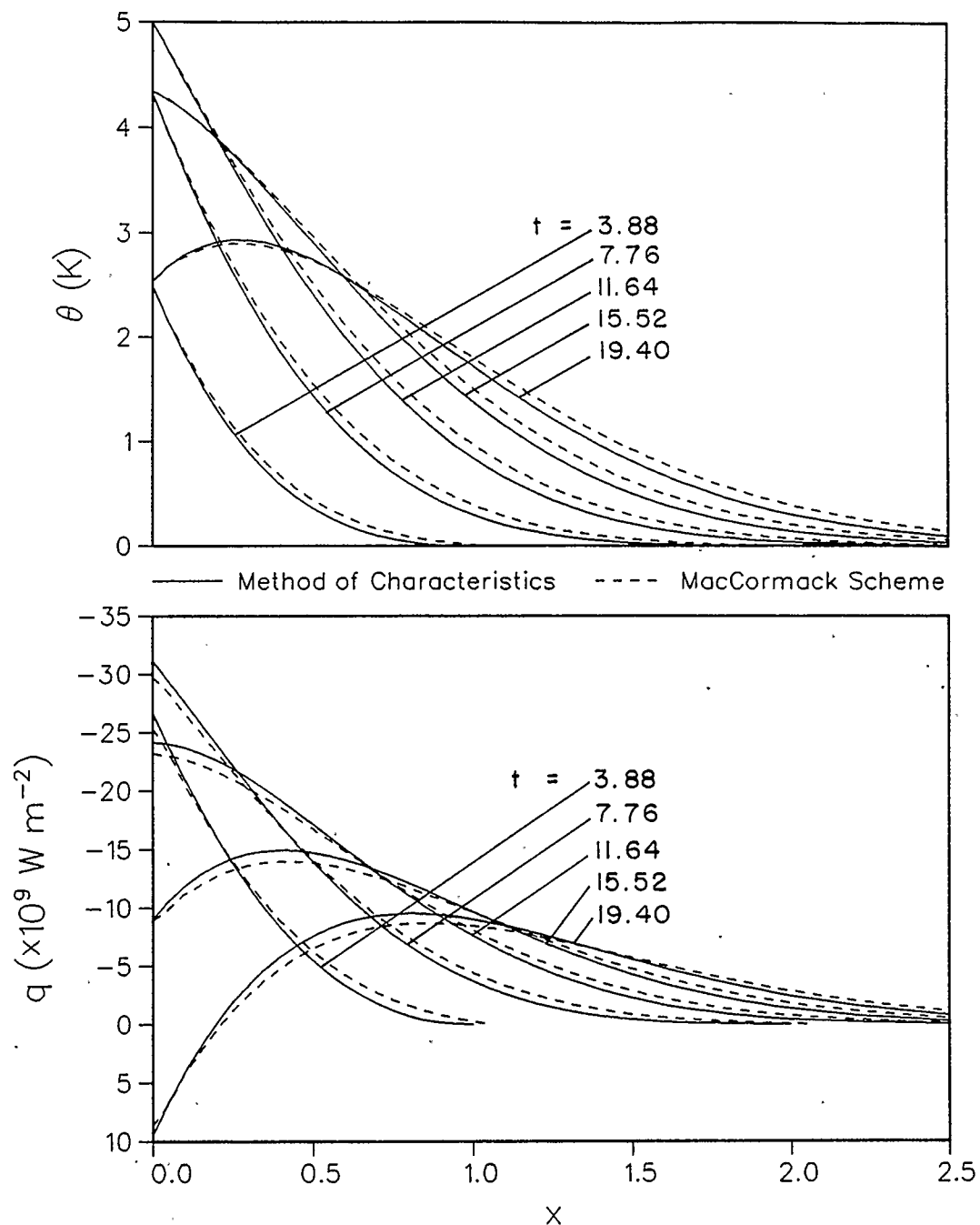


Figure 6.15b Temperature and heat flux response of SICOR to pulsive-sine stress and temperature inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $\omega = 2.61 \text{ E } 10$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.241$, $\Delta t = 0.1942$).

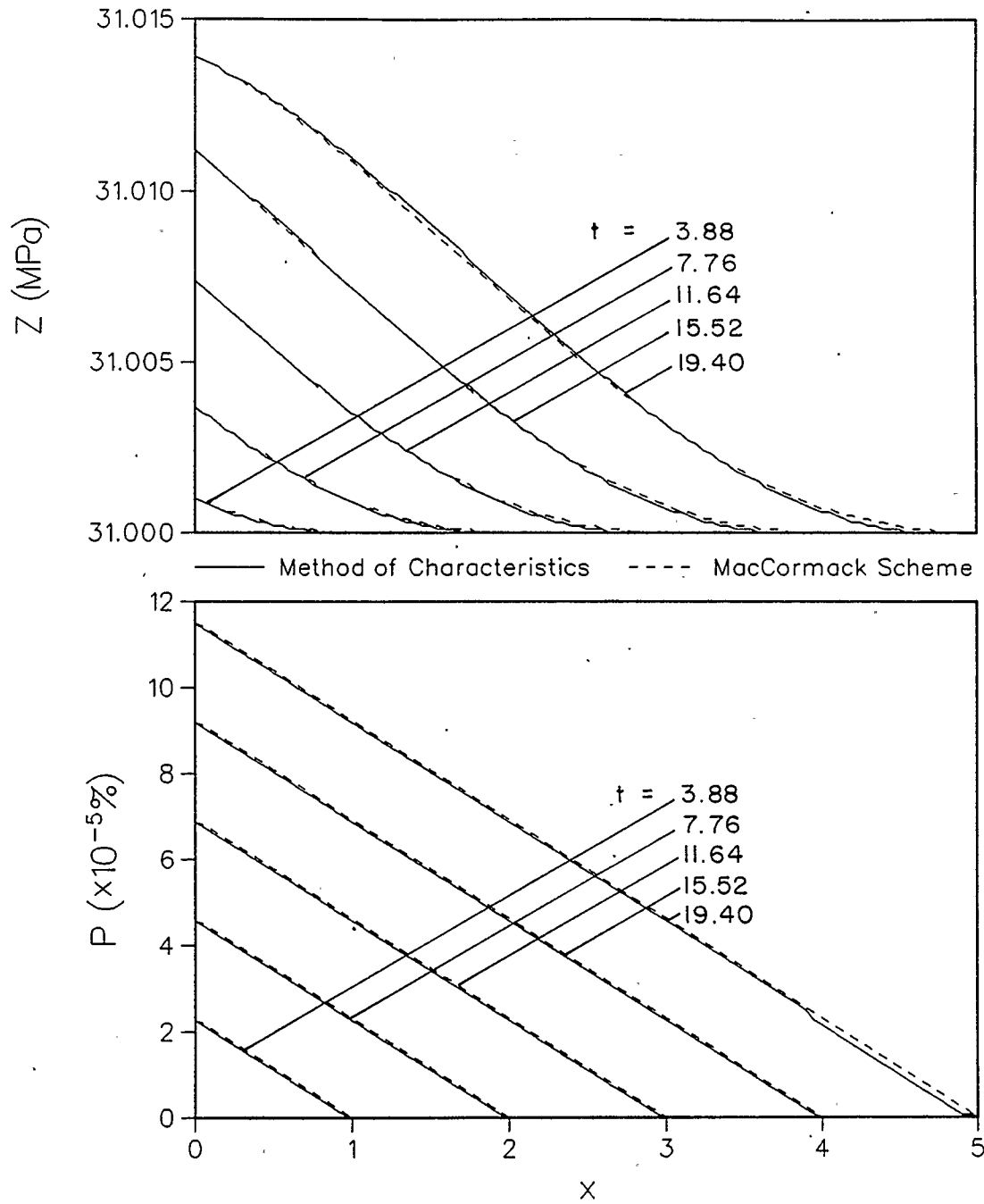


Figure 6.15c Strain hardening and plastic strain response of SICOR to pulsed-sine stress and temperature inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $\omega = 2.61 \text{ E } 10$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.241$, $\Delta t = 0.1942$).

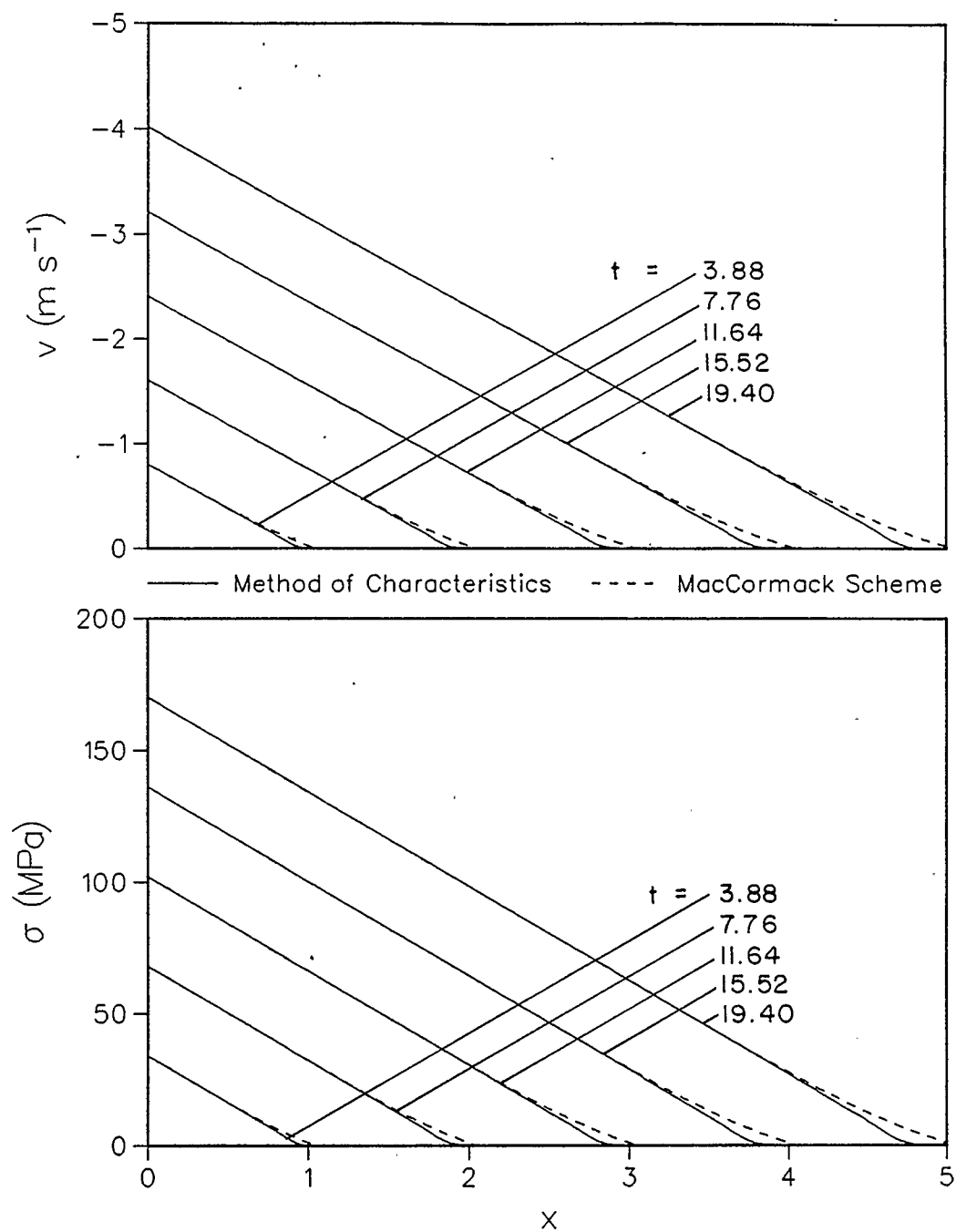


Figure 6.16a Velocity and stress response of SICOR to terminated-ramp stress and temperature inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $\omega = 2.61 \text{ E } 10$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.234$, $\Delta t = 0.1942$).

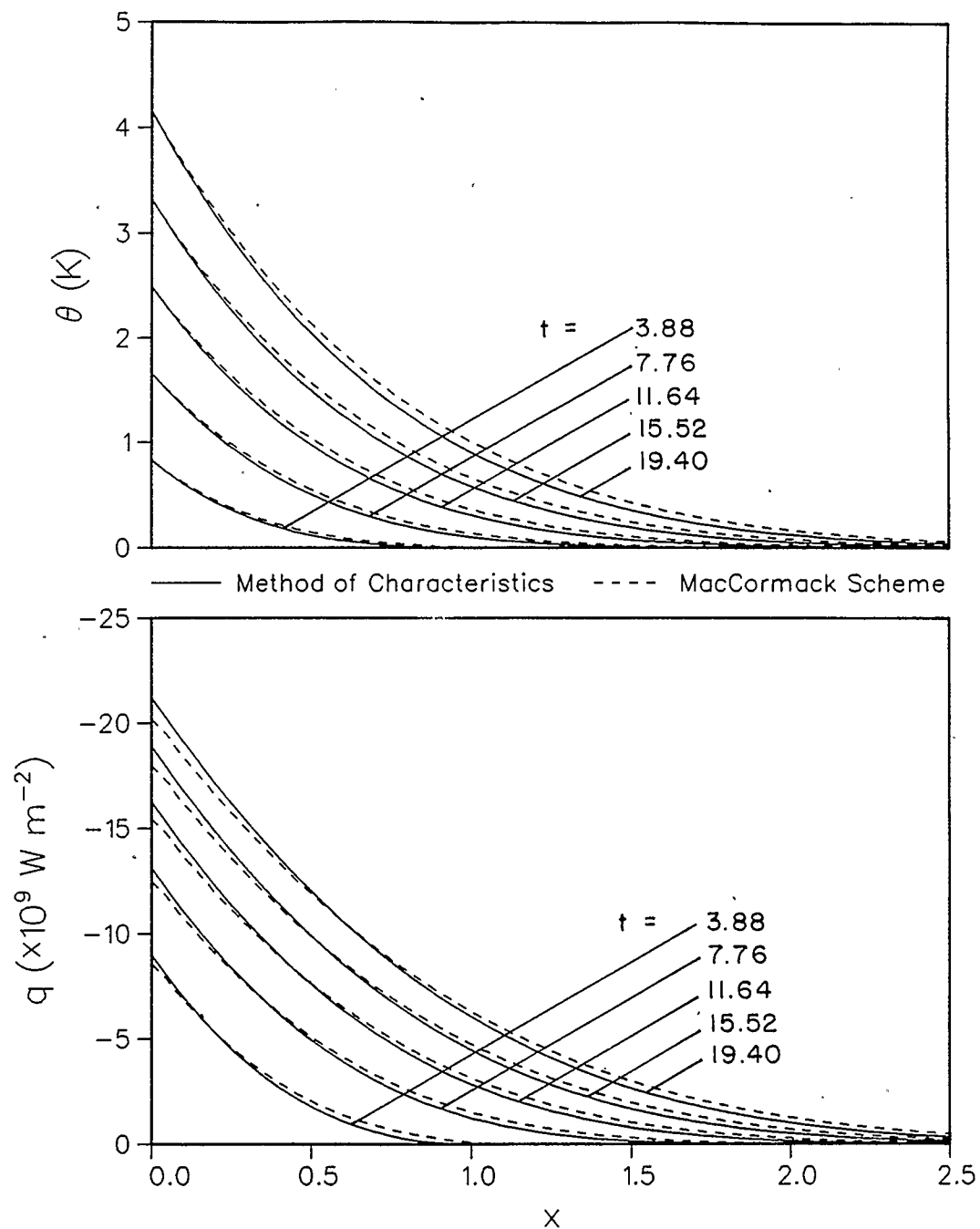


Figure 6.16b Temperature and heat flux response of SICOR to terminated-ramp stress and temperature inputs ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $\omega = 2.61 \text{ E } 10$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.234$, $\Delta t = 0.1942$).

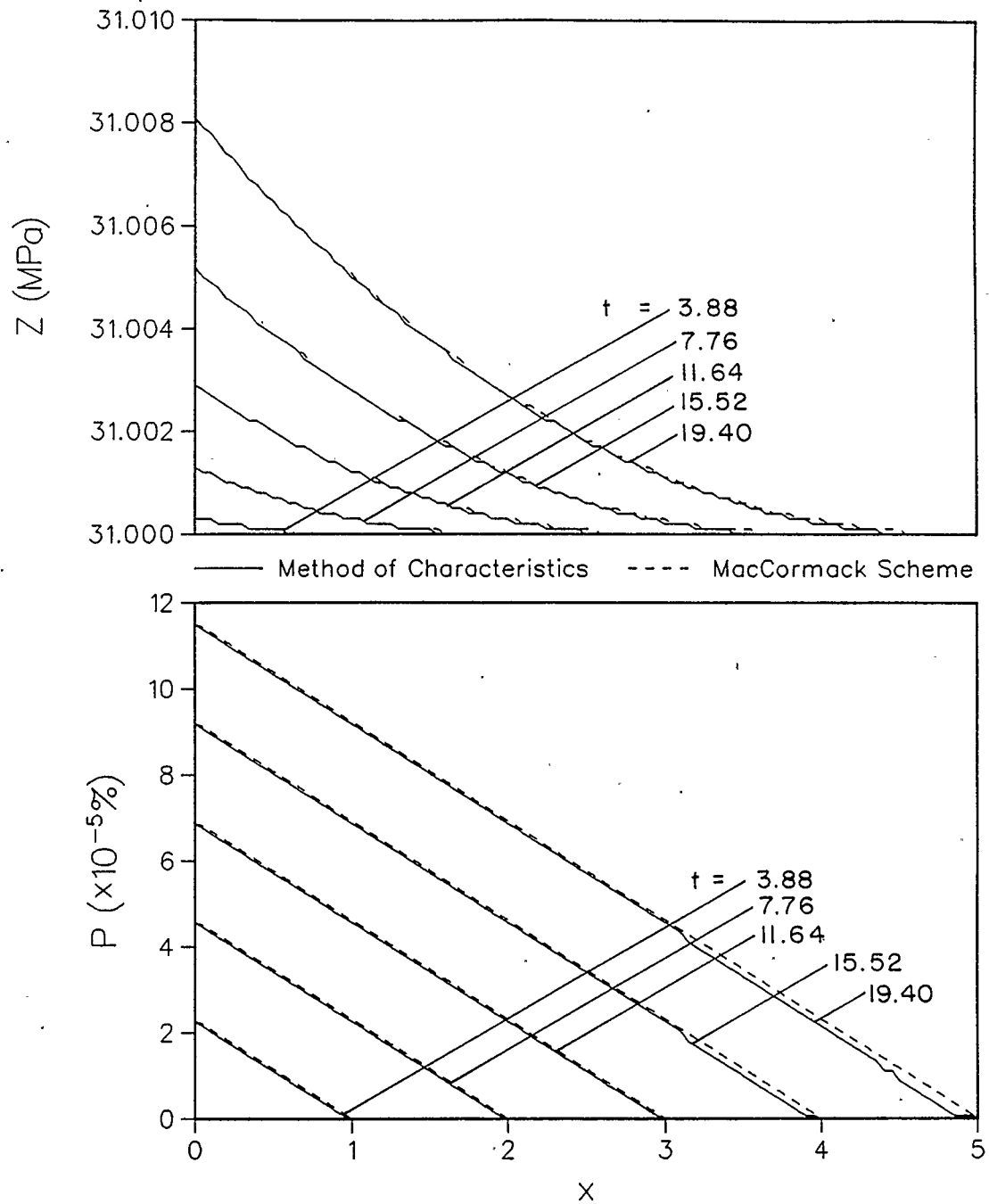


Figure 6.16c Strain hardening and plastic strain response of SICOR to terminated-ramp stress and temperature inputs ($\sigma_0 = 205$ MPa, $\omega = 2.61 \text{ E } 10$, $D_0 = 1.0 \text{ E } 03$, $X_{DF} = 0.234$, $\Delta t = 0.1942$, $\theta_0 = 5$ K).

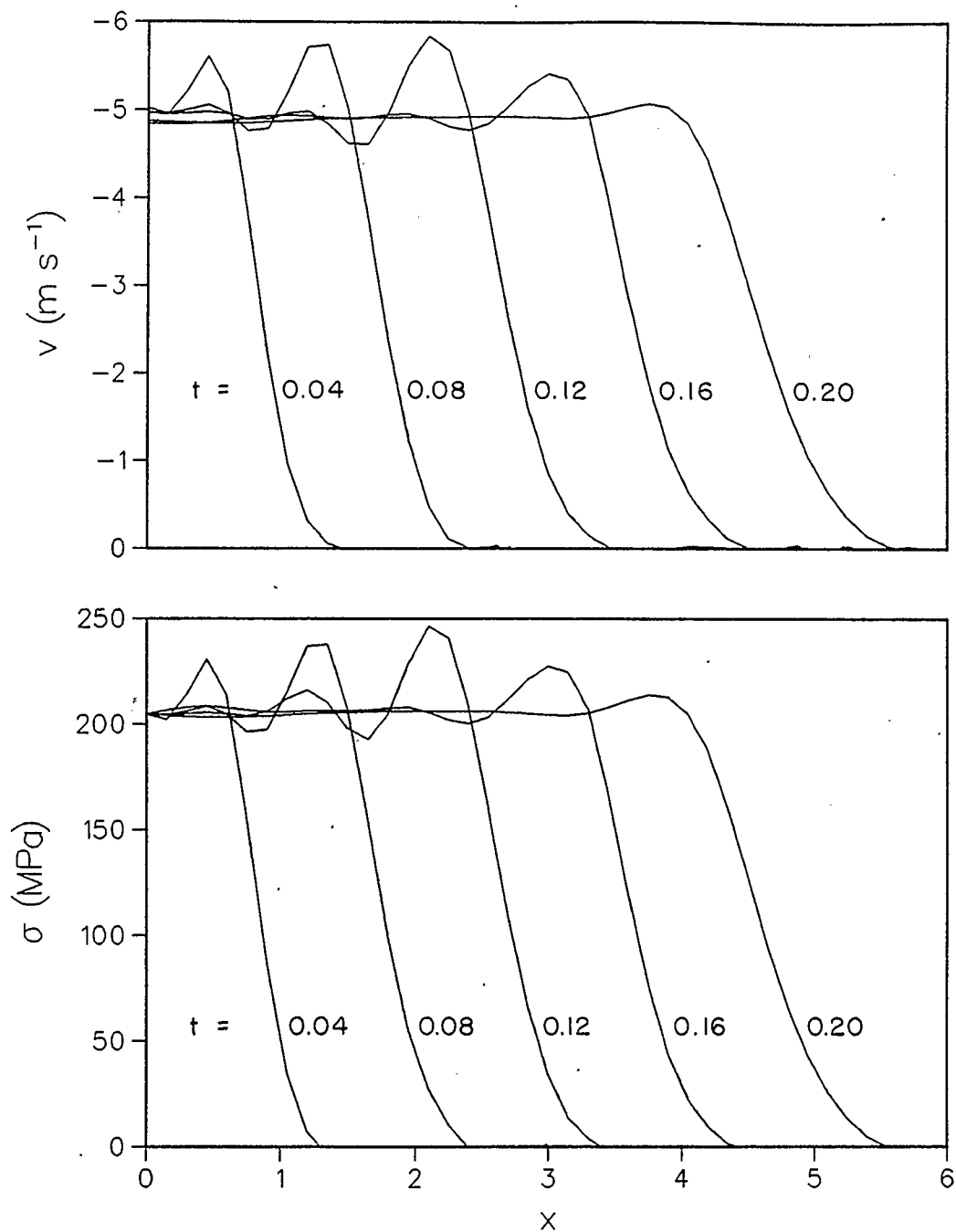


Figure 6.17a Velocity and stress response of SICOR to stress and temperature step inputs for a very high leading wave velocity ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 04$, $\tau_0 = 0.074$, $X_{DF} = 10.743$, $\Delta t = 0.00194$).

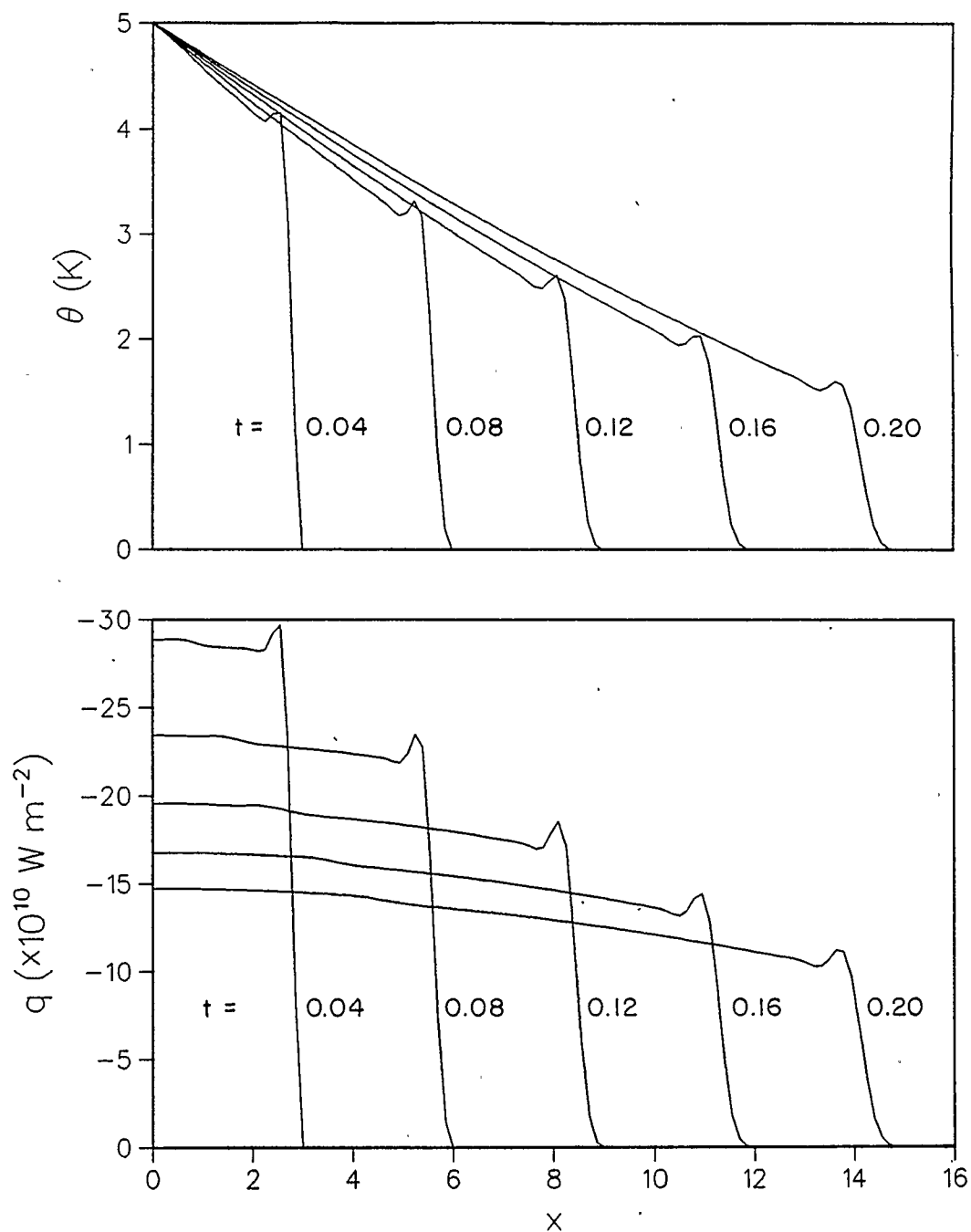


Figure 6.17b Temperature and heat flux response of SICOR to stress and temperature step inputs for a very high leading wave velocity ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 04$, $\tau_0 = 0.074$, $x_{DF} = 10.743$, $\Delta t = 0.00194$).

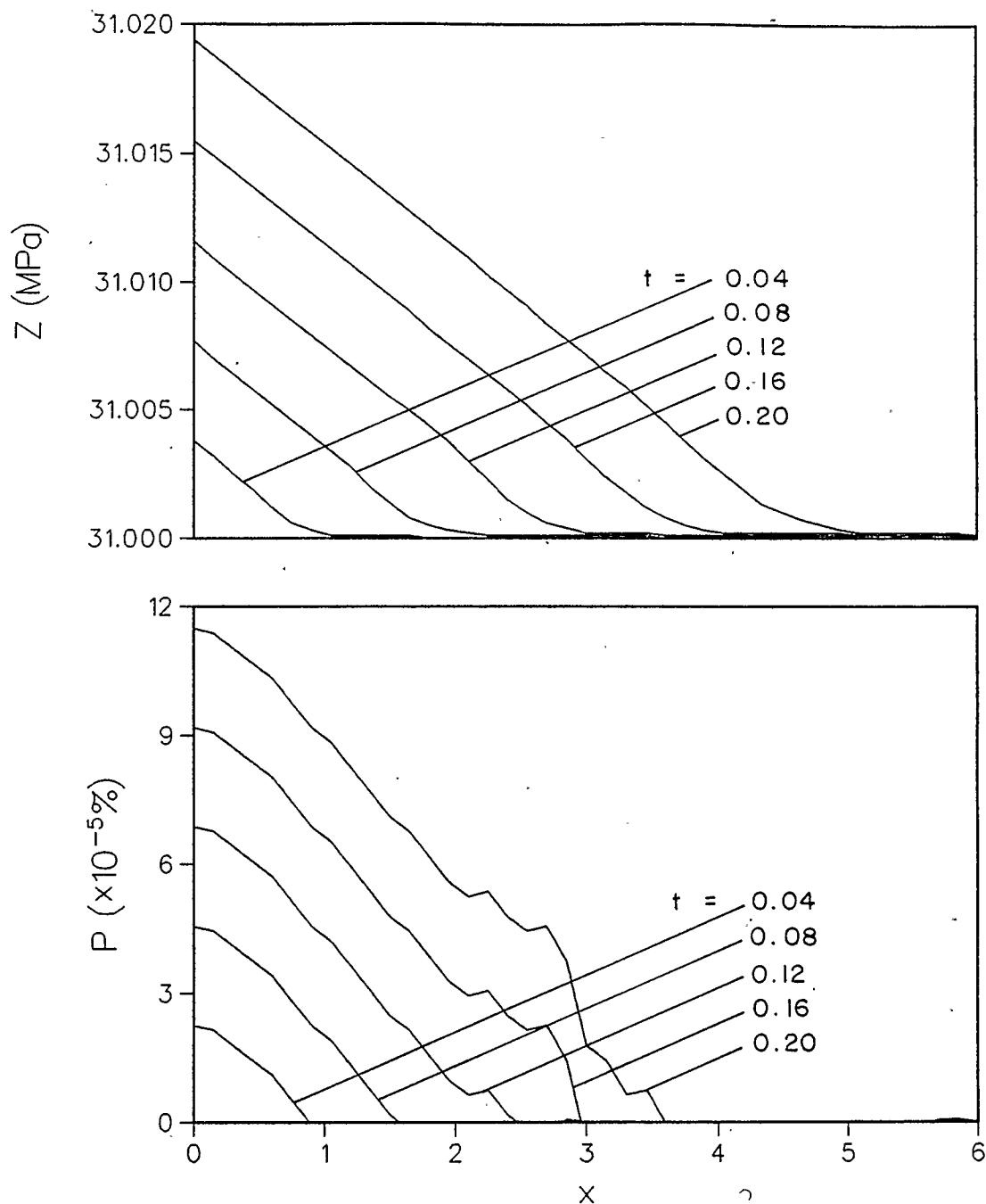


Figure 6.17c Strain hardening and plastic strain response of SICOR to stress and temperature step inputs for a very high leading wave velocity ($\sigma_0 = 205$ MPa, $\theta_0 = 5$ K, $D_0 = 1.0 \text{ E } 04$, $\tau_0 = 0.074$, $X_{DF} = 10.743$, $\Delta t = 0.00194$).

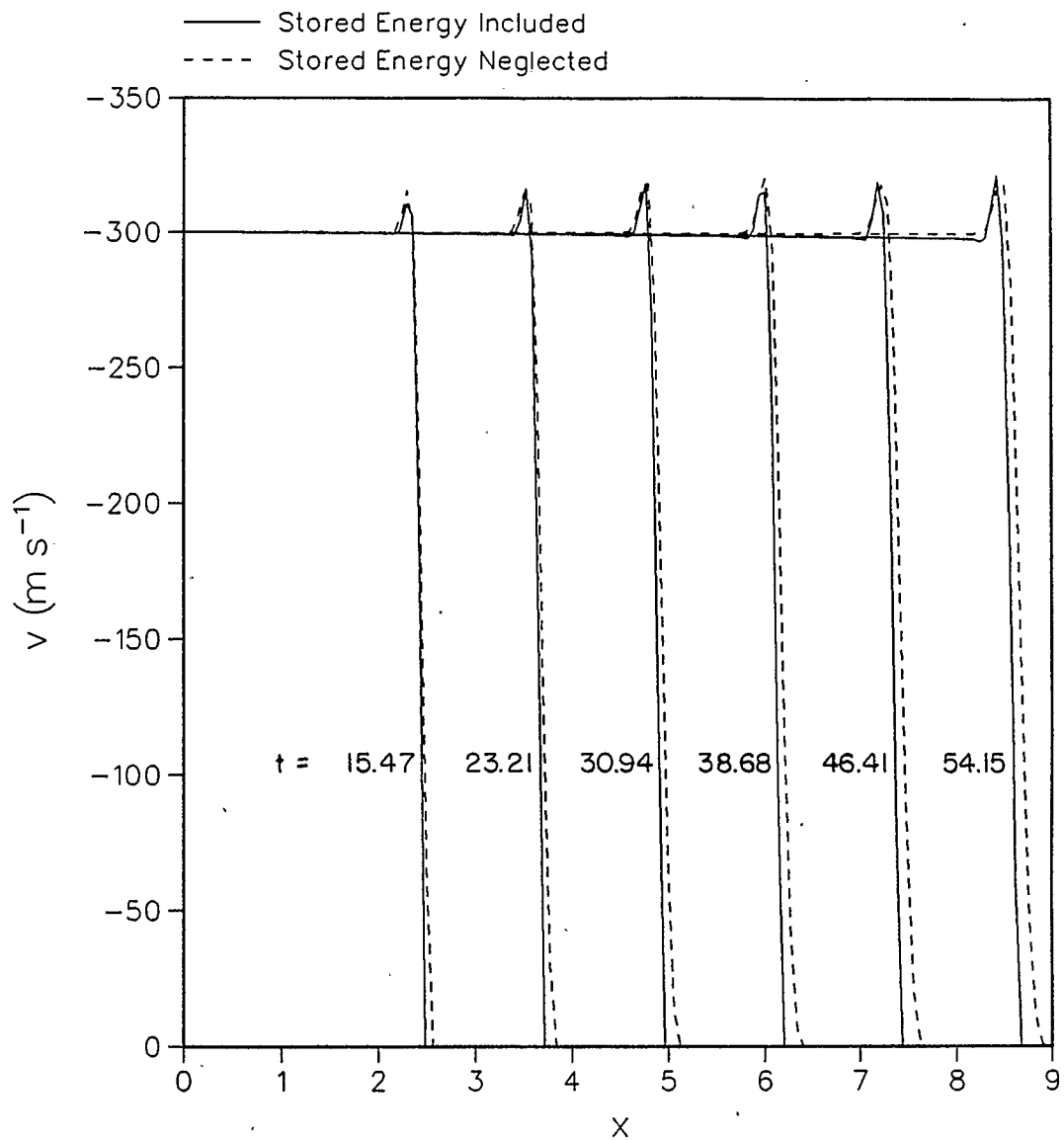


Figure 6.18a Influence of stored energy of cold work on the velocity response of SIAR to velocity and temperature step inputs ($v_0 = -300 \text{ ms}^{-1}$, $\theta_0 = 10 \text{ K}$, $\tau_0 = 1.47 \text{ E } 05$, $D_0 = 1.0 \text{ E } 05$, $x_{DF} = 0.00158$, $\Delta t = 0.387$).

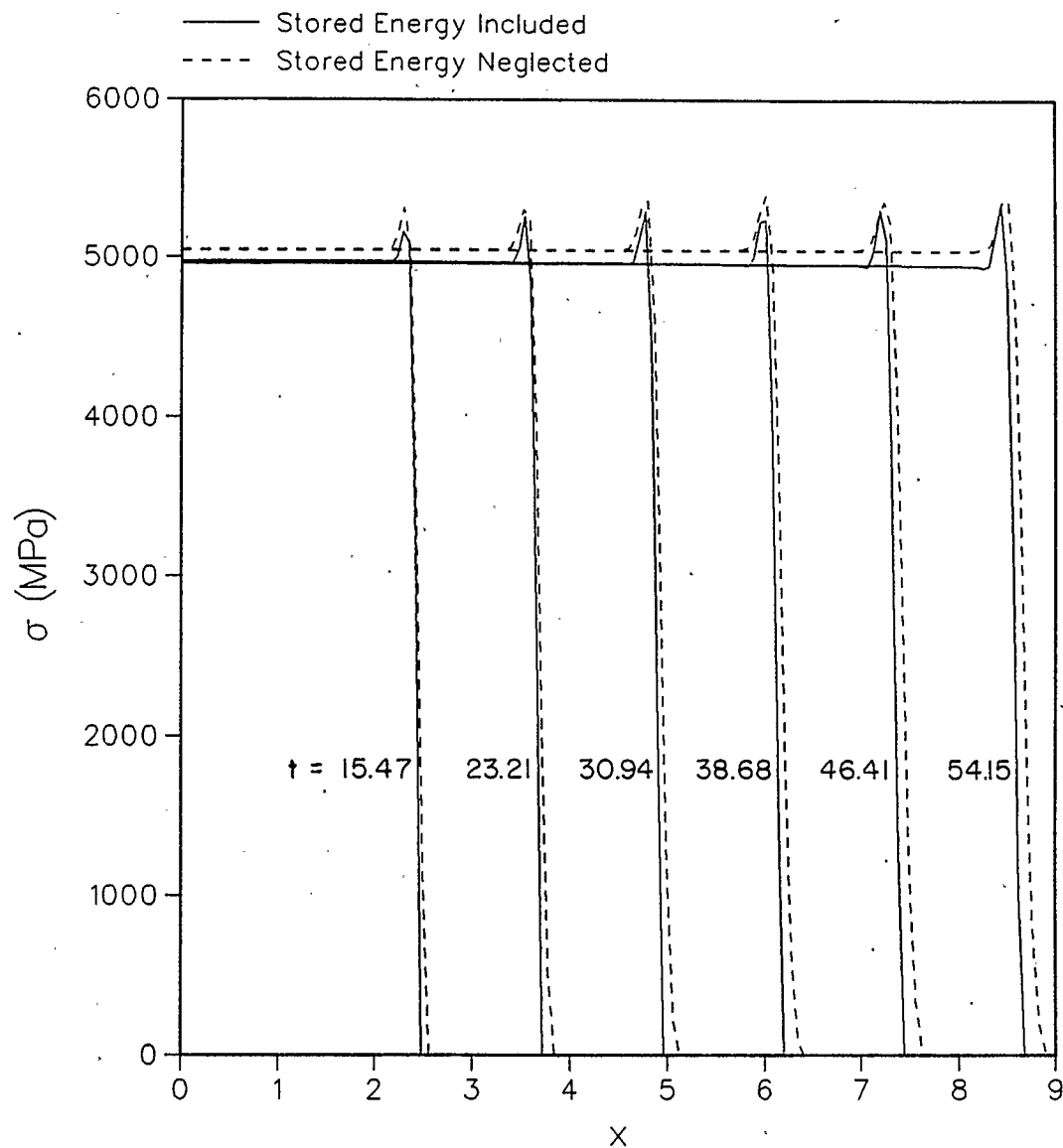


Figure 6.18b Influence of stored energy of cold work on the stress response of SIAR to velocity and temperature step inputs ($v_0 = -300 \text{ ms}^{-1}$, $\theta_0 = 10 \text{ K}$, $\tau_0 = 1.47 \text{ E } 05$, $D_0 = 1.0 \text{ E } 05$, $X_{DF} = 0.00158$, $\Delta t = 0.387$).

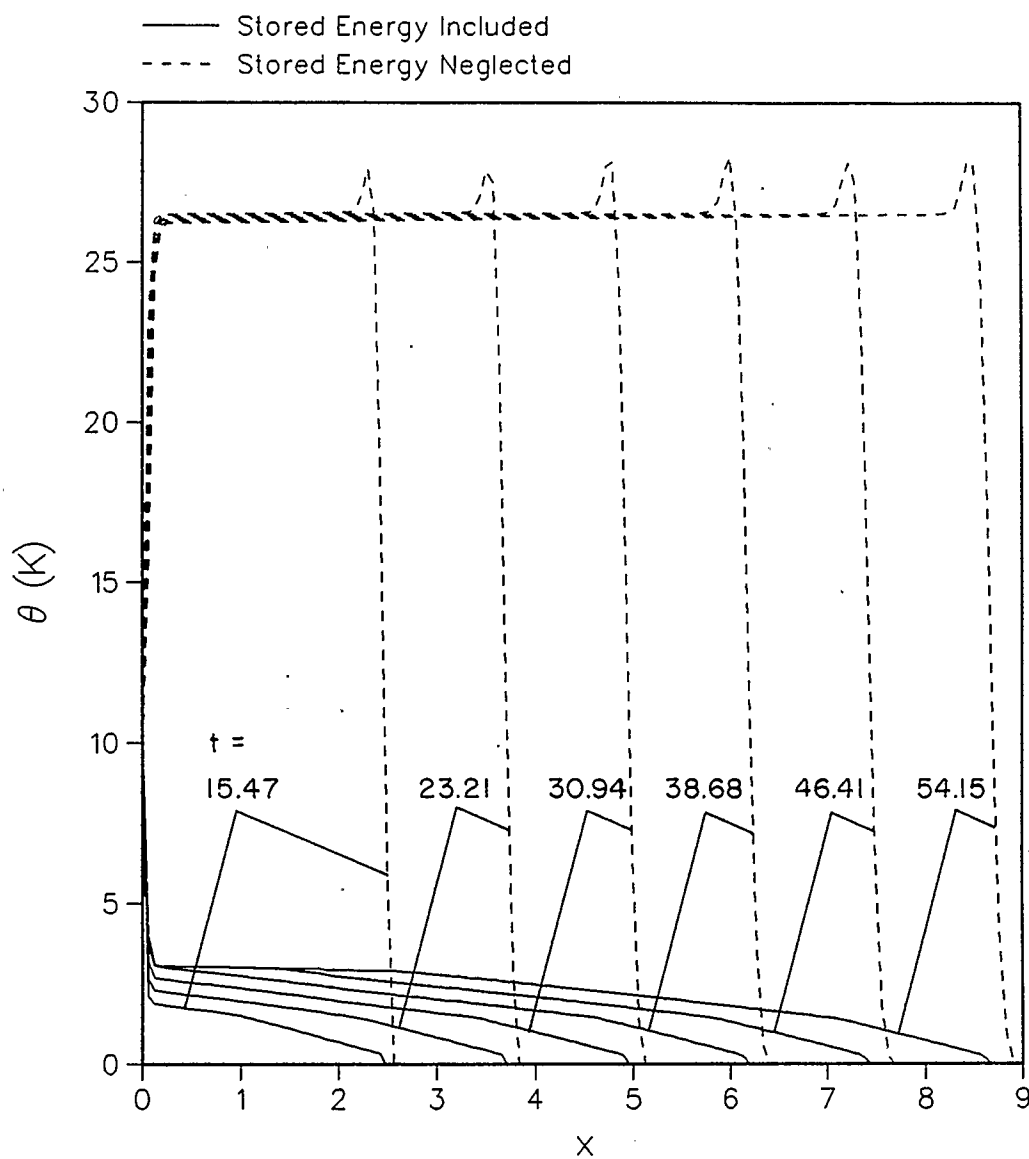


Figure 6.18c Influence of stored energy of cold work on the temperature response of SIAR to velocity and temperature step inputs ($v_0 = -300 \text{ ms}^{-1}$, $\theta_0 = 10 \text{ K}$, $\tau_0 = 1.47 \text{ E } 05$, $D_0 = 1.0 \text{ E } 05$, $x_{DF} = 0.00158$, $\Delta t = 0.387$).

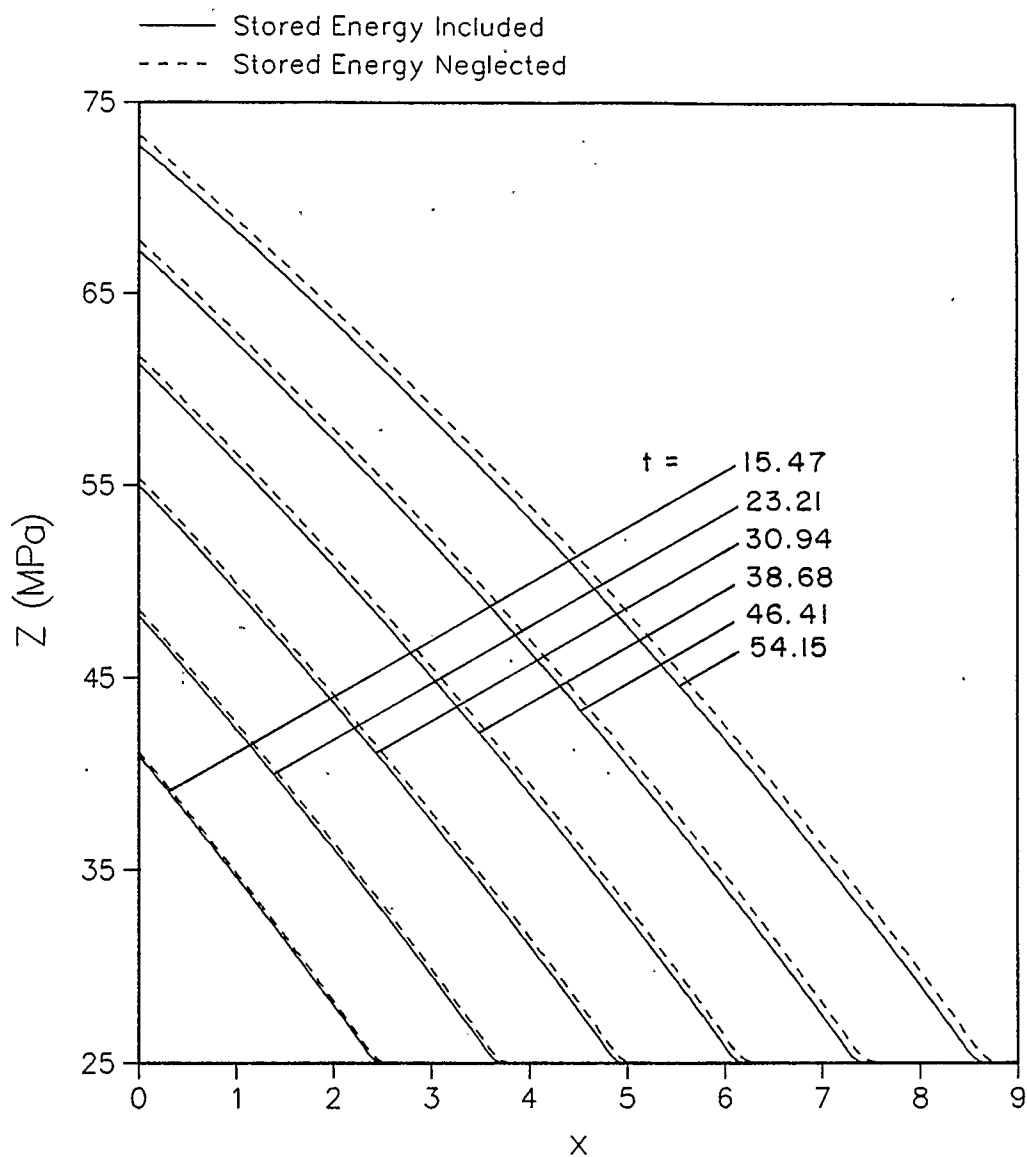


Figure 6.18d Influence of stored energy of cold work on the strain hardening response of SIAR to velocity and temperature step inputs ($v_0 = -300 \text{ ms}^{-1}$, $\theta_0 = 10 \text{ K}$, $\tau_0 = 1.47 \text{ E } 05$, $D_0 = 1.0 \text{ E } 05$, $X_{DF} = 0.00158$, $\Delta t = 0.387$).

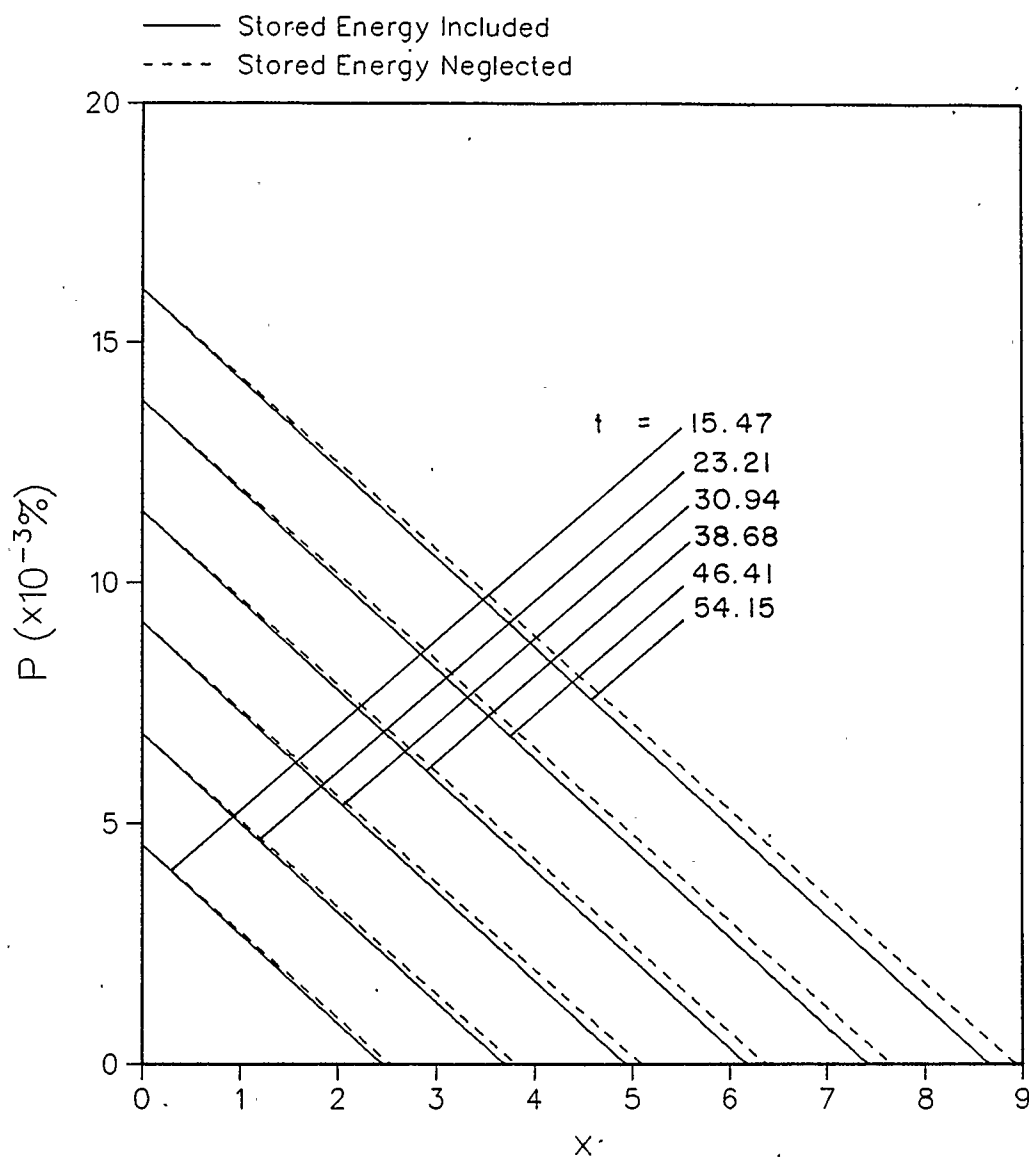


Figure 6.18e Influence of stored energy of cold work on the plastic strain response of SIAR to velocity and temperature step inputs ($v_0 = -300 \text{ ms}^{-1}$, $\theta_0 = 10 \text{ K}$, $\tau_0 = 1.47 \text{ E } 05$, $D_0 = 1.0 \text{ E } 05$, $X_{DF} = 0.00158$, $\Delta t = 0.387$).

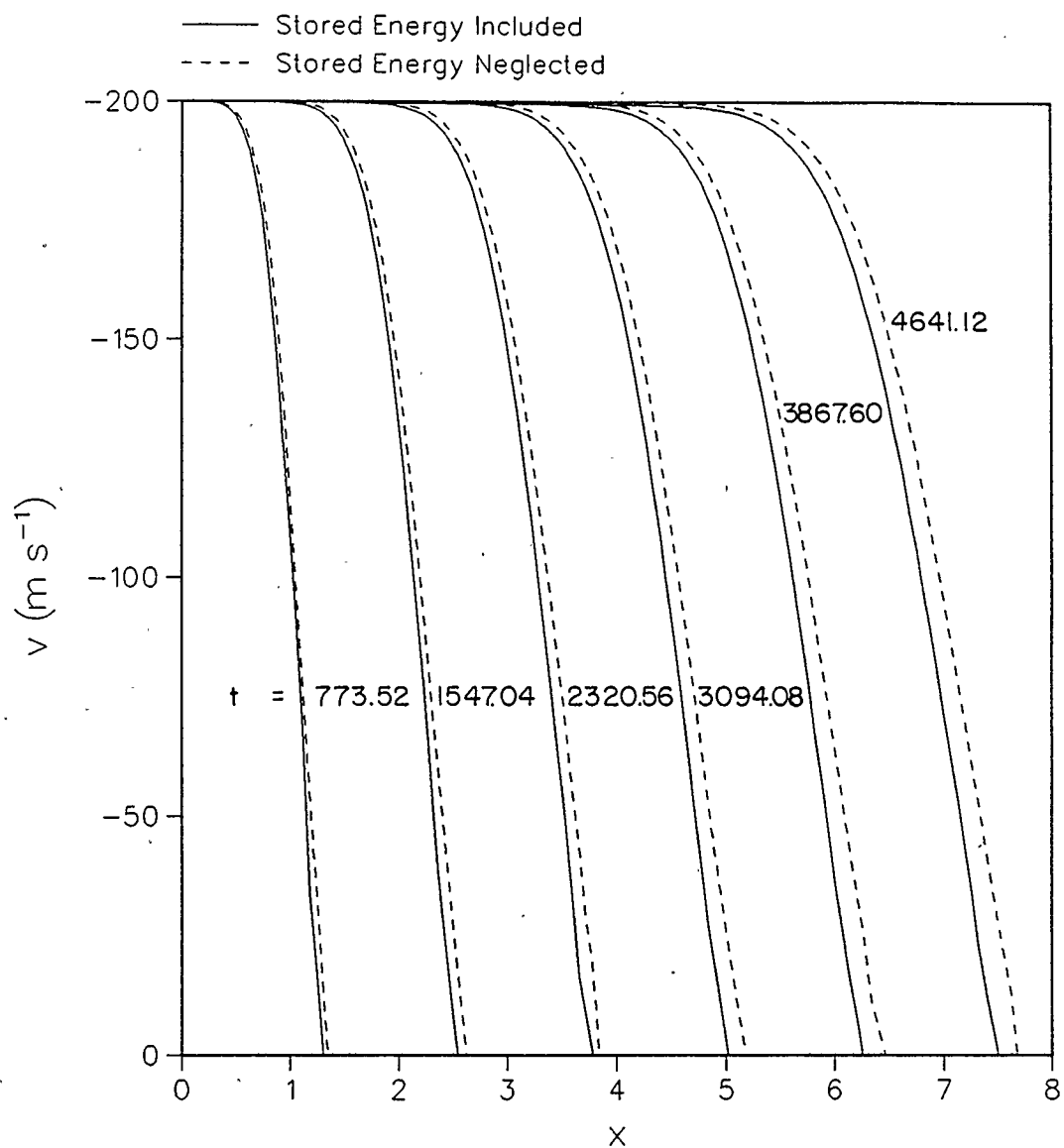


Figure 6.19a The effect of irrecoverable energy storage on the velocity response of SIAR to velocity only step input in the absence of second-sound and heat-flow effects ($v_0 = -200 \text{ ms}^{-1}$, $D_0 = 1.0 \text{ E } 04$, $X_{DF} = 0.00154$, $\Delta t = 38.7$).

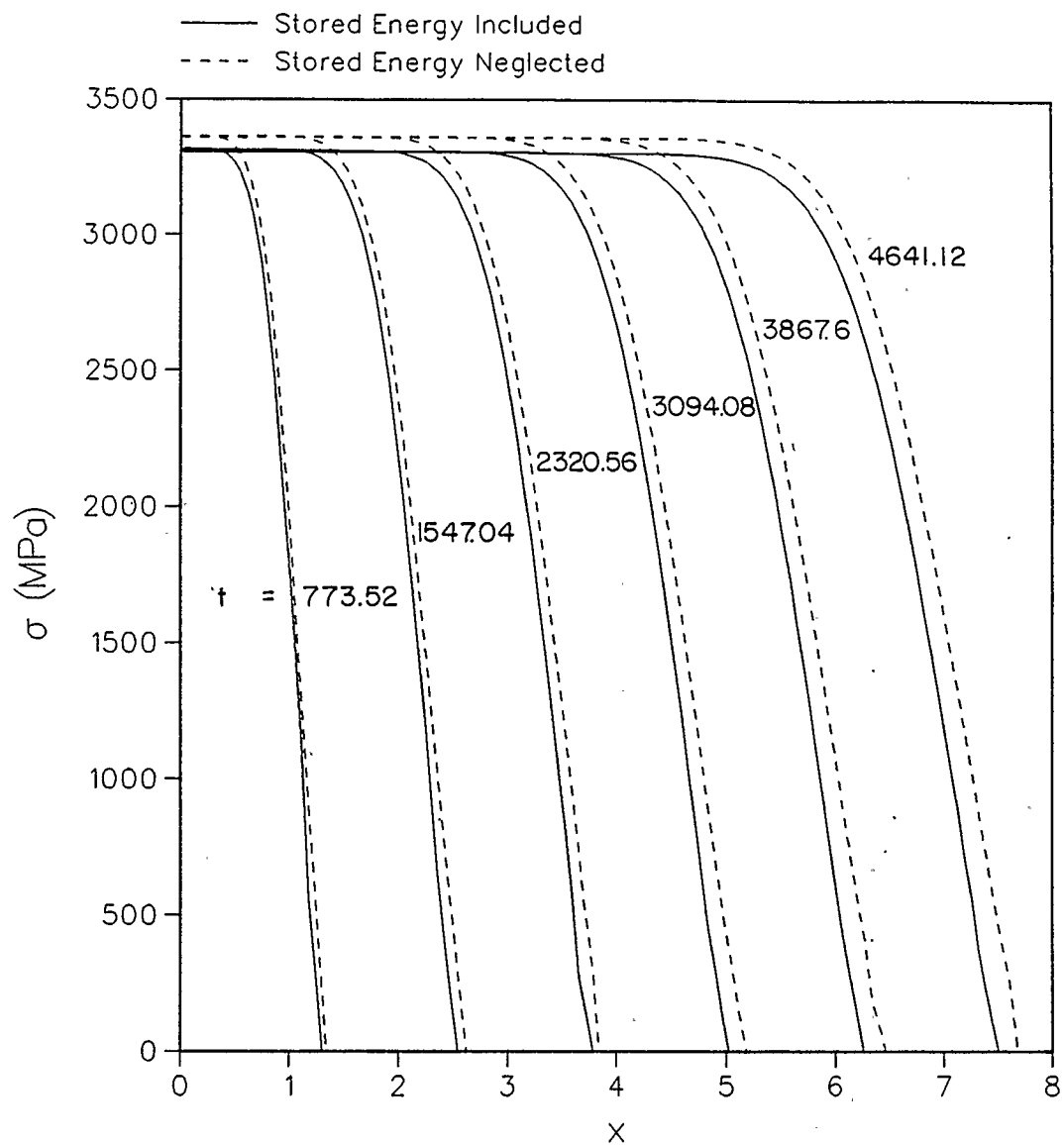


Figure 6.19b The effect of irrecoverable energy storage on the stress response of SIAR to velocity only step input in the absence of second-sound and heat-flow effects ($v_0 = -200 \text{ ms}^{-1}$, $D_0 = 1.0 \text{ E } 04$, $X_{DF} = 0.00154$, $\Delta t = 38.7$).

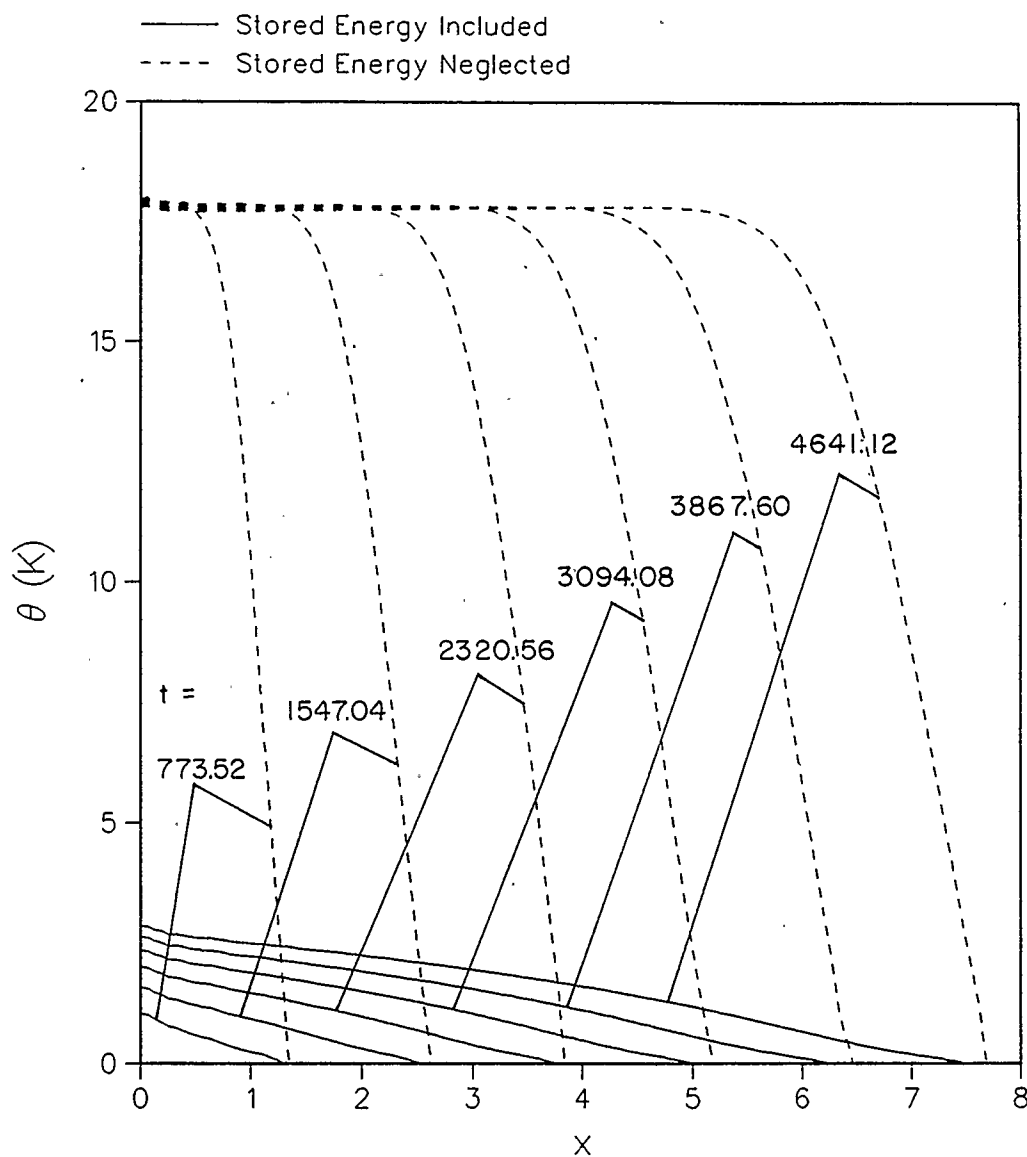


Figure 6.19c The effect of irrecoverable energy storage on the temperature response of SIAR to velocity only step input in the absence of second-sound and heat-flow effects ($v_0 = -200 \text{ ms}^{-1}$, $D_0 = 1.0 \text{ E } 04$, $X_{DF} = 0.00154$, $\Delta t = 38.7$).

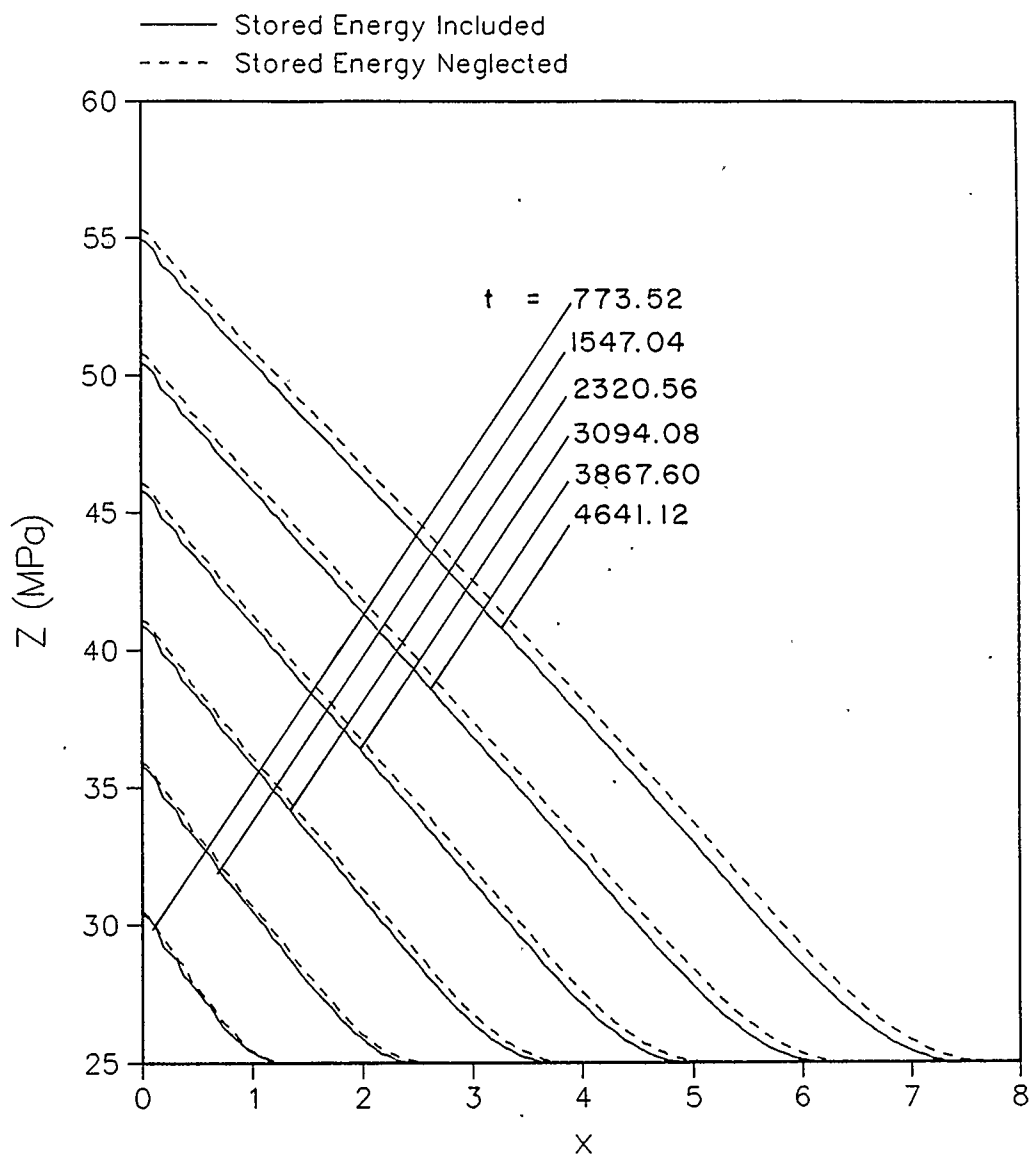


Figure 6.19d The effect of irrecoverable energy storage on the strain hardening response of SIAR to velocity only step input in the absence of second-sound and heat-flow effects ($v_0 = -200 \text{ ms}^{-1}$, $D_0 = 1.0 \text{ E } 04$, $X_{DF} = 0.00154$, $\Delta t = 38.7$).

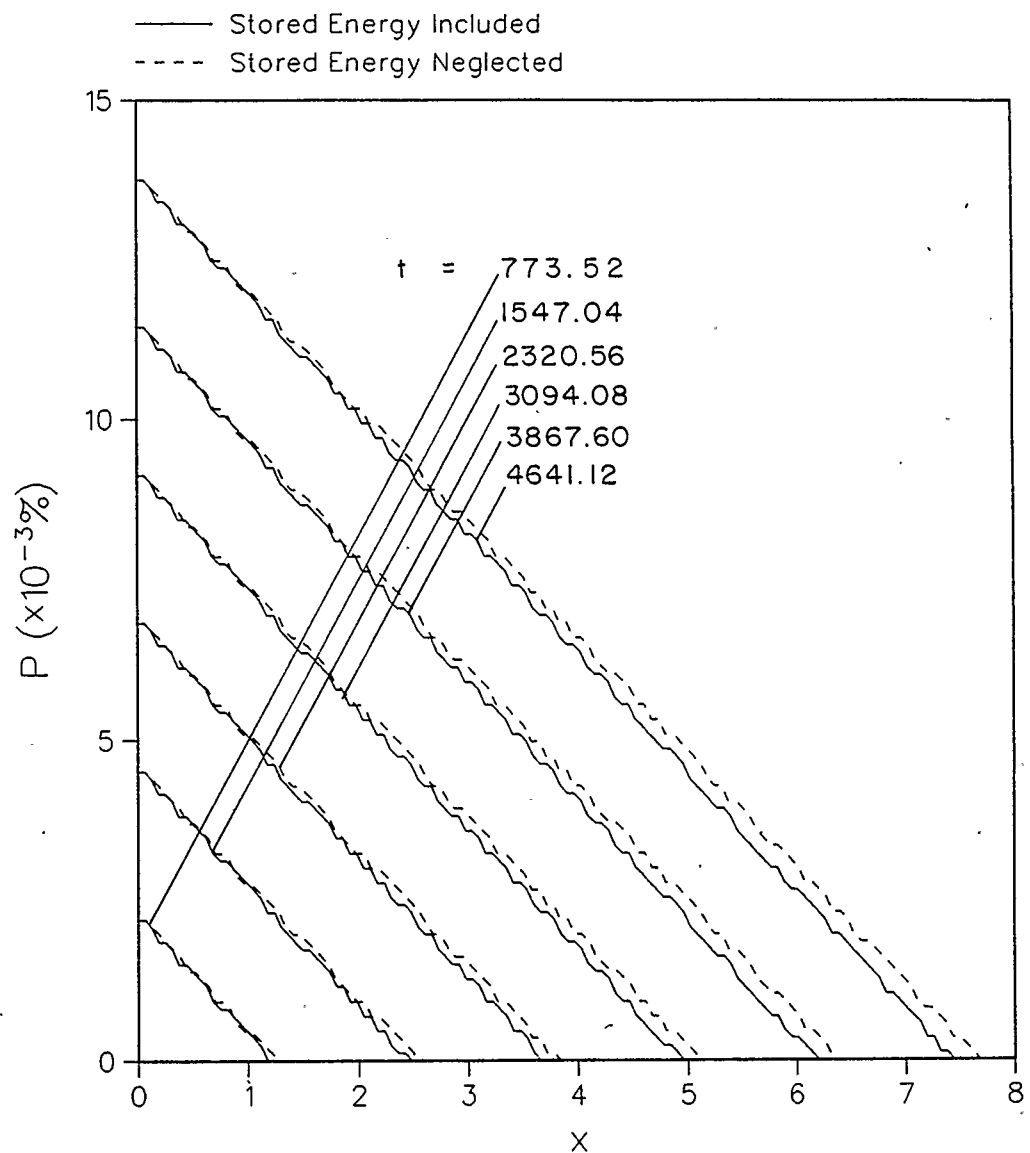


Figure 6.19e The effect of irrecoverable energy storage on the plastic strain response of SIAR to velocity only step input in the absence of second-sound and heat-flow effects ($v_0 = -200 \text{ ms}^{-1}$, $D_0 = 1.0 \text{ E } 04$, $X_{DF} = 0.00154$, $\Delta t = 38.7$).

6.3 Discussion of Results

All results involving the propagation of shock waves, for example Figure 6.2a, show the excellent shock resolution profiles of the numerical method of characteristics whereas there are evidences of shock smearing in the MacCormack finite difference scheme due to the phenomenon of numerical dispersion. Application of available shock capturing schemes such as the ones discussed in Chapter 5 did not improve the shock resolution capabilities of the MacCormack scheme. The author believes that this is due to the fact that the problems studied in this work are inherently dissipative thus not being able to benefit from additional dissipation introduced as artificial viscosity via conventional shock-capturing schemes. The observed numerical dispersions were most pronounced for velocity and stress responses but the responses of the temperature, heat flux, strain hardening, and plastic strain are better as can be seen in Figures 6.2b, 6.2c, 6.5a, and 6.5c, for example.

For the cases involving acceleration waves - that is responses to pulsive sine and terminated ramp inputs, there are excellent agreements between the characteristic and MacCormack algorithms for all variables. This can be easily seen from Figures 6.7a-c and 6.8a-c for aluminum, and Figures 6.15a-c and 6.16a-c for copper. Therefore, the MacCormack scheme is recommended for applications involving continuous inputs since algorithms based on this scheme are far easier to design and considerably cheaper to implement.

The initial heat flux responses are usually very high but die down and attain steady-state values after longer time periods as can be seen in Figures 6.2b and 6.10b. It can also be seen that for suddenly

imposed velocity or stress impacts, the heat flux magnitudes are greatest at the impacted ends for all times. These two observations show that in short-time response studies, non-adiabatic analyses are required especially at or near points of applications of impacts. The heat flux responses to mechanical-only inputs are very localized as can be seen in Figures 6.4b, 6.6b, 6.11b, and 6.14b.

As expected, for identical input conditions, the heat flux response levels of copper are generally higher than those of aluminum because copper has a higher coefficient of thermal conductivity - compare, for example, Figure 6.2b and Figure 6.10b, or Figure 6.7b and Figure 6.15b.

It is interesting to note that the terminated ramp input gives linear responses of velocity and stress but nonlinear responses in temperature, heat flux, and even strain hardening. Figures 6.8a-c and Figures 6.16a-c illustrate this observation.

For very small values of the thermal relaxation time, the jumps in temperature and heat flux are more pronounced. Whereas, no jumps in θ or q can be noticed in Figures 6.2b and 6.10b for a τ_0 of 3.8×10^{-12} s, appreciable jumps in θ and q for $\tau_0 = 3.8 \times 10^{-13}$ s can be observed for identical impact conditions in Figures 6.9b and 6.17b. It is also significant that the jumps in the thermal deformation variables are most pronounced at times that are shorter than or of the same order as the thermal relaxation time.

Evidence of the ability of the constitutive model developed in this work to simulate thermomechanical coupling effects is given by the results displayed in Figures 6.4b, 6.6b, 6.11b, 6.12a, and 6.14b. These results illustrate that stress impacts or velocity impacts would

generate thermal fields and that a temperature impact would give rise to velocity and stress fields. In particular, there is evidence of temperature rise due to conversion of inelastic mechanical work to heat energy which are most pronounced near the impacted ends where the plastic strains, of course, attain their maximum values. This also shows that the law of conservation of energy is capable of predicting temperature rises in inelastic deformation processes.

Figures 6.18a-e and 6.19a-e illustrate the influence of the stored energy of cold work on the various responses. First, it may be observed that neglecting the irrecoverably stored energy slightly overestimates the responses of the mechanical deformation variables: v , σ , Z , P . The overestimation becomes more pronounced as time increases as can be seen in Figures 6.18a and 6.19a, for example. Thus, it is believed that appreciable overestimation of these variables would be observed for very large times. Figures 6.18c and 6.19c clearly show that neglecting the stored energy of cold work leads to appreciable overestimation of the temperature rise in the material. This is consistent with physical expectations since neglecting the stored energy is equivalent to assuming that all the plastic mechanical work is converted into heat energy. It was also found that neglecting the stored energy of cold work overestimates the wave speeds as illustrated in Tables 6.3a and 6.3b.

Although for nonlinear problems, the shock waves do not necessarily propagate along the characteristic curves, it was found in this work that the shock waves appear to propagate along the characteristic directions. This is because the velocities of the shock waves (V_G and V_L) computed from the Rankine-Hugoniot conditions,

Table 6.3a Effect of stored energy of cold work on the initial wave velocities in an aluminum rod for different values of the thermal relaxation time.

Thermal relaxation time, τ_0 (s)	Lagging wave velocity, v_5 (ms ⁻¹)		Leading wave velocity, v_3 (ms ⁻¹)	
	Stored energy included	Stored energy neglected	Stored energy included	Stored energy neglected
3.8 E -13	6147.87	6139.44	11627.10	16086.90
3.8 E -12	3369.39	4902.60	6153.66	6370.49
2.0 E -11	1468.71	2179.97	6153.57	6244.91
1.0 E -10	656.827	976.37	6153.55	6235.55

Table 6.3b Effect of stored energy of cold work on the initial wave velocities in a copper rod for different values of the thermal relaxation time.

Thermal relaxation time, τ_0 (s)	Lagging wave velocity, v_5 (ms ⁻¹)		Leading wave velocity, v_3 (ms ⁻¹)	
	Stored energy included	Stored energy neglected	Stored energy included	Stored energy neglected
3.8 E -13	4756.13	4752.28	14296.40	17523.10
3.8 E -12	4520.33	4640.33	4756.75	5674.99
2.0 E -11	1983.85	2381.27	4758.21	4820.39
1.0 E -10	881.278	1067.92	4756.19	4806.91

Table 6.4a Comparison of the initial velocities of the shock waves calculated from the jump conditions and the wave velocities computed from the numerical algorithms for an aluminum rod when the stored energy is neglected.

Thermal relaxation time, τ_0 (s)	Lagging wave velocity (ms ⁻¹)		Leading wave velocity (ms ⁻¹)		Uncoupled wave velocities (ms ⁻¹)	
	V_G	V_5	V_L	V_3	Purely mechanical, V_M	Purely thermal, V_T
3.8 E -13	6140.28	6139.44	16021.80	16086.90	6153.29	16050.60
3.8 E -12	4876.95	4902.60	6343.20	6370.49	6153.29	5075.66
2.0 E -11	2168.71	2179.97	6236.40	6244.91	6153.29	2212.43
1.0 E -10	975.11	976.37	6235.63	6235.55	6153.29	989.43

Table 6.4b Comparison of the initial velocities of the shock waves calculated from the jump conditions and the wave velocities computed from the numerical algorithms for a copper rod when the stored energy is neglected.

Thermal relaxation time, τ_0 (s)	Lagging wave velocity (ms^{-1})		Leading wave velocity (ms^{-1})		Uncoupled wave velocities (ms^{-1})	
	V_G	V_5	V_L	V_3	Purely mechanical, V_M	Purely thermal, V_T
3.8 E -13	4752.42	4752.28	17449.80	17523.10	4756.13	17508.90
3.8 E -12	4640.16	4640.33	5662.26	5674.99	4756.13	5536.81
2.0 E -11	2369.90	2381.27	4815.81	4820.39	4756.13	2413.44
1.0 E -10	1062.88	1067.92	4803.63	4806.91	4756.13	1079.32

equations (4.46), and the values of the characteristic speeds (V_5 and V_3) are almost identical as illustrated in Tables 6.4a and 6.4b. All wave velocities are computed at the origin of the solution domain. The tables also show that the two wave velocities differ from the wave velocities corresponding to the purely mechanical (V_M) or purely thermal (V_T) theories.

Some wiggles are noticed in the strain hardening responses. These are slightly noticeable in Figures 6.2c and 6.10c for example, but are more seriously pronounced in Figures 6.7c and 6.8c. These are believed to be due to numerical problems associated with the stiffness of the evolution equations.

It was found by numerical experimentations that for both algorithms, the CFL criterion was necessary but insufficient for stability. The time step was found to be sensitive to the values of the thermal relaxation time, τ_0 , and the parameter $D_0(s^{-1})$ which essentially determines the magnitude of the plastic strain rate. It was observed that a time step smaller than τ_0 was required for the numerical stability of each of the computational algorithms. This requirement considerably limited the computations reported to relatively short time response studies since a very small time step demands a very large number of computations in order to proceed far in time.

CHAPTER 7CONCLUSIONS

Novel thermodynamically-consistent constitutive equations for the study of the propagation of inelastic waves are developed in this thesis. Essential features of dissipative effects such as heat generation, heat flow, thermomechanical coupling, and irrecoverable inelastic energy storage are incorporated in the model. Also included in the development are rate dependence and isotropic hardening. The approach consists of a systematic application of the theory of continuum thermodynamics with internal state variables, the results of materials science and mechanics experiments, and mathematical analysis. It is clearly illustrated by examples that an explicit, yet physically motivated, quantification of the irrecoverable portion of the free energy functional is feasible. A general framework under which the procedure may be globally employed for the characterization of the thermomechanical behavior of inelastic solids is given.

The nonlinear material model presented allows for the coupling of thermoelastic and thermoinelastic variables and automatically gives the dissipative part of the stress thereby eliminating the need for a separate dissipation potential. The model is also applicable over a wide range of temperatures since no assumption is made concerning the relative magnitudes of the incremental and reference temperatures.

The following main conclusions may be drawn from the development of the constitutive equations and the design and implementation of the computational algorithms.

- (1) The law of conservation of energy can adequately deal with the

issue of balance of work and energy even in the presence of dissipative effects. Thus, there is no need for *ad hoc* assumptions that serve to pre-empt the application of this fundamental principle of continuum mechanics.

- (ii) It is unnecessary to resort to *ab initio* quantitative guesses concerning the interconversion of mechanical work into heat energy. This issue automatically takes care of itself in a systematic application of the law of conservation of energy together with physically-motivated constitutive laws that account for the stored energy of cold work.
- (iii) In a plastically deforming material, the ratio of the energy irrecoverably stored to the energy converted into heat is not a constant but a variable that depends on the thermodynamic state of the deformation process.
- (iv) Neglecting the stored energy of cold work in inelastic analysis slightly overestimates the stress and velocity responses but leads to an appreciable overestimation of the temperature rise in the body.
- (v) Incorporation of the stored energy of cold work phenomenon decreases the wave speeds thus confirming the dissipative nature of the process of irrecoverable energy storage.
- (vi) There exist two coupled nonlinear thermomechanical waves propagating with distinct velocities in the positive X direction; the wave velocities are different from the purely mechanical or purely thermal wave velocities.
- (vii) The thermoinelastic waves propagate at the thermoelastic wave speeds in the absence of second sound effects. This is

consistent with earlier experimental findings discussed in the text.

- (viii) The algorithm based on the numerical method of characteristics is more complicated and involves much larger computation times than the algorithm based on the MacCormack finite difference scheme. However, the numerical method of characteristics gives sharper resolutions of the shock profiles.
- (ix) The algorithm based on the MacCormack finite difference scheme is recommended for numerical simulations of acceleration waves or other time-dependent inputs that are continuous with respect to the primary dependent variables. This recommendation is based on the observation that the MacCormack scheme gives very accurate results with negligible numerical dispersion for smooth inputs while it is easier to design and cheaper to implement.
- (x) For both computational algorithms, the CFL stability criterion is necessary but insufficient for stability. The time step required for stability is sensitive to the smallest characteristic time of the physical process. For the problems considered in this thesis, in particular, the time step was found to be sensitive to the thermal relaxation time and the magnitude of the plastic strain rate.
- (xi) Heat flux responses attain steady-state values after sufficiently large times but are significant for short time response studies of fast dynamical systems.

As far as the author knows, no elaborate quantitative analysis of inelastic wave propagation that encompasses non-isothermal,

non-adiabatic, and coupled effects, and that involves so many dependent variables as was done in this work has been reported in the literature. It is hoped that the results and conclusions given above will provide further insight into the methodology of inelastic constitutive modelling in general and the theory of inelastic wave propagation in particular. It is also expected that the work will be exploited for improving the design of plastic wave experiments and the proper interpretation of experimental data especially in the presence of high strain rates.

7.1 Recommendations for Further Work

Further work is needed in the experimental determination of the stored energy of cold work for a wider variety of loading conditions and for more metals and metallic alloys. This will allow the application of the procedure developed in this work to multidimensional stress states and to the characterization of other materials.

Inclusion of more internal state variables such as directional or kinematic hardening will be desirable for situations involving finite geometries so that loading and unloading phenomena caused by wave reflections may be accurately modelled.

As discussed in Chapter 4, conventional forms of evolution equations for internal state variables lead to vanishing jumps of the internal state variables. In the light of the fact that this is not generally consistent with the physical behavior of inelastic deformation processes, it is recommended that serious considerations be given the development of evolution equations that include divergence terms.

Development of shock-capturing schemes that are more suitable for nonconservative systems of equations would certainly improve the

shock resolution capabilities of the MacCormack finite difference scheme.

It will be interesting to search for numerical algorithms that demand less stringent stability requirements so that computations can proceed faster and further in time.

In summary, the author believes that any exploitation of advances in the various branches of knowledge illustrated in Figure 1.1 will significantly contribute to progress in the study of wave propagation in inelastic solids.

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APPENDIX

DETERMINATION OF THE MATERIAL PARAMETERS B_{4R} and B_{5R}

The detailed determination of the values of the quantities B_{4R} and B_{5R} which are used as the auxiliary conditions for the solution of equations (3.30e) and (3.30f) is presented in this appendix.

Recall that the explicit representation for the stress is given by

$$\sigma = A_{11} - [3\lambda(\theta) + 2\mu(\theta)]\alpha(\theta)\theta + [\lambda(\theta) + 2\mu(\theta)]E + B_4(\theta)Z + B_5(\theta)P. \quad (A1)$$

Consider a piece of material to be in the reference state R defined in equation (3.8) as

$$R = \{E = E_R, Z = Z_R = Z_0, P = P_R; \theta\}. \quad (A2)$$

Let the state R_0 be associated with a reference undeformed configuration in which the differential temperature (θ) assumes a zero value, that is,

$$R_0 = \{E = 0, Z = Z_0, P = 0, \theta = 0\}. \quad (A3)$$

This stress-free configuration implies that at state R_0 , the value of the stress is zero, that is,

$$\sigma \Big|_{R_0} = 0. \quad (A4)$$

Substituting (A3) and (A4) into (A1) gives

$$A_{11} + B_{4R} Z_0 = 0. \quad (A5)$$

Now, consider the same piece of material to be in another stress-free undeformed configuration in which the uniform differential temperature is $\theta = 1$ K. This equilibrium configuration, R_1 , is defined as

$$R_1 = \{E = 0, Z = Z_0, P = 0, \theta = 1 \text{ K}\}. \quad (\text{A6})$$

In (A6), it should be noted that the value of the strain hardening parameter corresponding to state R_1 remains essentially the same as the value for state R_0 . This is because the strain hardening parameter is insensitive to very small changes in temperature.

The expression for $B_4(\theta)$ may be recalled as

$$B_4(\theta) = B_{4R} \left(1 + \frac{\theta}{T_R}\right)^{1 - \lambda_1 - \lambda_2 T_R} \exp(\lambda_2 \theta). \quad (\text{A7})$$

From equation (A7), the value of $B_4(\theta)$ at this latter reference configuration (R_1) is

$$B_4(\theta) \Big|_{R_1} = B_{41} = B_{4R} \left(1 + \frac{1}{T_R}\right)^{1 - \lambda_1 - \lambda_2 T_R} \exp(\lambda_2), \quad (\text{A8})$$

or

$$B_{41} = B_{4R} S, \quad (\text{A9a})$$

where

$$S = \left(1 + \frac{1}{T_R}\right)^{1 - \lambda_1 - \lambda_2 T_R} \exp(\lambda_2). \quad (\text{A9b})$$

It should be noted that S is known because λ_1 , λ_2 , and T_R are known.

Since state R_1 is also stress-free, that is,

$$\sigma \Big|_{R_1} = 0, \quad (\text{A10})$$

and there is no appreciable variation of the thermoelastic material properties $\lambda(\theta)$, $\mu(\theta)$, and $\alpha(\theta)$ for small increments of temperature, satisfaction of the expression for stress at state R_1 requires that:

$$A_{11} - (3\lambda_R + 2\mu_R)\alpha_R + B_{41}Z_0 = 0, \quad (\text{A11a})$$

or, on using equation (A9a) in equation (A11a),

$$A_{11} - (3\lambda_R + 2\mu_R)\alpha_R + SB_{4R}Z_0 = 0. \quad (\text{A11b})$$

Solving equations (A5) and (A11b) simultaneously gives the two unknowns as

$$A_{11} = (3\lambda_R + 2\mu_R)\alpha_R \left[1 - \exp(\lambda_2) \left(1 + \frac{1}{T_R} \right) \right]^{1 - \lambda_1 - \lambda_2 T_R^{-1}}, \quad (\text{A12})$$

$$B_{4R} = - \left[\frac{(3\lambda_R + 2\mu_R)\alpha_R}{Z_0} \right] \cdot \left[1 - \exp(\lambda_2) \left(1 + \frac{1}{T_R} \right) \right]^{1 - \lambda_1 - \lambda_2 T_R^{-1}}. \quad (\text{A13})$$

Next, consider the approximate isothermal stress-strain curve of a plastically deformed material to be as shown in Figure A1 below at the reference temperature $\theta = 0$.

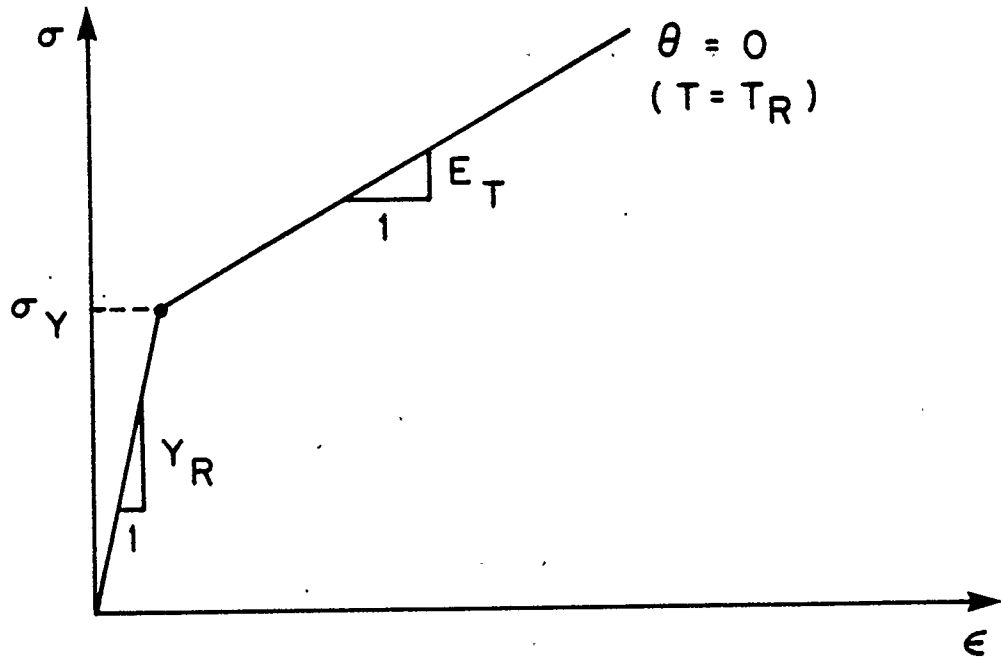


Figure A1 Isothermal stress-strain curve at the reference temperature.

From equation (A1), it is easy to see that

$$\frac{\partial \sigma}{\partial P} = B_5(\theta), \quad (A14)$$

so that

$$\left. \frac{\partial \sigma}{\partial P} \right|_{\substack{\theta = 0 \\ T = T_R}} = B_{5R}. \quad (A15)$$

Thus, from equation (A15), it can be seen that B_{5R} is the rate of change of the stress with the plastic strain at the reference temperature. It follows that B_{5R} is the slope of the isothermal stress-plastic strain curve.

Invoking the additive decomposition assumption of the total strain into elastic and plastic parts and assuming that the elastic deformation obeys Hooke's law, the stress-plastic strain curve can be constructed from the stress-total strain curve given in Figure A1 as follows. The stress-strain relation in the plastic region of Figure A1 is given by

$$\sigma = \sigma_Y + E_T \epsilon - E_T \epsilon_Y, \quad (A16)$$

where σ_Y is the yield stress and ϵ_Y is the corresponding strain. The two assumptions above imply that

$$\epsilon = E + P, \quad (A17)$$

$$\sigma = Y_R E, \quad (A18a)$$

$$\text{and} \quad \sigma_Y = Y_R \epsilon_Y. \quad (A18b)$$

Substituting equations (A17), (A18a), and (A18b) into (A16) gives

$$\sigma = \sigma_Y + \left(\frac{Y_R E_T}{Y_R - E_T} \right) P. \quad (A19)$$

Equation (A19) reveals that, approximately, the stress-plastic strain curve is as shown in Figure A2.

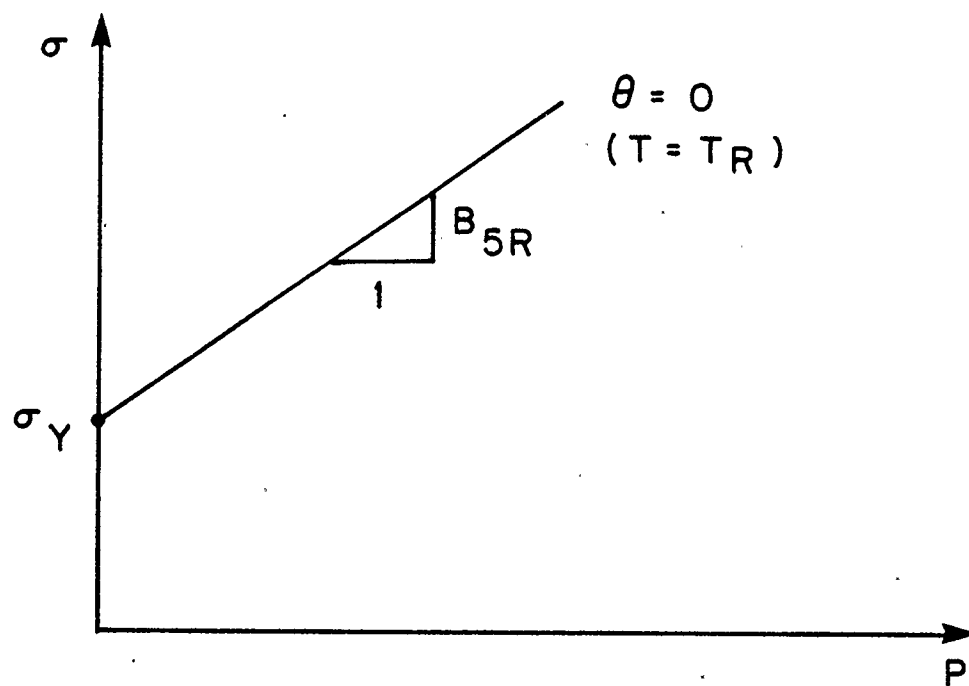


Figure A2 Derived isothermal stress-plastic strain curve at the reference temperature.

Thus, it can be seen that the value of the constant B_{5R} is approximately determined as

$$B_{5R} = \frac{Y_R E_T}{Y_R - E_T} \quad (A20)$$