THE UNIVERSITY OF CALGARY

A Constitutive Theory and Wave Propagation in Thermoplastic Solids

BY

XIANG-YAO QIU

A THESIS
SUBMITTED TO THE FACULTY OF GRADUATE STUDIES
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE
DEGREE OF DOCTOR OF PHILOSOPHY

DEPARTMENT OF MECHANICAL ENGINEERING

CALGARY, ALBERTA

MAY, 1991

ISBN 0-315-71177-9

THE UNIVERSITY OF CALGARY
FACULTY OF GRADUATE STUDIES

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a thesis entitled "A Constitutive Theory and Wave Propagation in Thermoplastic Solids", submitted by Xiang-Yao Qiu in partial fulfillment of the requirements for the degree of Doctor of Philosophy.

Mansa Singh

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

Dr. S. Dost
Department of Mechanical Engineering
University of Victoria

M. Epstein

Dr. M. Epstein
Department of Mechanical Engineering

N.G. Shrive.

Dr. N.G. Shrive
Department of Civil Engineering

R.S. Dhaliwal

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

R.N. Dubey

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

27 May, 1991

ABSTRACT

The theory of normality is extended to include both thermal and plastic effects. Some restrictions imposed on the free energy function are obtained. The relation between the free energy function and dissipation function is clarified. A theorem for constituting the two leading functions of thermodynamics is justified. By employing the concept of internal state variables and taking into account the dissipative nature of plastic deformation, strain hardening and temperature effects, the constitutive equations for thermoplastic solids are developed based upon the extended theory of normality and the field theory of irreversible thermodynamics.

Different combinations of free energy function and dissipation function are introduced for different properties of materials under consideration. Because both the free energy function and dissipation function have been employed, self-compatibility of the derived equations is assured. The developed model is temperature-dependent, and the material properties considered allow the constitutive equations for a wide temperature-range application.

A particularly selected rate-sensitive constitutive equation-set is employed to study plastic wave propagation problem in a semi-infinite rod. The resulting equations are numerically solved by utilizing CYBER-175 computer. Two different numerical integration procedures are involved. One is the characteristics and the other is of finite difference. For different boundary conditions the two methods generate physically meaningful results. In these results, mechanical and thermal coupling is clearly displayed.

ACKNOWLEDGEMENTS

I wish to express my sincere gratitude and appreciation to my supervisor, Dr. M.C. Singh, for his guidance, encouragement and support during the course of this research.

My thanks to Dr. S. Dost for his encouragement and support during early period of my program.

Instruction and interests in my academic progress from Dr. M. Epstein is highly appreciated.

The cooperation of the staff of Academic Computing Services is sincerely appreciated. I am also grateful for the allocation of super-computing funds without which the numerical work of this research could never be finished.

The financial assistance coming from Department of Mechanical Engineering and Graduate Studies is gratefully acknowledged. Only with it could the work be completed.

To my mother Fenglan

TABLE OF CONTENTS

TABLE OF CONTENTS (cont'd)

TABLE OF CONTENTS (cont'd)

LIST OF FIGURES

LIST OF FIGURES(cont'd)

LIST OF FIGURES(cont'd)

LIST OF FIGURES(cont'd)

NOMENCLATURE

Symbol

Roman Letters	Meaning
A	An arbitrary physical quantity
$\underset{\sim}{A}$	Squire matrix
A_{ij}	Elements of matrix $\underset{\sim}{A}$
$\mathcal{B}$	A body of continuum
D_1	Analytical function
D_2	Analytical function
D_3	Analytical function
D_4	Analytical function
D_5	Analytical function
C	Velocity of wave
$C(\theta)$	Temperature-dependent material property
$C^{+}_{(i)}$	Characteristics curves corresponding to positive eigenvalues
$C^{-}_{(i)}$	Characteristics curves corresponding to negative eigenvalues
D	Material derivative
$K(\theta)$	Analytical function of temperature
D_i'	Coefficients in the system of basic equations
$\bar{d}$	Small amount
d_{ij}	Components of strain rate tensor
$\underset{\sim}{E}$	Elastic strain tensor
$\mathbf{F}$	Force vector
$F(\theta)$	Analytical function of temperature

Roman Letters	Meaning
$F_k^{(d)}$	Dissipative forces
$\mathbf{f}$	Body force per unit volume
$\mathbf{g}$	Gradient of temperature
H	Strain hardening parameter
$K_1(\theta)$	Analytical function of temperature
$K_2(\theta)$	Analytical function of temperature
$m_i(\theta)$	Analytical function of temperature
$H(\cdot)$	Heaviside function
K	Kinetic energy
k	Heat conduction coefficient
$K(\theta)$	Temperature-dependent material property
$l^{(i)}$	The ith left eigenvector
P	Rate of work
Q	Heat energy
$\mathbf{q}$	Heat flow
q_i	Components of heat flow
R	Heat flow or equivalent heat flow
R_1	Analytical function
R_2	Analytical function
R_3	Analytical function
R_4	Analytical function
R_5	Analytical function
R_6	Analytical function
R_7	Analytical function
$\mathbf{S}$	Entropy vector
s	Entropy

Roman Letters	Meaning
s	Boundary surface
S(t)	Sine function
T	Increment of temperature
T_i	Surface traction components
t	Time
t′	Real time
U	Internal energy
u	Internal energy per unit volume
v	Volume
V_i	The ith eigenvalue
v_i	Velocity components
W	Work
W_p	Plastic work
W_1	Analytical function
W_2	Analytical function
W_3	Analytical function
W_4	Analytical function
W_5	Analytical function
W_6	Analytical function
W_7	Analytical function
x	Eulerian coordinate
x	Lagrangian coordinate
x′	Real distance
Y	Vector of dependent variables

Greek Letters	Meaning
α	The value of Δt over Δx;
	internal state variables
β	Thermodynamic force tensor
ε	Strain tensor
θ	Absolute temperature
Λ	Analytical function
λ	Lamé constant;
	eigenvalue
μ	Lamé constant
$\mu<\cdot>$	McAuley bracket
ν	Outward normal of a surface element;
	coefficient of normality in velocity space;
	Poisson's ratio
ν'	Coefficient of normality in force space
ρ	Density
σ	Stress tensor
ϕ	Dissipation function
Φ	Dissipation function per unit volume
Φ'	Dissipation function per unit volume in force space
Ψ	Free energy function per unit volume
ω	Angular velocity

Symbol	Meaning
$\underset{\sim}{\cdot}$	Vector
$\underline{\cdot}$	Squire matrix

Subscripts	Meaning
(1)	The first invariant of a second-order tensor
(2)	The second invariant of a second-order tensor
t	Derivative with respect to t
x	Derivative with respect to x
R	Reference

Superscripts	Meaning
(p)	Plastic
(e)	Elastic

CHAPTER 1

INTRODUCTION

1.1 Significance of Field Theory of Thermodynamics

The field theory of mechanics can be dated back to the 18th century when fluids were studied by Euler and to the 19th century when solids were studied by Cauchy. Compared with this fact the theory of thermodynamics established by Carnot, Mayer and Clausius is a younger science, and the development of its field theory has just been existing for several decades.

For a long time the objective in the study of thermodynamics has been to consider a finite portion of matter. This situation covers nearly entire published literature and it is still almost true for today's works, where one usually assumes that the state under consideration is the same through the entire volume of the body. From mechanics point of view this simply means that the body is in a homogeneous state. With this assumption, if we try to solve a mechanics problem to obtain the values of dependent variables such as stress and strain, which are associated with thermodynamics dependent variables like temperature, heat flow *etc.* we would be unable even to solve very simple problems like a circular bar subject to torsion or a cantilever beam subject to transverse loading and non-uniform temperature distributions, without using the field theory of thermodynamics. Lack of the field theory even at the middle of this century has resulted in a far reaching negative consequences.

Reversible process is one of the fundamental concepts in classical thermodynamics. Suppose we consider a finite portion of a continuum. Mechanical and thermodynamic states within this portion generally differ from point to point, and the state usually changes even when it is isolated from its surroundings. For instance, at least the temperature will tend to be uniform as time goes on; the process is accompanied by an increase of entropy, and therefore, is irreversible. To minimize the irreversibility, classical thermodynamics has to restrict itself to infinitely slow processes, or in other words, to the states that are in the immediate vicinity of equilibrium. Under this assumption most processes are considered reversible, and as a consequence classical thermodynamics claims that every sufficiently slow process is reversible. While the assumption has produced many conclusions in practice, a counter example concludes obviously that plastic deformation of a solid is always irreversible, no matter how slow it may be.

As continuum mechanics deals with motions in which many thermodynamic processes may be involved, it is closely related to thermodynamics. However, as the reasons mentioned above the classical theory can not be directly applied to continuum mechanics, unless a refined theory or so called field theory of thermodynamics is available.

1.2 Balance of Linear Momentum

Suppose a body of continuum, $\mathfrak{B}$ shown in Fig.1.1, is under examination. Its volume is denoted by v, and its surface whose exterior normal is ν is denoted by s. Now let us consider the balance law of momentum associated with the body.

If $\mathbf{f}$ is the body force per unit mass, and $\mathbf{t}_{(\nu)}$ is the stress

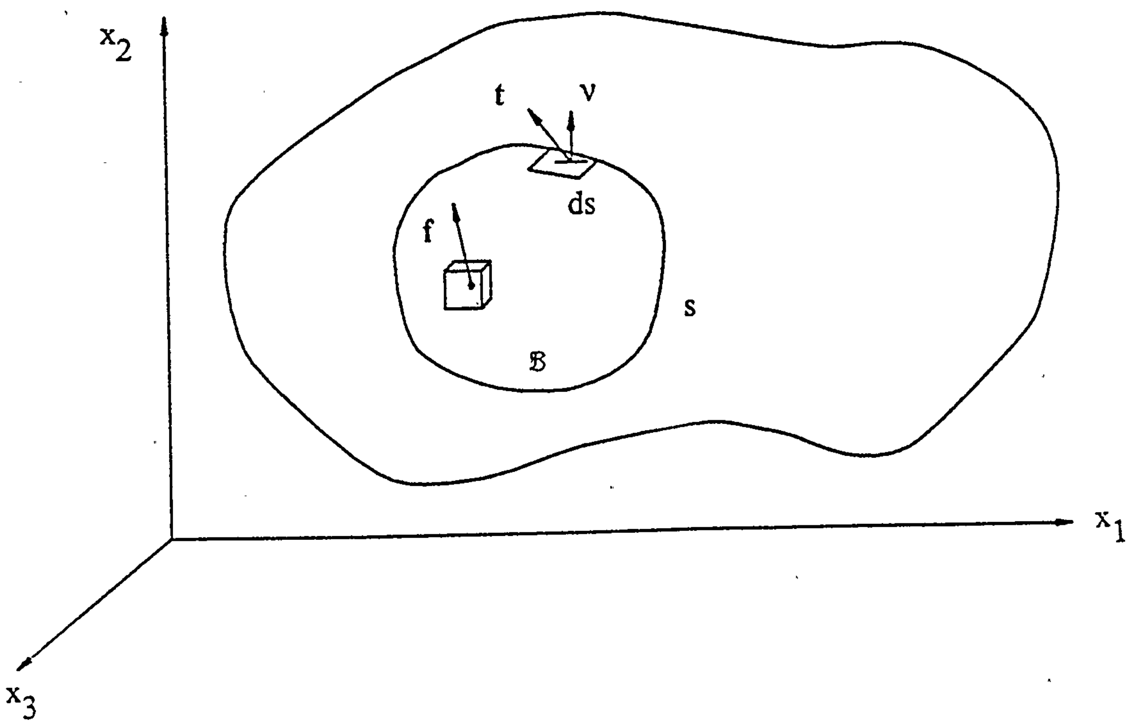

Fig. 1.1 A body of continuum

vector acting on the surface element ds whose exterior normal vector is v, then the resultant external force F acting on the body is given by the following expression:

$$F = \int_{s} \mathbf{t}_{(\mathrm{v})}\, ds + \int_{v} \rho\, \mathbf{f}\, dv \quad . \tag{1.1}$$

According to the law of balance of linear momentum, which asserts that the time rate of change of momentum is equal to the resultant force F acting on the body, we have:

$$\frac{D}{Dt} \int_{v} \rho\, \mathbf{v}\, dv = F \quad , \tag{1.2}$$

where $\frac{D}{Dt}$ stands for material derivative. Combining equation (1.1) with (1.2) yields the expression for global balance of linear momentum:

$$\frac{D}{Dt} \int_{v} \rho\, \mathbf{v}\, dv = \int_{s} \mathbf{t}_{(\mathrm{v})}\, ds + \int_{v} \rho\, \mathbf{f}\, dv \quad . \tag{1.3}$$

When the indicated differentiation on the left hand side is carried out, and the local form of mass conservation is noticed, equation (1.3) can be written in the form of

$$\int_{v} \rho\, \dot{\mathbf{v}}\, dv = \int_{s} \mathbf{t}_{(\mathrm{v})}\, ds + \int_{v} \rho\, \mathbf{f}\, dv \quad , \tag{1.4}$$

or

$$\int_{v} \rho\, \dot{\mathrm{v}}_{\mathrm{i}}\, dv = \int_{s} \mathrm{t}_{(\mathrm{v})\mathrm{i}}\, ds + \int_{v} \rho\, \mathrm{f}_{\mathrm{i}}\, dv \quad . \tag{1.4b}$$

Here the dot also means material derivative. By the stress principle of Euler and Cauchy [1.44] we have:

$$t_{(\nu)i} = \sigma_{ij}\, \nu_j \quad , \tag{1.5}$$

where σ_{ij} is the stress tensor and ν_j is the components of the unit vector along the outer normal to the surface of the region v.

Substituting equation (1.5) in (1.4b) and applying Gauss' theorem to convert the surface integral into volume integral, we obtain:

$$\int_{v} [\sigma_{ij,i} + \rho\, (f_j - \dot{v}_j)]\, dv = 0 \quad . \tag{1.6}$$

For equation (1.6) to be valid for any arbitrary volume v, the necessary and sufficient condition is vanishing of the integrand. Hence

$$\sigma_{ij,i} + \rho\, (f_j - \dot{v}_j) = 0 \quad . \tag{1.7}$$

Equation (1.7) expresses the local form of the law of balance of momentum, and is the equation of motion.

1.3 Conservation of Energy

For considering conservation of energy let us re-examine the ways by which the energy of a non-isolated system can be altered. By definition, the amount of energy transferred to a system as work, W, associated with some infinitesimal changes in the position of the system is:

$$đW = \mathbf{F} \cdot \mathbf{dx} = F_i\, dx_i \quad , \tag{1.8}$$

where **F** is a force vector exerted by the surroundings on the system and **dx** is the vector of infinitesimal displacement. $\bar{d}$ means this term is not necessarily an exact differential.

The rate at which work is done on the system can be expressed as below:

$$P = \frac{\bar{d}W}{dt} = \mathbf{F}\cdot \frac{d\mathbf{x}}{dt} = \mathbf{F}\cdot \mathbf{v} = F_i\, v_i \quad . \tag{1.9}$$

When this equation is applied to body $\mathcal{B}$ and the force is expressed with body force and surface traction, it takes the form of:

$$P = \int_s \mathbf{t}_{(\nu)}\cdot\, \mathbf{v}\; ds + \int_v \rho\; \mathbf{f}\cdot\mathbf{v}\; dv \quad , \tag{1.10}$$

or

$$P = \int_s \sigma_{ij}\; \nu_j\; v_i\; ds + \int_v \rho\; f_i\; v_i\; dv \; . \tag{1.11}$$

Heat, like work, is a form of energy being transferred in a thermodynamic process. However, usually heat transfer is not visible. If **q** with components q_i is heat flow entering the system, the rate of heat input is

$$\dot{Q} = - \int_s q_i\; \nu_i\; ds = - \int_v q_{i,i}\; dv \quad . \tag{1.12}$$

Beside the energy forms mentioned above, kinetic energy is another one which is often involved in a thermomechanic process. The kinetic energy K contained in body $\mathcal{B}$ is defined by:

$$K = \frac{1}{2} \int_{v} \rho \, v_i \, v_i \, dv \quad . \tag{1.13}$$

Similarly, the internal energy is expressed in the form of

$$U = \int_{v} \rho \, u \, dv \quad , \tag{1.14}$$

where u is the internal energy per unit mass of body $\mathbb{B}$.

According to the principle of conservation of energy, for the continuous medium contained in v, the time rate of kinetic energy K and internal energy U is equal to the rate of heat and the rate of work, therefore, we have:

$$\dot{K} + \dot{U} = \dot{Q} + P \quad . \tag{1.15}$$

Substituting equations (1.11) through (1.14) in equation (1.15), carrying out the indicated differentiation and using Gauss' theorem to convert the surface integrals into volume integrals, it is possible to obtain the local form of principle of conservation of energy:

$$\rho \, \dot{u} = \sigma_{ij} \, d_{ij} - q_{i,i} \quad , \tag{1.16}$$

where d_{ij} is the deformation rate tensor.

1.4 Irreversible Thermodynamics

The second law of thermodynamics postulates that any process which would reduce entropy of an isolated system is impossible to occur.

Processes which do not violate the second law can be classified as reversible and irreversible. Let us consider a process taking place within an isolated system. In what we shall call the forward direction the change in state of the system is such that the entropy increases. Then for the backward process, that is the reverse change of the state, the entropy would decrease. The backward process is therefore impossible, and the forward process is irreversible. If the entropy is unchanged, however, during the forward process, it will be unchanged during the backward process, and the process can go in either direction without violating the second law; such a process is called reversible. It can be seen that the key point of a reversible process within an isolated system is that it produces no entropy. That is what we have learnt from the classical thermodynamics. To make the theory applicable to continuum mechanics, we need to extend it with two more features. First, we should be able to count entropy in a more precise way and then to establish its evolution equation for an isolated system for any interesting process. And second, the formulation involved must be suitable for non-uniform systems, that is the theory must be of field form. These two items will be the main objectives of the theory of irreversible thermodynamics in which we are interested. Since these features are beyond the scope of classical thermodynamics some additional hypotheses have to be introduced.

The first assumption is that entropy is a function of state in irreversible processes as well as in reversible processes. Obviously, the assumption is significant for the development of irreversible thermodynamics. Its justification has been studied by Prigogine [1.45]. Having compared the results due to this assumption with those of statistical mechanics for some particular models of non-uniform gases, the author shows that the domain of validity of the assumption covers that of validity of linear phenomenological laws such as Fourier's law of heat conduction, Fick's law of mass diffusion, *etc.*

The second assumption consists of extending the second law of thermodynamics locally to every portion of a continuum, either uniform or non-uniform. It may be explained as follows. For precise accounts, it should be noticed that entropy is an extensive quantity, therefore it must be subject to a law of balance: for a given set of particles occupying a domain v the total change of entropy must be equal to the total amount of entropy transferred to these particles through the boundary plus that produced inside this domain. Referring to body $\mathcal{B}$, Fig 1.1 , we may have:

$$\frac{D}{Dt}\int_{v} \rho\ s\ dv = -\int_{s} \dot{\mathbf{S}}\cdot\mathbf{dA} + \frac{D}{Dt}\int_{v} \rho\ (s^{(i)})\ dv \quad , \tag{1.17}$$

where s is the specific entropy per unit mass, $s^{(i)}$ is the entropy source or internal entropy production per unit mass. $\dot{\mathbf{S}}$ is the entropy flow vector on the boundary . $\mathbf{dA}$ is a surface element of boundary s. Its direction is represented by the outward normal. The dot between $\dot{\mathbf{S}}$ and $\mathbf{dA}$ implies scalar product. The material derivative $\frac{D}{Dt}$ is taken with respect to a given set of particles. On transforming the first term of the right hand side into a volumetric integral, reducing the material derivative of an integral, realizing that domain v is arbitrary and using the continuity condition of entropy we are able to obtain the following equation:

$$\rho \frac{Ds}{Dt} = - \operatorname{div} \dot{\mathbf{S}} + \rho \frac{Ds^{(i)}}{Dt} , \tag{1.18}$$

or

$$\frac{Ds^{(i)}}{Dt} = \frac{Ds}{Dt} + \operatorname{div} \dot{s} , \tag{1.19}$$

where

$$\dot{\mathbf{S}} = \rho \dot{s} = \frac{\mathbf{q}}{\theta} , \tag{1.20}$$

in which $\mathbf{q}$ is the heat flow vector, and θ is the local absolute temperature.

Equation (1.18) or (1.19) serves as the relation among total entropy rate, entropy flow due to heat conduction and internal entropy production which is essentially related to the second law of thermodynamics. The law may be stated as follows:

$$\frac{Ds^{(i)}}{Dt} = 0 \quad \text{corresponding to reversible processes;} \tag{1.21a}$$

$$\frac{Ds^{(i)}}{Dt} > 0 \quad \text{corresponding to irreversible processes;} \tag{1.21b}$$

$$\frac{Ds^{(i)}}{Dt} < 0 \quad \text{never occurs in nature.} \tag{1.21c}$$

Combining equation (1.21b) with equations (1.19) and (1.20) generates the Clausius-Duhem inequality:

$$\theta \frac{Ds}{Dt} > \frac{1}{\rho} \frac{g_i}{\theta} q_i - \frac{1}{\rho} q_{i,i} , \tag{1.22}$$

where $g_i = \theta_{,i}$. (1.23)

CHAPTER 2

BACKGROUND OF PLASTIC WAVE PROPAGATION

2.1 Historical Background

Studying plastic waves in solids has had an unusually controversial history concerning whether the geometry, loading, boundary and initial conditions could be precisely defined. However, one of the most controversial topics has been around the velocity of wave front since 1951 when Bell did his experiments on incremental wave propagation in plastically prestressed rods of mild steel [2.37]. The specimen rod was pulled in simple tension until yielding occurred, Then a longitudinal tensile wave was generated by dropping a sleeved ring onto the end of the rod. At the same time the longitudinal wave was recorded by strain gauges attached to the specimen rod. The significant result of these experiments was that the wave front propagated at the velocity of an elastic rod. This fact appeared to contradict the rate independent theory of plastic wave propagation in rods, developed by von Karman and Duwez [1.6], Taylor [1.2], Rakhmatulin [1.22] and White and Griffis [1.10]. According to that theory the wave front should propagate at the plastic wave speed of $c=((d\sigma/d\varepsilon)/\rho)^{1/2}$, in which $d\sigma/d\varepsilon$ is the slope of the stress-strain curve at the prestressed state, and ρ is the mass density of the rod. Such a fundamental disagreement between theory and experiment was clearly unacceptable. When many investigators tried to clear the discrepancy, Sternglass and Stuwart [2.38] repeated the experiment and obtained the same result with copper rods. Later on, some other researchers conducted the similar experiments on different materials with different designs, but all these experiments showed that the wave front velocity corresponded to the elastic wave.

As the experiments were accepted to be well-founded, efforts were directed towards re-examination of the theory. Several researchers, *e.g.* Craggs [2.48] and Hill [2.49], considered plane plastic wave propagation as a better explanation. In their researches, the strain rate independent theories based on the commonly used form of plasticity constitutive equations were still used. The result obtained showed that under plane plastic wave consideration, there were three wave speeds of propagation involved, and the fastest one was lying between the elastic shear wave and elastic longitudinal wave speed. Based upon the result, there was speculation that elastic wave speed was observed in experiments because three-dimensional effect was neglected in a one dimensional rod. However, when a better numerical solution for plane strain case was obtained by Clifton [2.39] and an approximate axi-symmetric solution obtained by Hunter and Johnson [2.40], the explanation from three-dimensional theory became doubtful. The newer result showed that the theoretical disturbance which could propagate at elastic speeds would be too small to be observed as wave front at the experiment. It was more clear when torsion case was re-examined, where the wave front propagated also at an elastic wave speed but no three-dimensional effect included. Thus a broad agreement formed that three-dimensional effect was not, at least, the main reason for wave front of incremental disturbance propagated at elastic speed through a pre-stressed region.

Soklovsky [2.41] and Malvern [2.42] introduced a one-dimensional plasticity wave theory which included the part of rate dependent strain. The theory was based upon the assumption that when a load is applied to a crystalline solid, the instantaneous response is elastic, then inelastic process begins, mainly by the glide motion of dislocation, and plastic deformation occurs. Because the instantaneous response is elastic, the incremental wave propagates at elastic speed.

Although there were some other interpretations for Bell's tests, the following conclusion is broadly acceptable that rate dependent theory of plasticity does include the feature of instantaneous elastic response, which is consistent with the experimental observation that in a plastically prestressed rod the wave front of an incremental disturbance propagates with elastic speed.

The model of wave propagation in a plastic material consists of balances of momentum and energy, compatibility, heat conduction, and the most active of all, the constitutive relation between stress and strain. In classical elasticity this relation is described with two Lamé constants which are sufficient to set up the law. In plasticity, however, two constants are far from enough to completely describe the features of stress-strain relation. As a matter of fact, a lot of varieties of constitutive laws have fully been evolved by diiffenrent research workers [2.12], [2.15], [2.23], [2.17], [2.19] *etc.* Because of the variety and the directness of its influence on the analytical results, controversy on plastic wave propagation had concentrated on the nature of the constitutive law from the very beginning (see, *e.g.* Cristescu and Suliciu [4.1]). This fact tells us how important is the development of plasticity constitutive theory to the problem of plastic wave propagation.

Although criterion for the yielding of plastic solid such as soil was suggested by Coulomb in 1773. It was not considered to be a significant investigation concerning metal deformation. The plasticity theory as a scientific study may be justly regarded as beginning in 1864, when Tresca published his experiments on punching and extrusion and stated that a metal yielded plastically when the maximum shear stress reached a certain value. For the first time he realized that initiation of plastic deformation was governed primarily by shear stress.

Tresca's yield criterion was utilized by Saint-Venant to determine the stress distribution in a cylinder of perfectly plastic material. Then Lévy adopted the idea of perfectly plastic material from Saint-Venant to establish three dimensional relations between stress and strain rate.

After a long period of time , early this century von Mises proposed another yield criterion on the basis of mathematical consideration. It was interpreted afterwards by Hencky as that yield occurred when the elastic shear strain energy attained a critical value. Von Mises also independently proposed equations similar to Lévy's. The Lévy-Mises theory is sometimes regarded as "flow rule".

During the time period between the two world wars some important advances were made by German researchers. While Prandtl and Reuss made allowance for the elastic components of strain to be included, Schmidt and Odquist showed how work-hardening could be brought into the framework of Lévy-Mises' stress-strain relations. Besides, at about the same time Hencky proposed a rival plasticity theory which was analytically convenient for the problems where plastic strain was small. Hencky's equations lead to approximately correct result only for simple loading paths; sometimes it is regarded as "deformation theory".

After more than a century's efforts, all the contributors working in the area of classical plasticity, typically represented by Lévy-Mises' theory, seem to have laid its foundation. However, up to the present time, for each specific subject in plasticity, confusion seems no less than understanding. While too many questions are contrasted with too few answers, there seems still a long way to go before being able to say it is a well developed branch of solid mechanics.

The backward situation is basically due to the complicated features of plastic deformation process.

It is understandable if we say that physical non-linearity is an impediment to the progress of plasticity theory. With this inconvenience even when Hencky's "simple" theory is employed, the solutions for practically interesting problems are still limited. The main difficulty brought to us by non-linearity is that it makes the well-established mathematically linear theory of analysis lose its power. Even for solving a pretty simple problem we probably have to take numerical procedure, which, in many cases, would diminish our field of vision.

Another feature of non-linearity relates to large deformation which is sometimes called geometrical non-linearity. Since plastic deformation of metals can be notably large, to solve such a problem one has to use the geometrical relations based on finite displacement consideration, which surely makes any practically interesting problem even harder to be solved.

One of the important characteristics of plastic deformation is its irreversibility. In classical thermodynamics, while a process is under study, it is assumed that if the process is very slow it can be treated as a reversible process. Unfortunately, this hypothesis does not hold for a plastic deformation process. No matter how slow it is, plastic deformation is definitely irreversible. It may be said that plastic deformation is an inherently irreversible process. The irreversibility endows the material with a memory of the whole history it has experienced, and therefore makes the plastic deformation path-dependent. At least up to now, no successful modelling has been achieved to clearly describe the dependency. As a result, it is difficult to comprehend under what circumstances the simpler "deformation theory" would just reach the limit of the domain of its applicability.

To treat such inherently irreversible processes the theory of irreversible thermodynamics has to be utilized. As mentioned in Chapter 1, unlike classical thermodynamics in which uniform systems are studied, combined with continuum mechanics the irreversible thermodynamics deals with a continuous field, therefore sometimes it is called field theory of irreversible thermodynamics. This theory had not been well-established until the 50′s or 60′s of this century, thus it was impossible to utilize the theory of irreversible thermodynamics solving plasticity problems before that age.

Plastic deformation results in strain hardening. The concept was introduced into Lévy-von Mises′ theory in the 30′s. But not until the material science acquired enough knowledge, was it possible for scientists to comprehend its mechanisms. The up-to-date theory of material science has revealed the connection between hardening and micro structure movements of metallic materials. Nevertheless, a realistic model relating various variations of micro scale to macro-hardening still remains open.

The deformation-induced heat further complicates the nature of the problem. As a result the heat causes temperature and therefore stress re-distribution, deteriorates mechanical behavior or even bring about phase movement of a metallic material. For this complexity it is not surprising that the research in plastic deformation-induced heat is decades behind plasticity itself.

With all these difficulties comes today's plasticity. Looking back on it we feel some aspects concerning the advance are still worth notice: despite the theory itself keeps on being improved, the research methodology adopted has experienced a notable evolution. While Tresca worked out his yield criteria based on the experimental results, von Mises, Plandtl, Reuss and others employed mathematical techniques for improving the theory. Today's plasticity, consisting of relations of stress and strain, expression of dissipative energy, influence of micro scale variation on hardening *etc.* has become a system. Any amendment motivated either by experimental results or mathematical consideration in one aspect may alter its other features, therefore the methodology of continuum mechanics must be used to assure the consistency inside the whole system and no contradiction with fundamental laws.

2.2 Review of the Related Literature of Thermoplasticity

It is known from the preceding section that plastic deformation is a very complex process. The main feature of the process is its irreversibility, which always keeps company with energy dissipation. For such a complicated thermodynamic process any attempt to describe every detail with perfectness is not possible. From the published literature it is seen that different aspects have been considered important and worth study by different authors, and differences of their backgrounds and brand of era result in different methodology to be used. For instance, in studying constitutive theory of so-called Maxwellian materials, Nunziato and Drumheller [2.25] started their formulation with assuming the type of stress-strain relation. When theories of thermodynamics, especially, Clausius-Duhem inequality is applied, the restricting conditions which the constitutive model must observe are obtained. It is interesting that the authors have shown when the equilibrium state is considered both stress and temperature can be directly obtained from internal energy function.

In addition to stress-strain relation assumed to be in differential forms, the assumed law can also be in an integral form [2.6], [2.26], wherein there is a hypothesis that the entire history of the independent constitutive variables influence the constitutive response aspect of the material in a principle like fading memory. This kind of treatment has been very successful in obtaining some important results in viscoelasticity [2.50]. However, when non-linear kernels are involved as in the case of viscoplasticity the situation will be quite different and it is hard to expect the method to be so fruitful as it has been in the linear case.

The two methods mentioned above start with assumed stress-strain relations and then utilize the theory of irreversible thermodynamics to pursue the desired results. Another feasible procedure is quite different. First, it recognizes the deformation is an irreversible thermodynamic process, then independent and internal state variables, which characterize the process, and related thermodynamics functionals are prescribed. Application of fundamental thermodynamics theory to the system leads to the desired constitutive relations.

It seems not enough to regard the method of assuming thermodynamic functionals just as an inverse of that assuming the type of stress-strain relation. As a matter of fact the former has some notable advantages compared with its rival. When it is used, more or less, the research work of constitutive law of thermoplasticity becomes a systematic job, and the resulted relations are ensured to be self-consistent. Because of these features it has been adopted by a great number of authors since the 60′s when the theory of irreversible thermodynamics became popular.

No matter which one is chosen and employed to establish the constitutive relations for a thermoplastic deformation process, the obtained results must be subject to re-examination. They should not contradict the conclusions which have proved to be valid. When they are introduced in a plastic wave propagation problem the output should be physically reasonable.

To study a system with irreversible thermodynamics requires choosing a set of variables to characterize the system. Some of these variables have appeared in classical thermodynamics, and the others are introduced for a closer examination. The variables characterizing the internal state of the system are called internal state variables, or simply, internal variables. The concept of internal state variables may date back to half century ago when Onsager published his conspicuous articles [3.32], [3.33]. Since then, quite a few of works have been followed by Eckart [2.33], Biot [2.28], Ziegler [2.32] and Schapery *et al.* [2.16]. However, among those authors Coleman and Gurtin [2.5] seem to be the first who laid a solid foundation for studying thermoplastic behavior of materials with the concept of internal state variables. Their article has been cited repeatedly by different writers.

Since the 60's of this century, a great number of works about plastic deformation behavior of materials employing the theory of irreversible thermodynamics have been undertaken. It is impossible to make an overall review within few lines, but only those which are directly related to our interest will be discussed below.

First, we would like to mention the works of Kratochvil and Dillon [2.12], [2.19]. Therein the authors constructed analysis framework for plastic behavior of materials, using Coleman-Gurtin's theory. Rate-dependent phenomenon was studied and the internal state variables were considered to be the average quantities of micro structural re-arrangement. Thermodynamics functional such as free energy was examined, but no explicit expression was given.

In early 1970's Rice [2.15], [1.17] presented his framework combining continuum mechanics and irreversible thermodynamics for establishing constitutive relations concerning plastic deformation. In these works emphasis was given to the connection between macroscopic deformation mechanisms and micro scale re-arrangement of metallic materials. Although the author believed that many other mechanisms like diffusion, phase changes could be treated in the same manner, the main concern was the deformation caused by slip mechanism. In these articles no detail of expressions of the leading thermodynamics functionals was mentioned.

While many researchers built their frameworks of theory on the normality principle, Lehman [2.23] argued that revision of stress-strain relation based on normality was necessary, if the loading path was much different from the proportional. With this idea, not only was plastic deformation as global process, but also the generation, re-distribution of lattice defects were considered.

Although a great number of writers assuming thermodynamics functionals as a start point have used normality principle, the works about the theory itself are rarely reported. Ziegler [3.34], Ziegler and Wehrli [3.17] have presented a normality framework, in which according to the authors' opinion, the theory can be utilized to construct constitutive equations of heat conduction, thermoelasticity, gases, visco-liquids and isothermal plasticity. Actually, being compared with other works regarding normality and its application, this one built strictly from the field theory of thermodynamics shows its remarkable consistency. The addition of the dissipation functional therein is never superfluous, but makes designation of phenomenological relation between stress and strain more versatile.

Nevertheless, the theory has not been used widely by the researchers in the related area. This may be due to the fact that it does not include thermal effects in plastic deformation process. It is well known that a distinguishing feature of plastic deformation as an irreversible process is that a part of plastic work becomes heat energy and is dissipated. Having failed to account for thermal effects means neglecting one of the fundamental features of plastic deformation process and would lower the value of the theory.

Another point worth noting is that since the 60's many researchers in this area have been working for establishing the relations between micro structure rearrangements and macro plastic behaviour of metallic materials. In their works the concept adopted from science of materials has been used in the constitutive theories of plastic deformation, *e.g.* Gilman [1.46], Kratochvil [2.12], [2.19], [2.20], Rice [2.15], Perzyna [2.34], Lehman [2.9] *et al.* Through these studies it is believed that the generation, motion and interaction of dislocations of metallic materials is the most important factor among the micro structure re-arrangements which contribute to strain hardening properties of the materials. Unfortunately, the evolution aspect of strain hardening property is not included in Ziegler's framework. It seems that the main concern there is about the strictness of normality and its widespread applications.

Since more work to be done is related to the normality, we feel it necessary to give an outline below.

2.3 Outline of Normality Theory

A thermodynamic state of a point of continuum can generally be described by a set of independent variables ε_{ij} and temperature θ. If the deformation process, however, is irreversible, or entropy productive, more additional variables may be needed to describe the state. In that case we can introduce an additional set of variables into the problem which is under consideration to characterize different states of the continuum. The variables so introduced are generally related to the internal state of the continuum. They are denoted by α_{ij} in the following derivation.

Combining equations of energy conservation (1.16) and entropy production (1.19), (1.20), the following equation is obtained:

$$\rho(\dot{u} - \theta\,\dot{s}) = \sigma_{ij}\dot{\varepsilon}_{ij} - \frac{\theta,_i}{\theta} q_i - \rho\,\theta\cdot\dot{s}^{(i)} \quad . \tag{2.1}$$

If a function which is called free energy function is defined as:

$$\psi = u - \theta s \quad , \tag{2.2}$$

equation (2.1) takes the form of

$$\rho \left(\frac{\partial \psi}{\partial \varepsilon_{ij}}\right) \dot{\varepsilon}_{ij} + \rho \left(\frac{\partial \psi}{\partial \alpha_{ij}}\right) \dot{\alpha}_{ij} = \sigma_{ij} \dot{\varepsilon}_{ij} - \frac{\theta_{,i}}{\theta} q_i - \rho \theta \dot{s}^{(i)} . \tag{2.3}$$

Now that the stress tensor may be obtained from the following equation:

$$\sigma_{ij} = \rho \frac{\partial \psi}{\partial \varepsilon_{ij}} \quad . \tag{2.4}$$

The internal thermodynamic force tensor can be decomposed into quasi-conservative and dissipative parts as below:

$$\beta_{ij} = \beta_{ij}^{(q)} + \beta_{ij}^{(d)} \quad , \tag{2.5}$$

where by definition, the quasi-conservative part is

$$\beta_{ij}^{(q)} = \rho \frac{\partial \psi}{\partial \alpha_{ij}} \quad , \tag{2.6}$$

and $\beta_{ij}^{(d)}$ is the dissipative part. For the reason that β_{ij} do not show up in the energy equation (1.17) explicitly, the total β_{ij} should vanish:

$$\beta_{ij}^{(q)} + \beta_{ij}^{(d)} = 0 \quad . \tag{2.7}$$

Substituting equation (2.4) through (2.7) in equation (2.3) yields:

$$\beta_{ij}^{(d)}\dot{\alpha}_{ij} - \left(\frac{\theta_{,i}}{\theta}\right) q_i = \rho\, \theta\, \dot{s}^{(i)} = \rho\, \phi \quad , \tag{2.8}$$

where

$$\phi = \theta\, \dot{s}^{(i)} \quad , \tag{2.9}$$

is the specific dissipation function. According to the second law of thermodynamics ϕ can never be negative.

If we consider ρ, the material density a constant as in most cases of solid mechanics, the free energy and dissipation rate of unit volume can be expressed as:

$$\Psi = \rho\, \psi \quad , \tag{2.10}$$

$$\Phi = \rho\, \phi \quad . \tag{2.11}$$

Then equation (2.8) can be written as:

$$\Phi = \beta_{ij}^{(d)}\, \dot{\alpha}_{ij} - \left(\frac{\theta_{,i}}{\theta}\right) q_i \quad . \tag{2.12}$$

Again, the second law asserts that

$$\Phi \geq 0 \quad . \tag{2.13}$$

If it is assumed that the dissipation function is only dependent on the "velocities" as it appears in equation (2.12), having $\dot{\alpha}_k$ stand for $\dot{\alpha}_{ij}$ (conjugate with $\beta_{ij}^{(d)}$), q_i (conjugate with $-\frac{\theta,i}{\theta}$), where k runs from 1 to 9, and $F_k^{(d)}$ stand for the corresponding dissipative force, equation (2.12) can be written as

$$\Phi = F_k^{(d)} \dot{\alpha}_k \quad . \tag{2.14}$$

Furthermore, if Φ is a given single-valued differentiable function in the velocity space, then equation (2.14) has a unique solution for $F_k^{(d)}$, which is:

$$F_k^{(d)} = \nu \frac{\partial \Phi}{\partial \dot{\alpha}_k} \quad , \tag{2.15}$$

where

$$\nu = \Phi \left(\frac{\partial \Phi}{\partial \dot{\alpha}_m} \dot{\alpha}_m\right)^{-1} \quad . \tag{2.16}$$

And the normality asserts that

$$\dot{\alpha}_k > 0 \quad , \tag{2.17}$$

$$F_k^{(d)} > 0 \quad , \tag{2.18}$$

$$\frac{\partial \Phi}{\partial \dot{\alpha}_k} > 0 \quad . \tag{2.19}$$

The surface Φ ($\dot{\alpha}_k$) = constant is star-shaped and convex in the velocity space.

The duality is also true, if the dissipation function is given in the force space as following

$$\Phi' = \dot{\alpha}_k \, \dot{F}_k^{(d)} \quad , \tag{2.20}$$

then the solution is unique as

$$\dot{\alpha}_k = \nu' \frac{\partial \Phi' (F_i^{(d)})}{\partial F_k^{(d)}} \quad , \tag{2.21}$$

where

$$\nu' = \Phi' (\frac{\partial \Phi'}{\partial F_m^{(d)}} F_m^{(d)})^{-1} \quad , \tag{2.22}$$

And similarly

$$\dot{\alpha}_k > 0 \quad , \tag{2.17}$$

$$F_k^{(d)} > 0 \quad , \tag{2.18}$$

$$\frac{\partial \Phi'}{\partial F_k^{(d)}} > 0 \quad . \tag{2.23}$$

2.4 Objectives of This Research

When a solid body deforms elastically, its temperature may go up or down instantly, depending upon whether it is compressed or dilated. Since there is no energy dissipated, the process is said to be reversible. As loading is increased the body will deform plastically, and it is found that the plastic deformation is a typically irreversible process. No theory of classical plasticity yet, either Lévy-Mises-Reuss' flow rule or Hencky's deformation theory takes into account the dissipated heat energy. The classical plasticity seems independent of thermodynamics.

The combination of continuum mechanics with thermodynamics yields the field theory of thermodynamics, or continuum thermodynamics. With this theory it is possible to consider quantitatively the dissipated heat energy induced from plastic deformation process. The theoretical analysis shows that plastic deformation always accompanies temperature rising. Unfortunately, this important fact has not been strictly introduced into the theory of normality to construct a consistent framework, therefore, the first objective of this research is to extend the fundamental theory of normality which is based on isothermal plasticity regime to that based on thermoplasticity, and then employing the developed framework to study the constitutive relations of different metallic materials.

Studying plastic wave propagation or dynamics of thermo-plasticity, in which balance of momentum, conservation of energy, compatibility of deformation, heat conduction and constitutive relation of stress and strain are involved, is another objective of this research. The obtained constitutive equations will be examined with dynamic modeling environment, and at the same time, the important phenomena of plastic wave propagation in one-dimensional system will be investigated in detail.

For comparison, two numerical methods of integration, namely characteristics and finite difference, will be employed to obtain the solutions of the concerned problem.

2.5 Organization of the Dissertation

This dissertation consists of six chapters. Chapter 1 introduces the field theory of thermodynamics, including the law of energy conservation and the second law of irreversible thermodynamics. These theories are utilized in the development of our constitutive equations.

In Chapter 2, the background of plastic wave propagation is discussed. The literature related to our subject is reviewed. Besides, an outline of Ziegler's normality theory is presented.

Chapter 3 deals with the theoretical development of this research. The restriction imposed on Helmholtz free energy function and the relation between free energy function and dissipation function are derived. A theorem concerning the leading thermodynamics function is justified. Then the developed theory is used to study the constitutive relations of thermoplasticity for two kinds of metallic materials. The obtained results for mild steel are applied to the plastic wave propagation problem presented in the next chapter.

In Chapter 4, the problem of plastic wave propagation in a semi-infinite rod is studied. The system of the equations governing the problem and the associated characteristics analysis are presented. Then the jump conditions are given at the end of the chapter.

In Chapter 5, the computational algorithms solving the system of equations are introduced. Two integration methods are considered. One is the characteristics method, and the other is the two-sub-step finite difference method. Since the computational procedure for interior grid points is different from that for boundary grid points both methods are treated differently at interior and boundary points.

In Chapter 6, the information about boundary and initial conditions is given, and the numerical results are presented and discussed. The main body of the dissertation concludes with Chapter 6, where the conclusions of this research and recommendation for further work are addressed.

CHAPTER 3

DEVELOPMENT OF CONSTITUTIVE THEORY OF THERMOPLASTICITY

3.1 The Restriction Imposed on Helmholtz Free Energy Function

Before further discussion on our subject we need to determine the state variables which are employed in the analysis. Since the selection of the variables has some arbitrariness, at the beginning we will do it with a broad point of view. As modeling is further developed more specification of independent state variables may become necessary and natural.

To make it distinct let us divide the independent variables into two groups. One of them consists of internal state variables, which characterize the variation happening inside the material and are closely connected to dissipation process. The other is used to describe the state of the material and consists of free state variables. Following Coleman and Gurtin [2.5], and Ziegler *et al.* [3.17] we choose ε, θ and $\mathbf{g}$ as independent variables, where ε is the total strain tensor, θ is the absolute temperature of the system, and $\mathbf{g}$ is the gradient of the temperature. In addition, $\alpha_{(i)}$ are used to denote a set of internal variables.

As soon as the independent variables have been selected, the fundamental leading thermodynamics functions Ψ and Φ, which are free energy and dissipation function respectively, may be expressed as function of the independent variables. It should be pointed out that the "independent" variables themselves are functions of spatial coordinates and time, actually, they are "dependent" variables, therefore, the fundamental functions should be called functionals.

However, for simplicity, we still call them functions, and the free energy function can be written as

$$\Psi = \Psi \, (\varepsilon_{ij}, \, \theta, \, g_i, \, \alpha_i) \quad . \tag{3.1}$$

By the definition of the free energy which is

$$\Psi = U - S \, \theta \quad , \tag{3.2}$$

and equation (1.16) which represents the principle of energy conservation or the first law of thermodynamics, the following equation can be readily obtained:

$$\dot{\Psi} + S \, \dot{\theta} + \theta \, \dot{S} = \sigma_{ij} \, \dot{\varepsilon}_{ij} - q_{i,i} \tag{3.3}$$

where S is entropy, σ_{ij} is stress tensor, and $\mathbf{q}$ is heat flow. Equation (3.3) expresses the requirement of energy conservation. Besides, a thermodynamic process is possible to occur only if it meets the restriction imposed by the second law, which is expressible by Clausius-Duhem inequality (1.22). With $S = \rho \cdot s$ it takes the following form:

$$\theta \, \dot{S} > \frac{g_i}{\theta} \, q_i - \frac{\partial q_i}{\partial x_i} \quad . \tag{3.4}$$

Substituting (3.4) in (3.3) we obtain

$$\dot{\Psi} + S \, \dot{\theta} - \sigma_{ij} \, \dot{\varepsilon}_{ij} + \frac{g_i}{\theta} \, q_i < 0 \quad . \tag{3.5}$$

Assuming the free energy function expressed in (3.1) is differentiable with respect to its arguments, we have

$$\dot{\Psi} = \frac{\partial \Psi}{\partial \varepsilon_{ij}} \dot{\varepsilon}_{ij} + \frac{\partial \Psi}{\partial \theta} \dot{\theta} + \frac{\partial \Psi}{\partial g_i} \dot{g}_i + \frac{\partial \Psi}{\partial \alpha_i} \dot{\alpha}_i \quad . \tag{3.6}$$

Combining (3.5) and (3.6) yields

$$\left(\frac{\partial \Psi}{\partial \varepsilon_{ij}} - \sigma_{ij} \right) \dot{\varepsilon}_{ij} + \left(\frac{\partial \Psi}{\partial \theta} + S \right) \dot{\theta}$$

$$+ \frac{\partial \Psi}{\partial \alpha_i} \dot{\alpha}_i + \frac{\partial \Psi}{\partial g_i} \dot{g}_i + \frac{g_i}{\theta} q_i < 0 \quad . \tag{3.7}$$

According to the second law of thermodynamics inequality (3.7) holds for any deformation process, where $\dot{\varepsilon}_{ij}$, $\dot{\theta}$, $\dot{g}_i$ could vary independently. For (3.7) to be valid we must have:

$$\sigma_{ij} = \frac{\partial \Psi}{\partial \varepsilon_{ij}} \quad , \tag{3.8}$$

$$S = - \frac{\partial \Psi}{\partial \theta} \quad , \tag{3.9}$$

$$\frac{\partial \Psi}{\partial g_i} = 0 \quad , \tag{3.10}$$

where (3.10) implies that Ψ is a function independent of **g**. With equations (3.8) through (3.10) being valid inequality (3.7) becomes

$$\frac{\partial \Psi}{\partial \alpha_i} \dot{\alpha}_i + \frac{g_i}{\theta} q_i < 0 \quad . \tag{3.11}$$

Assuming that validity of the law of heat conduction is independent of the changes of internal state variables we have:

$$\frac{g_i}{\theta} q_i < 0 \quad , \tag{3.12}$$

Inequality (3.12) asserts that for a real process which can occur in nature, the gradient of temperature and the heat flow always have opposite signs. In other words, as is well known the heat energy is always transferred in the direction from the higher temperature to the lower.

Then from independence of heat conduction and internal state variables we obtain:

$$\frac{\partial \Psi}{\partial \alpha_i} \dot{\alpha}_i < 0 \quad . \tag{3.13}$$

Although inequality (3.11) has been obtained elsewhere such as [4.6], the deduction (3.13) and the important fact behind it have been neglected. As a result, errors may be brought into the expression of the free energy function.

For simplicity, the signs of the internal variables are so defined that α_i are positive and during an irreversible thermodynamic process $\dot{\alpha}_i$ are greater than zero [3.34]. This requirement can be easily satisfied when a monotonic process is considered. If a process is non-monotonic, however, the characteristic physical quantity may change its sign during the whole process. In such circumstances the whole process should be divided into several sub-processes. Each of them is monotonic and may be considered as an independent thermodynamic process, for which the above mentioned requirement is satisfied.

The combination of (3.13) and (2.17) yields the following inequality and theorem.

$$\frac{\partial \Psi}{\partial \alpha_i} < 0 \quad . \tag{3.14}$$

Theorem 3.1: The free energy function is a decreasing function of the internal state variables.

When the irreversibilities of thermodynamic processes are examined, an essential question may arise: does the irreversibility diminish the free energy in the system? Theorem 3.1 answers the question in the affirmative and implies the free energy contained in the real system is less than that in the system which were with "less" or "no" irreversibility.

As a simple example we may consider a bar subject to tension. Let us assume the selected independent variables to characterize the system are temperature, total strain and an internal state variable which is plastic strain. For such a system when the total strain is fixed, the case with more plastic strain will contain less free energy. In other words, when total strain is constant, the case with more plastic strain recovers less strain energy when the system is unloaded.

3.2 Effects of Temperature

From the discussion in Chapter 2 it is seen that the theory of plasticity is still in its developing stage. In order to do some research work in that area we have to assign some limitation to ourselves. In the following discussion it is assumed again that the material is plastically incompressible; Baushinger effect is ignored; the change of temperature would not cause the processes such as phase change, recovering *etc.* to occur.

Generally speaking, increasing temperature has several effects on the system. First of all, the higher temperature directly increases the internal energy of the system. Second, it changes the mechanical properties of the material, and third, it causes re-distribution of strain and stress field. Hereinafter, we will concentrate our attention to the last issue.

Our discussion will eventually take into account thermoplastic effects, however, for a better understanding we will start our discussion with a thermoelastic case.

It is well known that if a solid body, subjected to a uniform temperature increase, can expand freely, there will be no stress developed inside. If, however, the temperature increase is non-uniform or the expansion is restrained, stresses and corresponding strains will be developed inside the body. For further development the strains concerned are distinctly defined as follows.

Definition: The strain developed independently of stress is called free strain, and *that developed due to stress is called constrained strain.*

With this definition we can see that if a body subjected to a uniform temperature increase can expand freely, there is only free strain existing; however, if the temperature is not uniform or the expansion is restrained, there will be both free and restrained strains existing. In other words, the effect of temperature generates both free expansion and stressed strain which co-exists with stress developed inside the body. The stress so developed, depending upon the selected coordinate system, can be normal or shear or both normal and shear stress. This simply means that temperature rising can develop shear stress and constrained shear strain inside the solid body even when it is isotropic. This is the basic picture concerning thermoelasticity. However, an important fact which should be noticed is that the effect of temperature never produces "free distortion strain" inside an isotropic body.

Now let us examine the construction of free energy function for a linearly isotropic body. From thermoelasticity point of view two state parameters are decisive, which are temperature and elastic strain. By all possible combinations the free energy function would have the form as follows:

$$\Psi = \Psi_1(\theta) + \Psi_2(\varepsilon) + \Psi_3(\varepsilon, \theta) \quad , \tag{3.15}$$

where $\Psi_1(\theta)$ is corresponding to thermal internal energy of the system. It is related to temperature changes only. $\Psi_2(\varepsilon)$ is the strain energy corresponding to the stressed strains due to both loading and restrained thermal expansion. $\Psi_3(\varepsilon,\theta)$, representing the coupling of temperature changes and stressed strain is our main concern. Physically, this coupling means the work done by the stress tensor during thermal free expansion, or in the words of the definition, it is the strain energy of stress tensor and free strain. Since temperature changes produce no free distortion strain, Ψ_3 is only related to dilatation part of the stress tensor and thermal free expansion. It can be shown that

$$\Psi_3 = -(3\lambda + 2\mu)\, \varepsilon_{(1)}\, k\, (\theta - \theta_R) \quad . \tag{3.16}$$

This fact may be explained in a different way. Physically, it can be said that a deviatoric stress tensor does no work during a thermal free expansion, or mathematically, the inner product of a deviatoric stress and another tensor of free dilatation strain is zero. Thus we may state as below:

Statement: For an isotropic body there is no explicit coupling between temperature change and distortion in the evaluation of strain energy.

After examining the coupling effect between distortion and temperature change in the elastic range we are ready to study the same problem in thermoplasticity. It has been noticed since the very beginning that distortion plays a major role in plasticity. Tresca first found that shearing caused plastic yield. Then the theory developed by Lévy and Mises confirmed that plastic deformation was governed by the relationship between deviatoric stresses and the increments of distortion strains. All of this means plastic deformation is of distortion in nature. As we already know in the elastic range, the free thermal expansion directly contributes to dilatation. By the same reasoning we can conclude that for a plastically incompressible isotropic material, temperature changes generate no "free plastic strain", and finally, the following statement is justified.

Statement: For evaluation of the energy, there is no explicit coupling between temperature change and plastic deformation.

The statement is significant for evaluating the free energy and dissipative energy. In constituting the two leading functions, which are free energy function and dissipation function, it suggests that there be no explicit coupling terms appearing in their expressions.

3.3 Selection of Internal State Variable

As we have noticed, plastic deformation of a metallic material is a complicated process in which many microscopic mechanisms, such as twinning, void growth, and dislocation *etc.* may be involved. If our knowledge of material science enabled us to comprehend the evolution law of every such mechanism and the combination relation of its contribution to the free energy and dissipation functions, a great number of internal state variables would be used to specify the effect of each mechanism individually. However, if some of them remain, at least at the time being, obscure, a smaller number of internal state variables will be employed and only the major concerned factors or their comprehensive influence will be considered. Thus, the number of internal state variables selected shows how much we know the system and indicates the degree of freedom with which the thermoplastic system is examined.

As soon as the number of internal state variables has been determined, we are faced with the problem of selecting the physical variables which are to be considered as basic unknowns. For instance, let us assume the strain is under consideration. The total strain can be divided into two parts: the elastic part and the plastic part, and . is the sum of the two parts so long as the small deformation is considered. Then, in order to describe the deformation state we may either choose elastic and plastic strains or plastic and total strains as independent variables.

One of the important features concerning plastic deformation of metallic materials is the strain hardening effect. If thermoplasticity can be successfully applied to engineering problems with the sophisticated continuum mechanics theories and as many as possible micro structure features included, the hardening effect should be within the scope of our examination. As for answering the question whether hardening should be chosen as an internal state variable deliberation is necessary to make the system of equations to be consistent.

In analyzing behaviors of elastic-viscoplastic materials Kratochvil and Dillon [3.14] employed the free energy function of following form

$$\Psi = \frac{1}{2} \mu_0 \sigma^2 + \nu \alpha - k T(\ln \frac{T}{T_R} - 1) \quad , \tag{3.17}$$

where σ is the stress, T is absolute temperature, T_R the reference temperature, μ_0, ν, k are material constants, and α is an internal state variable characterizing the defect arrangement. It is noteworthy that hardening effect was brought in by α, but plastic strain was not introduced simultaneously as another independent internal state variable.

Kim and Oden [3.6] presented the following expression for free energy function:

$$\Psi = \frac{1}{2} [\lambda \ (trE)^2 + 2 \ \mu \ tr(\underset{\sim}{E}^2)] - Z_1 W_p - \frac{1}{m} (Z_1 - Z_0)\exp(-mW_p), \qquad (3.18)$$

where λ and μ are Lame's constants of elasticity, $\underset{\sim}{E}$ is elastic strain tensor, W_p is plastic work. The same as in (3.17), the authors did not consider thermoelastic effect. Another point noteworthy is that only one internal state variable W_p has been used, while Z the hardening variable is introduced as conjugate of the plastic work.

It is believed that in above articles the authors have recognized there is only one degree of freedom in the internal state space when plastic hardening is considered, therefore introducing one internal state variable is enough. It can be either the hardening parameter or plastic work or something else. But if more than one were employed to characterize the plastic deformation system with isotropic hardening, the introduced state variables would not be independent of each other, therefore erroneous conclusion would result.

Moreover, it is clear from these two expressions that the gradient of temperature is not an argument of the free energy function; it only appears in the equation of heat conduction.

With these considerations, the variables adopted as independent in this research work are ε, ε_p and θ. Here ε stands for the total strain tensor, ε_p the plastic strain tensor and θ absolute temperature.

3.4 Constitutive Relations of Thermoplasticity

3.4.1 The Free Energy Function

According to the theory of normality the constitutive equations are derived from free energy function Ψ and dissipation function

Φ. The free energy function Ψ is, generally, a function of the basic independent variables ε_{ij}, $\varepsilon_{ij}^{(p)}$ and θ. It can be expressed in the following form:

$$\Psi = \Psi\ (\varepsilon_{ij},\ \varepsilon_{ij}^{(p)},\ \theta) \tag{3.19}$$

For a better approximation of limited-term expansion of Taylor series, the independent variables may be equivalently substituted with $\varepsilon_{ij}^{(e)}$, the elastic part of strain, $\varepsilon_{ij}^{(p)}$, the plastic part of strain and θ, the temperature. In so doing we have the free energy function Ψ as follows:

$$\Psi = \Psi\ (\varepsilon_{ij}^{(e)},\ \varepsilon_{ij}^{(p)},\ \theta)\ . \tag{3.20}$$

If the material is assumed to be isotropic, the free energy function Ψ will be a function of $\varepsilon_{(1)}^{(e)}$, $\varepsilon_{(2)}^{(e)}$, $\varepsilon_{(3)}^{(e)}$, $\varepsilon_{(1)}^{(p)}$, $\varepsilon_{(2)}^{(p)}$, $\varepsilon_{(3)}^{(p)}$ and θ, where the subscripts (1), (2) and (3) stands for the first, the second and the third invariants, respectively. Then Ψ can be re-written as

$$\Psi = \Psi\ (\varepsilon_{(1)}^{(e)},\ \varepsilon_{(2)}^{(e)},\ \varepsilon_{(3)}^{(e)},\ \varepsilon_{(1)}^{(p)},\ \varepsilon_{(2)}^{(p)},\ \varepsilon_{(3)}^{(p)},\ \theta)\ . \tag{3.21}$$

Expanding Ψ into a Taylor series with respect to the reference configuration where $\varepsilon_{(1)}^{(e)}$, $\varepsilon_{(2)}^{(e)}$, $\varepsilon_{(3)}^{(e)}$, $\varepsilon_{(1)}^{(p)}$, $\varepsilon_{(2)}^{(p)}$, $\varepsilon_{(3)}^{(p)}$, and $T = \theta - \theta_R$ are zero, taking the small amount such as $\varepsilon_{(1)}^{(e)}, \ldots, \varepsilon_{(3)}^{(p)}$, or T as the increment and neglecting the terms which are higher than the second order, we obtain the following expression:

$$\Psi = \Psi_0 + \frac{\partial \Psi}{\partial \varepsilon^{(e)}_{(1)}} \varepsilon^{(e)}_{(1)} + \frac{\partial \Psi}{\partial \varepsilon^{(p)}_{(1)}} \varepsilon^{(p)}_{(1)} + \frac{\partial \Psi}{\partial \theta} T + \frac{1}{2} \frac{\partial^2 \Psi}{\partial \varepsilon^{(e)2}_{(1)}} \varepsilon^{(e)2}_{(1)}$$

$$+ \frac{1}{2} \frac{\partial^2 \Psi}{\partial \varepsilon^{(p)2}_{(1)}} \varepsilon^{(p)2}_{(1)} + \frac{1}{2} \frac{\partial^2 \Psi}{\partial \theta^2} T^2 + \frac{\partial^2 \Psi}{\partial \varepsilon^{(e)}_{(1)} \partial \varepsilon^{(p)}_{(1)}} \varepsilon^{(e)}_{(1)} \varepsilon^{(p)}_{(1)}$$

$$+ \frac{\partial^2 \Psi}{\partial \varepsilon^{(e)}_{(1)} \partial \theta} \varepsilon^{(e)}_{(1)} T + \frac{\partial \Psi}{\partial \varepsilon^{(e)}_{(2)}} \varepsilon^{(e)}_{(2)} + \frac{\partial \Psi}{\partial \varepsilon^{(p)}_{(2)}} \varepsilon^{(p)}_{(2)} . \tag{3.22}$$

In equation (3.22) if T, $\varepsilon^{(p)}_{(1)}$ and $\varepsilon^{(p)}_{(2)}$ are identically zero, Ψ degenerates to that for an elastic case:

$$\Psi = \Psi_0 + \frac{\partial \Psi}{\partial \varepsilon^{(e)}_{(1)}} \varepsilon^{(e)}_{(1)} + \frac{1}{2} \frac{\partial^2 \Psi}{\partial \varepsilon^{(e)2}_{(1)}} \varepsilon^{(e)2}_{(1)} + \frac{\partial \Psi}{\partial \varepsilon^{(e)}_{(2)}} \varepsilon^{(e)}_{(2)} . \tag{3.23}$$

For the free energy function, which is the strain energy function in an elastic case, expressed in equation (3.23) to be positive definite, its second term must vanish.

If we assume that the plastic deformation of the material is incompressible, all the terms containing $\varepsilon^{(p)}_{(1)}$ in equation (3.22) vanish. As a result we have:

$$\Psi = \Psi_0 + \frac{\partial \Psi}{\partial \theta} T + \frac{1}{2} \frac{\partial^2 \Psi}{\partial \varepsilon^{(e)2}_{(1)}} \varepsilon^{(e)2}_{(1)} + \frac{1}{2} \frac{\partial^2 \Psi}{\partial \theta^2} T^2 + \frac{\partial^2 \Psi}{\partial \varepsilon^{(e)}_{(1)} \partial \theta} \varepsilon^{(e)}_{(1)} T$$

$$+ \frac{\partial \Psi}{\partial \varepsilon^{(e)}_{(2)}} \varepsilon^{(e)}_{(2)} + \frac{\partial \Psi}{\partial \varepsilon^{(p)}_{(2)}} \varepsilon^{(p)}_{(2)} . \tag{3.24}$$

For a thermoelastic case concerned, there is no plastic term in the expression of the free energy function, and it takes the form:

$$\Psi = \Psi_0 + \frac{\partial \Psi}{\partial \theta} T + \frac{1}{2} \frac{\partial^2 \Psi}{\partial \varepsilon_{(1)}^{(e)2}} \varepsilon_{(1)}^{(e)2} + \frac{1}{2} \frac{\partial^2 \Psi}{\partial \theta^2} T^2 + \frac{\partial^2 \Psi}{\partial \varepsilon_{(1)}^{(e)} \partial \theta} \varepsilon_{(1)}^{(e)} T$$

$$+ \frac{\partial \Psi}{\partial \varepsilon_{(2)}^{(e)}} \varepsilon_{(2)}^{(e)} \tag{3.25}$$

It can be shown that if the material properties are independent of temperature, the thermoelastic free energy function assumes the following form [3.17]:

$$\Psi = \Psi_0 - S_0 T + \frac{\lambda}{2} \varepsilon_{(1)}^{(e)2} + \mu \, \varepsilon_{(2)}^{(e)} - (3\lambda + 2\mu) \, k \, \varepsilon_{(1)}^{(e)} T$$

$$- \frac{\rho c}{2\theta_R} T^2 \, . \tag{3.26}$$

The comparison of (3.23) with (3.26) yields the following set of equations:

$$\frac{\partial \Psi}{\partial \theta} = - S = - \left(S_0 + (3\lambda + 2\mu) \, k \, \varepsilon_{(1)}^{(e)} + \frac{\rho c}{\theta_R} T \right) \tag{3.27}$$

$$\frac{\partial^2 \Psi}{\partial \theta^2} = - \frac{\rho c}{\theta_R} \, , \tag{3.28}$$

$$\frac{\partial^2 \Psi}{\partial \varepsilon_{(1)}^{(e)2}} = \lambda \, , \tag{3.29}$$

$$\frac{\partial^2 \Psi}{\partial \varepsilon_{(1)}^{(e)} \partial \theta} = - (3\lambda + 2\mu) \, k \, , \tag{3.30}$$

$$\frac{\partial \Psi}{\partial \varepsilon_{(2)}^{(e)}} = \mu \, . \tag{3.31}$$

Setting $$\frac{\partial\Psi}{\partial\varepsilon^{(p)}_{(2)}} = H \ , \tag{3.32}$$

which is a hardening parameter, with equations (3.27) through (3.32) noticed, equation (3.24) can be written as

$$\Psi = \Psi_0 - S_0\, T + \frac{\lambda}{2}\, \varepsilon^2_{(1)} + \mu\, (\varepsilon - \varepsilon^{(p)})_{(2)} + H\, \varepsilon^{(p)}_{(2)}$$

$$- (3\lambda + 2\mu)\, k\, \varepsilon_{(1)} T - \frac{\rho c}{2\theta_R}\, T^2 \ , \tag{3.33}$$

in which ε is the total strain. Equation (3.33) is the expression of free energy function for linearly elastic and plastic strain hardening materials of non-isothermal situation.

Generally speaking, the coefficients of Taylor series in equation (3.24) are state-dependent. This fact means that both sides of equations (3.27) through (3.32) are functions of the independent variables, which are ε, $\varepsilon^{(p)}$ and θ. Actually, however, most of them but H show little change as deformation goes up, while every one apparently depends on temperature. When thermoplasticity is concerned, the dependency of properties of materials on temperature must be taken into account. Thus, the free energy function takes the following form:

$$\Psi(\theta) = \Psi_0 - S_0\, (\theta - \theta_R) + \frac{1}{2}\, \lambda(\theta)\, \varepsilon^2_{(1)} + \mu(\theta)\, (\varepsilon - \varepsilon^{(p)})_{(2)}$$

$$+ H\, (\theta, W_p)\, \varepsilon^{(p)}_{(2)} - D(\theta)\, \varepsilon_{(1)}\, (\theta - \theta_R)$$

$$- F(\theta)\, (\theta - \theta_R)^2 \ , \tag{3.34}$$

where

$$D(\theta) = (3\lambda(\theta) + 2\mu(\theta))\ k(\theta) \quad , \tag{3.35}$$

and

$$F(\theta) = \frac{1}{2\theta_R}\ \rho(\theta)\ c(\theta)\ . \tag{3.36}$$

3.4.2 The Meaning of Dissipation Function

In [3.17], Ziegler *et al.* consider the cases of thermoelasticity and isothermal plasticity. The theory of normality is used to obtain the corresponding constitutive equations. The article is certainly motivational, yet since plastic deformation irreversibly transfers some part of mechanical energy into heat, thermal effects in plasticity is inherent, therefore, we feel it essential for our research to have the free energy function include thermal effects in developing plasticity theory as it is shown in equation (3.34), from which by the field theory of thermodynamics we are able to obtain the expression of entropy function as below:

$$S = -\frac{\partial\Psi}{\partial\theta} = S_0 - \frac{1}{2}\lambda'(\theta)\ \varepsilon_{(1)}^2 - \mu'(\theta)(\varepsilon - \varepsilon^{(p)})_{(2)}$$
$$- \frac{\partial H(\theta,W_p)}{\partial\theta}\varepsilon_{(2)}^{(p)} + D'(\theta)\ \varepsilon_{(1)}(\theta - \theta_R) + D(\theta)\ \dot{\varepsilon}_{(1)}$$
$$+ F'(\theta)(\theta - \theta_R)^2 + 2\ F(\theta)(\theta - \theta_R)\ , \tag{3.37}$$

where the prime stands for derivative.

On the other hand,from equation (1.19) we have the following expression for the specific rate of entropy increase:

$$\dot{S} = \dot{S}^{(i)} - \left(\frac{q_i}{\theta}\right)_{,i} \quad , \tag{3.38}$$

which states that the rate of change of entropy consists of a reversible and an irreversible part. The reversible part is the entropy supply from the outside of the element, and the irreversible part, interpreted as an entropy production within the element, is never negative.

Equation (3.38) can be written as

$$\theta \dot{S} = \Phi + \frac{\theta_{,i}}{\theta} q_i - q_{i,i} \quad , \tag{3.39}$$

where $\Phi = \theta \dot{S}^{(i)}$ is defined as dissipation function. This function consists of two parts. One of them, Φ_1 is corresponding to mechanical irreversible process, and the other, $\Phi_2 = -\frac{\theta_{,i}}{\theta} q_i$ is due to heat conduction, therefore, equation (3.39) is simplified as

$$\theta \dot{S} = \Phi_1 - q_{i,i} \tag{3.40}$$

Recall equation (1.16), which we have for the expression of rate of change of internal energy, shown as below:

$$\dot{U} = \rho \dot{u} = \sigma_{ij} \dot{\varepsilon}_{ij} - q_{i,i} \quad . \tag{3.41}$$

Combination of equation (3.40) with equation (3.41) yields:

$$\Phi_1 = \sigma_{ij} \dot{\varepsilon}_{ij} + \theta \dot{S} - \dot{U} \, . \tag{3.42}$$

However, by the definition of free energy function we have

$$\dot{U} = \dot{\theta}\ S + \theta\ \dot{S} + \dot{\Psi}\ . \qquad (3.43)$$

Substituting equation (3.43) in (3.42) generates the interesting expression for Φ_1.

$$\Phi_1 = \sigma_{ij}\ \dot{\varepsilon}_{ij} - (\dot{\theta}\ S + \dot{\Psi})\ . \qquad (3.44)$$

As S and Ψ are related with each other by equation (3.9), our equation (3 .44) establishes a relationship between the mechanically dissipative power and the rate of change of free energy. This equation is important not only because it directly relates the two leading thermodynamic functions, but also because it can be conveniently employed to derive the plasticity constitutive equations. In other words, the equation is an alternative way other than normality for establishing the constitutive equations.

The first term on the right hand side of equation (3.44) is easily to be recognized as total mechanical power. The second term can be changed as below on the basis of equation (3.9)

$$\dot{\Psi} + S\ \dot{\theta} = (\ \dot{\Psi} - \frac{\partial\Psi}{\partial\theta}\ \dot{\theta}\ )\ , \qquad (3.45)$$

which is the rate of change of free energy due to the factors other than temperature.

As a matter of fact, from equation (3.34) the expression of the rate of change of the free energy is

$$\dot{\Psi} = -\ S_0\ \dot{\theta} + \frac{1}{2}\ \lambda'(\theta)\ \dot{\theta}\ \varepsilon^2_{(1)} + \mu'(\theta)\ \dot{\theta}\ (\varepsilon - \varepsilon^{(p)})_{(2)}$$

$$+ \frac{\partial H}{\partial \theta} \dot{\theta} \varepsilon^{(p)}_{(2)} - D'(\theta) \dot{\theta} (\theta - \theta_R) \varepsilon_{(1)} - D(\theta) \dot{\theta} \varepsilon_{(1)}$$

$$- F'(\theta) \dot{\theta} (\theta - \theta_R)^2 - 2 F(\theta) \dot{\theta} (\theta - \theta_R)$$

$$+ \lambda(\theta) \varepsilon_{(1)} \dot{\varepsilon}_{(1)} + 2 \mu(\theta) (\varepsilon - \varepsilon^{(p)})(\dot{\varepsilon} - \dot{\varepsilon}^{(p)})$$

$$+ 2 H(\theta, W_p) \varepsilon^{(p)} \dot{\varepsilon}^{(p)} - D(\theta)(\theta - \theta_R) \dot{\varepsilon}_{(1)}$$

$$+ \frac{\partial H}{\partial W_p} \frac{dW_p}{dt} \varepsilon^{(p)}_{(2)} \quad . \tag{3.46}$$

Equation (3.37) allows us to obtain the following expression:

$$\dot{\theta} S = S_0 \dot{\theta} - \frac{1}{2} \lambda'(\theta) \dot{\theta} \varepsilon^2_{(1)} - \mu'(\theta) \dot{\theta} (\varepsilon - \varepsilon^{(p)})_{(2)}$$

$$- \frac{\partial H}{\partial \theta} \dot{\theta} \varepsilon^{(p)}_{(2)} + D'(\theta) \dot{\theta} (\theta - \theta_R) \varepsilon_{(1)} + D(\theta) \dot{\theta} \varepsilon_{(1)}$$

$$+ F'(\theta) \dot{\theta} (\theta - \theta_R)^2 + 2 F(\theta) \dot{\theta} (\theta - \theta_R) \ . \tag{3.47}$$

Then from equations (3.46) and (3.47) we have

$$\dot{\Psi} + \dot{\theta} S = \lambda(\theta) \varepsilon_{(1)} \dot{\varepsilon}_{(1)} + 2 \mu(\theta) (\varepsilon - \varepsilon^{(p)})(\dot{\varepsilon} - \dot{\varepsilon}^{(p)})$$

$$+ 2 H(\theta, W_p) \varepsilon^{(p)} \dot{\varepsilon}^{(p)} - D(\theta)(\theta - \theta_R) \dot{\varepsilon}_{(1)}$$

$$+ \frac{\partial H}{\partial W_p} \frac{dW_p}{dt} \varepsilon^{(p)}_{(2)} \quad . \tag{3.48}$$

Realizing $\varepsilon = \varepsilon^{(e)} + \varepsilon^{(p)}$, and $\varepsilon_{(1)} = \varepsilon^{(e)}_{(1)}$ the above equation can be written as

$$\dot{\Psi} + \dot{\theta}\, S = \frac{\partial}{\partial t}\, [\, \frac{1}{2}\, \lambda(\theta)\, \varepsilon_{(1)}^{(e)2} + \mu(\theta)\, \varepsilon^{(e)2} - D(\theta)(\theta - \theta_R)\, \varepsilon_{(1)}^{(e)}$$

$$+ H(\theta, W_p)\, \varepsilon_{(2)}^{(p)}\,] \quad . \tag{3.49}$$

Now it is seen that the second term on the right hand side of equation (3.44) is nothing but the recoverable part of the mechanical power. Then the meaning of equation (3.44) is clear. It says the mechanically dissipative power is the difference between the total mechanical power and the recoverable part. Of course, this is nothing surprising, yet it does show that after so much manipulation the dissipation function keeps its clear physical meaning.

The stress tensor can be directly derived from the free energy function (3.34) on the basis of equation (3.8):

$$\sigma_{ij} = \frac{\partial \Psi}{\partial \varepsilon_{ij}} = \lambda(\theta)\, \varepsilon_{(1)}\, \delta_{ij} + 2\, \mu(\theta)(\varepsilon_{ij} - \varepsilon_{ij}^{(p)})$$

$$- D(\theta)(\theta - \theta_R)\, \delta_{ij} \quad . \tag{3.50}$$

The deviatoric part of the stress tensor, which is responsible for plastic deformation is then obtained as:

$$\sigma'_{ij} = 2\, \mu(\theta)(\varepsilon'_{ij} - \varepsilon_{ij}^{(p)}) \,, \tag{3.51}$$

where the prime means deviatoric.

With all these results ready, equation (3.44) is reduced to the following form:

$$\Phi_1 = 2\,\mu(\theta)(\varepsilon'_{ij} - \varepsilon^{(p)}_{ij})\,\dot{\varepsilon}^{(p)}_{ij} - 2\,H(\theta,\,W_p)\,\varepsilon^{(p)}_{ij}\,\dot{\varepsilon}^{(p)}_{ij}$$

$$- \frac{\partial H}{\partial W_p}\,\frac{dW_p}{d\,t}\,\varepsilon^{(p)}_{(2)}\ . \qquad (3.52)$$

To make a better understanding of equation (3.52) let us consider a simple case. For the materials whose hardening parameter H is independent of W_p [3.17], the last term vanishes, and with equation (3.51) noticed, the dissipation function becomes

$$\Phi_1 = \sigma'_{ij}\,\dot{\varepsilon}^{(p)}_{ij} - 2\,H\,\varepsilon^{(p)}_{ij}\dot{\varepsilon}^{(p)}_{ij}\ , \qquad (3.53)$$

from which it is seen that the entire amount of plastic deformation power has not been dissipated. The second term, part $2H\varepsilon^{(p)}_{ij}\dot{\varepsilon}^{(p)}_{ij}$ is not dissipated.

3.4.3 Constitutive Equations for Linear Dissipation Materials

In elasticity where the processes are reversible, the free energy is a potential function, and usually is a function of "position" characterized by strain tensor. Anyway, it is not a function of "velocity", therefore, there is no time factor involved. In thermoplasticity, however, things are completely different. Because the processes are irreversible, the factor of time is always involved. An attempt to employ the free energy function alone to describe the dissipative processes and to obtain the constitutive equations seems no longer a proper way, because the evolution equation of the internal variable can not be directly derived from the assumed free energy function. It is because of this reason that Ziegler and Wehrli [3.17] introduced the dissipation function in the velocity space.

In the preceding section the constructive features of function Φ_1 have been discussed. It is believed that there should be no temperature term explicitly involved in the function. According to the theory of normality the dissipation function is defined in the velocity space of internal state variables [3.17]. For the materials with linear dissipation, the function can be chosen as follows

$$\Phi_1 = C(\theta)\ (2\ \dot{\varepsilon}^{(p)}_{(2)})^{\frac{1}{2}} \quad , \tag{3.54}$$

where $C(\theta)$ is a temperature-dependent material property. The subscript (2) stands for the second invariant.

As mentioned before, Φ_2, the other part of the dissipation function concerns the process of heat conduction, for which the selected "velocity" is heat flow or "equivalent heat flow" depending upon which law of heat conduction is adopted, and the the conjugated "force" is $(-\frac{g}{\theta})$. In order the law of heat conduction is to be satisfied, for isotropic materials the dissipation function due to heat conduction is assumed as:

$$\Phi_2 = \left(\frac{1}{k(\theta)\theta} \right) R_i R_i \quad , \tag{3.55}$$

where $k(\theta)$ is a temperature-dependent material property, and $\mathbf{R}$ is heat flow *i.e.* $\mathbf{R} \equiv \mathbf{q}$ when Fourier's heat conduction law is adopted; or equivalent heat flow $R \equiv q + \tau \frac{dq}{dt}$ if Cattaneo's hyperbolic heat conduction law is employed.

A hypothesis employed in this research is that the constitutive laws for plasticity and for heat conduction are independent of each other, therefore we have

$$\Phi = \Phi_1 + \Phi_2 = C(\theta)(\ 2\ \dot{\varepsilon}^{(p)}_{(2)}\ )^{\frac{1}{2}} + (\ \frac{1}{k(\theta)\theta}\ )\ R_i R_i\ . \qquad (3.56)$$

With free energy function described by equation (3.34), dissipation function by (3.56) all the constitutive equations concerning the dependent variables can be derived from the leading functions according to the theory of thermomechanics.

First of all, the relation among stress, total strain, plastic strain and difference of temperature can be readily established as given in equation (3.50), and the expression of entropy is given by equation (3.37).

Heat conduction is a dissipative process, therefore, the establishment of the constitutive relation governing the process is related to the dissipation function. By equations (2.15) and (2.16) the following equation between the "velocity" and the "force" is obtained:

$$-\frac{\theta_{,i}}{\theta} = \Phi_2(\ \frac{\partial \Phi_2}{\partial R_k}\ R_k\ )^{-1}\ \frac{\partial \Phi_2}{\partial R_i}\ . \qquad (3.57)$$

Substituting equation (3.55) in equation (3.57) yields either one of the following equations, depending upon which law of heat conduction is adopted:

$$q_i = - k(\theta)\ \theta,_i \quad , \tag{3.58}$$

or

$$q_i + \tau\ \dot{q}_i = - k(\theta)\ \theta,_i \ . \tag{3.59}$$

In addition to those obtained above, the most important one is the plasticity constitutive equations, which can be obtained either by by normality equations (2.4) through (2.7) and (2.14), (2.15), (2.16) or directly by our equation (3.44), and the result is:

$$\sigma'_{ij}\{1 + J(m_1(\theta),\ m_2(\theta),...,m_i(\theta),\ W_p)\varepsilon^{(p)}_{(2)}\} - 2\ H\ (\theta,\ w_p)\ \varepsilon^{(p)}_{ij}$$

$$= C(\theta)\ (\tfrac{1}{2}\ \dot{\varepsilon}^{(p)}_{(2)})^{-\frac{1}{2}}\ \dot{\varepsilon}^{(p)}_{ij} \ , \tag{3.60}$$

where

$$J(m_1(\theta),\ m_2(\theta),...,m_i(\theta),\ W_p) = - \frac{\partial H(\theta\ , W_p)}{\partial W_p} \tag{3.61}$$

is the softening rule of strain hardening parameter of the material, and $m_1(\theta)$, $m_2(\theta),...,m_i(\theta)$ are the material properties depending upon the temperature. The softening rule serves as an interface between the constitutive theory and the related experimental works. A simple example of this rule has been given by Bodner and Parton [3.18] as well as Bodner and Aboudi [1.26], where only the isothermal case is examined, and based upon the experimental observation exponential law is considered suitable for metallic materials such as copper, aluminum and titanium with variable strain hardening properties.

Many authors have been trying to introduce strain hardening effects into the theory of plasticity since Schmidt and Odquist succeeded in revising Lévy-Mises plasticity theory of perfect material. Ziegler and Wehrli [3.17] introduced a simple parameter into the free energy function of isothermal plasticity, in which the strain hardening parameter, instead of being a function of plastic work, is taken as a constant. Of course, it only represents a simple model, yet the authors have realized that strain hardening is contributive to the free energy function. Bodner *et al.* [1.26], [3.18] have been considering the strain hardening parameter as a function of plastic work. Similarly to Schmidt and Odquist, Bodner *et al* use the flow rule of plasticity to obtain the desired equations, and as a result, the thermal effects can not be naturally taken into account.

Trying to obtain a consistent set of constitutive equations of thermoplasticity is a major objective of this research. As a consiquence the expressions for the leading functions, equations (3.34), (3.54) and (3.55); the expression for entropy, equation (3.37); for stress, equation (3.50); for heat conduction, equation (3.58) or (3.59) and most important, for thermoplasticity constitutive relation, equations (3.60) and (3.63) are obtained. All these equations are consistent with one another.

3.4.4 Constitutive Equations for Non-Linear Dissipation Materials

Experiments have shown that metallic materials like mild steel *e.g.* Steel 1010 are very rate-sensitive. Cowper and Symonds [3.35] and Bodner and Symonds [3.36] presented a relation between stress and rate of strain, based on Manjoine's test data. For the reason that the formula is only applicable to isothermal case and empirically based it does not reveal any information concerning thermodynamic features of plastic deformation. It is worthwhile to re-examine the process with the theory of thermomechanics. Referring to [3.17], let us have the non-linear dissipation function of the following form:

$$\Phi_1 = K_1(\theta)[1 + K_2(\theta)(\dot{\varepsilon}^{(p)}_{(2)})^{\frac{1}{n(\theta)}}]\,(2\,\dot{\varepsilon}^{(p)}_{(2)})^{\frac{1}{2}} \;, \tag{3.62}$$

and the free energy function

$$\Psi = \Psi_0 - S_0\,T + \frac{1}{2}\,\lambda(\theta)\,\varepsilon^2_{(1)} + \mu(\theta)(\,\varepsilon - \varepsilon^{(p)})_{(2)}$$

$$- D(\theta)\,\varepsilon_{(1)}\,T - F(\theta)\,T^2 \,. \tag{3.63}$$

With the leading functions given above the expression of entropy can be found on the basis of equation (3.9) as:

$$S = S_0 - \frac{1}{2}\frac{d\lambda(\theta)}{d\theta}\,\varepsilon^2_{(1)} - \frac{d\mu(\theta)}{d\theta}\,(\varepsilon - \varepsilon^{(p)})_{(2)} + D(\theta)\,\varepsilon_{(1)}$$

$$+ \frac{dD(\theta)}{d\theta}\,\varepsilon_{(1)}\,T + 2\,F(\theta)\,T + \frac{dF(\theta)}{d\theta}\,T^2 \,, \tag{3.64}$$

and the plastic constitutive relation on the basis of equation (3.44) is:

$$\sigma'_{ij} = K_1(\theta)\,[1 + K_2(\theta)\,(\dot{\varepsilon}^{(p)}_{(2)})^{\frac{1}{n(\theta)}}](\frac{1}{2}\,\dot{\varepsilon}^{(p)}_{(2)})^{-\frac{1}{2}}\,\dot{\varepsilon}^{(p)}_{ij} \,. \tag{3.65}$$

For one-dimensional case equation (3.65) assumes the following form:

$$\dot{\varepsilon}^{(p)} = G(\theta)\left(\frac{\sigma}{\sigma_0(\theta)} - 1\right)^{k(\theta)} \quad , \tag{3.66}$$

where

$$G(\theta) = \sqrt{\tfrac{2}{3}}\,[K_2(\theta)]^{-\frac{n(\theta)}{2}} \quad , \tag{3.67}$$

$$\sigma_0(\theta) = \sqrt{3}\,K_1(\theta) \quad , \tag{3.68}$$

and

$$K(\theta) = \frac{n(\theta)}{2} \quad . \tag{3.69}$$

To gain some physical understanding let us consider a simple case of deformation-induced heat. Around the centre part of the sample, the equation is simplified as:

$$\theta\,\dot{S} = \Phi_1 \quad . \tag{3.72}$$

Substituting equations (3.62) and (3.64) in (3.70) yields the following relation between the increase of temperature and the deformation rate:

$$\frac{\sigma_0(\theta)}{\sqrt{3}}\left\{1 + \left(\frac{3}{2}\right)^{\frac{1}{2k(\theta)}}\left(G(\theta)\right)^{\frac{1}{k(\theta)}}\left(\dot{\varepsilon}^{(p)}_{(2)}\right)^{\frac{1}{2k(\theta)}}\right\}\left(2\dot{\varepsilon}^{(p)}_{(2)}\right)^{\frac{1}{2}}$$

$$= \left\{\left(-\frac{1}{2}\frac{d^2\lambda(\theta)}{d\theta^2}\,\varepsilon^2_{(1)} - \frac{d^2\mu(\theta)}{d\theta^2}\,\varepsilon^{(e)}_{(2)} + 2\,\frac{dD(\theta)}{d\theta}\,\varepsilon_{(1)}\right.\right.$$

$$\left. + \frac{d^2D(\theta)}{d\theta^2}\,\varepsilon_{(1)}\,T + 4\,\frac{dF(\theta)}{d\theta}\,T + 2\,F(\theta) + \frac{d^2F(\theta)}{d\theta^2}\,T^2\right)\dot{T}$$

$$+\left(D(\theta)\,\dot{\varepsilon}_{(1)} + \frac{dD(\theta)}{d\theta}\,T\,\dot{\varepsilon}_{(1)} - \frac{d\lambda(\theta)}{d\theta}\,\varepsilon_{(1)}\dot{\varepsilon}_{(1)}\right.$$

$$- 2 \frac{d\mu(\theta)}{d\theta} \varepsilon_i^{(e)} \dot{\varepsilon}_i^{(e)} \Big) \Big\} \Big(\theta_R + T \Big) . \tag{3.71}$$

It can be seen from equation (3.71) that plastic deformation corresponding to term $\dot{\varepsilon}_{(2)}^{(p)}$ on the left hand side of equation (3.71) will cause an increase of temperature. While in elastic region in which $\dot{\varepsilon}_{(2)}^{(p)} = 0$, equation (3.71) implies that a positive $\dot{\varepsilon}_{(1)}$ *i.e.* expansion corresponds to a negative $\dot{T}$. The elastic body behaves as an ideal gas, expansion causes decrease of temperature.

The isothermal form of equation (3.66) is called Cowper-Symonds formula. The constitutive relation (3.66) is employed for study of wave propagation in a uniaxial solid in this research.

CHAPTER 4

PLASTIC WAVE PROPAGATION IN A SEMI-INFINITE ROD

4.1 Introduction

It is well known that the action of impulsively applied loads is not distributed instantaneously through the body, but is transferred from particle to particle in a wave manner.

The theory of plastic wave propagation deals with motions of disturbances in metallic solids when the stresses are large enough to cause plastic strains in the material. The theory was originally motivated by the necessity of protection from an explosive attack during World War II. Now it has found widespread applications in different areas. In spite of its importance in practical applications, study of plastic wave propagation along with the associated plastic constitutive relations is considered significant for the reason that a sound constitutive law must generate the results which can be proved correct.

In this chapter, the problem of plastic wave propagation in a semi-infinite rod is examined, and a uniaxial model is utilized. The reason of this usage is its simplicity and feasibility, yet it illustrates the main features of the problem without much undue mathematical complications. The chapter begins with the description of the motion. When the fundamental laws are applied, the equation of motion, the equation for energy conservation are obtained. Then associated with the geometric compatibility equation, the Cattaneo's hyperbolic heat conduction and the constitutive equation are derived. the system of equations which govern the problem is thus established.

Characteristics analysis of the system is undertaken following the establishment of the system of equations. The statement of the problem is completed by prescribing initial and boundary conditions. The jump conditions at the wave fronts, which are essential for determining the values of discontinuities, are discussed thereafter.

4.2 Description of the Problem

Many practical problems for deformable media may be simplified by means of appropriate justifiable assumptions, so that the medium can be regarded as a one-dimensional geometric object. Also, there are many dynamic problems for which it is justifiable to assume the dependent variables depend upon only one space variable and time. These physical situations, when occurring in the field of propagation of disturbances, lead to the theory of one-dimensional waves.

In the development of the theory of one-dimensional wave, some fundamental assumptions are made in the outset. First of all, the cross-section of the rod is assumed to remain plane and normal to the axis of the rod during the dynamic deformation. Second, the inertia forces corresponding to the motion of the rod in transverse directions are negligible. Then the problem can be readily treated as a uniaxial one.

The rod is composed of material particles each of which is called a particle for simplicity. The instantaneous geometric location of a particle will be spoken of as a point. At the beginning, to label a particle we choose a coordinate system x, which is called as Lagrangian coordinate system. At a later time t, the particle with label x is moved to another point. Its position is denoted by coordinate x, which is called as Eulerian coordinate. Then the motion of the particle is described by the following relation:

$$x = x\ (\mathrm{x,t}) \quad . \tag{4.1}$$

Equation (4.1) is said to be Lagrangian description of motion. It implies that a material particle which initially had a label coordinate x is at position x at time t. With this information the displacement function can be written as

$$u = u\ (\mathrm{x,t}) = x - \mathrm{x} \quad , \tag{4.2}$$

Infinitesimal strain is then expressible as

$$\varepsilon = \varepsilon(\mathrm{x,t}) = \frac{\partial u(\mathrm{x,t})}{\partial \mathrm{x}} \quad . \tag{4.3}$$

The velocity of the particle can be obtained as the derivative of displacement function with respect to time t.

$$v = v(\mathrm{x,t}) = \frac{\partial u(\mathrm{x,t})}{\partial t} \quad . \tag{4.4}$$

Assuming function u(x,t) to be smooth enough, its alternate derivative respect to x and t does not depend upon the order of differentiation, and we have

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial v}{\partial \mathrm{x}} \ , \tag{4.5}$$

known as the geometric compatibility equation. In addition, there are some other governing equations which can be derived from the fundamental balance laws of continuum mechanics.

The law of balance of momentum generates the equation of motion (1.7). In one-dimensional case it is in the form

$$\frac{\partial \sigma}{\partial x} = \rho \frac{\partial v}{\partial t} - f \ , \tag{4.6}$$

where σ stands for stress, ρ is mass density of the material, and f is the body force per unit volume.

The balance of angular momentum is automatically satisfied since there is only one stress component involved, and the symmetry of stress tensor is automatically ensured.

Because constant density is assumed, conservation of mass gives no further governing equation, but is identically satisfied.

The law of energy conservation or the first law of thermodynamics plays an important role in a thermomechanic process. The law asserts that the time rate of the internal energy equals the sum of inputs of external power and heat flow. According to equations (1.16) the first law can be represented by the following form

$$\dot{U} = \sigma \frac{\partial \varepsilon}{\partial t} - \frac{\partial q}{\partial x} \ . \tag{4.7}$$

Besides, as we discussed in Chapter 3, the system gets some restrictions imposed by the second law of thermodynamics. Among them the most impressive one is

$$\frac{d|p|}{dt} \geq 0 \ , \tag{4.8}$$

where and thereafter p stands for plastic strain.

The relations (4.5) through (4.8) are utilized in establishing a system of governing equations.

4.3 System of Equations Governing the Problem of Wave Propagation

The requirements of balance of momentum, compatibility, energy conservation, heat conduction and the relation between stress and rate of plastic strain form the system of equations governing the problem of wave propagation in a semi-infinite rod. Based on equations (4.5), (4.6), (4.7) associated with equations (3.59) and (3.68) the system of equations can be listed below:

$$\rho \frac{\partial v}{\partial t} - \frac{\partial \sigma}{\partial x} = f \tag{4.9a}$$

the equation of motion,

$$D_2 \frac{\partial \sigma}{\partial t} + D_5 \frac{\partial T}{\partial t} + \frac{\partial p}{\partial t} - \frac{\partial v}{\partial x} = 0 \tag{4.9b}$$

the geometric compatibility equation,

$$D_1 \frac{\partial \sigma}{\partial t} + D_3 \frac{\partial T}{\partial t} - D_4 \frac{\partial p}{\partial t} + \frac{\partial q}{\partial x} = 0 \tag{4.9c}$$

the equation of energy conservation,

$$\tau_0 \frac{\partial q}{\partial t} + k \frac{\partial T}{\partial x} + q = 0 \tag{4.9d}$$

the Cattaneo's hyperbolic heat conduction equation, and

$$\frac{\partial p}{\partial t} - F = 0 \tag{4.9e}$$

the constitutive equation. The coefficients D_k(k=1, 2,..., 5) are functions of temperature, stress and plastic strain. F is the expression of the right hand side of equation (3.68).

4.4 Characteristics Analysis of the System

Equations (4.9) may be re-written as:

$$\left[A_0 \right] \left\{ Y_t \right\} + \left[B_0 \right] \left\{ Y_x \right\} = \left\{ C_0 \right\}, \tag{4.10}$$

where

$$\left[A_0 \right] = \begin{pmatrix} \rho & 0 & 0 & 0 & 0 \\ 0 & D_2 & D_5 & 0 & 1 \\ 0 & D_1 & D_3 & 0 & -D_4 \\ 0 & 0 & 0 & \tau_0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \tag{4.11a}$$

$$\left[B_0 \right] = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & k & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{4.11b}$$

$$\left\{ Y_t \right\}^T = \left[\frac{\partial v}{\partial t} \ \frac{\partial \sigma}{\partial t} \ \frac{\partial T}{\partial t} \ \frac{\partial q}{\partial t} \ \frac{\partial p}{\partial t} \right], \tag{4.11c}$$

$$\left\{ Y_x \right\}^T = \left[\frac{\partial v}{\partial x} \quad \frac{\partial \sigma}{\partial x} \quad \frac{\partial T}{\partial x} \quad \frac{\partial q}{\partial x} \quad \frac{\partial p}{\partial x} \right] , \tag{4.11d}$$

$$\left\{ C_0 \right\}^T = \left[f \quad 0 \quad 0 \quad -q \quad F \right] ; \tag{4.11e}$$

and superscript T stands for transpose of the column matrix.

Equation (4.10) may be simplified by left-multiplying both sides with A_0^{-1}, the inverse of A_0. In so doing the equations become

$$\left\{ Y_t \right\} + \left[A_0 \right]^{-1} \left[B_0 \right] \left\{ Y_x \right\} = \left[A_0 \right]^{-1} \left\{ C_0 \right\} , \tag{4.12}$$

where, as given in appendix A

$$\left[A_0 \right]^{-1} = \begin{pmatrix} \frac{1}{\rho} & 0 & 0 & 0 & 0 \\ 0 & \frac{D_3}{\tilde{D}} & -\frac{D_5}{\tilde{D}} & 0 & -\frac{(D_3+D_4D_5)}{\tilde{D}} \\ 0 & -\frac{D_1}{\tilde{D}} & \frac{D_2}{\tilde{D}} & 0 & \frac{(D_1+D_2D_4)}{\tilde{D}} \\ 0 & 0 & 0 & \frac{1}{\tau_0} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} . \tag{4.13}$$

Substituting (4.13) in (4.12) yields

$$\left\{ Y_t \right\} + \left[A \right] \left\{ Y_x \right\} = \left\{ C \right\} , \tag{4.14}$$

or simply

$$\underset{\sim}{Y}_t + \underset{-}{A}\ (\underset{\sim}{Y})\ \underset{\sim}{Y}_x = \underset{\sim}{C}\ (\underset{\sim}{Y})\ , \tag{4.15}$$

where

$$\left[\, A \,\right] = \begin{pmatrix} 0 & -\frac{1}{\rho} & 0 & 0 & 0 \\ -\frac{D_3}{\tilde{D}} & 0 & 0 & -\frac{D_5}{\tilde{D}} & 0 \\ \frac{D_1}{\tilde{D}} & 0 & 0 & \frac{D_2}{\tilde{D}} & 0 \\ 0 & 0 & \frac{k}{\tau_0} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{4.16}$$

$$\left\{ C \right\}^T = \left[\frac{f}{\rho} \quad -\frac{(D_3+D_4D_5)F}{\tilde{D}} \quad \frac{(D_1+D_2D_4)F}{\tilde{D}} \quad -\frac{q}{\tau_0}\ F \right], \tag{4.17}$$

and

$$\tilde{D} = D_2\ D_3\ -\ D_1\ D_5\ . \tag{4.18}$$

For obtaining the eigenvalues of equations (4.15) the characteristic equation is expressible as

$$\det\ (\ \underline{A} - \lambda\ \underline{I}\ ) = 0\ . \tag{4.19}$$

Substituting equation (4.16) in equation (4.19) and accomplishing the required operation we obtain

$$\lambda\ \{\ \lambda^4 - (\ \frac{D_3}{\tilde{D}}\ \frac{1}{\rho} + \frac{k}{\tau_0}\ \frac{D_2}{\tilde{D}}\ )\ \lambda^2 + \frac{k}{\tau_0\ \rho\ \tilde{D}}\ \} = 0\ . \tag{4.20}$$

The solution of equation (4.20) generates the eigenvalues which are

$$\lambda^{(1)} = 0 \quad , \tag{4.21a}$$

$$\lambda^{(2,3)} = \pm V_2 \ , \tag{4.21b}$$

$$\lambda^{(4,5)} = \pm V_3 \ , \tag{4.21c}$$

where

$$V_2 = \left\{ C \left(1 + \sqrt{1-R} \right) \right\}^{\frac{1}{2}} , \tag{4.22a}$$

$$V_3 = \left\{ C \left(1 - \sqrt{1-R} \right) \right\}^{\frac{1}{2}} , \tag{4.22b}$$

$$C = \frac{1}{2\tilde{D}} \left(\frac{k}{\tau_0} D_2 + \frac{D_3}{\rho} \right) , \tag{4.22c}$$

$$R = \frac{4 \ \tilde{D} \rho \tau_0 k}{(D_3 \tau_0 + \rho k D_2)^2} \ . \tag{4.22d}$$

The system of the partial differential equations is hyperbolic if its associated eigenvalues $\lambda^{(i)}(i=1, 2, ..., 5)$ are real. This requirement is satisfied if

$$C \ (\sigma, \theta, p \ ) > 0 \quad , \tag{4.23}$$

and

$$R \ (\sigma, \theta, p \ ) < 1 \quad . \tag{4.24}$$

In other words, equations (4.23) and (4.24) assure of the hyperbolicity of the system of equations, therefore, they are referred to as hyperbolicity conditions. The eigenvalues given by equations (4.22) are called as characteristic speeds, which reflect the fact that thermal and plastic deformations are coupled with each other.

When τ_0, the relaxation time tends to zero, the equation of heat conduction becomes that of Fourier, and equations (4.9) become singular. With T and q deleted, equations (4.9a), (4.9b) and (4.9e) can be re-organized to be a degenerated equation-system. The main eigenvalue of this system, which reflects the velocity of wave propagation is

$$\lambda = \left(\frac{1}{\rho D_2}\right)^{\frac{1}{2}}, \tag{4.25}$$

which is the velocity of elastic wave propagation. This result is consistent with Bell's experiments [2.37]. The fact means that rate dependent type constitutive equations are capable of predicting the speed of plastic wave propagation. In the history of controversy, this was the reason for some people preferring it to the constitutive equations of rate-independent type.

4.5 Statement of the Problem

The governing equations (4.9) for the problem may be written in the following form:

$$\frac{\partial v}{\partial t} - \frac{1}{\rho}\frac{\partial \sigma}{\partial x} - \frac{1}{\rho} f = 0 \tag{4.26}$$

$$\frac{\partial \sigma}{\partial t} - D_1' (\sigma,T,p) \frac{\partial v}{\partial x} + D_2' (\sigma,T,p) \frac{\partial T}{\partial t} + D_3' (\sigma,T,p) \frac{\partial p}{\partial t} = 0 \tag{4.27}$$

$$\frac{\partial \sigma}{\partial t} + D_4' \, (\sigma,T,p) \, \frac{\partial T}{\partial t} - D_5' \, (\sigma,T,p) \, \frac{\partial p}{\partial t} + D_6' \, (\sigma,T,p) \, \frac{\partial q}{\partial x} = 0 \qquad (4.28)$$

$$\frac{\partial q}{\partial t} + \frac{k}{\tau_0} \frac{\partial T}{\partial x} + \frac{q}{\tau_0} = 0 \qquad (4.29)$$

$$\frac{\partial p}{\partial t} - F(\sigma,T,p) = 0 \quad , \qquad (4.30)$$

where $D_1' = D_3'$, and D_j'(j =1, 2,...,6) are related to D_k via equations (4.9). The solution for the basic unknowns will uniquely and continuously depend upon the initial values, if the initial and boundary conditions are properly prescribed. Following Orisamolu [4.6], these conditions are chosen as below.

Initial conditions:

$$v(x,0) = v_I(x)$$

$$\sigma(x,0) = \sigma_I(x)$$

$$T(x,0) = 0 \qquad \text{or} \qquad \theta(x,0) = \theta_0$$

$$q(x,0) = q_I(x)$$

$$p(x,0) = p_I(x) \qquad (4.31a,b,c,d,e)$$

Boundary conditions:

Case (A): $\quad \theta(0,t) = \theta_0(t)$,

$$\sigma(0,t) = \sigma_0(t) \tag{4.32a,b}$$

Case (B): $\theta(0,t) = \theta_0(t)$

$$v(0,t) = v_0(t) \ . \tag{4.33a,b}$$

The performed numerical work has shown that the problem is properly stated, and the values of following unknowns are obtainable:

$v(x,t)$, $\sigma(x,t)$, $T(x,t)$, $q(x,t)$ and $p(x,t)$.

Other dependent functions such as free energy, internal energy, entropy *etc.* if necessary, may be obtained from the fundamental ones.

4.6 Jump Conditions at the Wavefront

A wave propagating through the rod is a smooth curve in the (x,t) plane with property that the dependent variables v, σ, T, q, p and their derivatives are continuous with respect to x and t everywhere except at the wavefront. The continuous variations of the dependent variables are governed by the system of equations (4.9). However, discontinuities or jumps exist across the wavefront, and the quantities of the discontinuities must be determined separately.

Quite a few researchers have studied the wave propagation problem, in which the hyperbolic heat conduction equation is employed and internal state variables are involved. Cristescu and Suliciu [4.1] have presented the relevant literature. In Chapter VII, [4.1], the authors show that for such a hyperbolic system, there exist acceleration waves, and the corresponding jump conditions across the wavefront can be accordingly determined.

A regular curve in the (x,t) plane is called an acceleration wave if the dependent variables such as v, σ, T, q and p are continuous across this curve, but their derivatives with respect to x and t have jump discontinuities when crossing it. As $\{y\}^T = \{ v,\sigma,T,q,p \}$ are continuous functions, Hadamard's kinematic compatibility conditions, which have to be satisfied when crossing the curve, are expressible in the form

$$\left[\frac{\partial y}{\partial t}\right] + v_w\left[\frac{\partial y}{\partial x}\right] = 0 \;, \tag{4.34}$$

where v_w is the propagating velocity of the wave, and the brackets [ ], in this section, denote the jump of the quantity inside. On the basis of equation (4.34), we have

$$\left[\frac{\partial v}{\partial x}\right] = \bar{v} \;,$$

$$\left[\frac{\partial v}{\partial t}\right] = -v_w\,\bar{v} \;,$$

$$\left[\frac{\partial \sigma}{\partial x}\right] = \bar{\sigma} \;,$$

$$\left[\frac{\partial \sigma}{\partial t}\right] = -v_w\,\bar{\sigma} \;,$$

$$\left[\frac{\partial T}{\partial x}\right] = \bar{T} \;,$$

$$\left[\frac{\partial T}{\partial t}\right] = -v_w\,\bar{T} \;,$$

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

$$[\frac{\partial q}{\partial t}] = -v_w \, \bar{q} \quad ,$$

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

$$[\frac{\partial p}{\partial t}] = -v_w \, \bar{p} \quad , \qquad (4.35a\text{-}j)$$

where $\bar{v}$, $\bar{\sigma}$, $\overline{T}$, $\bar{q}$ and $\bar{p}$ are jumps across the wavefront; their values are to be determined.

As equations (4.9) are quasi-linear, the coefficients D_i($i=1,...,5$) do not contain the derivatives of the dependent variables; neither does function F, the expression on the right hand side of equation (3.66). Assuming the body force is continuous everywhere and applying the jump operation to equations (4.9), we obtain the Hadamard's dynamic and geometric compatibility equations as below.

$$\rho \, v_w \, \bar{v} + \bar{\sigma} = 0 \quad ,$$

$$\bar{v} + D_2 \, v_w \, \bar{\sigma} + D_5 \, v_w \, \overline{T} = 0 \quad ,$$

$$D_1 \, v_w \, \bar{\sigma} + D_3 \, v_w \, \overline{T} - \bar{q} = 0 \quad ,$$

$$k \, \overline{T} - \tau_0 \, v_w \, \bar{q} = 0 \quad ,$$

$$\bar{p} = 0 \quad . \qquad (4.36a\text{-}c)$$

The first four equations can be written as

$$[\underset{\sim}{C}]\ \{\ \bar{v}\ \bar{\sigma}\ \bar{T}\ \bar{q}\ \}^{T} = 0 \quad , \tag{4.37}$$

where

$$[\underset{\sim}{C}] = \begin{bmatrix} \rho\, v_w & 1 & 0 & 0 \\ 1 & D_2 v_w & D_5 v_w & 0 \\ 0 & D_1 v_w & D_3 v_w & -1 \\ 0 & 0 & k & -\tau_0 v_w \end{bmatrix} , \tag{4.38}$$

with $\quad \det\, [\underset{\sim}{C}] = \rho\, v_w^2\ (\ k\, D_2 + \tau_0\, v_w\, \tilde{D}\ ) + k\, D_1\, \tau_0\, v_w^2\ .$ (4.39)

Because equations (4.37) are non-singular, the quantities of jumps can always be evaluated.

Since there are two positive eigenvalues involved ((4.22a) and (4.22b)), the coupled waves propagate with leading and trailing wavefronts, whose velocities may be denoted by v_{wl} and v_{wt} respectively. The total jumps of the derivatives of the dependent variables are the sum at the two wavefronts, therefore, we have the following results:

$$[\frac{\partial v}{\partial x}] = \bar{v}_l + \bar{v}_t\ ,$$

$$[\frac{\partial v}{\partial t}] = -(\ v_{wl}\ \bar{v}_l + v_{wt}\ \bar{v}_t)\ ,$$

$$[\frac{\partial \sigma}{\partial x}] = \bar{\sigma}_l + \bar{\sigma}_t$$

$$[\frac{\partial \sigma}{\partial t}] = -(\ v_{wl}\ \bar{\sigma}_l + v_{wt}\ \bar{\sigma}_t)\ ,.$$

$$[\frac{\partial T}{\partial x}] = \overline{T}_l + \overline{T}_t \ ,$$

$$[\frac{\partial T}{\partial t}] = -(v_{wl} \overline{T}_l + v_{wt} \overline{T}_t) \ ,$$

$$[\frac{\partial q}{\partial x}] = \overline{q}_l + \overline{q}_t \ ,$$

$$[\frac{\partial q}{\partial t}] = -(v_{wl} \overline{q}_l + v_{wt} \overline{q}_t) \ ,$$

$$[\frac{\partial p}{\partial x}] = 0 \ ,$$

$$[\frac{\partial p}{\partial t}] = 0 \ . \qquad (4.40a\text{-}j)$$

The values of $\overline{v}_l$, $\overline{v}_t$, $\overline{\sigma}_l$, $\overline{\sigma}_t$, $\overline{T}_l$, $\overline{T}_t$, $\overline{q}_l$, $\overline{q}_t$ are determined by equations (4.37) at the leading and trailing wavefronts respectively.

CHAPTER 5

DEVELOPMENT OF COMPUTATIONAL ALGORITHMS

5.1 Preface

The principle of numerical integration of hyperbolic equation was first presented by Massau [5.16] at the end of last century. Because these kinds of partial differential equations relate to many important phenomena such as vibration in engineering, various waves in mechanics, supersonic aerodynamic flow *etc.* its numerical integration has attracted much attention.

When compared with other kinds of partial differential equations the hyperbolic equations have some particular features. First, there is discontinuity existing in the solution. This fact makes it more difficult to solve it than others. Another feature is that there are characteristics with which it is possible to utilize some particular methods of integration like Massau's to obtain numerical result.

The existing numerical procedures for integration of hyperbolic partial differential equations include two difference methods. One of them is the characteristic method. In this method, first of all, the characteristics are worked out, then the original equations are changed into ordinary differential equations along the characteristics.Numerical integration of the equations generates the solution of the problem along the characteristics. The values of unknowns at the positions out of the characteristics may be obtained by the interpolation technique.

It has been asserted [5.14] that the accuracy of Massau's method for a hyperbolic system is comparable to that of the Euler method for ordinary differential equations. There are also some variants of the characteristic method, which give greater accuracy. For instance, the extrapolation method by Busch and Esser *et al* [5.15] has proven to be particularly useful. The method uses higher order difference quotients, therefore is much more involved than Massau's. Before using such a procedure one should also consider the cost of the increased accuracy.

Two types of nets can be employed for numerical integration of hyperbolic equations. For one of them, like Massau's, both integration and net grid are along characteristics. In order to obtain the values of the unknowns at certain points in the x-t space one has to utilize interpolation procedures, therefore, outputting the calculated results at certain time and positions are not very convenient.

For the other net type, the grid is formed by constant-time and constant-position lines. The values at the points which do not coincide with the grid nodes are obtained via interpolation. Integration procedures are still along characteristics. Although the slopes of characteristics vary from point to point due to non-linearity of the system, the interpolation easily provides the necessary data for the next integration step with tolerated error. This procedure has proved to be very convenient and efficient.

In addition to the method of integrating the equations along characteristics a finite difference procedure is also applicable. In this procedure a partial differential equation is reduced into a finite difference equation in terms of the unknowns at grid nodes. The equation is then employed to evaluate the desired unknowns at the grid nodes.

5.2 Integration of the System via Characteristics Method

A feasible computational algorithm based on characteristics method will be provided in this section. As the system of partial differential equations developed in Chapter 4 is highly non-linear, the eigenvalues, and therefore the slopes of the characteristic lines vary from point to point. Under these circumstances, the most convenient and efficient grid system to choose is the constant-time grid. In our development presented below, the original system is, at first, transferred into ordinary differential equations which hold along the characteristic lines; then these ordinary differential equations are integrated with prescribed auxiliary conditions. Recall that the original partial differential equations as obtained in equations (4.26) through (4.30) are:

$$\frac{\partial v}{\partial t} - \frac{1}{\rho}\frac{\partial \sigma}{\partial x} - \frac{1}{\rho} f = 0 \ ,$$

$$\frac{\partial \sigma}{\partial t} - D_1'(\sigma,\theta,p)\frac{\partial v}{\partial x} + D_2'(\sigma,\theta,p)\frac{\partial \theta}{\partial t} + D_3'(\sigma,\theta,p)\frac{\partial p}{\partial t} = 0 \ ,$$

$$\frac{\partial \sigma}{\partial t} + D_4'(\sigma,\theta,p)\frac{\partial \theta}{\partial t} - D_5'(\sigma,\theta,p)\frac{\partial p}{\partial t} + D_6'(\sigma,\theta,p)\frac{\partial q}{\partial x} = 0 \ ,$$

$$\frac{\partial q}{\partial x} + \frac{k}{\tau_0}\frac{\partial \theta}{\partial x} + \frac{q}{\tau_0} = 0 \ ,$$

$$\frac{\partial p}{\partial t} - F(\sigma,\theta,p) = 0 \ . \qquad (5.1a\text{-}e)$$

This system is represented by:

$$\underset{\sim}{Y}_t + \underline{A}(\underset{\sim}{Y})\,\underset{\sim}{Y}_x = \underset{\sim}{C}(\underset{\sim}{Y}) \ , \qquad (5.2)$$

where matrix $\underset{\sim}{\underline{A}}(Y)$ and vector $\underset{\sim}{C}(\underset{\sim}{Y})$ were determined by equation (4.16) and equation (4.17), respectively.

With the eigenvalues given by equations (4.21) and (4.22) the corresponding characteristics are determined by the following equations:

$$\text{for} \quad \lambda^{(1)} = 0 \qquad \frac{dx_1}{dt} = 0 \quad ; \tag{5.3a}$$

$$\text{for} \quad \lambda^{(2)} = V_2(\underset{\sim}{Y}) \qquad \frac{dx_2}{dt} = V_2(\underset{\sim}{Y}) \quad ; \tag{5.3b}$$

$$\text{for} \quad \lambda^{(3)} = -V_2(\underset{\sim}{Y}) \qquad \frac{dx_3}{dt} = -V_2(\underset{\sim}{Y}) \quad ; \tag{5.3c}$$

$$\text{for} \quad \lambda^{(4)} = V_3(\underset{\sim}{Y}) \qquad \frac{dx_4}{dt} = V_3(\underset{\sim}{Y}) \quad ; \tag{5.3d}$$

$$\text{for} \quad \lambda^{(5)} = -V_3(\underset{\sim}{Y}) \qquad \frac{dx_5}{dt} = -V_3(\underset{\sim}{Y}) \ . \tag{5.3e}$$

It can be seen from equation (5.3a) that its corresponding characteristics in the x-t space is a straight line parallel to the t axis. For the other four, however, their slopes in the space are non-linear functions of the basic unknown vector $\underset{\sim}{Y}$ whose values vary from point to point, therefore, the characteristic lines are curvilinear.

For equations (5.2), the left eigenvectors associated with matrix $\underline{A}(\underset{\sim}{Y})$ are found from the following relation:

$$\underset{\sim}{l}^{(i)}(\underset{\sim}{Y})\ \underset{\sim}{\underline{A}}(\underset{\sim}{Y}) = \lambda^{(i)}(\underset{\sim}{Y})\ \underset{\sim}{l}^{(i)}(\underset{\sim}{Y}) \ , \tag{5.4}$$

where $\underset{\sim}{l}^{(i)}(\underset{\sim}{Y})$ stands for the ith left eigenvector. In Appendix B all the eigenvectors have been determined as:

$$\underset{\sim}{l}^{(1)} = [0 \quad 0 \quad 0 \quad 0 \quad 1] \quad , \tag{5.5a}$$

$$\underset{\sim}{l}^{(2)} = \begin{Bmatrix} 1 \\ -\dfrac{1}{\rho V_2} \\ \dfrac{\rho V_2^2 \tilde{D} - D_3}{\rho V_2 D_1} \\ \dfrac{\tau_0}{\rho k} \left(\dfrac{\rho V_2^2 \tilde{D} - D_3}{D_1}\right) \\ 0 \end{Bmatrix}^T \tag{5.5b}$$

$$\underset{\sim}{l}^{(3)} = \begin{Bmatrix} 1 \\ \dfrac{1}{\rho V_2} \\ -\dfrac{\rho V_2^2 \tilde{D} - D_3}{\rho V_2 D_1} \\ \dfrac{\tau_0}{\rho k} \left(\dfrac{\rho V_2^2 \tilde{D} - D_3}{D_1}\right) \\ 0 \end{Bmatrix}^T . \tag{5.5c}$$

$$\underset{\sim}{l}^{(4)} = \left\{ \begin{array}{c} 1 \\ \\ -\dfrac{1}{\rho V_3} \\ \\ \dfrac{\rho V_3^2 \tilde{D} \quad - D_3}{\rho V_3 D_1} \\ \\ \dfrac{\tau_0}{\rho k} \left(\dfrac{\rho V_3^2 \tilde{D} \; - D_3}{D_1} \right) \\ \\ 0 \end{array} \right\}^T \tag{5.5d}$$

$$\underset{\sim}{l}^{(5)} = \left\{ \begin{array}{c} 1 \\ \\ \dfrac{1}{\rho V_3} \\ \\ -\dfrac{\rho V_3^2 \tilde{D} \quad - D_3}{\rho V_3 D_1} \\ \\ \dfrac{\tau_0}{\rho k} \left(\dfrac{\rho V_3^2 \tilde{D} \; - D_3}{D_1} \right) \\ \\ 0 \end{array} \right\}^T \tag{5.5e}$$

On the basis of partial differential equations (5.2) and equations (5.3) of the characteristic lines, the ordinary differential equations holding along each of the characteristic lines can be determined by the left eigenvectors. Left multiplying equations (5.2) and utilizing equations (5.4) we obtain

$$\underset{\sim}{l}^{(i)}(\underset{\sim}{Y})\ \underset{\sim}{Y}_t + \underset{\sim}{l}^{(i)}(\underset{\sim}{Y})\ \lambda^{(i)}(\underset{\sim}{Y})\ Y_x = \underset{\sim}{l}^{(i)}(\underset{\sim}{Y})\ \underset{\sim}{C}(\underset{\sim}{Y})\ . \tag{5.6}$$

Making use of equations (5.3), we can re-write equations (5.6) as:

$$\underset{\sim}{l}^{(i)}(\underset{\sim}{Y})\ \frac{d\underset{\sim}{Y}}{dt} = \underset{\sim}{l}^{(i)}(Y)\ \underset{\sim}{C}(\underset{\sim}{Y}) \qquad i=1,2,\ \ldots,5\ . \tag{5.7}$$

These are the desired ordinary differential equations which hold along the characteristics. The explicit form is expressed as:

$$\frac{dp}{dt} = F \qquad \text{along } \frac{dx}{dt} = 0\ ; \tag{5.8a}$$

$$\frac{dv}{dt} - \left(\frac{1}{\rho V_2}\right)\frac{d\sigma}{dt} + \left(\frac{\rho V_2^2\tilde{D} - D_3}{\rho V_2 D_1}\right)\frac{d\theta}{dt} + \frac{\tau_0}{\rho k}\left(\frac{\rho V_2^2\tilde{D} - D_3}{D_1}\right)\frac{dq}{dt}$$

$$= \frac{1}{\rho} f + \frac{1}{\rho V_2}\left(\frac{D_3+D_4D_5}{\tilde{D}}\right) F + \frac{\rho V_2^2\tilde{D} - D_3}{\rho V_2 D_1}\left(\frac{D_1+D_2D_4}{\tilde{D}}\right) F$$

$$- \frac{q}{\rho k}\left(\frac{\rho V_2^2\tilde{D} - D_3}{D_1}\right) \qquad \text{along } \frac{dx}{dt} = V_2\ ; \tag{5.8b}$$

$$\frac{dv}{dt} + \left(\frac{1}{\rho V_2}\right)\frac{d\sigma}{dt} - \left(\frac{\rho V_2^2\tilde{D} - D_3}{\rho V_2 D_1}\right)\frac{d\theta}{dt} + \frac{\tau_0}{\rho k}\left(\frac{\rho V_2^2\tilde{D} - D_3}{D_1}\right)\frac{dq}{dt}$$

$$= \frac{1}{\rho} f - \frac{1}{\rho V_2}\left(\frac{D_3 + D_4 D_5}{\tilde{D}}\right) F - \frac{\rho V_2^2\tilde{D} - D_3}{\rho V_2 D_1}\left(\frac{D_1 + D_2 D_4}{\tilde{D}}\right) F$$

$$- \frac{q}{\rho k}\left(\frac{\rho V_2^2\tilde{D} - D_3}{D_1}\right) \qquad \text{along } \frac{dx}{dt} = -V_2 \; ; \qquad (5.8c)$$

$$\frac{dv}{dt} - \left(\frac{1}{\rho V_3}\right)\frac{d\sigma}{dt} + \left(\frac{\rho V_3^2\tilde{D} - D_3}{\rho V_3 D_1}\right)\frac{d\theta}{dt} + \frac{\tau_0}{\rho k}\left(\frac{\rho V_3^2\tilde{D} - D_3}{D_1}\right)\frac{dq}{dt}$$

$$= \frac{1}{\rho} f + \frac{1}{\rho V_3}\left(\frac{D_3 + D_4 D_5}{\tilde{D}}\right) F + \frac{\rho V_3^2\tilde{D} - D_3}{\rho V_3 D_1}\left(\frac{D_1 + D_2 D_4}{\tilde{D}}\right) F$$

$$- \frac{q}{\rho k}\left(\frac{\rho V_3^2\tilde{D} - D_3}{D_1}\right) \qquad \text{along } \frac{dx}{dt} = V_3 \; ; \qquad (5.8d)$$

$$\frac{dv}{dt} + \left(\frac{1}{\rho V_3}\right)\frac{d\sigma}{dt} - \left(\frac{\rho V_3^2\tilde{D} - D_3}{\rho V_3 D_1}\right)\frac{d\theta}{dt} + \frac{\tau_0}{\rho k}\left(\frac{\rho V_3^2\tilde{D} - D_3}{D_1}\right)\frac{dq}{dt}$$

$$= \frac{1}{\rho} f - \frac{1}{\rho V_3}\left(\frac{D_3 + D_4 D_5}{\tilde{D}}\right) F - \frac{\rho V_3^2\tilde{D} - D_3}{\rho V_3 D_1}\left(\frac{D_1 + D_2 D_4}{\tilde{D}}\right) F$$

$$- \frac{q}{\rho k}\left(\frac{\rho V_3^2\tilde{D} - D_3}{D_1}\right) \qquad \text{along } \frac{dx}{dt} = -V_3 \; . \qquad (5.8e)$$

The above equations are to be numerically integrated along the characteristics.

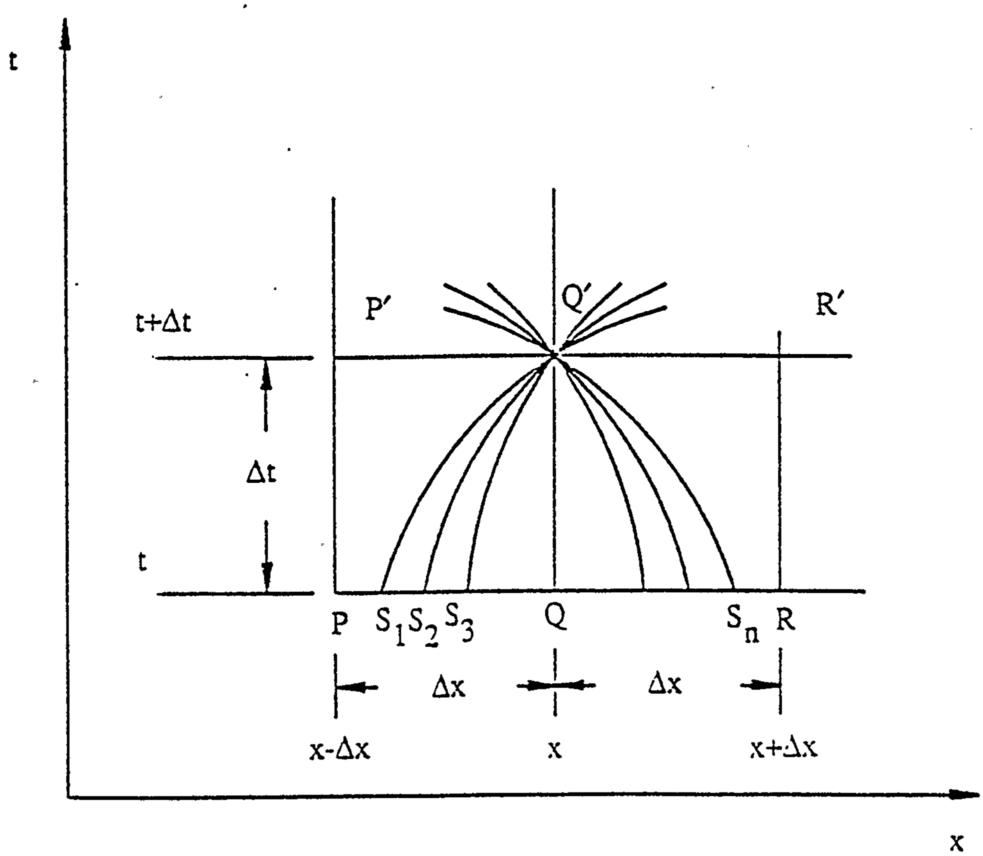

Fig. 5.1 Characteristics at a typical point Q′

5.3 Outline of the Numerical Procedure via Characteristics Method

Since solutions in closed analytical form are seldom possible for our quasi-linear system, to solve the problem we now turn to finite difference method. Among various numerical procedures of finite difference method which exist we would like to present that due to Courant *et al.*[5.12]. This method has the advantage of being straightforward and general in its application, but particularly suitable for initial-boundary value problem of quasi-linear hyperbolic system which has two independent and n dependent variables. To outline the method let us examine the representative points in the x-t plane illustrated in Fig. 5.1. Suppose the values of the vector Y at point p are denoted by Y(p), then the initial data at time t will give the values of the vectors Y(P), Y(Q), Y(R). Now it is required to determine the values of the vectors at the next moment $t+\Delta t$, that is the values of Y(P′), Y(Q′) and Y(R′). For arbitrary values of net intervals Δx, Δt the n characteristics passing through Q′ when traced backwards in time will intersect the line through PR at points $S_1,\dots,S_n$ all of which may not lie between P and R. That is, in general, line segment PR does not contain the whole domain of dependence of the point Q′. However, since the solution is required to be evaluated at the mesh points and all the initial data specified within the domain of dependence $S_1,\dots,S_n$ will influence the solution at Q′; it is clear that for simplicity Δx and Δt must be so chosen that line segment $S_1,\dots,S_n$ lies within the line segment PR. This condition is of fundamental importance and will be expressed more conveniently. Since in the finite difference approximation no knowledge of the solution between net points is available, simplification of the requirements regarding the domain of dependence of

Q' is taken as follows. The Δx and Δt are so selected that at all points of interest the tangents to the characteristics at Q' when traced backwards in time intersect the line through P and R at points always between P and R. Satisfaction of this condition ensures that the domain of dependence is contained within the segment PR. Geometrically, this condition may be conveniently expressed by :

$$\max \mid \lambda^{(i)}(Q') \mid < \frac{\Delta x}{\Delta t}, \qquad i=1,2,\ldots,n \quad . \tag{5.9}$$

for all points Q' under consideration.

Inequality (5.9) imposes an important condition which must be satisfied when net sizes are selected.

The method of Courant *et al.* was revised by M. Lister [5.5] with three obvious improvements. First, Lister introduced a second-order approximation by trapezoidal rule formula, that substantially enhanced the precision of the solution. Second, in the article particular attention was paid to the boundary points with which proper algorithm was re-developed, and third, it gave the concrete quadratic interpolation procedures matching with the second order process. To apply the procedures to the present problem let us begin with the interior points.

5.4 Algorithms for the Interior Grid Points by Characteristics Method

Now let us consider an interior grid point P shown in Fig. 5.2 where C_1 is the characteristics curve corresponding to $\lambda^{(1)}$. The intersect of C_1 with axis x is denoted by C. C_2^+, C_2^-, C_4^+, C_4^- are the characteristics curves passing through point P. These curves corresponding to $\lambda^{(2)}$, $\lambda^{(3)}$, $\lambda^{(4)}$, $\lambda^{(5)}$ intersect the x-axis at S_2, S_3, S_4 and S_5

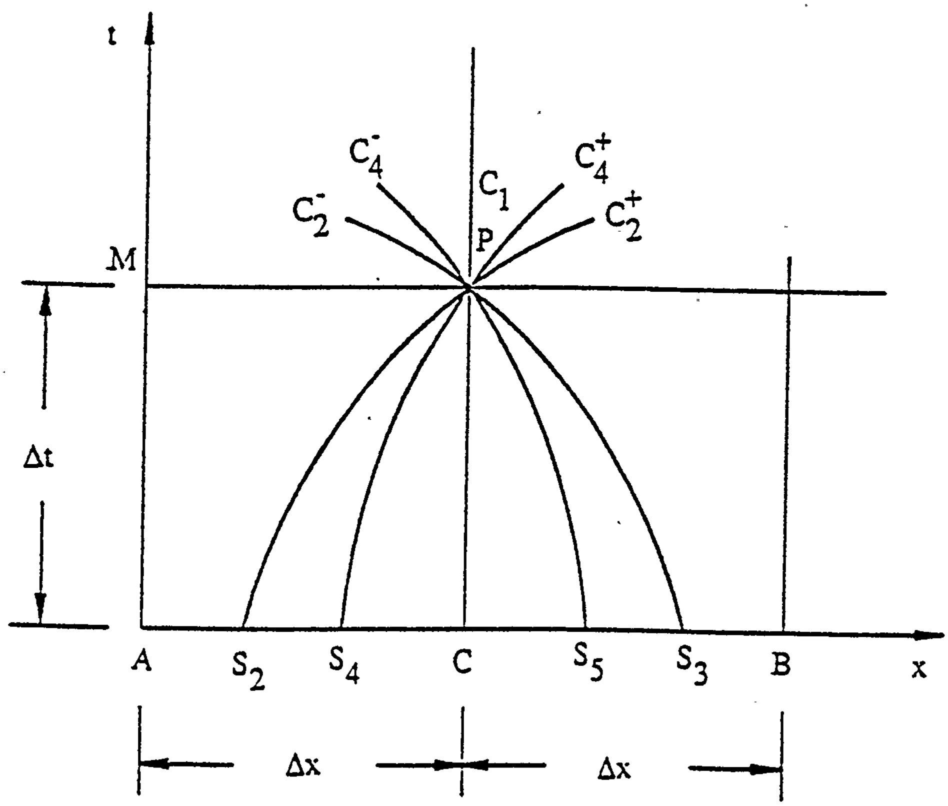

Fig 5.2 A typical interior grid point P

respectively. Our grid size is so designed by taking inequality (5.9) into account, which guarantees that the points S_2, S_3, S_4 and S_5 are within the segment AB. In section 5.2 the ordinary differential equations (5.8) which hold along C_2^+, C_2^-, C_4^+, C_4^- and C_1 have been established. Now the solution at point P is to be obtained by the numerical integration of equations (5.8) and taking into account the values at points S_2, S_3, S_4, S_5 and C. It will generate five simultaneous equations which are just enough for the solution of the five unknowns, v, σ, θ, q and p.

Along each characteristics line the integral can be approximated with finite difference. The first-order approximation is expressed as:

$$\int_{x_0}^{x_1} f(x)\, dx = f(x_0)(x_1 - x_0) \quad , \tag{5.10}$$

which is equivalent to supposing that the integrand keeps its value at x_0. The second-order approximation is:

$$\int_{x_0}^{x_1} f(x)\, dx = \frac{1}{2}\,[f(x_0) + f(x_1)](x_1 - x_0) \quad , \tag{5.11}$$

which is equivalent to assuming the integrand is the average value at x_0 and x_1.

If, say, equation (5.11) is employed to evaluate the integral from S_2, S_3, S_4, S_5 or C, the values of dependent variables at S_2, S_3, S_4, S_5 must be known. However, for an interior point like P, all the information available is at the points A, B and C, obtainable either from previous step of calculation or initial condition assigned beforehand. To make the values of dependent variables at points S_2, S_3, S_4 and S_5 available a quadratic interpolation procedure as follows is utilized [5.5],

$$\underset{\sim}{Y}^{(k+1)}_{S_2} = \underset{\sim}{Y}_C + \frac{1}{4}\,\alpha\,(\underset{\sim}{Y}_A - \underset{\sim}{Y}_B)(V^{(k)}_{2S_2} + V^{(k)}_{2P})$$

$$+ \frac{1}{8}\,\alpha^2(\underset{\sim}{Y}_A + \underset{\sim}{Y}_B - 2\,\underset{\sim}{Y}_c)(V^{(k)}_{2S_2} + V^{(k)}_{2P})^2 \quad ; \qquad (5.12a)$$

$$\underset{\sim}{Y}^{(k+1)}_{S_4} = \underset{\sim}{Y}_C + \frac{1}{4}\,\alpha\,(\underset{\sim}{Y}_A - \underset{\sim}{Y}_B)(V^{(k)}_{3S_4} + V^{(k)}_{3P})$$

$$+ \frac{1}{8}\,\alpha^2(\underset{\sim}{Y}_A + \underset{\sim}{Y}_B - 2\,\underset{\sim}{Y}_c)(V^{(k)}_{3S_4} + V^{(k)}_{3P})^2 \quad ; \qquad (5.12b)$$

$$\underset{\sim}{Y}^{(k+1)}_{S_5} = \underset{\sim}{Y}_C - \frac{1}{4}\,\alpha\,(\underset{\sim}{Y}_A - \underset{\sim}{Y}_B)(V^{(k)}_{3S_5} + V^{(k)}_{3P})$$

$$+ \frac{1}{8}\,\alpha^2(\underset{\sim}{Y}_A + \underset{\sim}{Y}_B - 2\,\underset{\sim}{Y}_c)(V^{(k)}_{3S_5} + V^{(k)}_{3P})^2 \quad ; \qquad (5.12c)$$

$$\underset{\sim}{Y}^{(k+1)}_{S_3} = \underset{\sim}{Y}_C - \frac{1}{4}\,\alpha\,(\underset{\sim}{Y}_A - \underset{\sim}{Y}_B)(V^{(k)}_{2S_3} + V^{(k)}_{2P})$$

$$+ \frac{1}{8}\,\alpha^2(\underset{\sim}{Y}_A + \underset{\sim}{Y}_B - 2\,\underset{\sim}{Y}_c)(V^{(k)}_{2S_3} + V^{(k)}_{2P})^2 \quad ; \qquad (5.12d)$$

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

Before going any further, for the reason of convenience let us change the equations (5.8) into following forms:

$$\frac{dp}{dt} = F \qquad \text{along } \frac{dx}{dt} = 0 \ ; \tag{5.13a}$$

$$R_1\frac{dv}{dt} - R_2\frac{d\sigma}{dt} + R_3\frac{d\theta}{dt} + R_4\frac{dq}{dt} = R_7 F - R_6 q + R_5 f \tag{5.13b}$$

$$\text{along } \frac{dx}{dt} = V_2 \ ;$$

$$R_1\frac{dv}{dt} + R_2\frac{d\sigma}{dt} - R_3\frac{d\theta}{dt} + R_4\frac{dq}{dt} = -R_7 F - R_6 q + R_5 f \tag{5.13c}$$

$$\text{along } \frac{dx}{dt} = -V_2 \ ;$$

$$W_1\frac{dv}{dt} - W_2\frac{d\sigma}{dt} + W_3\frac{d\theta}{dt} + W_4\frac{dq}{dt} = W_7 F - W_6 q + W_5 f \tag{5.13d}$$

$$\text{along } \frac{dx}{dt} = V_3 \ ;$$

$$W_1\frac{dv}{dt} + W_2\frac{d\sigma}{dt} - W_3\frac{d\theta}{dt} + W_4\frac{dq}{dt} = -W_7 F - W_6 q + W_5 f \tag{5.13e}$$

$$\text{along } \frac{dx}{dt} = -V_3 \ ;$$

where the coefficients are defined as follows

$$R_1 = \rho V_2 D_1 \tilde{D} \ , \tag{5.14a}$$

$$R_2 = D_1 \tilde{D} \ , \tag{5.14b}$$

$$R_3 = \tilde{D}\,(\rho V_2^2\,\tilde{D} - D_3)\ , \tag{5.14c}$$

$$R_4 = \frac{\tau_0 V_2 \tilde{D}}{k}\,(\rho V_2^2 \tilde{D} - D_3)\ , \tag{5.14d}$$

$$R_5 = V_2 D_1 \tilde{D}\ , \tag{5.14e}$$

$$R_6 = \frac{R_4}{\tau_0}\ , \tag{5.14f}$$

$$R_7 = D_1(D_3 + D_4 D_5) + (D_1 + D_2 D_4)(\rho V_2^2 \tilde{D} - D_3)\ ; \tag{5.14g}$$

and

$$W_1 = \rho V_3 D_1 \tilde{D}\ , \tag{5.15a}$$

$$W_2 = D_1 \tilde{D}\ , \tag{5.15b}$$

$$W_3 = \tilde{D}\,(\rho V_3^2 \tilde{D} - D_3)\ , \tag{5.15c}$$

$$W_4 = \frac{\tau_0 V_3 \tilde{D}}{k}\,(\rho V_3^2 \tilde{D} - D_3)\ , \tag{5.15d}$$

$$W_5 = V_3^2 D_1 \tilde{D}\ , \tag{5.15e}$$

$$W_6 = \frac{W_4}{\tau_0}\ , \tag{5.15f}$$

$$W_7 = D_1(D_3 + D_4 D_5) + (D_1 + D_2 D_4)(\rho V_3^2 \tilde{D} - D_3)\ . \tag{5.15g}$$

To obtain a discrete form of differential equations (5.13) let us apply the finite difference method of second-order approximation, equation (5.11), which is equivalent to assuming that the coefficients of equation (5.13) remain constant along each segment of the characteristics curves such as S_2P, S_3P, S_4P or S_5P, and the value of the coefficient equals the average value at the two points such as S_2 and P, *etc.* Then the equations to be integrated are reduced to the following finite-difference forms:

$$p_P^{(k+1)} = p_C + \frac{1}{2}(F_C + F_P)\,\Delta t \quad , \tag{5.16a}$$

$$\begin{aligned}
&({}^1R_{S2}^{(k)} + R_{1P}^{(k)})\,v_P^{(k+1)} - ({}^2R_{S2}^{(k)} + R_{2P}^{(k)})\sigma_P^{(k+1)} + ({}^3R_{S2}^{(k)} + R_{3P}^{(k)})\theta_P^{(k+1)} \\
&+ ({}^4R_{S2}^{(k)} + R_{4P}^{(k)})q_P^{(k+1)} = ({}^1R_{S2}^{(k)} + R_{1P}^{(k)})\,v_{S2}^{(k)} - ({}^2R_{S2}^{(k)} + R_{2P}^{(k)})\sigma_{S2}^{(k)} \\
&+ ({}^3R_{S2}^{(k)} + R_{3P}^{(k)})\theta_{S2}^{(k)} + ({}^4R_{S2}^{(k)} + R_{4P}^{(k)})q_{S2}^{(k)} + \{(R_5\, f)_{S2}^{(k)} + (R_5\, f)_P^{(k)} \\
&- (R_6 q)_{S2}^{(k)} - (R_6\, q)_P^{(k)} + (R_7\, F)_{S2}^{(k)} + (R_7\, F)_P^{(k)}\}\,\Delta t \quad ,
\end{aligned} \tag{5.16b}$$

$$\begin{aligned}
&({}^1R_{S3}^{(k)} + R_{1P}^{(k)})\,v_P^{(k+1)} + ({}^2R_{S3}^{(k)} + R_{2P}^{(k)})\sigma_P^{(k+1)} - ({}^3R_{S3}^{(k)} + R_{3P}^{(k)})\theta_P^{(k+1)} \\
&+ ({}^4R_{S3}^{(k)} + R_{4P}^{(k)})q_P^{(k+1)} = ({}^1R_{S3}^{(k)} + R_{1P}^{(k)})\,v_{S3}^{(k)} + ({}^2R_{S3}^{(k)} + R_{2P}^{(k)})\sigma_{S3}^{(k)} \\
&- ({}^3R_{S3}^{(k)} + R_{3P}^{(k)})\theta_{S3}^{(k)} + ({}^4R_{S3}^{(k)} + R_{4P}^{(k)})q_{S3}^{(k)} + \{(R_5\, f)_{S3}^{(k)} + (R_5\, f)_P^{(k)} \\
&- (R_6 q)_{S3}^{(k)} - (R_6\, q)_P^{(k)} - (R_7\, F)_{S3}^{(k)} - (R_7\, F)_P^{(k)}\}\,\Delta t \quad ,
\end{aligned} \tag{5.16c}$$

$$({}^{1}W_{S4}^{(k)} + W_{1P}^{(k)})\, v_{P}^{(k+1)} - ({}^{2}W_{S4}^{(k)} + W_{2P}^{(k)})\sigma_{P}^{(k+1)} + ({}^{3}W_{S4}^{(k)} + W_{3P}^{(k)})\theta_{P}^{(k+1)}$$

$$+ ({}^{4}W_{S4}^{(k)} + W_{4P}^{(k)})q_{P}^{(k+1)} = ({}^{1}W_{S4}^{(k)} + W_{1P}^{(k)})v_{S4}^{(k)} - ({}^{2}W_{S4}^{(k)} + W_{2P}^{(k)})\sigma_{S4}^{(k)}$$

$$+ ({}^{3}W_{S4}^{(k)} + W_{3P}^{(k)})\theta_{S4}^{(k)} + ({}^{4}W_{S4}^{(k)} + W_{4P}^{(k)})q_{S4}^{(k)} + \{(W_5\, f)_{S4}^{(k)} + (W_5\, f)_{P}^{(k)}$$

$$- (W_6 q)_{S4}^{(k)} - (W_6\, q)_{P}^{(k)} + (W_7\, F)_{S4}^{(k)} + (W_7\, F)_{P}^{(k)}\}\ \Delta t\ , \tag{5.16d}$$

$$({}^{1}W_{S5}^{(k)} + W_{1P}^{(k)})\, v_{P}^{(k+1)} + ({}^{2}W_{S5}^{(k)} + W_{2P}^{(k)})\sigma_{P}^{(k+1)} - ({}^{3}W_{S5}^{(k)} + W_{3P}^{(k)})\theta_{P}^{(k+1)}$$

$$+ ({}^{4}W_{S5}^{(k)} + W_{4P}^{(k)})q_{P}^{(k+1)} = ({}^{1}W_{S5}^{(k)} + W_{1P}^{(k)})v_{S5}^{(k)} + ({}^{2}W_{S5}^{(k)} + W_{2P}^{(k)})\sigma_{S5}^{(k)}$$

$$- ({}^{3}W_{S5}^{(k)} + W_{3P}^{(k)})\theta_{S5}^{(k)} + ({}^{4}W_{S5}^{(k)} + W_{4P}^{(k)})q_{S5}^{(k)} + \{(W_5\, f)_{S5}^{(k)} + (W_5\, f)_{P}^{(k)}$$

$$- (W_6\, q)_{S5}^{(k)} - (W_6\, q)_{P}^{(k)} - (W_7\, F)_{S5}^{(k)} - (W_7\, F)_{P}^{(k)}\}\ \Delta t\ , \tag{5.16e}$$

where, for instance, ${}^{i}R_{Sj}^{(k)}$ stands for the value of R_i defined by equation (5.14) at point S_j during the kth iteration; ${}^{i}W_{jP}^{(k)}$ stands for the value of W_i defined by equation (5.15) at point j_p during the kth iteration, and so forth.

The values of the unknowns at point P, *e.g.* v_P, σ_P, θ_P and q_P are to be obtained from the above equations. Because of the non-linear nature of the system of equations, the coefficients of equations (5.16) remain unknown until the unknowns′ values v_P, σ_P,... are obtained. To be out of the dilemma and get the discrete equations solved, an iteration procedure is required. For initiating the iteration the initial values of the unknowns are needed. As a first order approximation it may be assumed that the values of the coefficients along the segments of the characteristics curves are the same as those at points S_2, S_4, C, S_5 and S_3. This simply means equation (5.10) is being utilized. By doing so the initial values of the unknowns for iteration can be obtained from the solution of the following equations:

$$p_P^{(0)} = p_C + F_C \Delta t \ , \tag{5.17a}$$

$${}^1R_{S2}^{(0)} v_P^{(0)} - {}^2R_{S2}\sigma_P^{(0)} + {}^3R_{S2}^{(0)}\theta_P^{(0)} + {}^4R_{S2}^{(0)} q_P^{(0)} = {}^1\Lambda_{S2} + {}^2\Lambda_{S2}\Delta t \ , \tag{5.17b}$$

$${}^1R_{S3}^{(0)} v_P^{(0)} + {}^2R_{S3}\sigma_P^{(0)} - {}^3R_{S3}^{(0)}\theta_P^{(0)} + {}^4R_{S3}^{(0)} q_P^{(0)} = {}^3\Lambda_{S3} + {}^4\Lambda_{S3}\Delta t \ , \tag{5.17c}$$

$${}^1W_{S4}^{(0)} v_p^{(0)} - {}^2W_{S4}^{(0)}\sigma_P^{(0)} + {}^3W_{S4}^{(0)}\theta_P^{(0)} + {}^4W_{S4}^{(0)} q_P^{(0)} = {}^5\Lambda_{S4} + {}^6\Lambda_{S4}\Delta t \ , \tag{5.17d}$$

$${}^1W_{S5}^{(0)} v_p^{(0)} + {}^2W_{S5}^{(0)}\sigma_P^{(0)} - {}^3W_{S5}^{(0)}\theta_P^{(0)} + {}^4W_{S5}^{(0)} q_P^{(0)} = {}^7\Lambda_{S5} + {}^8\Lambda_{S5}\Delta t \ , \tag{5.17e}$$

where superscript (0) stands for "initial", and

$${}^1\Lambda_{S2} = {}^1R_{S2} v_{S2}^{(0)} - {}^2R_{S2}^{(0)}\sigma_{S2}^{(0)} + {}^3R_{S2}^{(0)}\theta_{S2}^{(0)} + {}^4R_{S2}^{(0)} q_{S2}^{0} \ , \tag{5.18a}$$

$${}^2\Lambda_{S2} = (R_5 \ f)_{S2}^{(0)} - (R_6 \ q)_{S2}^{(0)} + (R_7 \ F)_{S2}^{(0)} \ , \tag{5.18b}$$

$${}^3\Lambda_{S3} = {}^1R_{S3} v_{S3}^{(0)} + {}^2R_{S3}^{(0)}\sigma_{S3}^{(0)} - {}^3R_{S3}^{(0)}\theta_{S3}^{(0)} + {}^4R_{S3}^{(0)} q_{S3}^{0} \ , \tag{5.18c}$$

$${}^4\Lambda_{S3} = (R_5 \ f)_{S3}^{(0)} - (R_6 \ q)_{S3}^{(0)} - (R_7 \ F)_{S3}^{(0)} \ , \tag{5.18d}$$

$$ {}^{5}\Lambda_{S4} = {}^{1}W_{S4}^{(0)} v_{S4}^{(0)} - {}^{2}W_{S4}^{(0)} \sigma_{S4}^{(0)} + {}^{3}W_{S4}^{(0)} \theta_{S4}^{(0)} + {}^{4}W_{S4}^{(0)} q_{S4}^{0} \quad , \tag{5.18e} $$

$$ {}^{6}\Lambda_{S4} = (W_5\ f)_{S4}^{(0)} - (W_6\ q)_{S4}^{(0)} + (W_7\ F)_{S4}^{(0)} \quad , \tag{5.18f} $$

$$ {}^{7}\Lambda_{S5} = {}^{1}W_{S5}^{(0)} v_{S5}^{(0)} + {}^{2}W_{S5}^{(0)} \sigma_{S5}^{(0)} - {}^{3}W_{S5}^{(0)} \theta_{S5}^{(0)} + {}^{4}W_{S5}^{(0)} q_{S5}^{0} \quad , \tag{5.18g} $$

$$ {}^{8}\Lambda_{S5} = (W_5\ f)_{S5}^{(0)} - (W_6\ q)_{S5}^{(0)} + (W_7\ F)_{S5}^{(0)} \quad . \tag{5.18h} $$

The intermediate unknowns involved are obtained by the following linear interpolation equations:

$$ \underset{\sim}{Y}_{S2}^{(0)} = \underset{\sim}{Y}_C (1 - \alpha\ V_{2C}) + \alpha\ \underset{\sim}{Y}_A V_{2C} \quad , \tag{5.19a} $$

$$ \underset{\sim}{Y}_{S4}^{(0)} = \underset{\sim}{Y}_C (1 - \alpha\ V_{3C}) + \alpha\ \underset{\sim}{Y}_A V_{3C} \quad ; \tag{5.19b} $$

$$ \underset{\sim}{Y}_{S5}^{(0)} = \underset{\sim}{Y}_C (1 - \alpha\ V_{3C}) + \alpha\ \underset{\sim}{Y}_B V_{3C} \quad , \tag{5.19c} $$

$$ \underset{\sim}{Y}_{S3}^{(0)} = \underset{\sim}{Y}_C (1 - \alpha\ V_{2C}) + \alpha\ \underset{\sim}{Y}_B V_{2C} \quad . \tag{5.19d} $$

Equations (5.17) with (5.18) can be put in a matrix form :

$$ \underline{a}^{(0)} \underset{\sim}{u}_P^{(0)} = \underset{\sim}{h}^{(0)} \quad , \tag{5.20} $$

where $$ \underset{\sim}{u}_P^{(0)} = [v_P^{(0)}\ \sigma_P^{(0)}\ \theta_P^{(0)}\ q_P^{(0)}]^T \quad , \tag{5.21} $$

$$\underset{\sim}{h}^{(0)} = \begin{Bmatrix} {}^{1}\Lambda_{S2} + {}^{2}\Lambda_{S2}\,\Delta t \\ \\ {}^{3}\Lambda_{S3} + {}^{4}\Lambda_{S3}\,\Delta t \\ \\ \Lambda_{S4} + {}^{6}\Lambda_{S4}\,\Delta t \\ \\ {}^{7}\Lambda_{S5} + {}^{8}\Lambda_{S5}\,\Delta t \end{Bmatrix} \tag{5.22}$$

$$\underline{a}^{(0)} = \begin{bmatrix} {}^{1}R^{(0)}_{S2} & -{}^{2}R^{(0)}_{S2} & {}^{3}R^{(0)}_{S2} & {}^{4}R^{(0)}_{S2} \\ \\ {}^{1}R^{(0)}_{S3} & {}^{2}R^{(0)}_{S3} & -{}^{3}R^{(0)}_{S3} & {}^{4}R^{(0)}_{S3} \\ \\ {}^{1}W^{(0)}_{S4} & -{}^{2}W^{(0)}_{S4} & {}^{3}W^{(0)}_{S4} & {}^{4}W^{(0)}_{S4} \\ \\ {}^{1}W^{(0)}_{S5} & {}^{2}W^{(0)}_{S5} & -{}^{3}W^{(0)}_{S5} & {}^{4}W^{(0)}_{S5} \end{bmatrix} . \tag{5.23}$$

The solution of equations (5.20) gives us the initial values of the unknowns at an interior point P. Yet, care must be taken as the equations are ill-conditioned.

As soon as the initial values have been obtained, the main iteration equations are to be solved. They are

$$\underline{Q}^{(k)}\underset{\sim}{u}_{P}^{(k+1)} = \underset{\sim}{b}^{(k)} , \tag{5.24}$$

where $$\underset{\sim}{u}_P^{(k+1)} = [v_P^{(k+1)} \; \sigma_P^{(k+1)} \; \theta_P^{(k+1)} \; q_P^{(k+1)}]^T \quad , \tag{5.25}$$

$$Q_{11}^{(k)} = {}^1R_{S2}^{(k)} + R_{1P}^{(k)} \quad ,$$

$$Q_{12}^{(k)} = -\,({}^2R_{S2}^{(k)} + R_{2P}^{(k)}) \quad ,$$

$$Q_{13}^{(k)} = {}^3R_{S2}^{(k)} + R_{3P}^{(k)} \quad ,$$

$$Q_{14}^{(k)} = {}^4R_{S2}^{(k)} + R_{4P}^{(k)} \quad ,$$

$$Q_{21}^{(k)} = {}^1R_{S3}^{(k)} + R_{1P}^{(k)} \quad ,$$

$$Q_{22}^{(k)} = {}^2R_{S3}^{(k)} + R_{2P}^{(k)} \quad ,$$

$$Q_{23}^{(k)} = -\,({}^3R_{S3}^{(k)} + R_{3P}^{(k)}) \quad ,$$

$$Q_{24}^{(k)} = {}^4R_{S3}^{(k)} + R_{4P}^{(k)} \quad ,$$

$$Q_{31}^{(k)} = {}^1W_{S4}^{(k)} + W_{1P}^{(k)} \quad ,$$

$$Q_{32}^{(k)} = -\,({}^2W_{S4}^{(k)} + W_{2P}^{(k)}) \quad ,$$

$$Q_{33}^{(k)} = {}^3W_{S4}^{(k)} + W_{3P}^{(k)} \quad ,$$

$$Q_{34}^{(k)} = {}^4W_{S4}^{(k)} + W_{4P}^{(k)} \quad ,$$

$$Q_{41}^{(k)} = {}^{1}W_{S5}^{(k)} + W_{1P}^{(k)} \quad ,$$

$$Q_{42}^{(k)} = {}^{2}W_{S5}^{(k)} + W_{2P}^{(k)} \quad ,$$

$$Q_{43}^{(k)} = -\,({}^{3}W_{S5}^{(k)} + W_{3P}^{(k)}) \quad ,$$

$$Q_{44}^{(k)} = {}^{4}W_{S5}^{(k)} + W_{4P}^{(k)} \quad , \qquad (5.26a - p)$$

and

$$\begin{aligned} b_{1}^{(k)} = {} & ({}^{1}R_{S2}^{(k)} + R_{1P}^{(k)})\ v_{S2}^{(k)} - ({}^{2}R_{S2}^{(k)} + R_{2P}^{(k)})\ \sigma_{S2}^{(k)} \\ & + ({}^{3}R_{S2}^{(k)} + R_{3P}^{(k)})\ \theta_{S2}^{(k)} + ({}^{4}R_{S2}^{(k)} + R_{4P}^{(k)})\ q_{S2}^{(k)} \\ & + \{(R_5\ f)_{S2}^{(k)} + (R_5\ f)_{P}^{(k)} - (R_6\ q)_{S2}^{(k)} - (R_6\ q)_{P}^{(k)} \\ & + (R_7\ F)_{S2}^{(k)} + (R_7\ F)_{P}^{(k)}\}\ \Delta t \quad , \end{aligned} \qquad (5.27a)$$

$$\begin{aligned} b_{2}^{(k)} = {} & ({}^{1}R_{S3}^{(k)} + R_{1P}^{(k)})\ v_{S3}^{(k)} + ({}^{2}R_{S3}^{(k)} + R_{2P}^{(k)})\ \sigma_{S3}^{(k)} \\ & - ({}^{3}R_{S3}^{(k)} + R_{3P}^{(k)})\ \theta_{S3}^{(k)} + ({}^{4}R_{S3}^{(k)} + R_{4P}^{(k)})\ q_{S3}^{(k)} \\ & + \{(R_5\ f)_{S3}^{(k)} + (R_5\ f)_{P}^{(k)} - (R_6\ q)_{S3}^{(k)} - (R_6\ q)_{P}^{(k)} \\ & - (R_7\ F)_{S3}^{(k)} - (R_7\ F)_{P}^{(k)}\}\ \Delta t \quad , \end{aligned} \qquad (5.27b)$$

$$b_3^{(k)} = ({}^1W_{S4}^{(k)} + W_{1P}^{(k)})\, v_{S4}^{(k)} - ({}^2W_{S4}^{(k)} + W_{2P}^{(k)})\, \sigma_{S4}^{(k)}$$

$$+ ({}^3W_{S4}^{(k)} + W_{3P}^{(k)})\, \theta_{S4}^{(k)} + ({}^4W_{S4}^{(k)} + W_{4P}^{(k)})\, q_{S4}^{(k)}$$

$$+ \{(W_5\, f)_{S4}^{(k)} + (W_5\, f)_P^{(k)} - (W_6\, q)_{S4}^{(k)} - (W_6\, q)_P^{(k)}$$

$$+ (W_7\, F)_{S4}^{(k)} + (W_7\, F)_P^{(k)}\}\, \Delta t \quad , \tag{5.27c}$$

$$b_4^{(k)} = ({}^1W_{S5}^{(k)} + W_{1P}^{(k)})\, v_{S5}^{(k)} + ({}^2W_{S5}^{(k)} + W_{2P}^{(k)})\, \sigma_{S5}^{(k)}$$

$$- ({}^3W_{S5}^{(k)} + W_{3P}^{(k)})\, \theta_{S5}^{(k)} + ({}^4W_{S5}^{(k)} + W_{4P}^{(k)})\, q_{S5}^{(k)}$$

$$+ \{(W_5\, f)_{S5}^{(k)} + (W_5\, f)_P^{(k)} - (W_6\, q)_{S5}^{(k)} - (W_6\, q)_P^{(k)}$$

$$- (W_7\, F)_{S5}^{(k)} - (W_7\, F)_P^{(k)}\}\, \Delta t \quad . \tag{5.27d}$$

At any interior point like P equations (5.24) are solved iteratively until the precision requirement is satisfied.

5.5 Algorithms for the Boundary Grid Points by Characteristics Method

In Fig.5.3 a boundary point M with characteristics passing through is shown. It is clear that the situation for a typical boundary point like M is different from that of an interior point, therefore, the treatments for the two types of points must be different as well. Generally, for determination of the solution of the system some auxiliary conditions must be prescribed on the boundary. In this research they are considered as follows.

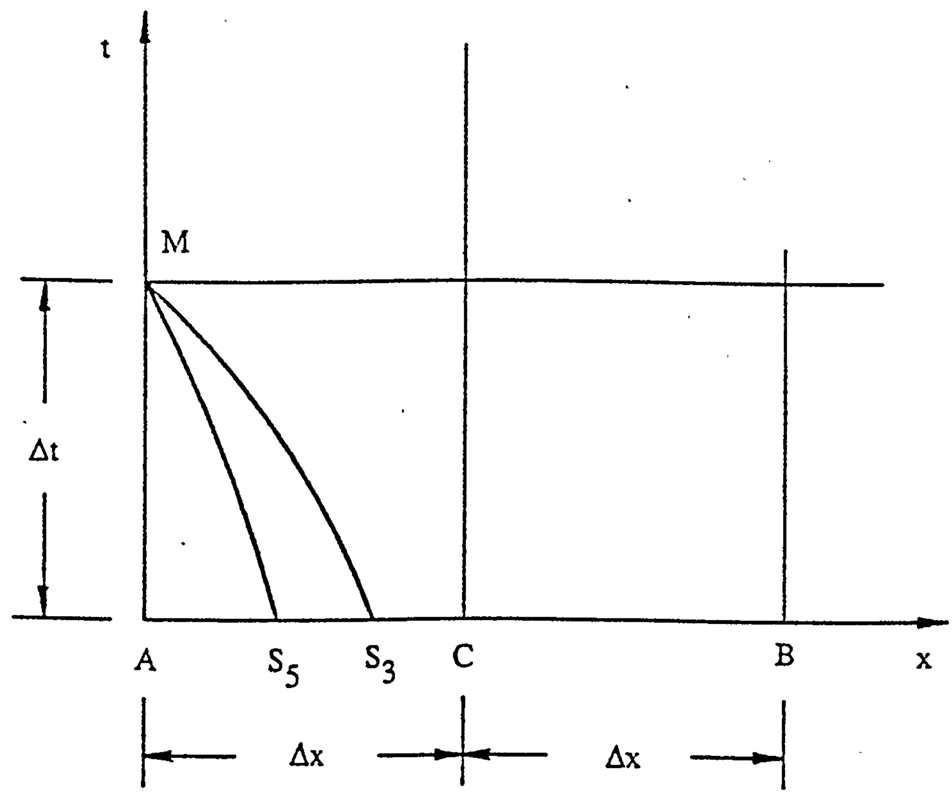

Fig.5.3 A boundary grid point M

Case (A): $\sigma(0,t)$ and $\theta(0,t)$ prescribed

Due to the non-linearity of the system, the solution at boundary points as well as at interior points requires iterative procedures. For the initial values of iteration the intermediate unknowns are obtained from the linear interpolation formulas:

$$\underset{\sim}{Y}_{S5}^{(0)} = \underset{\sim}{Y}_A(1 - \alpha V_{3A}) + \alpha \underset{\sim}{Y}_C V_{3A} , \tag{5.28a}$$

$$\underset{\sim}{Y}_{S3}^{(0)} = \underset{\sim}{Y}_A(1 - \alpha V_{2A}) + \alpha \underset{\sim}{Y}_C V_{3A} . \tag{5.28b}$$

Re-examination of equations (5.16c) and (5.16e) gives the following equations for determining the initial values of the unknowns at a boundary point:

$$\begin{aligned} {}^1R_{S3}^{(0)} v_M^{(0)} + {}^4R_{S3}^{(0)} q_M^{(0)} &= ({}^3\Lambda_{S3}^{(0)} + {}^4\Lambda_{S3}^{(0)} \Delta t \\ &- {}^2R_{S3}^{(0)} \sigma_M + {}^3R_{S3}^{(0)} \theta_M) , \end{aligned} \tag{5.29a}$$

$$\begin{aligned} {}^1W_{S5}^{(0)} v_M^{(0)} + {}^4W_{S5}^{(0)} q_M^{(0)} &= ({}^7\Lambda_{S5}^{(0)} + {}^8\Lambda_{S5}^{(0)} \Delta t \\ &- {}^2W_{S5}^{(0)} \sigma_M + {}^3W_{S5}^{(0)} \theta_M) . \end{aligned} \tag{5.29b}$$

The solutions of equations (5.29) generate $v_M^{(0)}$ and $q_M^{(0)}$, the initial values of velocity and heat flow supplementary to stress and temperature which are already prescribed.

As soon as the initial values of the unknowns are obtained, the main iteration procedure may be executed as follows.

At first the intermediate unknowns are determined via the three-point quadratic interpolation formulas:

$$\underset{\sim}{Y}_{S5}^{(k+1)} = \underset{\sim}{Y}_C - \frac{1}{4}(\underset{\sim}{Y}_A - \underset{\sim}{Y}_B)\{\alpha(V_{3S5}^{(k)} + V_{3M}^{(k)}) - 2\}$$

$$+ \frac{1}{8}(\underset{\sim}{Y}_A + \underset{\sim}{Y}_B - 2\underset{\sim}{Y}_C)\{\alpha(V_{3S5}^{(k)} + V_{3M}^{(k)}) - 2\}^2 \quad , \tag{5.30a}$$

$$\underset{\sim}{Y}_{S3}^{(k+1)} = \underset{\sim}{Y}_C - \frac{1}{4}(\underset{\sim}{Y}_A - \underset{\sim}{Y}_B)\{\alpha(V_{2S3}^{(k)} + V_{2M}^{(k)}) - 2\}$$

$$+ \frac{1}{8}(\underset{\sim}{Y}_A + \underset{\sim}{Y}_B - 2\underset{\sim}{Y}_C)\{\alpha(V_{2S3}^{(k)} + V_{2M}^{(k)}) - 2\}^2 \quad . \tag{5.30b}$$

The equations for the iterative values of v_M and q_M are of the form:

$$({}^1R_{S3}^{(k)} + R_{1M}^{(k)})v_M^{(k+1)} + ({}^4R_{S3}^{(k)} + R_{4M}^{(k)})q_M^{(k+1)} =$$

$$({}^3R_{S3}^{(k)} + R_{3M}^{(k)})\theta_M - ({}^2R_{S3}^{(k)} + R_{2M}^{(k)})\sigma_M$$

$$+ ({}^1R_{S3}^{(k)} + R_{1M}^{(k)})V_{S3}^{(k)} + ({}^2R_{S3}^{(k)} + R_{2M}^{(k)})\sigma_{S3}^{(k)}$$

$$-({}^3R_{S3}^{(k)} + R_{3M}^{(k)})\theta_{S3}^{(k)} + ({}^4R_{S3}^{(k)} + R_{4M}^{(k)})q_{S3}^{(k)}$$

$$+\{(R_5\ f)^{(k)}_{S3} + (R_5\ f)^{(k)}_{M} - (R_6\ q)^{(k)}_{S3}$$

$$-(R_6\ q)^{(k)}_{M} - (R_7\ F)^{(k)}_{S3} - (R_7\ F)^{(k)}_{M}\}\ \Delta t \quad , \tag{5.31a}$$

$$({}^1W^{(k)}_{S5} + W^{(k)}_{1M})v^{(k+1)}_{M} + ({}^4W^{(k)}_{S5} + W^{(k)}_{4M})q^{(k+1)}_{M} =$$

$$({}^3W^{(k)}_{S5} + W^{(k)}_{3M})\theta_M - ({}^2W^{(k)}_{S5} + W^{(k)}_{2M})\sigma_M$$

$$+ ({}^1W^{(k)}_{S5} + W^{(k)}_{1M})V^{(k)}_{S5} + ({}^2W^{(k)}_{S5} + W^{(k)}_{2M})\sigma^{(k)}_{S5}$$

$$-({}^3W^{(k)}_{S5} + W^{(k)}_{3M})\theta^{(k)}_{S3} + ({}^4W^{(k)}_{S5} + W^{(k)}_{4M})q^{(k)}_{S5}$$

$$+\{(W_5\ f)^{(k)}_{S5} + (W_5\ f)^{(k)}_{M} - (W_6\ q)^{(k)}_{S5}$$

$$-(W_6\ q)^{(k)}_{M} - (W_7\ F)^{(k)}_{S5} - (W_7\ F)^{(k)}_{M}\}\ \Delta t \quad . \tag{5.31b}$$

Equations (5.29) may be written in the matrix form as

$$\underset{=}{a}{}^{(k)}_{g}\ \underset{\sim}{a}{}^{(k+1)}_{rm} = \underset{\sim}{a}{}^{(k)}_{w} \quad , \tag{5.32}$$

where

$$\underset{\sim}{a}_{rm} = [\ v_M \quad q_M\ ]^T \tag{5.33a}$$

$$a^{(k)}_{g11} = {}^1R^{(k)}_{S3} + R^{(k)}_{1M} \tag{5.33b}$$

$$a^{(k)}_{g12} = {}^4R^{(k)}_{S3} + R^{(k)}_{4M} \tag{5.33c}$$

$$a_{g21}^{(k)} = {}^{1}W_{S5}^{(k)} + W_{1M}^{(k} \tag{5.33d}$$

$$a_{g22}^{(k)} = {}^{4}W_{S5}^{(k)} + W_{4M}^{(k)} \quad , \tag{5.33e}$$

$$\begin{aligned} a_{w1}^{(k)} = & ({}^{3}R_{S3}^{(k)} + R_{3M}^{(k)})\theta_M - ({}^{2}R_{S3}^{(k)} + R_{2M}^{(k)})\sigma_M \\ & +({}^{1}R_{S3}^{(k)} + R_{1M}^{(k)})v_{S3}^{(k)} + ({}^{2}R_{S3}^{(k)} + R_{2M}^{(k)})\sigma_{S3}^{(k)} \\ & -({}^{3}R_{S3}^{(k)} + R_{3M}^{(k)})\theta_{S3}^{(k)} + ({}^{4}R_{S3}^{(k)} + R_{4M}^{(k)})q_{S3}^{(k)} \\ & +\{(R_5\ f)_{S3}^{(k)} + (R_5\ f)_M^{(k)} - (R_6\ q)_{S3}^{(k)} \\ & -(R_6\ q)_M^{(k)} - (R_7\ F)_{S3}^{(k)} - (R_7\ F)_M^{(k)}\}\ \Delta t \quad , \end{aligned} \tag{5.33f}$$

$$\begin{aligned} a_{w2}^{(k)} = & ({}^{3}W_{S5}^{(k)} + W_{3M}^{(k)})\theta_M - ({}^{2}W_{S5}^{(k)} + W_{2M}^{(k)})\sigma_M \\ & +({}^{1}W_{S5}^{(k)} + W_{1M}^{(k)})v_{S5}^{(k)} + ({}^{2}W_{S5}^{(k)} + W_{2M}^{(k)})\sigma_{S5}^{(k)} \\ & -({}^{3}W_{S5}^{(k)} + W_{3M}^{(k)})\theta_{S5}^{(k)} + ({}^{4}W_{S5}^{(k)} + W_{4M}^{(k)})q_{S5}^{(k)} \\ & +\{(W_5\ f)_{S5}^{(k)} + (W_5\ f)_M^{(k)} - (W_6\ q)_{S5}^{(k)} \\ & -(W_6\ q)_M^{(k)} - (W_7\ F)_{S5}^{(k)} - (W_7\ F)_M^{(k)}\}\ \Delta t \quad . \end{aligned} \tag{5.33g}$$

Equations (5.32) are to be solved for every iteration to obtain the values of $v_M^{(k+1)}$ and $q_M^{(k+1)}$. The procedure is continued until a satisfactory solution is obtained.

Case (B): v(0,t) and θ(0,t) prescribed

When the particle velocity and the temperature are prescribed on the boundary grid points, the solution procedure is similar to Case (A) where the stress and temperature are given.

The intermediate values are evaluated from the following linear interpolation formulas:

$$\underset{\sim}{Y}_{S5}^{(0)} = \underset{\sim}{Y}_A(1 - \alpha V_{3A}) + \alpha \underset{\sim}{Y}_c V_{3A} \quad , \tag{5.34a}$$

$$\underset{\sim}{Y}_{S3}^{(0)} = \underset{\sim}{Y}_A(1 - \alpha V_{2A}) + \alpha \underset{\sim}{Y}_c V_{2A} \quad . \tag{5.34b}$$

The values of the unknowns for initiating the iterative procedure are determined from the following set of linear equations:

$$\begin{aligned}{}^2R_{S3}^{(0)}\sigma_M^{(0)} - {}^4R_{S3}^{(0)}q_M^{(0)} &= {}^3R_{S3}^{(0)}\theta_M - {}^1R_{S3}^{(0)}v_M \\ &+ {}^1R_{S3}^{(0)}v_{S3}^{(0)} + {}^2R_{S3}^{(0)}\sigma_{S3}^{(0)} - {}^3R_{S3}^{(0)}\theta_{S3}^{(0)} + {}^4R_{S3}^{(0)}q_{S3}^{(0)} \\ &+ \{(R_5\ f)_{S3}^{(0)} - (R_6\ q)_{S3}^{(0)} - (R_7\ F)_{S3}^{(0)}\}\ \Delta t \quad ,\end{aligned} \tag{5.35a}$$

$$\begin{aligned}{}^2W_{S5}^{(0)}\sigma_M^{(0)} - {}^4W_{S5}^{(0)}q_M^{(0)} &= {}^3W_{S5}^{(0)}\theta_M - {}^1W_{S5}^{(0)}v_M \\ &+ {}^1W_{S5}^{(0)}v_{S5}^{(0)} + {}^2W_{S5}^{(0)}\sigma_{S5}^{(0)} - {}^3W_{S5}^{(0)}\theta_{S5}^{(0)} + {}^4W_{S5}^{(0)}q_{S5}^{(0)} \\ &+ \{(W_5\ f)_{S5}^{(0)} - (W_6\ q)_{S5}^{(0)} - (W_7\ F)_{S5}^{(0)}\}\ \Delta t \quad .\end{aligned} \tag{5.35b}$$

As soon as the values of $\sigma_M^{(0)}$ and $q_M^{(0)}$ have been obtained from the solution of equations (5.35) we are ready to run the main iteration for evaluating the values of σ_M and q_M. For the main iteration the intermediate unknowns are obtained by the three-point quadratic interpolation formulas, equations (5.30). Then the main iteration based on equations (5.16c) and (5.16e) are expressed in the matrix form as

$$\underline{b}_g^{(k)} \; \underset{\sim}{b}_{rm}^{(k+1)} = \underset{\sim}{b}_w^{(k)} \quad , \tag{5.36}$$

where

$$\underset{\sim}{b}_{rm}^{(k)} = [\sigma_M^{(k+1)} \quad q_M^{(k+1)}]^T \quad , \tag{5.37a}$$

$$b_{g11}^{(k)} = {}^2R_{S3}^{(k)} + R_{2M}^{(k)} \quad , \tag{5.37b}$$

$$b_{g12}^{(k)} = {}^4R_{S3}^{(k)} + R_{4M}^{(k)} \quad , \tag{5.37c}$$

$$b_{g21}^{(k)} = {}^2W_{S5}^{(k)} + W_{2M}^{(k)} \quad , \tag{5.37d}$$

$$b_{g22}^{(k)} = {}^4W_{S5}^{(k)} + W_{4M}^{(k)} \quad , \tag{5.38e}$$

$$b_{w1}^{(k)} = ({}^3R_{S3}^{(k)} + R_{3M}^{(k)})\theta_M - ({}^1R_{S3}^{(k)} + R_{1M}^{(k)})v_M$$

$$+({}^1R_{S3}^{(k)} + R_{1M}^{(k)})v_{S3}^{(k)} + ({}^2R_{S3}^{(k)} + R_{2M}^{(k)})\sigma_{S3}^{(k)}$$

$$-({}^3R_{S3}^{(k)} + R_{3M}^{(k)})\theta_{S3}^{(k)} + ({}^4R_{S3}^{(k)} + R_{4M}^{(k)})q_{S3}^{(k)}$$

$$+\{(R_5\ f)_{S3}^{(k)} + (R_5\ f)_M^{(k)} - (R_6\ q)_{S3}^{(k)} - (R_6\ q)_M^{(k)}$$

$$-(R_7\ F)_{S3}^{(k)} - (R_7\ F)_M^{(k)}\}\ \Delta t\ , \tag{5.38f}$$

$$b_{w2}^{(k)} = ({}^3W_{S5}^{(k)} + W_{3M}^{(k)})\theta_M - ({}^1W_{S5}^{(k)} + W_{1M}^{(k)})v_M$$

$$+({}^1W_{S5}^{(k)} + W_{1M}^{(k)})v_{S5}^{(k)} + ({}^2W_{S5}^{(k)} + W_{2M}^{(k)})\sigma_{S5}^{(k)}$$

$$-({}^3W_{S5}^{(k)} + W_{3M}^{(k)})\theta_{S5}^{(k)} + ({}^4W_{S5}^{(k)} + W_{4M}^{(k)})q_{S5}^{(k)}$$

$$+\{(W_5\ f)_{S5}^{(k)} + (W_5\ f)_M^{(k)} - (W_6\ q)_{S5}^{(k)} - (W_6\ q)_M^{(k)}$$

$$-(W_7\ F)_{S5}^{(k)} - (W_7\ F)_M^{(k)}\}\ \Delta t\ . \tag{5.38f}$$

In each above-mentioned case, based on equation (5.16a) the plastic strain is calculated from the following equation:

$$p_M^{(k+1)} = p_A + \frac{1}{2}(F_A + F_M^{(k)})\ \Delta t\ . \tag{5.39}$$

5.6 Algorithms of Finite Difference for Interior Grid Points

Like other partial differential equations the equations of wave propagation can be solved with common finite difference method. Now let us recall the basic equations, equations (5.2):

$$\underset{\sim}{Y}_t + \underline{A}\ \underset{\sim}{Y}_x = \underset{\sim}{C}\ , \tag{5.40}$$

where

$$Y_t = [\ \frac{\partial v}{\partial t}\ \ \frac{\partial \sigma}{\partial t}\ \ \frac{\partial \theta}{\partial t}\ \ \frac{\partial q}{\partial t}\ \ \frac{\partial p}{\partial t}\ ]^T\ , \tag{5.41a}$$

$$Y_x = [\ \frac{\partial v}{\partial x}\ \ \frac{\partial \sigma}{\partial x}\ \ \frac{\partial \theta}{\partial x}\ \ \frac{\partial q}{\partial x}\ \ \frac{\partial p}{\partial x}\ ]^T . \tag{5.41b}$$

The elements other than zero of the square matrix $\underline{A}$ are as follows:

$$A_{12} = -\frac{1}{\rho} , \tag{5.42a}$$

$$A_{21} = -\frac{D_3}{\tilde{D}} , \tag{5.42b}$$

$$A_{24} = -\frac{D_5}{\tilde{D}} , \tag{5.42c}$$

$$A_{31} = \frac{D_1}{\tilde{D}} , \tag{5.42d}$$

$$A_{34} = \frac{D_2}{\tilde{D}} , \tag{5.42e}$$

$$A_{43} = \frac{k}{\tau_0} . \tag{5.42f}$$

Vector $\underset{\sim}{C}$ has the following elements:

$$C_1 = \frac{f}{\rho} \tag{5.43a}$$

$$C_2 = -\frac{(D_3+D_4D_5)}{\tilde{D}} F \tag{5.43b}$$

$$C_3 = \frac{(D_1+D_2D_4)}{\tilde{D}} F \tag{5.43c}$$

$$C_4 = -\frac{q}{\tau_0} \tag{5.43d}$$

$$C_5 = F \quad . \tag{5.43e}$$

To solve hyperbolic differential equations by finite difference method MacCormack has developed a procedure with alternative features [5.7]. The procedure includes two sub-steps. The first one is called "predictor" which is done under the condition that time is "fixed". The second sub-step is called "corrector" which is elaborately designed. The method was originally developed for solving field problem of supersonic flow. However, it has been shown that it can also be successfully applied to wave and dynamic problems of solid mechanics.

The modification of MacCormack method which is suitable for wave propagation problem is given as follows:

$$\overline{\underset{\sim}{Y}}{}_j^{n+1} = \overline{\underset{\sim}{Y}}{}_j^{n} - \frac{\Delta t}{\Delta x}\left[\underline{A}(\underset{\sim}{Y}{}_j^n)(\underset{\sim}{Y}{}_{j+1}^n - \underset{\sim}{Y}{}_j^n)\right] + \Delta t\ \underset{\sim}{C}(\underset{\sim}{Y}{}_j^n) \quad , \tag{5.44}$$

$$\underset{\sim}{Y}{}_j^{n+1} = \frac{1}{2}\left\{ \underset{\sim}{Y}{}_j^n + \overline{\underset{\sim}{Y}}{}_j^{n+1} - \frac{\Delta t}{\Delta x}\left[\underline{A}(\overline{\underset{\sim}{Y}}{}_j^{n+1})(\overline{\underset{\sim}{Y}}{}_j^{n+1} - \overline{\underset{\sim}{Y}}{}_{j-1}^{n+1})\right]\right.$$

$$\left. + \Delta t\ \underset{\sim}{C}(\overline{\underset{\sim}{Y}}{}_j^{n+1})\right\} \quad , \tag{5.45}$$

where n counts for time t and j for coordinate x. Equations (5.44) are for the predictor and equations (5.45) are for the corrector sub-steps respectively.

Expanding equations (5.44), we obtain

$$\begin{Bmatrix} \bar{v}_j^{n+1} \\ \bar{\sigma}_j^{n+1} \\ \bar{\theta}_j^{n+1} \\ \bar{q}_j^{n+1} \\ \bar{p}_j^{n+1} \end{Bmatrix} = \begin{Bmatrix} v_j^n \\ \sigma_j^n \\ \theta_j^n \\ q_j^n \\ p_j^n \end{Bmatrix} - \frac{\Delta t}{\Delta x} \begin{Bmatrix} A_{12}(\sigma_{j+1}^n - \sigma_j^n) \\ A_{21}(v_{j+1}^n - v_j^n) + A_{24}(q_{j+1}^n - q_j^n) \\ A_{31}(v_{j+1}^n - v_j^n) + A_{34}(q_{j+1}^n - q_j^n) \\ A_{43}(\theta_{j+1}^n - \theta_j^n) \\ 0 \end{Bmatrix}$$

$$+ \Delta t \begin{Bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{Bmatrix} , \tag{5.46}$$

which yields

$$\bar{v}_j^{n+1} = v_j^n - \frac{\Delta t}{\Delta x} A_{12} (\sigma_{j+1}^n - \sigma_j^n) + \Delta t \; C_1 \quad ,$$

$$\bar{\sigma}_j^{n+1} = \sigma_j^n - \frac{\Delta t}{\Delta x} [A_{21}(v_{j+1}^n - v_j^n) + A_{24}(q_{j+1}^n - q_j^n)] + \Delta t \; C_2 \quad ,$$

$$\bar{\theta}_j^{n+1} = \theta_j - \frac{\Delta t}{\Delta x} [A_{31}(v_{j+1}^n - v_j^n) + A_{34}(q_{j+1}^n - q_j^n)] + \Delta t \; C_3 \quad ,$$

$$\bar{q}_j^{n+1} = q_j^n - \frac{\Delta t}{\Delta x} A_{43}(\theta_{j+1}^n - \theta_j^n) + \Delta t \; C_4 \quad ,$$

$$\bar{p}_j^{n+1} = p_j^n + \Delta t \; C_5 \quad . \tag{5.47a,b,c,d,e}$$

Then from equations (5.45) the following equations of corrector are obtained:

$$v_j^{n+1} = \frac{1}{2}\,[v_j^n + \bar{v}_j^{n+1} - \frac{\Delta t}{\Delta x}\,\bar{A}_{12}(\bar{\sigma}_j^{n+1} - \bar{\sigma}_{j-1}^{n+1})$$

$$+ \Delta t\,\bar{C}_1\,] \quad , \tag{5.48a}$$

$$\sigma_j^{n+1} = \frac{1}{2}\,\{\sigma_j^n + \bar{\sigma}_j^{n+1} - \frac{\Delta t}{\Delta x}\,[\bar{A}_{21}(\bar{v}_j^{n+1} - \bar{v}_{j-1}^{n+1})$$

$$+ \bar{A}_{24}(\bar{q}_j^{n+1} - \bar{q}_{j-1}^{n+1}) + \Delta t\,C_2\} \;, \tag{5.48b}$$

$$\theta_j^{n+1} = \frac{1}{2}\,\{\theta_j^n + \bar{\theta}_j^{n+1} - \frac{\Delta t}{\Delta x}\,[\bar{A}_{31}(\bar{v}_j^{n+1} - \bar{v}_{j-1}^{n+1})$$

$$+ \bar{A}_{34}(\bar{q}_j^{n+1} - \bar{q}_{j-1}^{n+1}) + \Delta t\,\bar{C}_3\} \;, \tag{5.48c}$$

$$q_j^{n+1} = \frac{1}{2}\,\{q_j^n + \bar{q}_j^{n+1} - \frac{\Delta t}{\Delta x}\,\bar{A}_{43}(\bar{\theta}_j^{n+1} - \bar{\theta}_{j-1}^{n+1})$$

$$+ \Delta t\,\bar{C}_4\,\} \quad , \tag{5.48d}$$

$$p_j^{n+1} = \frac{1}{2}\,\{p_j^n + \bar{p}_j^{n+1} - \Delta t\,\bar{C}_5\,\} \quad . \tag{5.48e}$$

5.7 Algorithms of Finite Difference for Boundary Grid Points

At the points of boundary grid the predicted values $\underset{\sim}{Y}_{j-1}^{n+1}$ may not be available for the corrector. With the forward derivatives employed, the scheme then becomes as :

$$\underset{\sim}{Y}_0^{n+1} = \underset{\sim}{Y}_0^n - \frac{\Delta t}{\Delta x} [\underline{A}(\underset{\sim}{Y}_0^n)(\underset{\sim}{Y}_1^n - \underset{\sim}{Y}_0^n)] + \Delta t \, \underset{\sim}{C}(\underset{\sim}{Y}_0^n) \quad , \tag{5.49}$$

and

$$\underset{\sim}{Y}_0^{n+1} = \frac{1}{2} \{\underset{\sim}{Y}_0 + \underset{\sim}{Y}_0^{n+1} - \frac{\Delta t}{\Delta x} [\underline{A}(\underset{\sim}{Y}_0^{n+1})(\underset{\sim}{Y}_1^{n+1} - Y_0^{n+1})]$$

$$+ \Delta t \, C(\underset{\sim}{Y}_0^{n+1})\} \quad . \tag{5.50}$$

Expanding equations (5.49) we obtain the expression of the predictor for boundary grid points as :

$$\bar{v}_1^{n+1} = v_1^n - \frac{\Delta t}{\Delta x} A_{12}(\sigma_2^n - \sigma_1^n) + \Delta t \, C_1 \quad , \tag{5.51a}$$

$$\bar{\sigma}_1^{n+1} = \sigma_1^n - \frac{\Delta t}{\Delta x} [A_{21}(v_2^n - v_1^n)$$

$$+ A_{24}(q_2^n - q_1^n)] + \Delta t \, C_2 \quad , \tag{5.51b}$$

$$\bar{\theta}_1^{n+1} = \theta_1^n - \frac{\Delta t}{\Delta x} [A_{31}(v_2^n - v_1^n)$$

$$+ A_{34}(q_2^n - q_1^n)] + \Delta t \, C_3 \quad , \tag{5.51c}$$

$$\bar{q}_1^{n+1} = q_1^n - \frac{\Delta t}{\Delta x} A_{43}(\theta_2^n - \theta_1^n) + \Delta t \, C_4 \quad , \tag{5.51d}$$

$$\bar{p}_1^{n+1} = p_1^n + \Delta t \, C_5 \quad , \tag{5.51e}$$

where A_{ij} take their values at the boundary grid points.

Similarly, according to equations (5.50) the corrector for boundary grid points is expressed as :

$$v_1^{n+1} = \frac{1}{2} [v_1^n - \bar{v}_1^{n+1} - \frac{\Delta t}{\Delta x} \bar{A}_{12}(\bar{\sigma}_2^{n+1}$$

$$- \bar{\sigma}_1^{n+1}) + \Delta t\ \bar{C}_1] \quad , \tag{5.52a}$$

$$\sigma_1^{n+1} = \frac{1}{2} \{\sigma_1^n + \bar{\sigma}_1^{n+1} - \frac{\Delta t}{\Delta x} [\bar{A}_{21}(\bar{v}_2^{n+1} - \bar{v}_1^{n+1})$$

$$+ \bar{A}_{24}(\bar{q}_2^{n+1} - \bar{q}_1^{n+1})] + \Delta t\ \bar{C}_2 \} \quad , \tag{5.52b}$$

$$\theta_1^{n+1} = \frac{1}{2} \{\theta_1^n + \bar{\theta}_1^{n+1} - \frac{\Delta t}{\Delta x} [\bar{A}_{31}(\bar{v}_2^{n+1} - \bar{v}_1^{n+1})$$

$$+ \bar{A}_{34}(\bar{q}_2^{n+1} - \bar{q}_1^{n+1})] + \Delta t\ \bar{C}_3 \} \ , \tag{5.52c}$$

$$q_1^{n+1} = \frac{1}{2} [q_1^n + \bar{q}_1^{n+1} - \frac{\Delta t}{\Delta x} \bar{A}_{43}(\bar{\theta}_2^{n+1}$$

$$- \bar{\theta}_1^{n+1}) + \Delta t\ \bar{C}_4] \quad , \tag{5.52d}$$

$$p_1^{n+1} = \frac{1}{2} [p_1^n + \bar{p}_1^{n+1} + \Delta t\ \bar{C}_5] \quad . \tag{5.52e}$$

By utilizing equations (5.47), (5.48), (5.51) and (5.52) we are able to solve the basic equations (5.40) in either case of the boundary conditions prescribed.

CHAPTER 6

NUMERICAL RESULTS AND CONCLUSIONS

6.1 Preface

The coupled one-dimensional thermoplastic waves propagating in a semi-infinite mild steel rod have been studied in the chapters 4 and 5 under different combinations of time-dependent inputs. The numerical results are presented in this chapter.

Two algorithms of numerical integration discussed in the preceding chapter have been implemented with computer programs coded in FORTRAN-77 language and carried out on CYBER-175. For the generality of the results the programs are written in dimensionless form. Since the algorithms for the boundary grid points are different from those for the interior grid points, each program contains two different parts to deal with the different types of grid points.

As presented in the preceding chapter, the solution procedures for the two boundary conditions assigned in Case (A) and Case (B) are different, therefore different computational programs have to be utilized when using the method of characteristics. For each of these programs, according to the numbering rule the computer judges the types of grid points and then executes the appropriate subroutine.

Because the system is non-linear, an iterative procedure had to be imposed upon the two subroutines for both interior and boundary grid points. In addition, as the system is ill-conditioned, to obtain a convergent solution, "high accuracy linear system solution" coded as LSARG in Nosve, CYBER-175 was called in each iteration. With properly selected net size these two measures guaranteed convergence of the solutions; nevertheless, large number of iterations were still required for any boundary point.

The program of finite difference method is much more straightforward; yet, two different procedures were needed for different types of grid points. The program for interior grid points was based on equations (5.44) and (5.45), while the program for boundary grid points was based on equations (5.49) and (5.50).

6.2 Boundary Conditions Assigned in the Numerical Calculation

It is assumed that the rod is initially in unstressed state with known temperature and then the following forms of inputs are applied for Case (A).

(i) Stress and temperature increment are in the form of step input,

$$\sigma(0,t) = \sigma_0 \, H(t) \quad , \tag{6.1a}$$

$$T(0,t) = \theta_0 \, H(t) \quad , \tag{6.1b}$$

where H(t) is the Heaviside function defined as:

$$H(t) = \begin{cases} 1 & \text{if } t \geq 0 \ , \\ 0 & \text{if } t < 0 \ . \end{cases} \tag{6.2}$$

This type of input prescribes the impact condition at the boundary, through which the discontinuity propagates into the medium. In the figures, the boundary condition is coded as 1.

(ii) Stress and temperature increment are in the form of ramp input as

$$\sigma(0,t) = \sigma_0 \ \mu\langle t\rangle \quad , \tag{6.3a}$$

$$T(0,t) = \theta_0 \ \mu\langle t\rangle \quad , \tag{6.3b}$$

where $\mu\langle\cdot\rangle$ denotes the McAuley bracket defined as

$$\mu\langle t\rangle = \begin{cases} \frac{t}{t_0} & 0 < t \leq t_0 \\ 1 & t > t_0 \end{cases} \tag{6.4a,b}$$

This kind of input prescribes a continuous function, but its derivatives are discontinues at t=0 and t_0. The boundary condition is coded as 2 in the figures.

(iii) Stress and temperature increment inputs are of sinusoidal form as

$$\sigma(0,t) = \sigma_0 \ S(t) \quad , \tag{6.5a}$$

$$T(0,t) = \theta_0 \ S(t) \quad , \tag{6.5b}$$

where S(t) is the sine function defined as below

$$S(t) = \begin{cases} \text{Sin } \omega t & \text{if } t \leq \frac{\pi}{\omega} \, , \\ 0 & \text{if } t > \frac{\pi}{\omega} \, . \end{cases} \tag{6.6a,b}$$

Again, the input prescribes a continuous function for the dependent variables, but its derivatives are discontinues at t=0 and $t=\frac{\pi}{\omega}$. This boundary condition is coded as 3 in the figures.

(iv) Stress input alone is prescribed on the boundary as step function,

$$\sigma(0,t) = \sigma_0 H(t) \quad ,$$
$$T(0,t) = 0 \quad . \tag{6.7a,b}$$

This case is assigned with intent to show the temperature change due to mechanical deformation process. The boundary condition is coded as 4 in the figures.

Similar forms of inputs are considered in Case (B), where the increments of velocity and temperature are prescribed.

During the calculations the data of Steel SAE1010 were employed. Its physical properties at room-temperature are:

$$E = 2.0 \times 10^{11} \ (\mathrm{N\ M^{-2}}) \quad ,$$
$$\rho = 7.78 \times 10^{3} \ (\mathrm{kg\ M^{-3}}) \quad ,$$
$$\alpha = 1.25 \times 10^{-5} \ (\mathrm{K^{-1}}) \quad ,$$
$$k = 52.25 \ (\mathrm{W\ M^{-1}K^{-1}}) \quad ,$$
$$C = 522.5 \ (\mathrm{J\ kg^{-1}K^{-1}}) \quad ,$$
$$\nu = 0.32 \quad .$$

All the calculated results are expressed in Fig.6.1 through Fig 6.78. The solid lines are of the solutions by the method of characteristics, while the dashed are of the finite difference solution. B.C. stands for "boundary condition", where the first Roman letter other than H denotes the types of boundary conditions. "A" means that stress σ and temperature increment T are prescribed on the boundary, while "B" means that velocity v and temperature increment are prescribed on the boundary. The first Arabic numeral stands for the type of boundary conditions; 1 is the code of case (i);. 2 for case (ii) and so on. The second Arabic number gives the information of what the figure is for. 1 indicates that the figure is for velocity; 2 means the figure is for stress; 3 is for temperature; 4 is for heat flow and 5 for plastic strain. When the first letter under "B.C." is A or B, the figure is plotted with dependent variable versus distance x, while time t is the parameter whose values corresponding to different curves are denoted by t_1, t_2, *etc.* If the first letter under "B.C." is H, the figure is plotted with dependent variables versus time t, while distance (or position) x is the parameter whose values are denoted by x_1, x_2 and so on.

The following dimensionless time and distance have been employed:

$$t = \left(\frac{E}{\rho}\right)\left(\frac{\rho c}{k}\right) t' \;,$$

$$x = \left(\frac{E}{\rho}\right)^{\frac{1}{2}} \left(\frac{\rho c}{k}\right) x' \;, \qquad (6.8a,b)$$

where t' and x' denote the real time and distance respectively.

6.3 Description of the Results

All the results obtained from the numerical work show that both characteristics and finite difference methods have produced profiles of excellent resolution. It can be seen from Fig.6.1, Fig.6.2, Fig.6.31 and Fig.6.33 that the results obtained by the two methods are convergent and very close to each other. It can also be seen that for the basic responses like velocity, stress, and plastic strain the characteristics method usually gives a sharper solution. However, the situation for heat flow is different as is shown in Fig.6.39.

It is interesting to note that for the case of an end step input the values of dependent variables are continuous everywhere except on the boundary. This simply means that there is no discontinues shock waves except on the boundary, therefore, all the waves in the problem are of acceleration type. The conclusion can be justified by checking Fig.6.1 to Fig.6.10, Fig.6.30 to Fig.6.40, Fig.6.41 to Fig.6.50 and Fig.6.71 to Fig.6.80.

The comparisons of Fig.6.1, Fig.6.2, and Fig.6.5 with Fig.6.3 and Fig.6.4; of Fig.6.41, Fig.6.42, and Fig.6.45 with Fig.6.43 and Fig.6.44 reveal the fact that the fronts of mechanical waves such as velocity, stress, plastic strain and of thermal waves like temperature increment, heat flow are propagated with the same velocity. This fact shows the thermoplastic waves are coupled.

The thermal responses produced by mechanical input can be seen in Fig.6.33 and Fig.6.34 which indicates that due to the stress step input, each point in different position, *i.e.* with different value of x experiences a pulse of heat wave. After that pulse the heat wave diminishes and tends to a stable value. The fact can be observed in Fig.6.38 and Fig.6.39 which show the similar situation for the heat flow except that the range of variation is wider.

It may be noticed from Fig.6.6 and Fig.6.36 that the discontinuity corresponding to step input loses its sharpness when it is propagated in a plastic medium. Because the input is that of Heaviside function type, at x=0, it takes no time to reach its maximum value for each of the inputs. At x_1=0.16, however, by Fig.6.6 and Fig.6.36 it takes about 3 units of time for the velocity to reach its maximum value. At x_2=0.047, it takes about 5 units of time to do so. At x_3=0.08, it

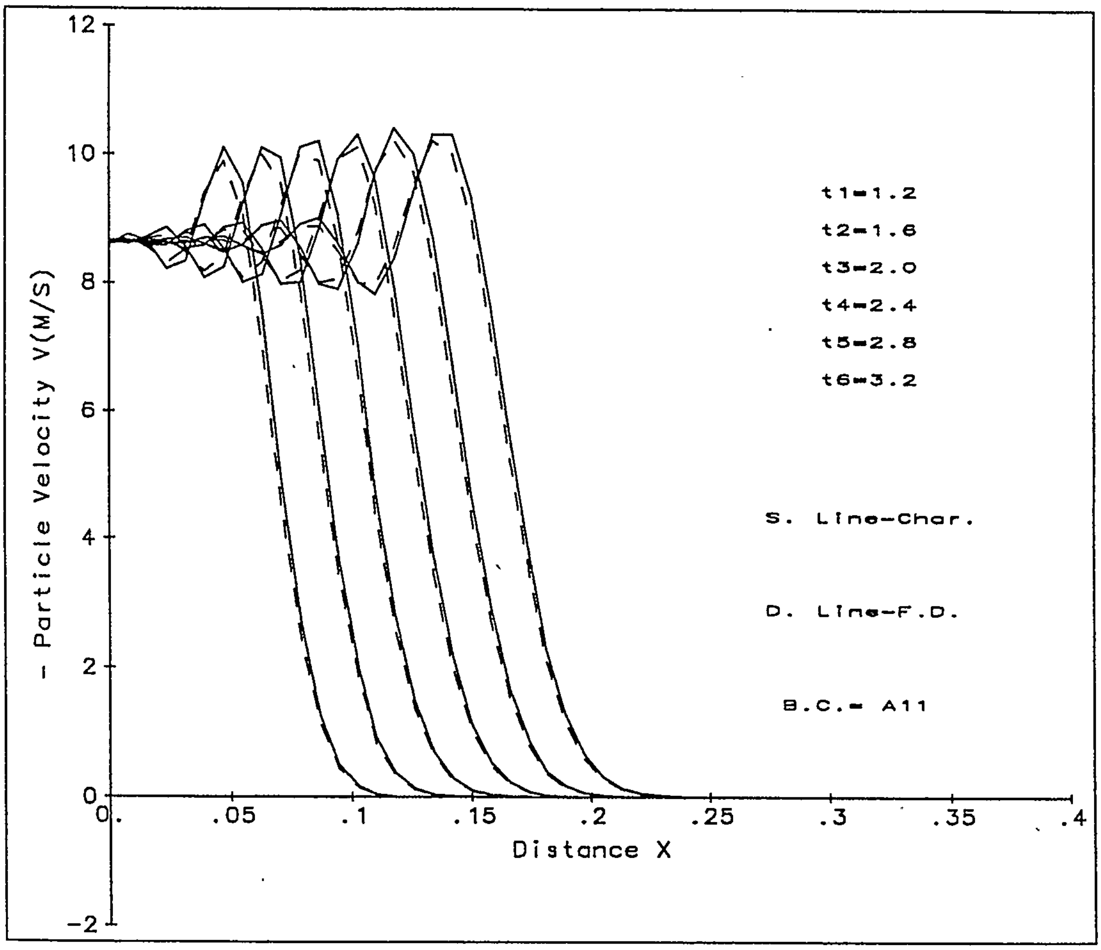

Fig. 6.1 Velocity distribution along x-axis due to stress and temperature step inputs (σ_0=340 MPA,θ_0=5K)

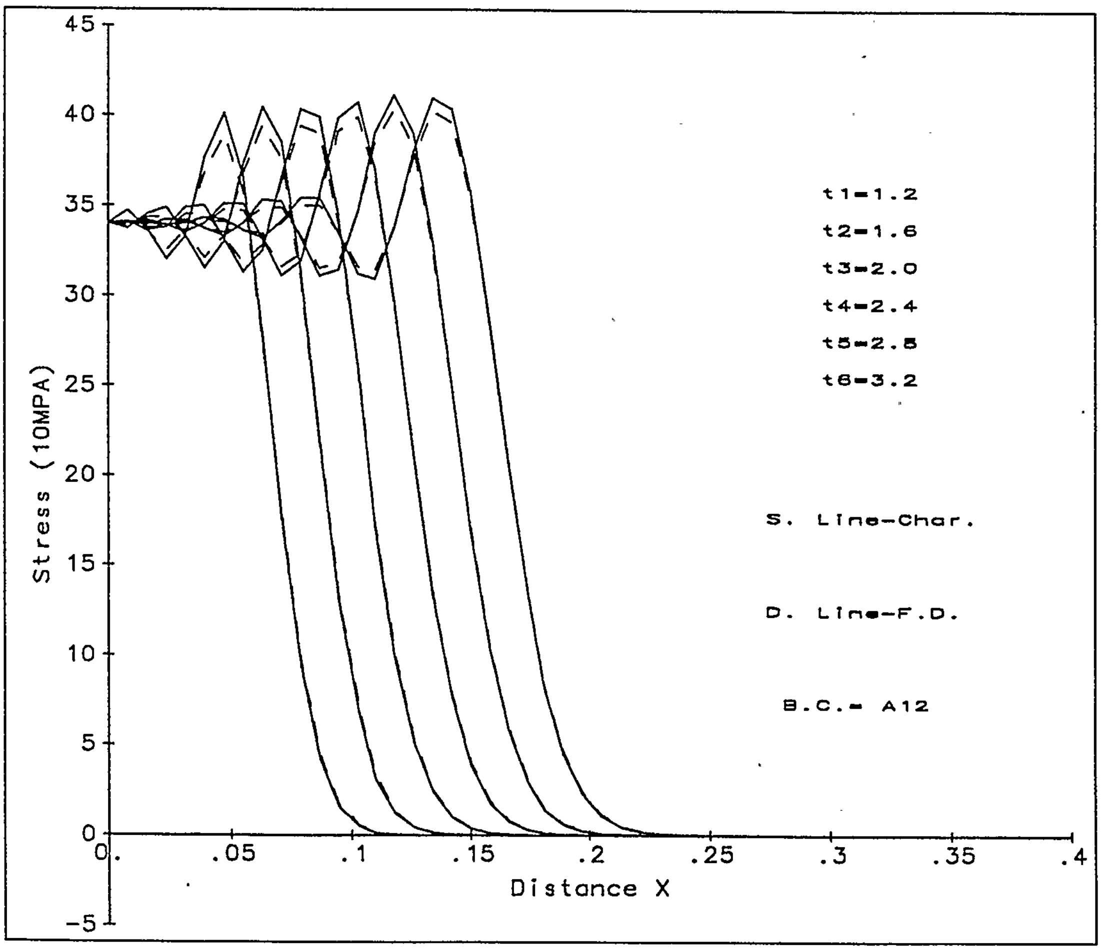

Fig. 6.2 Stress distribution along x-axis due to stress and temperature step inputs (σ_0=340 MPA,θ_0=5K)

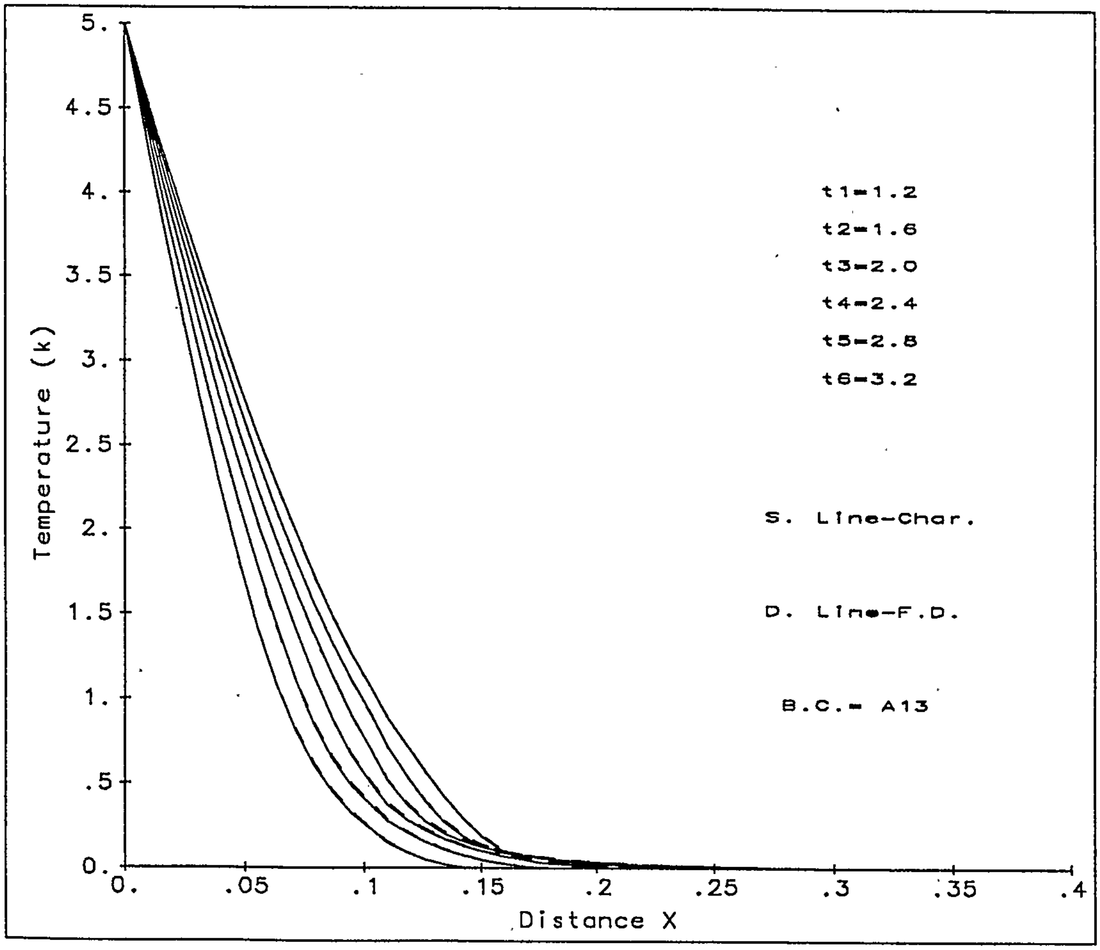

Fig. 6.3 Temperature distribution along x-axis due to stress and temperature step inputs (σ_0=340 MPA,θ_0=5K)

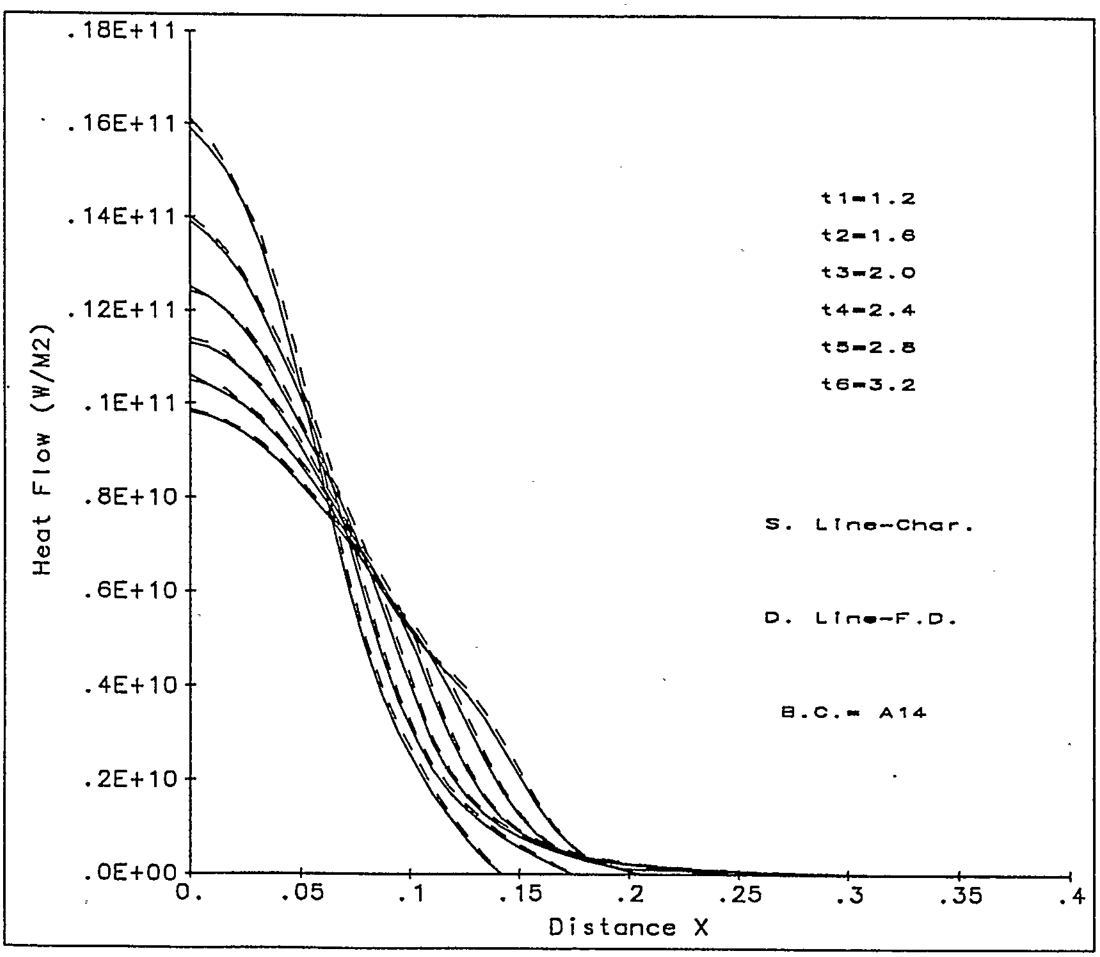

Fig. 6.4 Heat flow distribution along x-axis due to stress and temperature step inputs (σ_0=340 MPA,θ_0=5K)

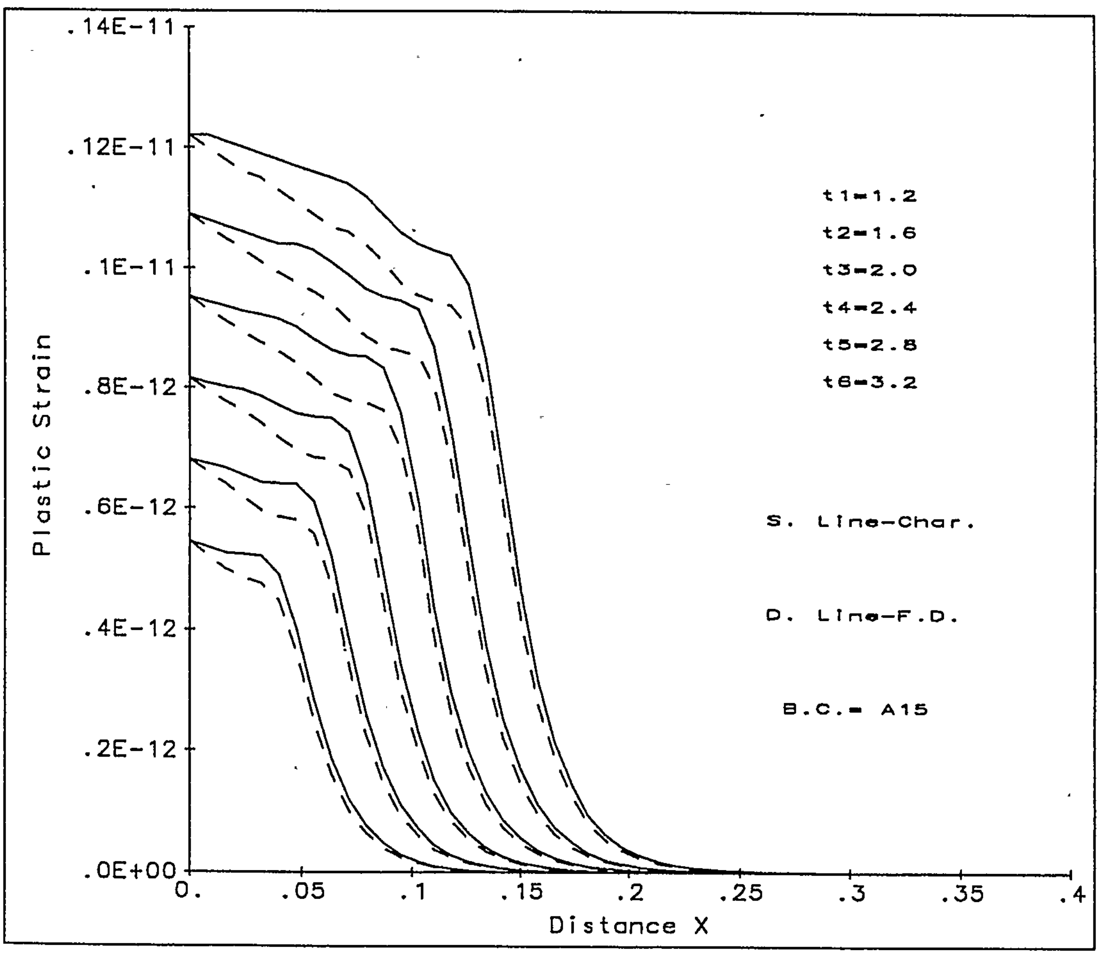

Fig. 6.5 Plastic strain distribution along x-axis due to stress and temperature step inputs (σ_0=340 MPA,θ_0=5K)

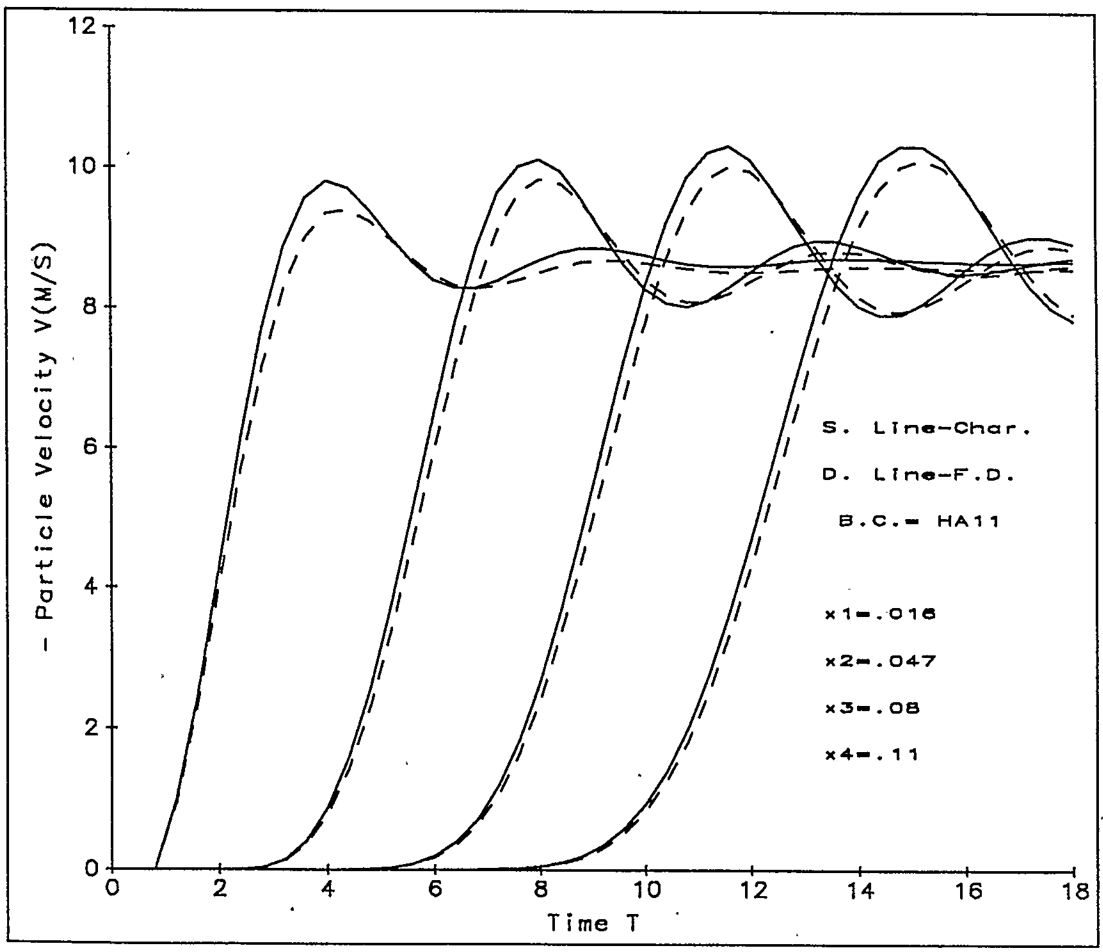

Fig. 6.6 Velocity response at certain positions due to stress and temperature step inputs (σ_0=340 MPA, θ_0=5K)

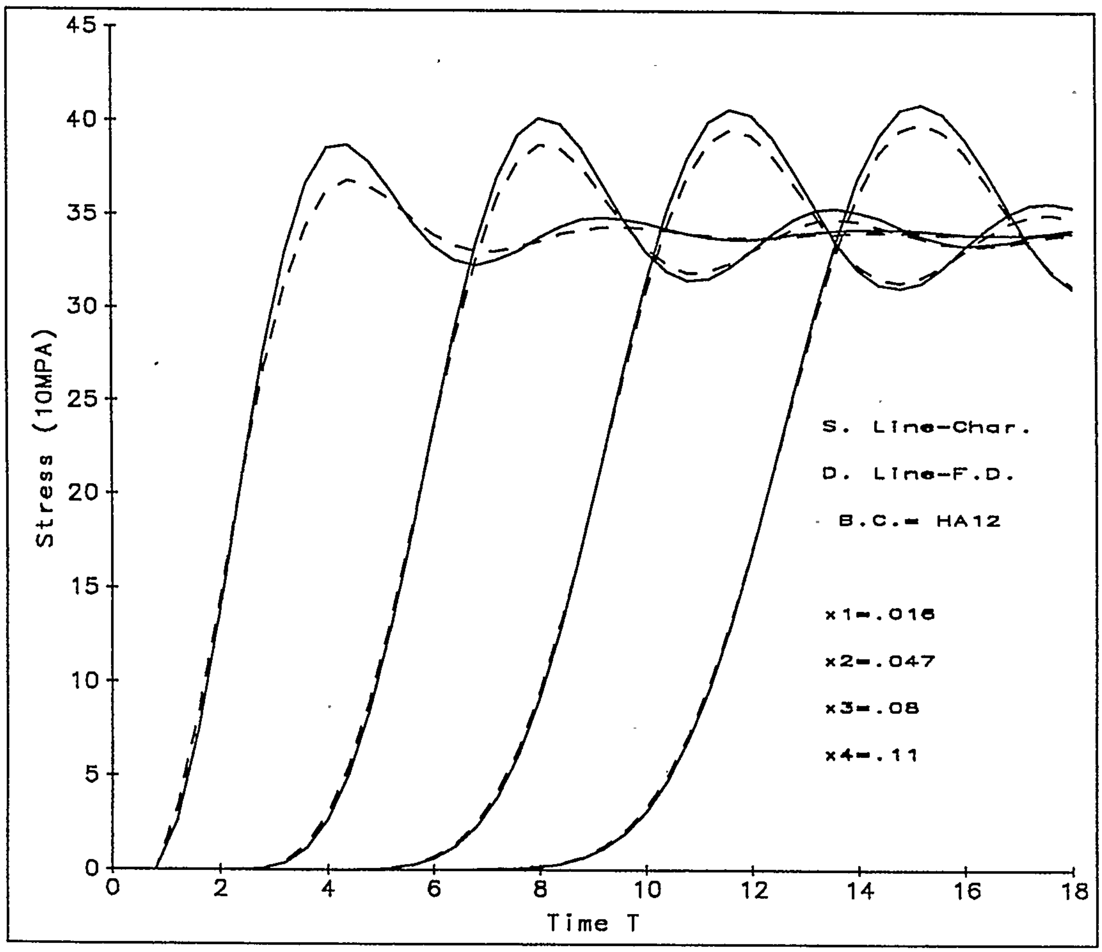

Fig. 6.7 Stress response at certain positions due to stress and temperature step inputs (σ_0=340 MPA,θ_0=5K)

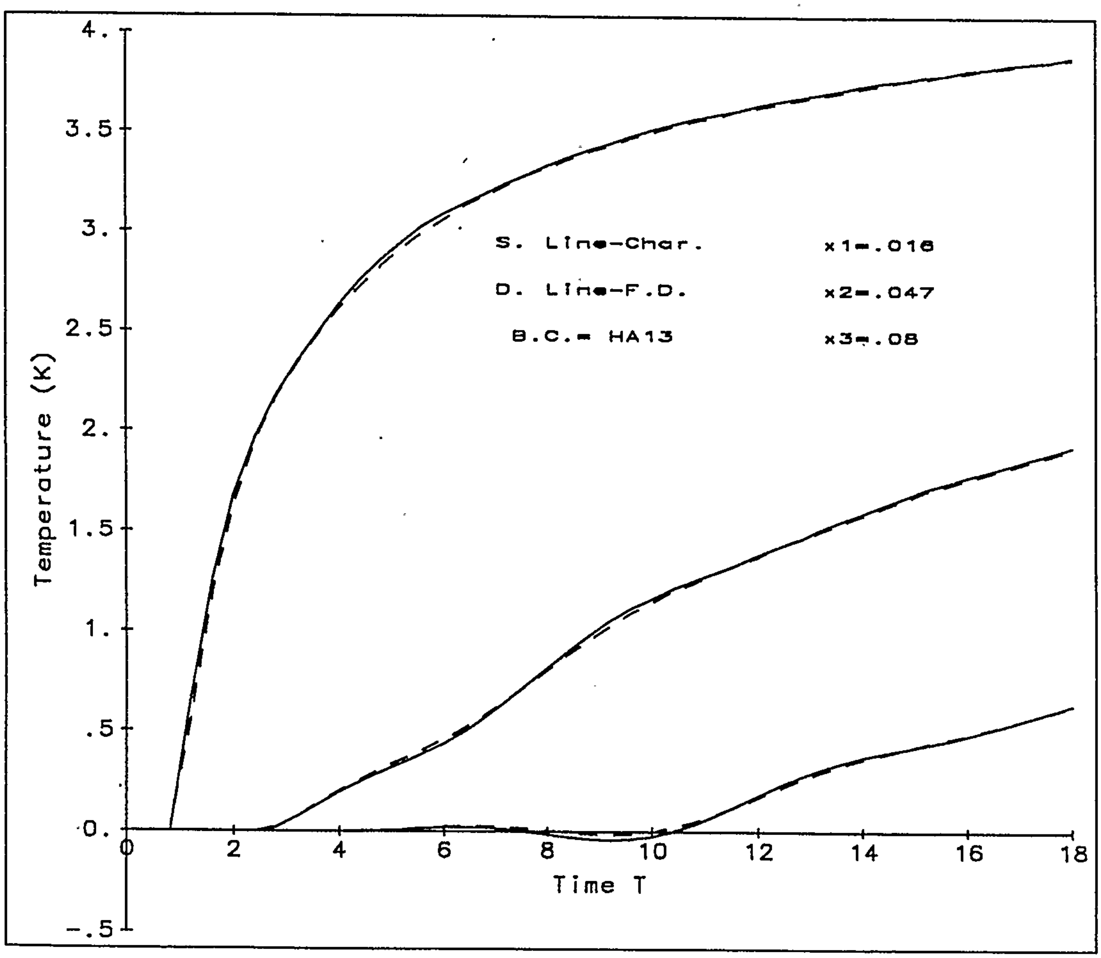

Fig. 6.8 Temperature response at certain positions due to stress and temperature step inputs (σ_0=340 MPA,θ_0=5K)

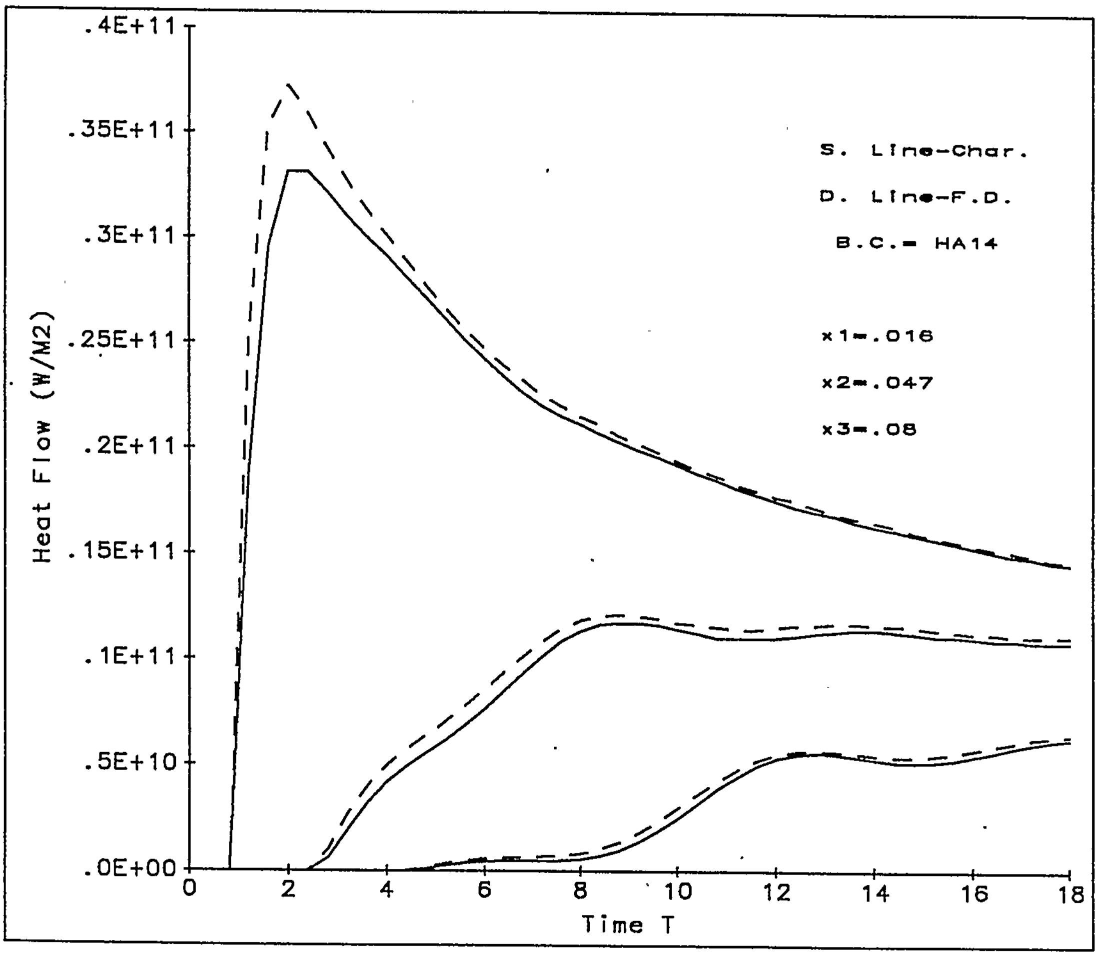

Fig. 6.9 Heat flow response at certain positions due to stress and temperature step inputs (σ_0=340 MPA,θ_0=5K)

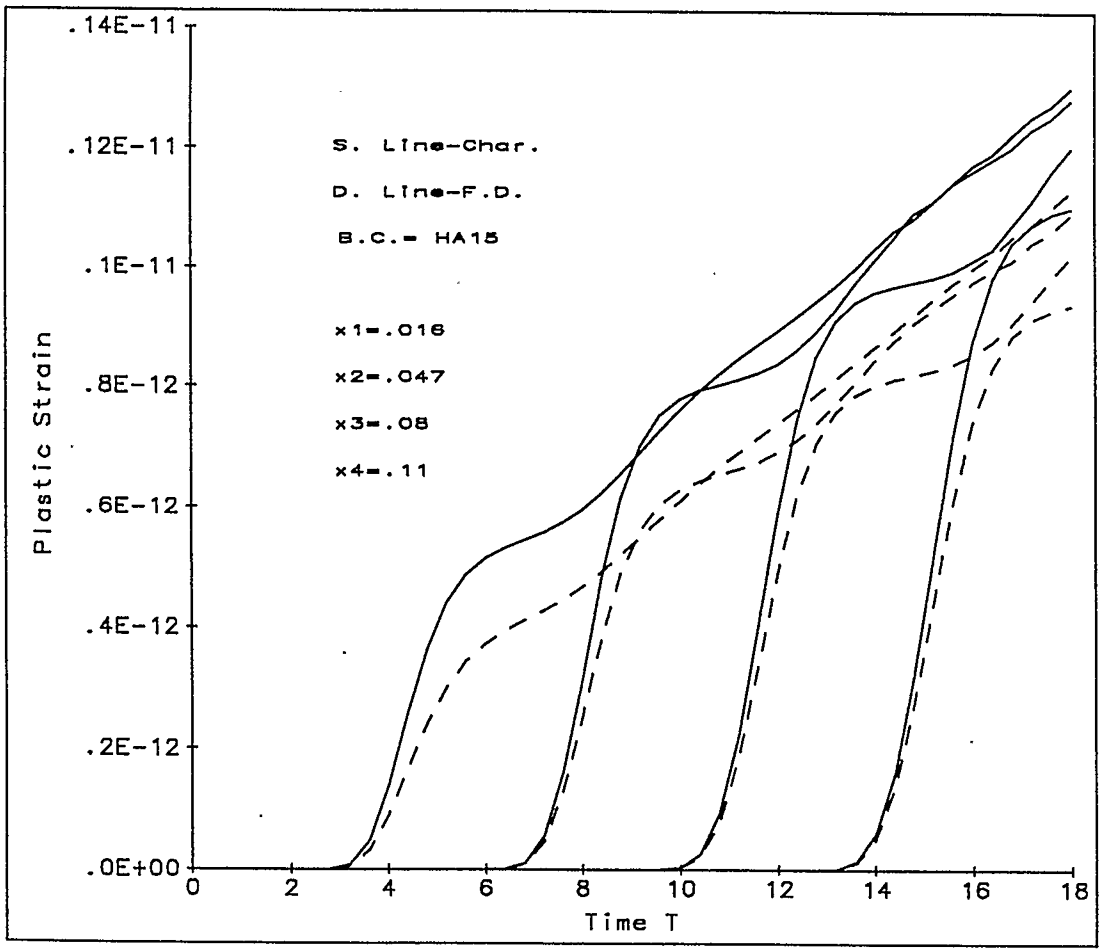

Fig. 6.10 Plastic strain response at certain positions due to stress and temperature step inputs (σ_0=340 MPA,θ_0=5K)

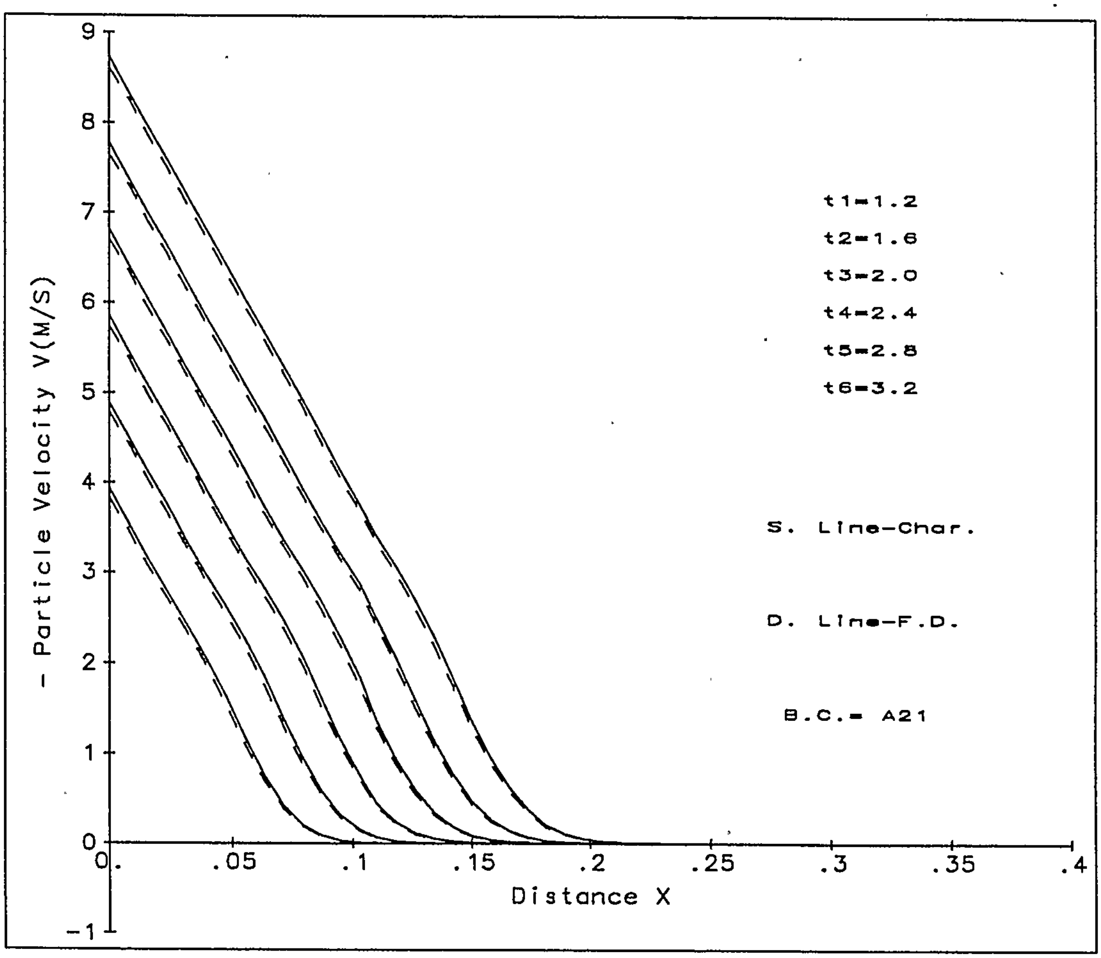

Fig. 6.11 Velocity distribution along x-axis due to stress and temperature ramp inputs (σ_0=340 MPA,θ_0=5K)

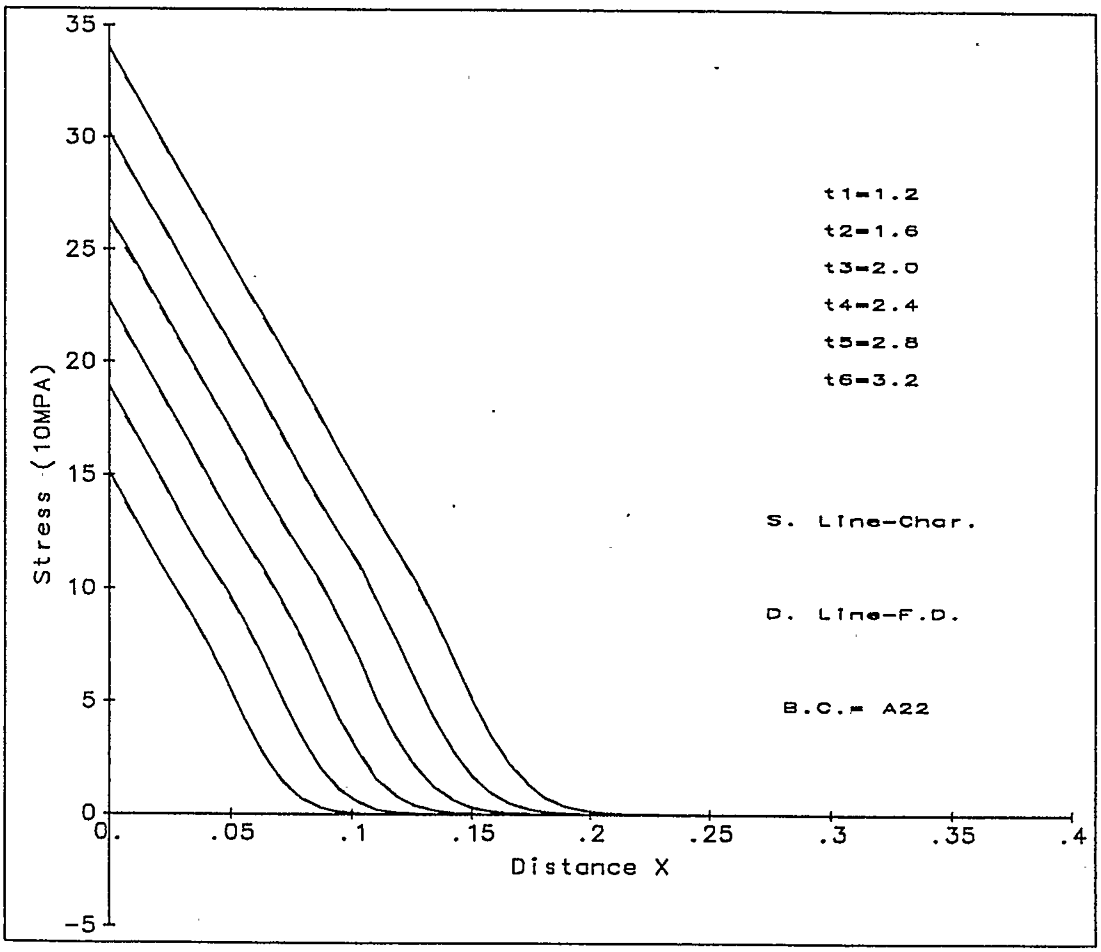

Fig. 6.12 Stress distribution along x-axis due to stress and temperature ramp inputs (σ_0=340 MPA,θ_0=5K)

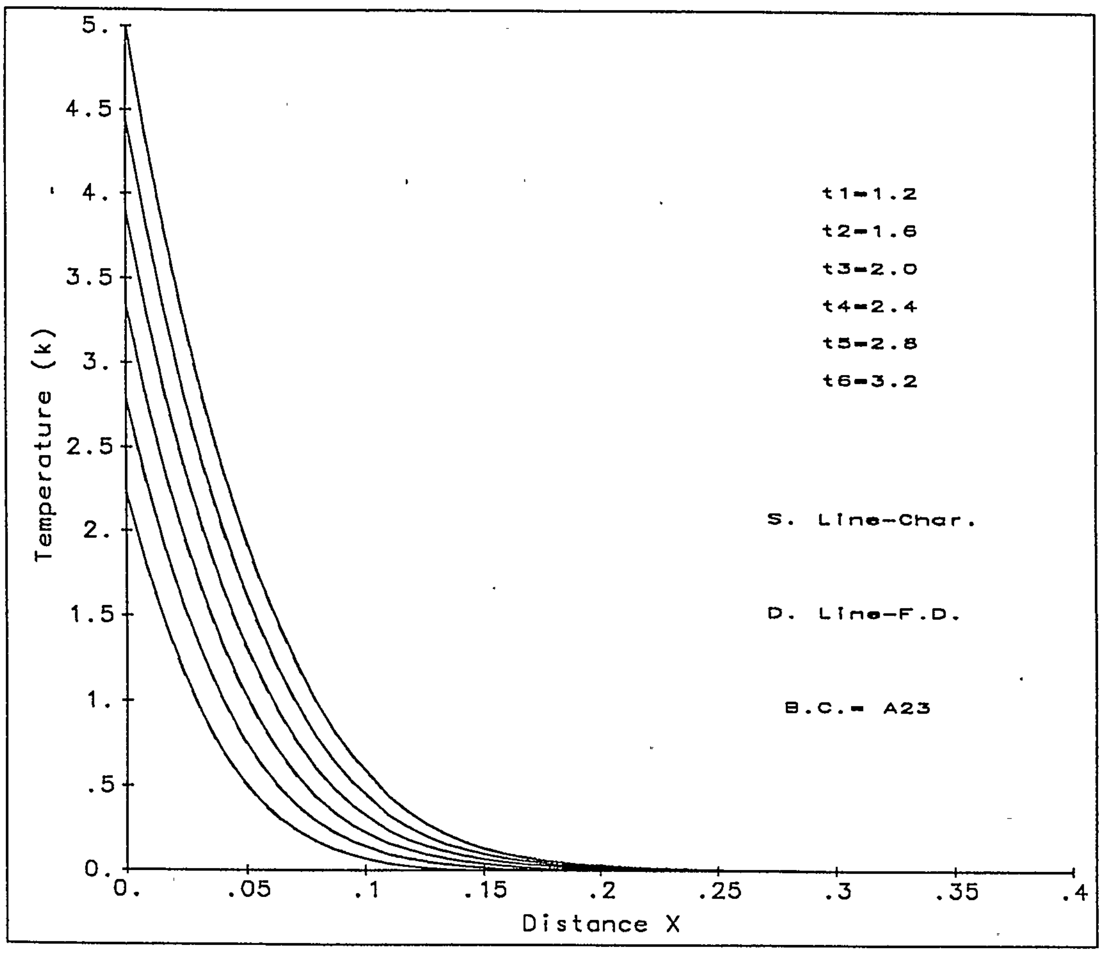

Fig. 6.13 Temperature distribution along x-axis due to stress and temperature ramp inputs (σ_0=340 MPA,θ_0=5K)

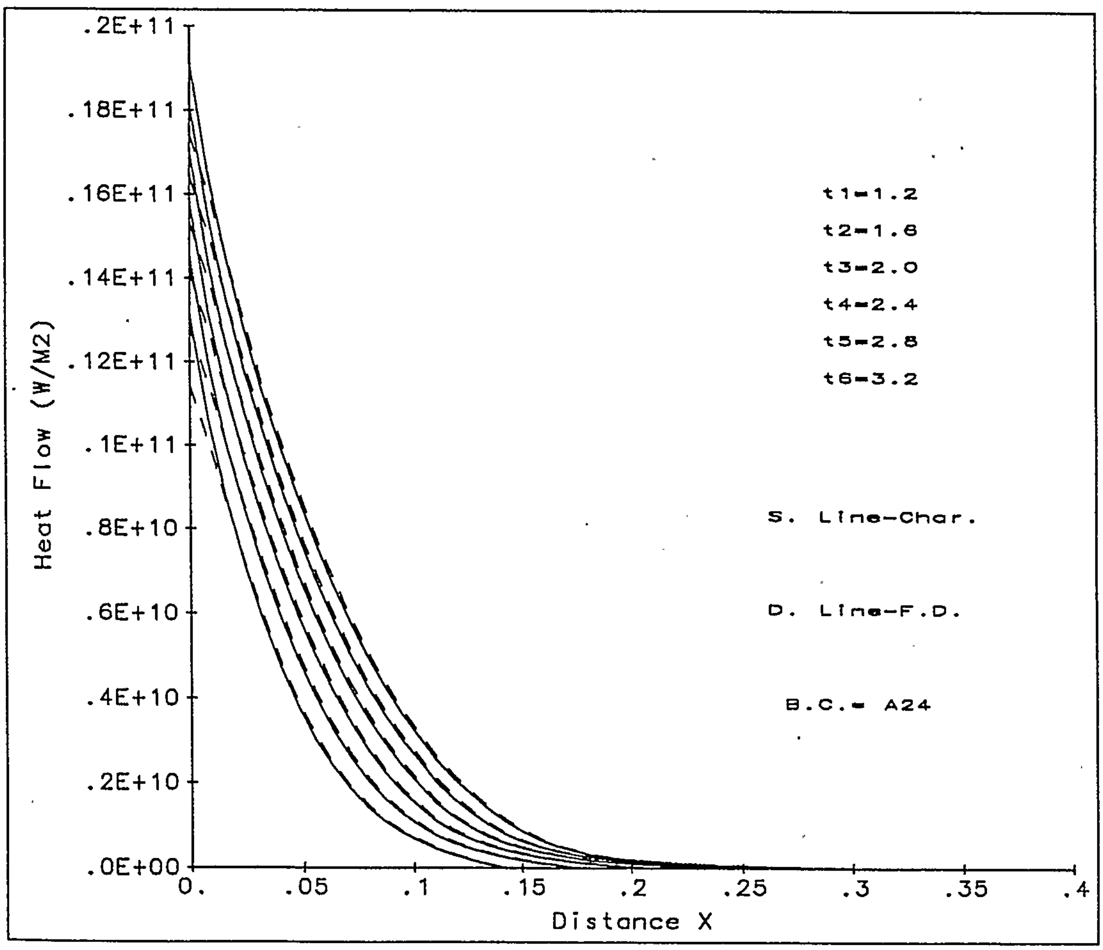

Fig. 6.14 Heat flow distribution along x-axis due to stress and temperature ramp inputs (σ_0=340 MPA,θ_0=5K)

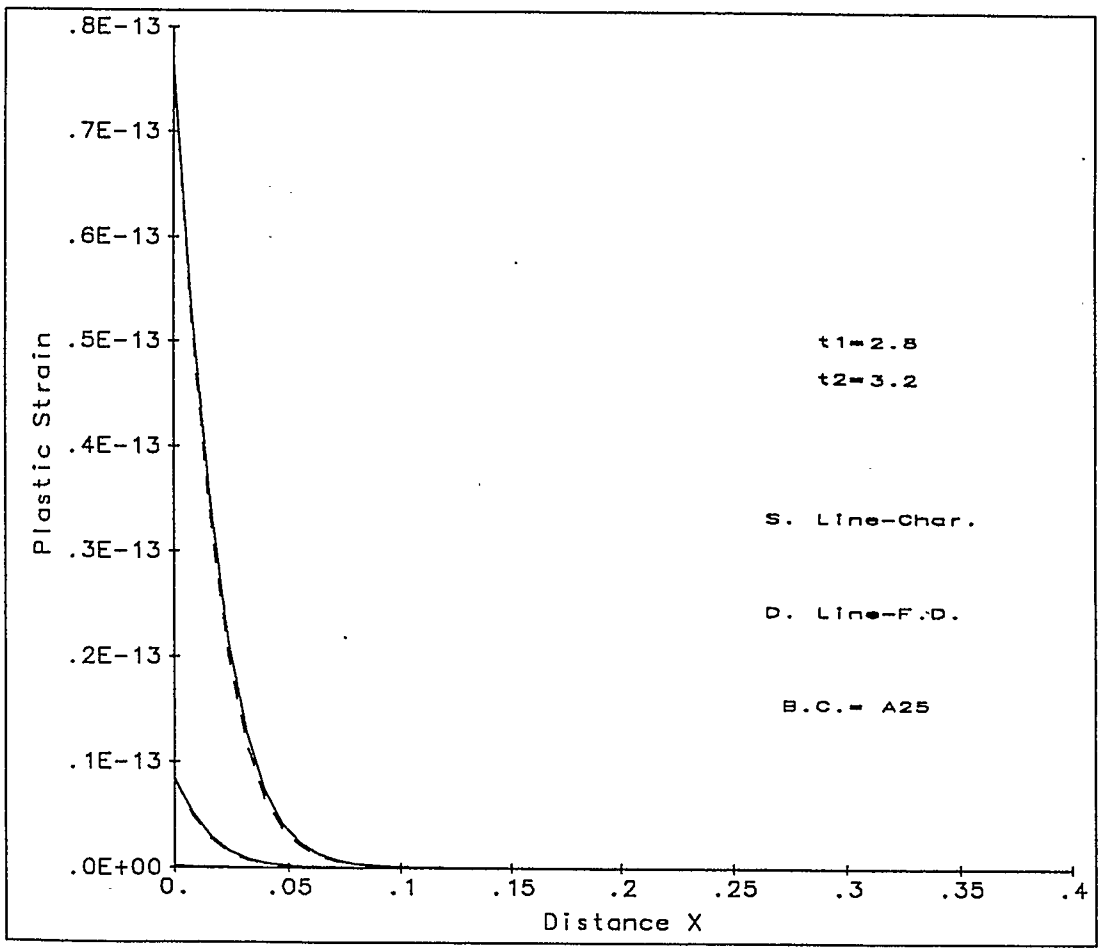

Fig. 6.15 Plastic strain distribution along x-axis due to stress and temperature ramp inputs (σ_0=340 MPA,θ_0=5K)

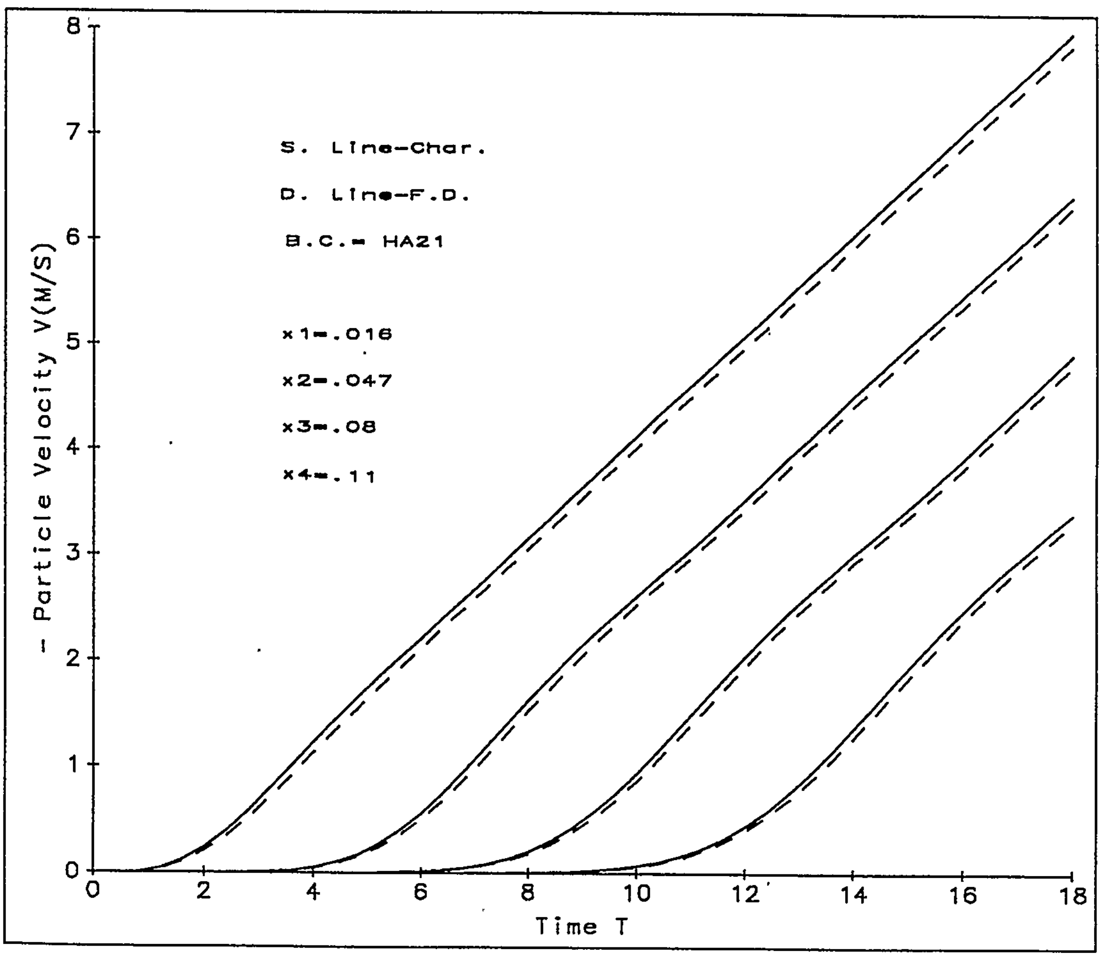

Fig. 6.16 Velocity response at certain positions due to stress and temperature ramp inputs (σ_0=340 MPA,θ_0=5K)

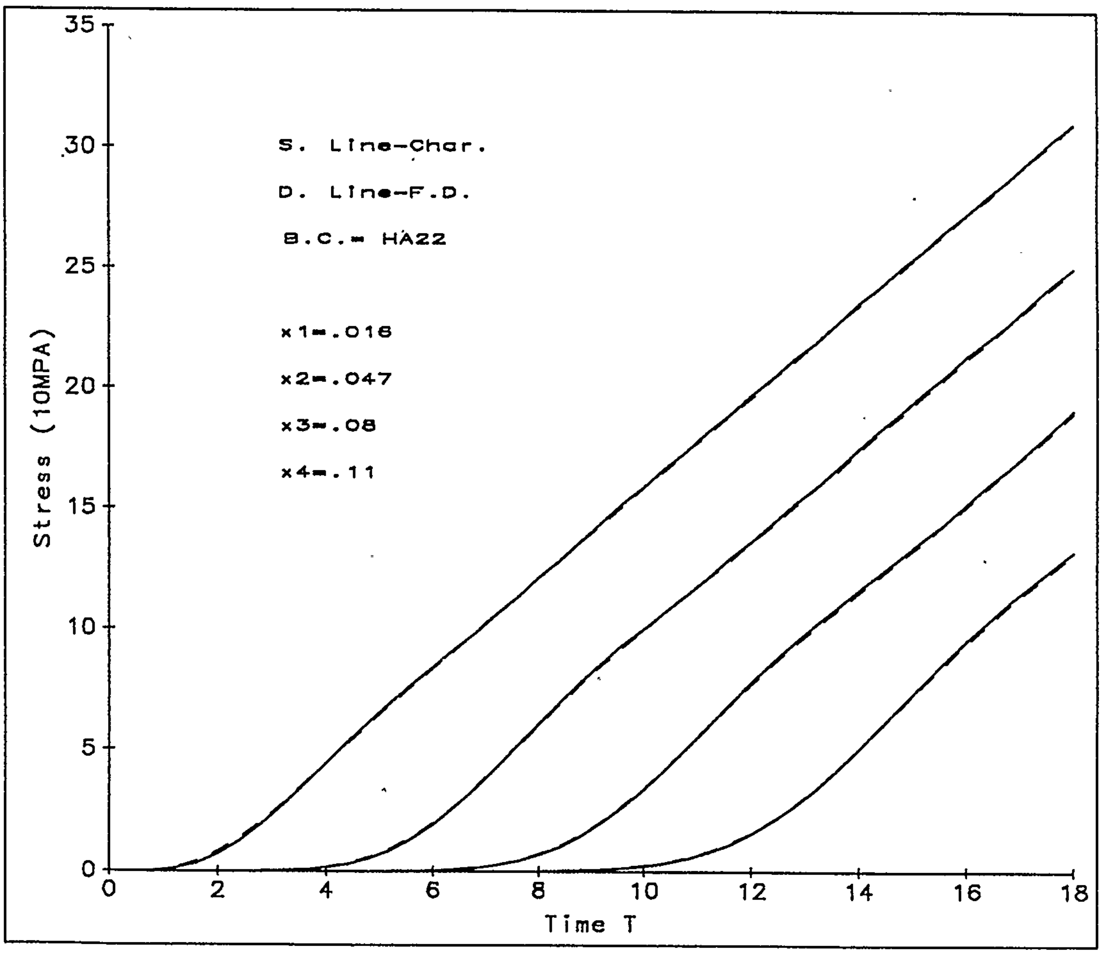

Fig. 6.17 Stress response at certain positions due to stress and temperature ramp inputs (σ_0=340 MPA,θ_0=5K)

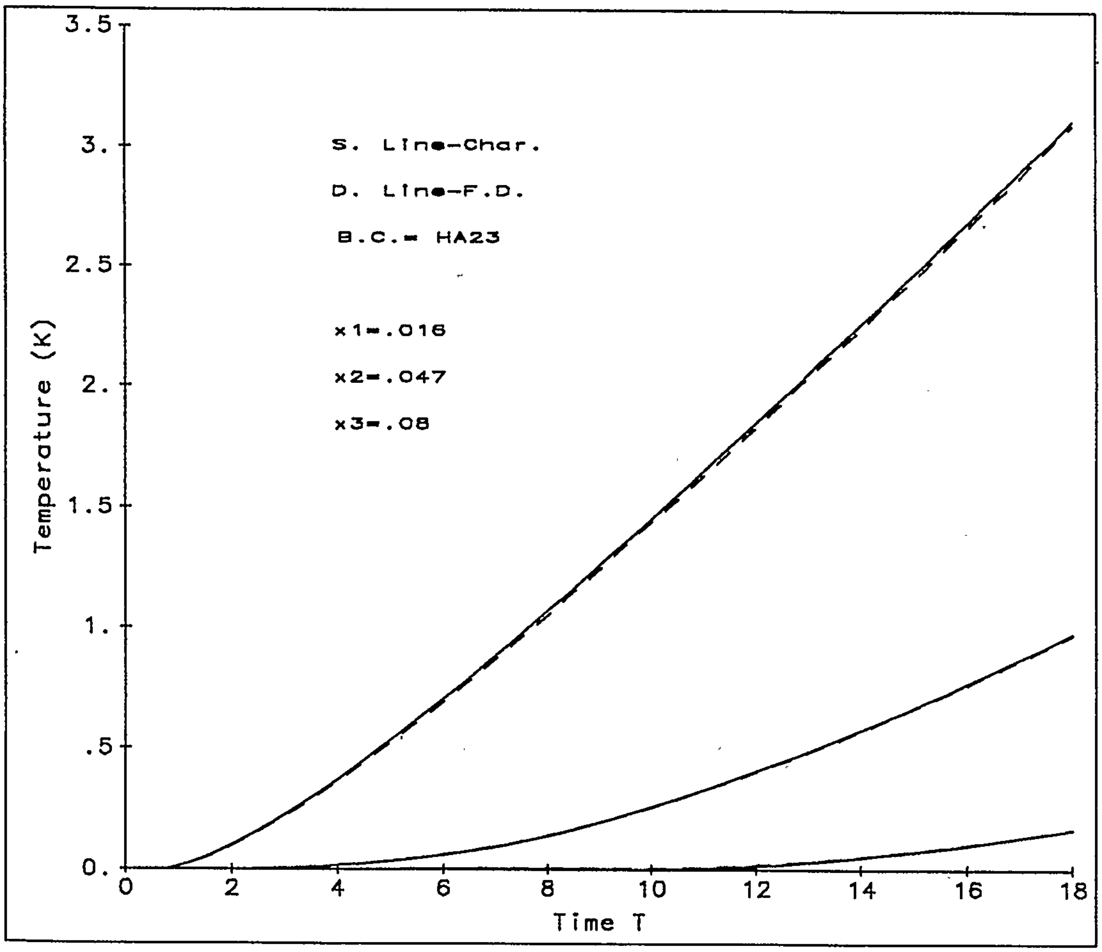

Fig. 6.18 Temperature response at certain positions due to stress and temperature ramp inputs (σ_0=340 MPA,θ_0=5K)

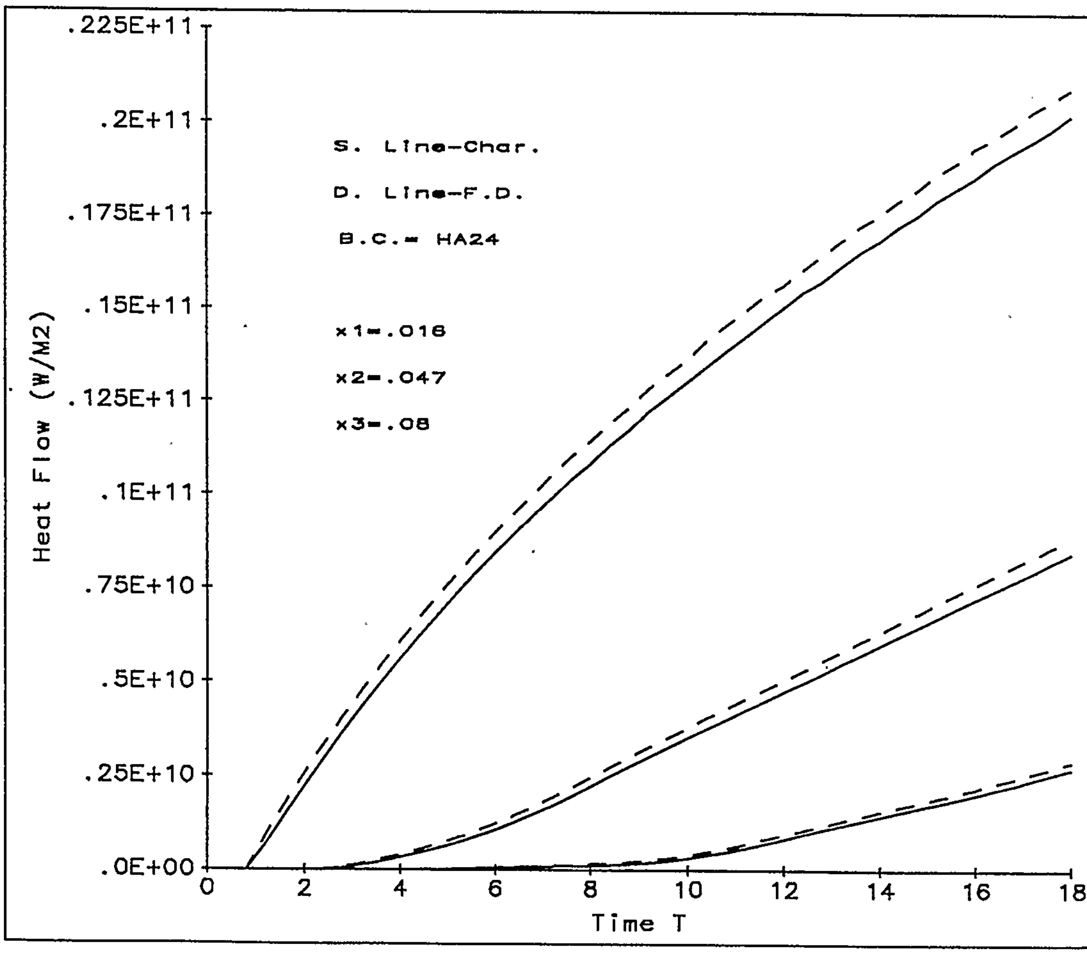

Fig. 6.19 Heat flow response at certain positions due to stress and temperature ramp inputs (σ_0=340 PA,θ_0=5K)

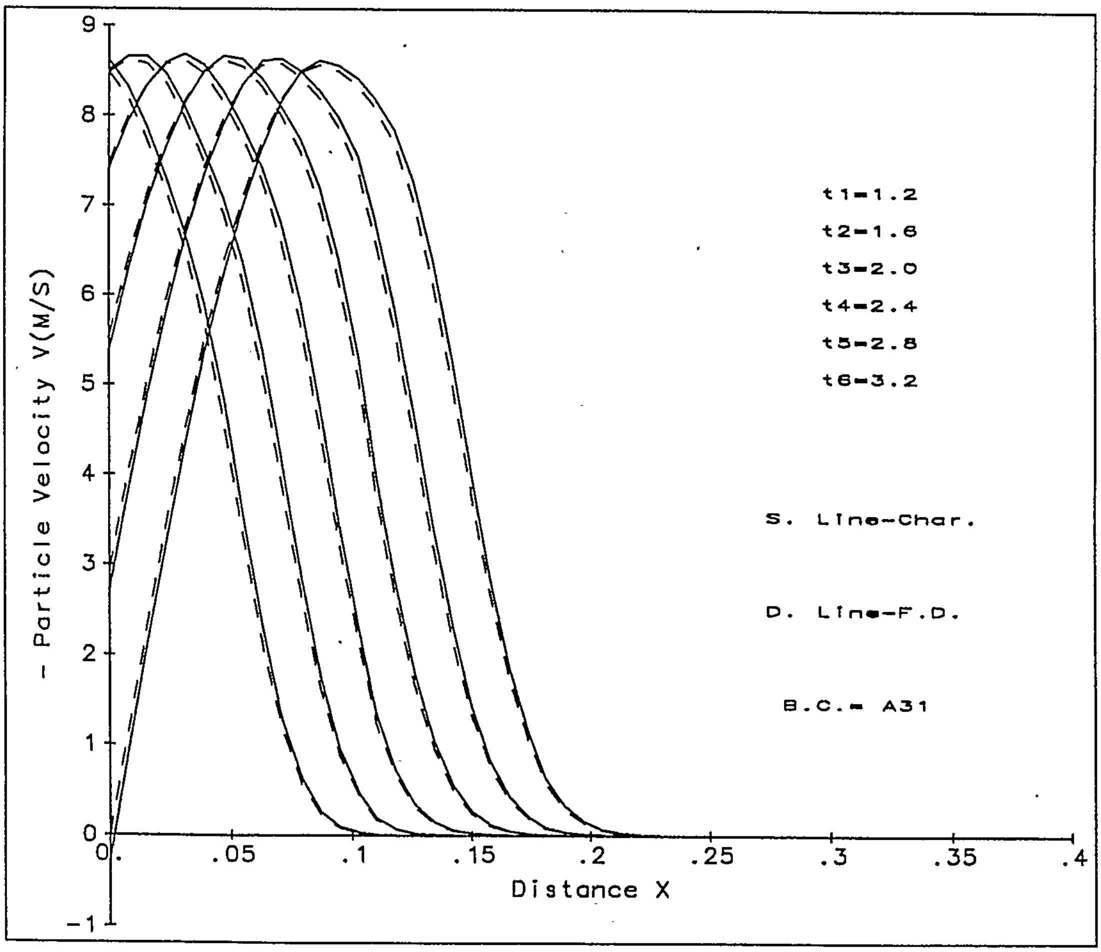

Fig. 6.21 Velocity distributions along x-axis due to stress and temperature sinusoid inputs (σ_0=340 MPA,θ_0=5K)

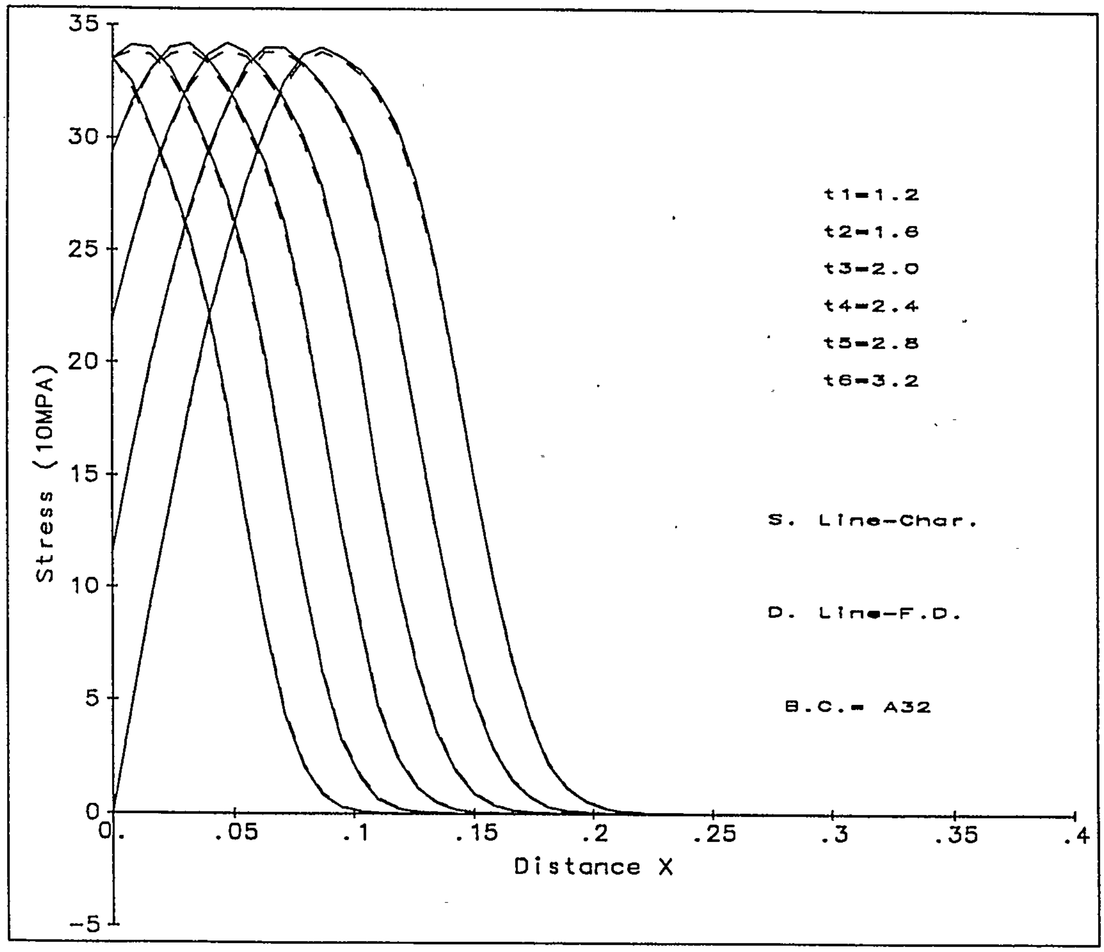

Fig. 6.22 Stress distribution along x-axis due to stress and temperature sinusoid inputs (σ_0=340 MPA,θ_0=5K)

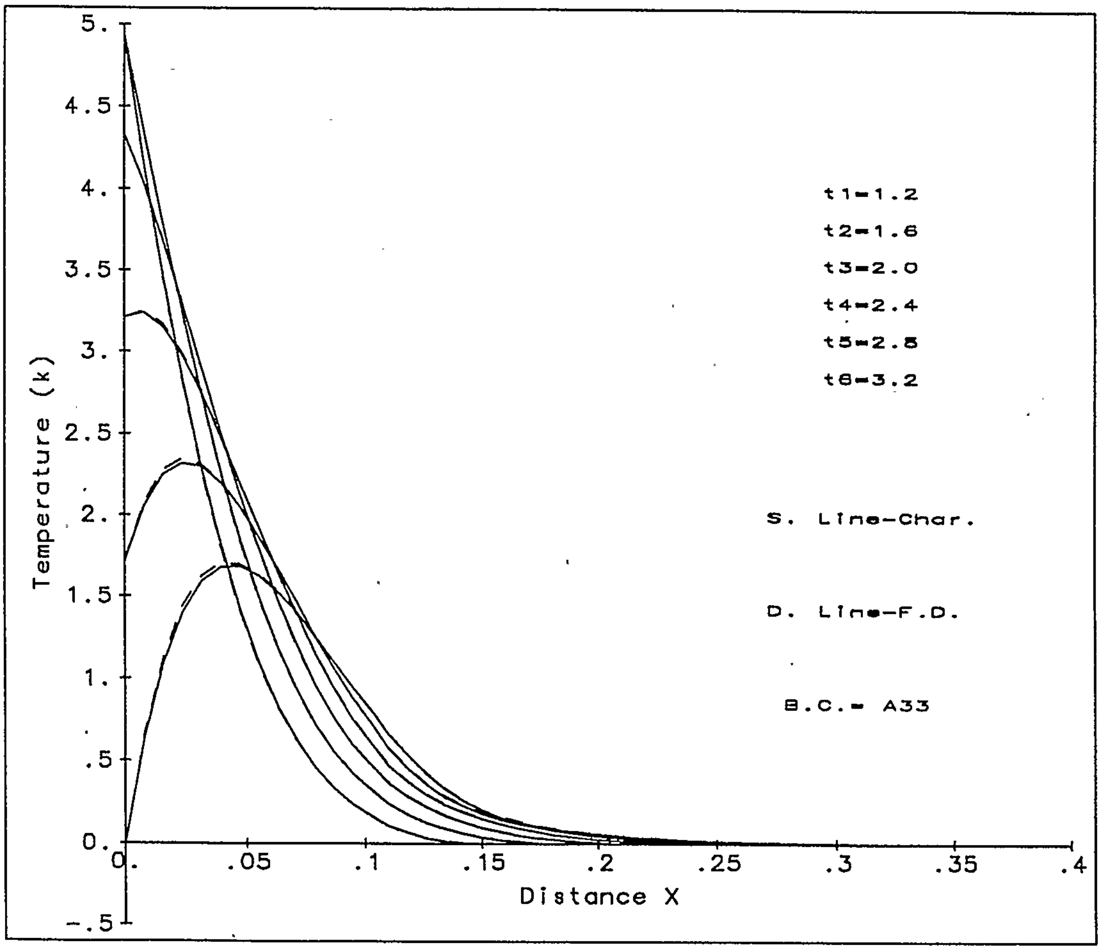

Fig. 6.23 Temperature distribution along x-axis due to stress and temperature sinusoid inputs (σ_0=340 MPA,θ_0=5K)

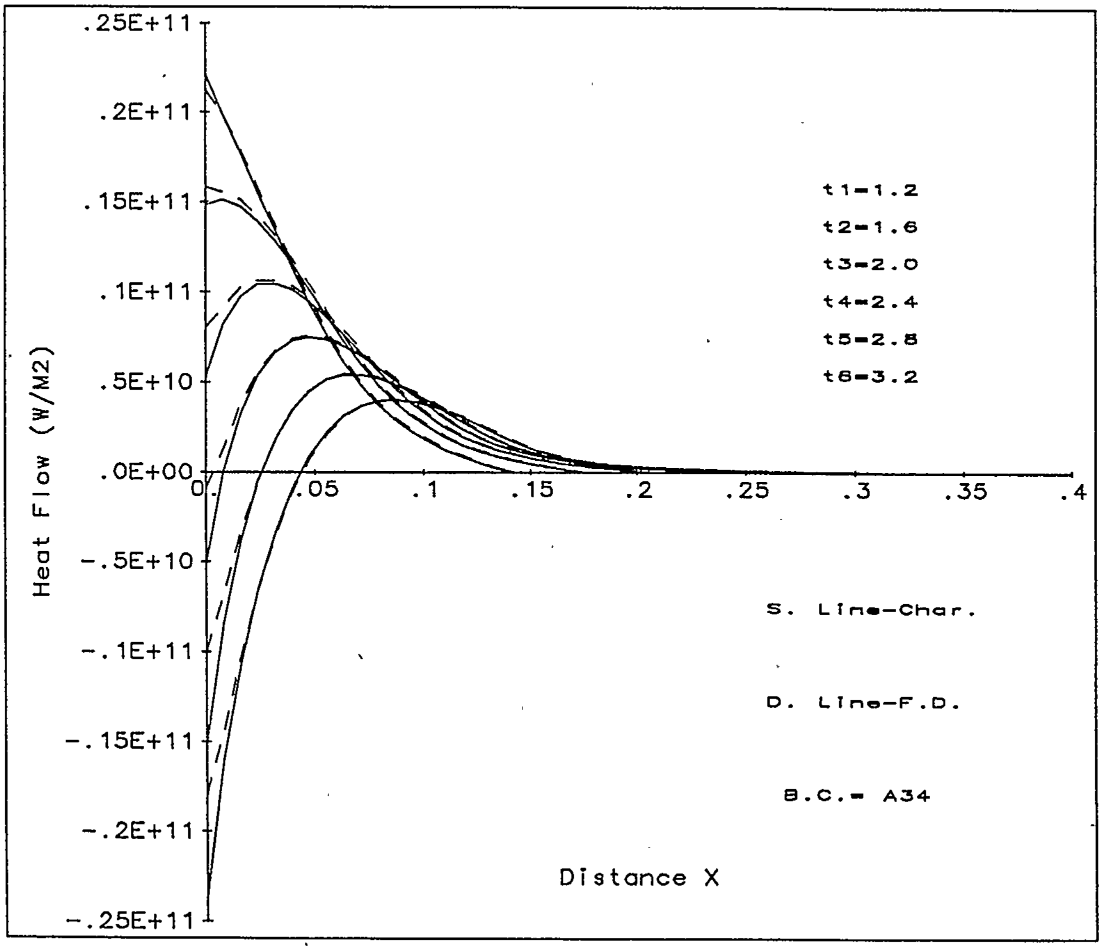

Fig. 6.24 Heat flow distribution along x-axis due to stress and temperature sinusoid inputs (σ_0=340 MPA,θ_0=5K)

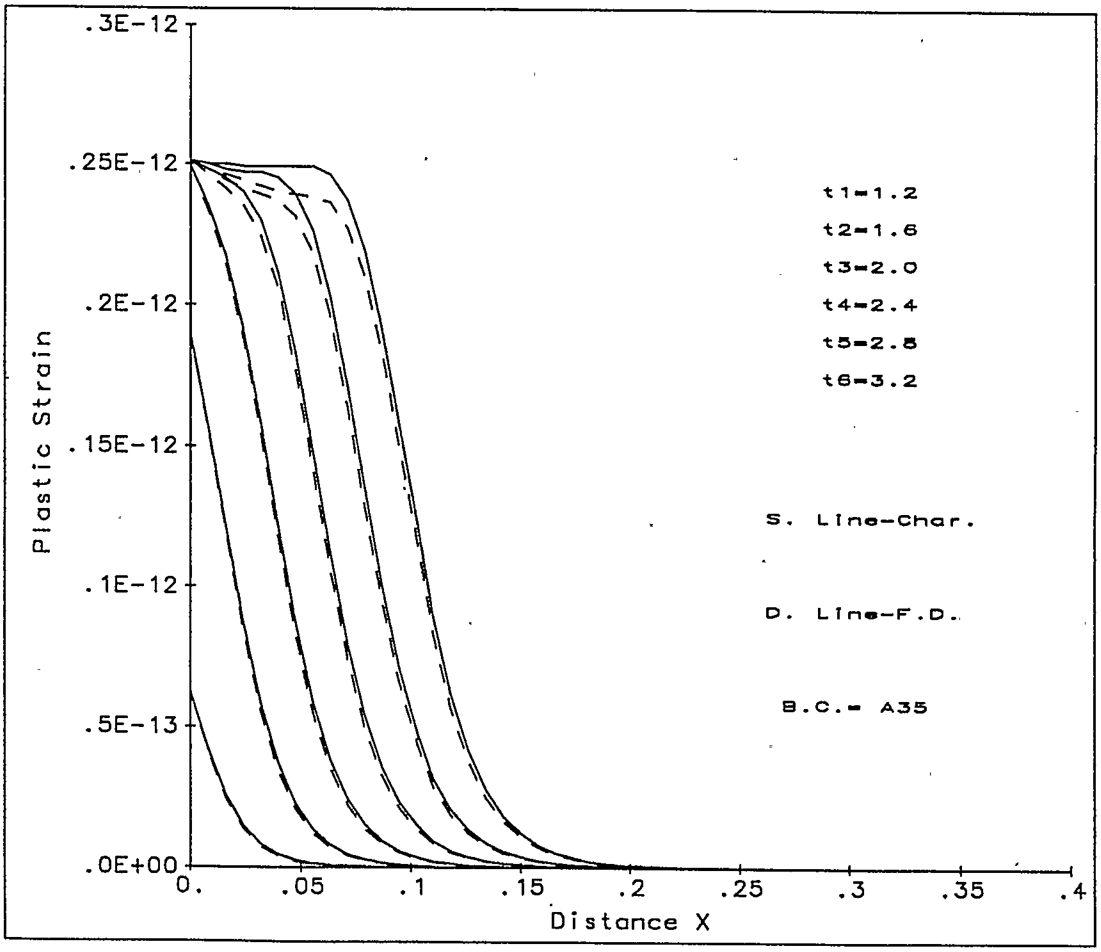

Fig. 6.25 Plastic strain distribution along x-axis due to stress and temperature sinusoid inputs (σ_0=340 MPA,θ_0=5K)

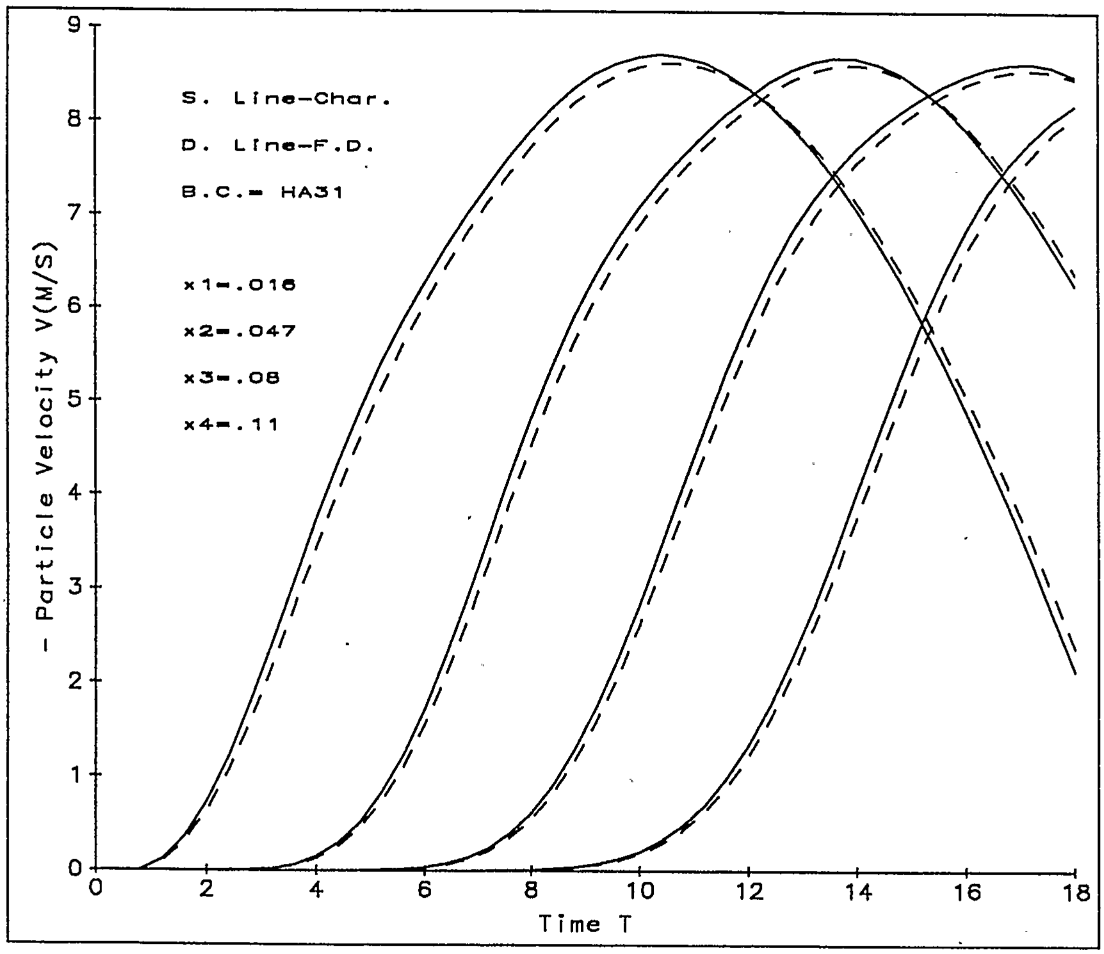

Fig. 6.26 Velocity response at certain positions due to stress and temperature sinusoid inputs (σ_0=340 MPA,θ_0=5K)

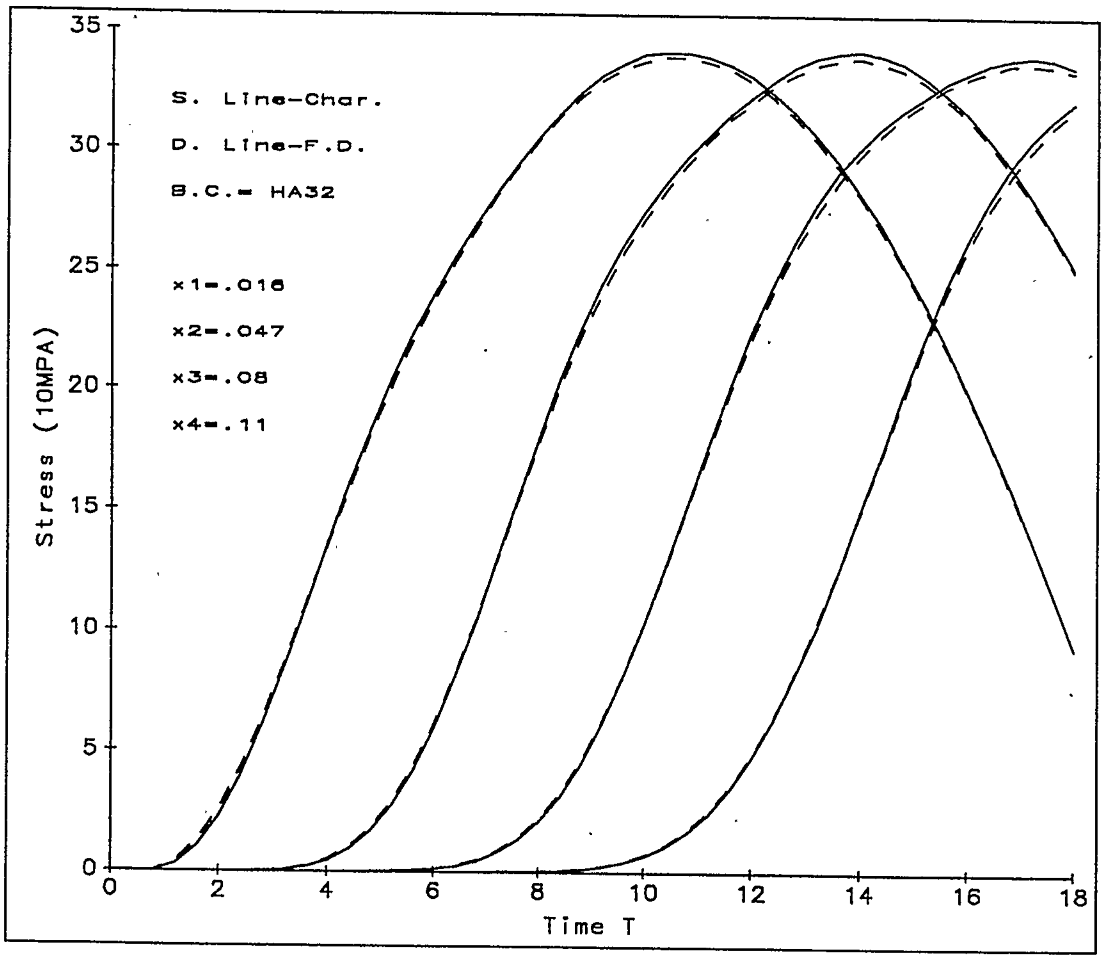

Fig. 6.27 Stress response at certain positions due to stress and temperature sinusoid inputs (σ_0=340 MPA,θ_0=5K)

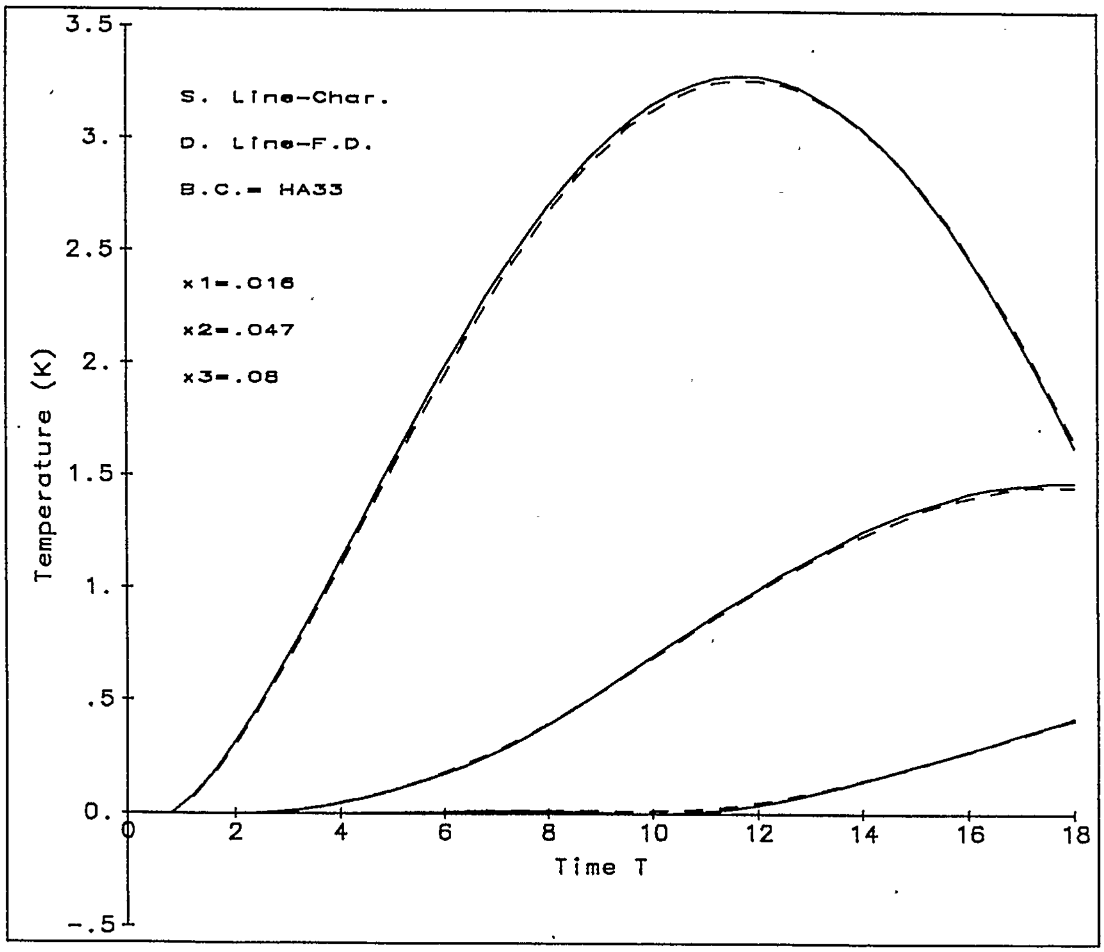

Fig.. 6.28 Temperature response at certain positions due to stress and temperature sinusoid inputs (σ_0=340 MPA,θ_0=5K)

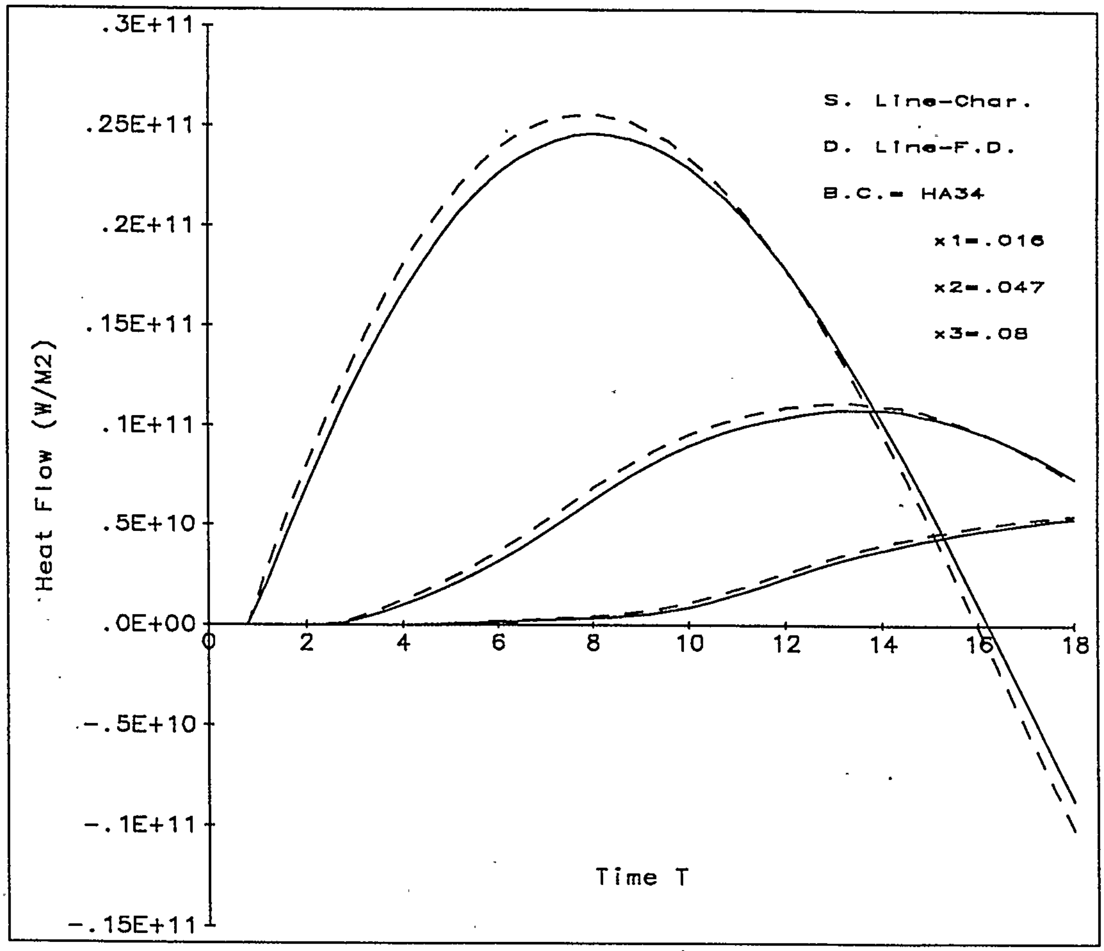

Fig. 6.29 Heat flow response at certain positions due to stress and temperature sinusoid inputs (σ_0=340 MPA,θ_0=5K)

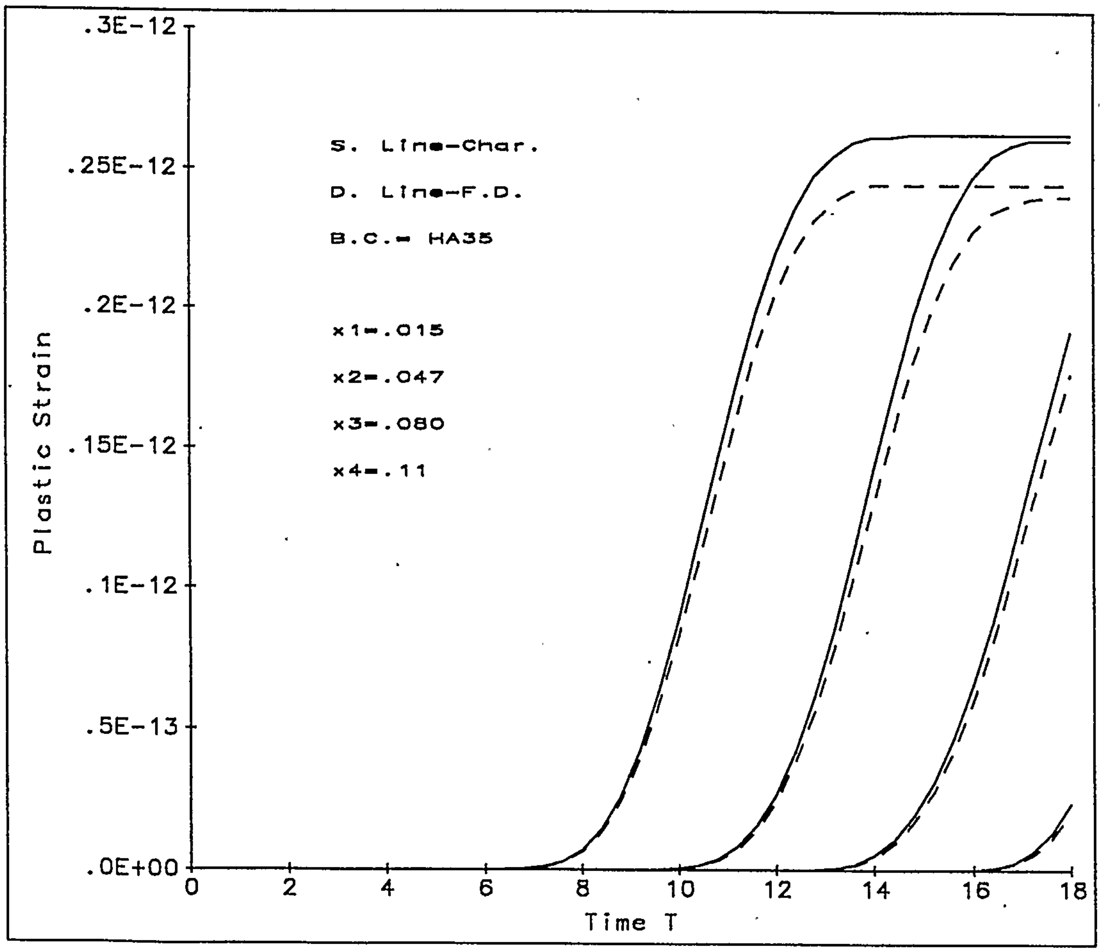

Fig. 6.30 Plastic strain response at certain positions due to stress and temperature sinusoid inputs (σ_0=340 MPA,θ_0=5K)

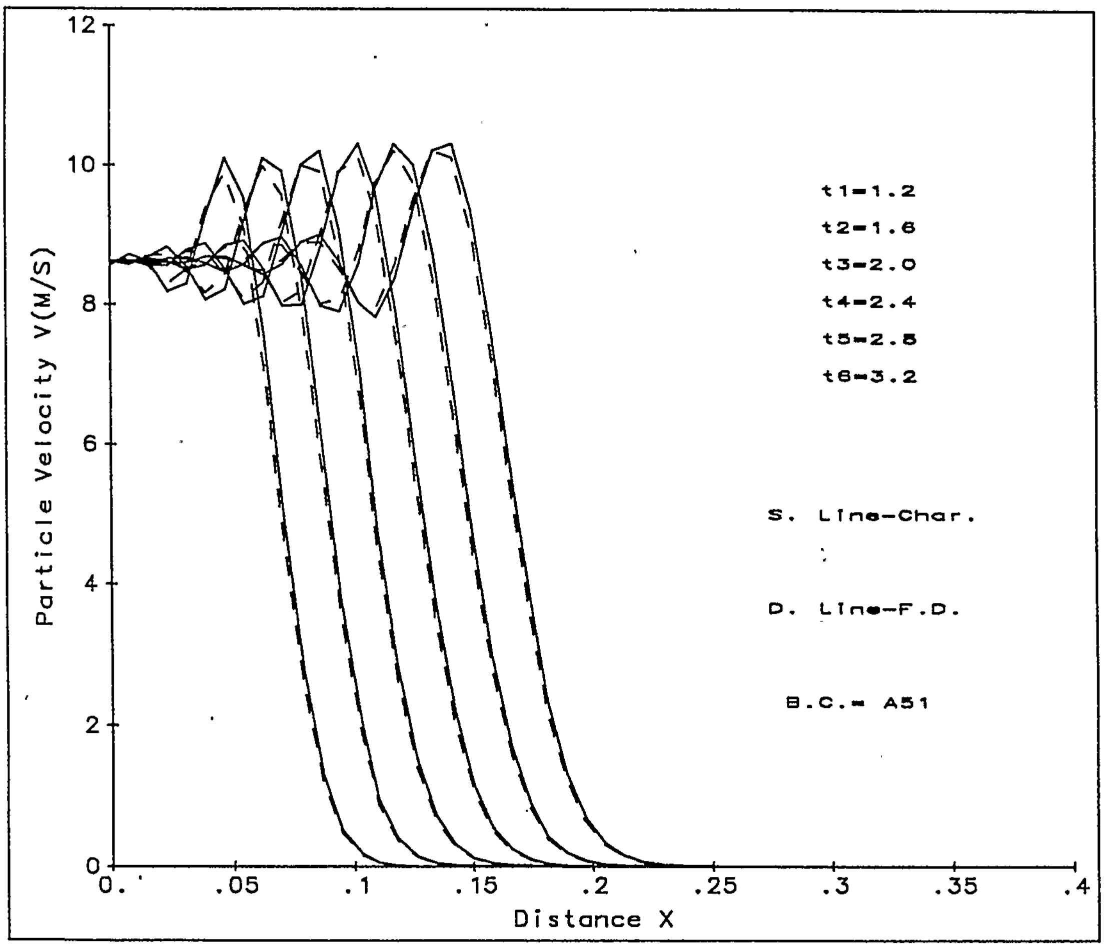

Fig. 6.31 Velocity distribution along x-axis due to stress step input alone (σ_0=340 MPA)

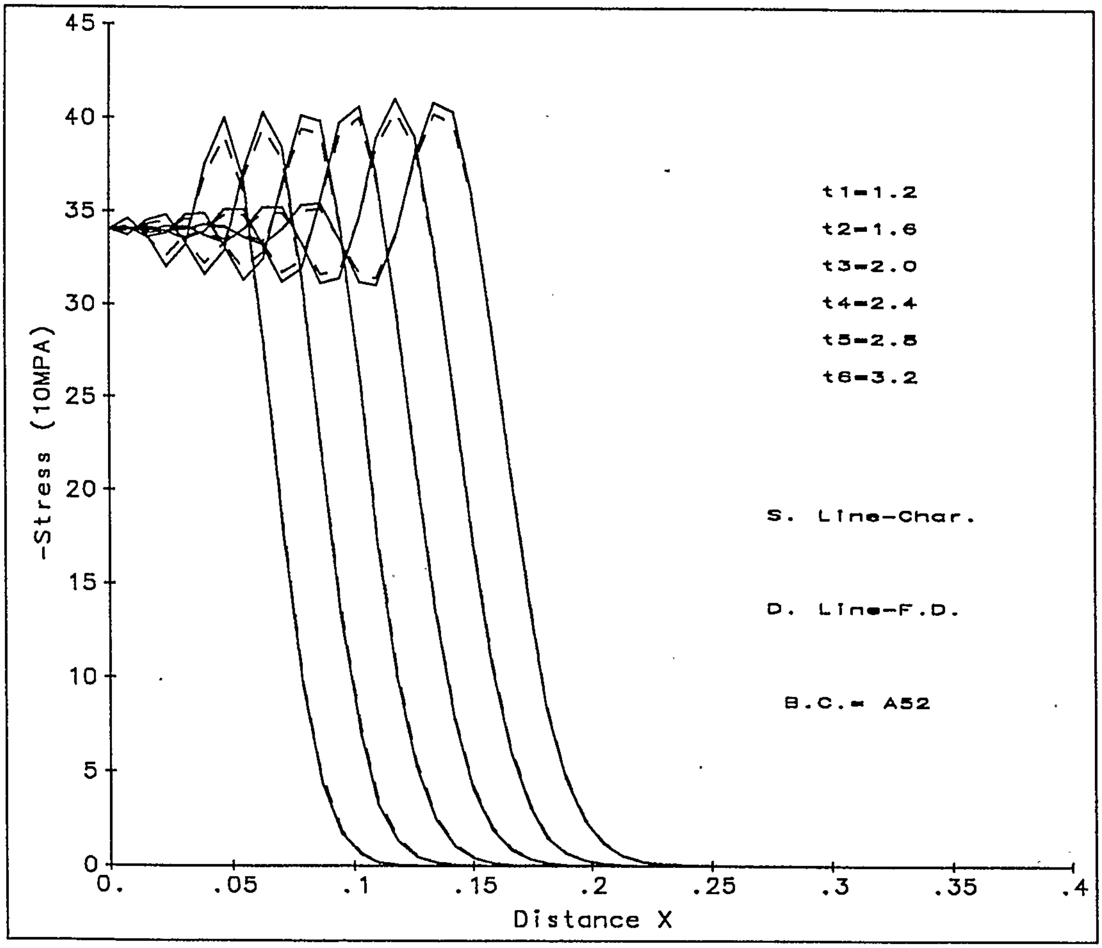

Fig. 6.32 Stress distribution along x-axis due to stress step input alone (σ_0=340 MPA)

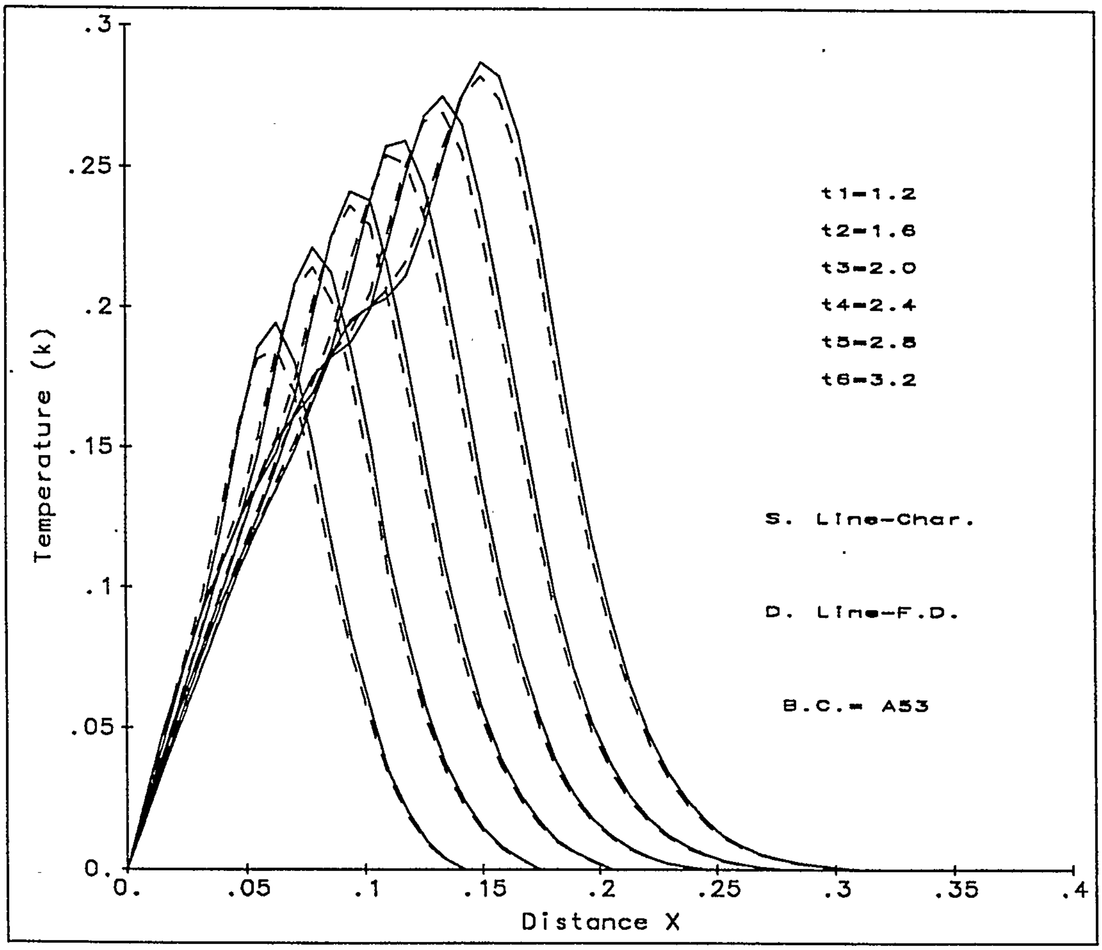

Fig. 6.33 Temperature distribution along x-axis due to stress step input alone (σ_0=340 MPA)

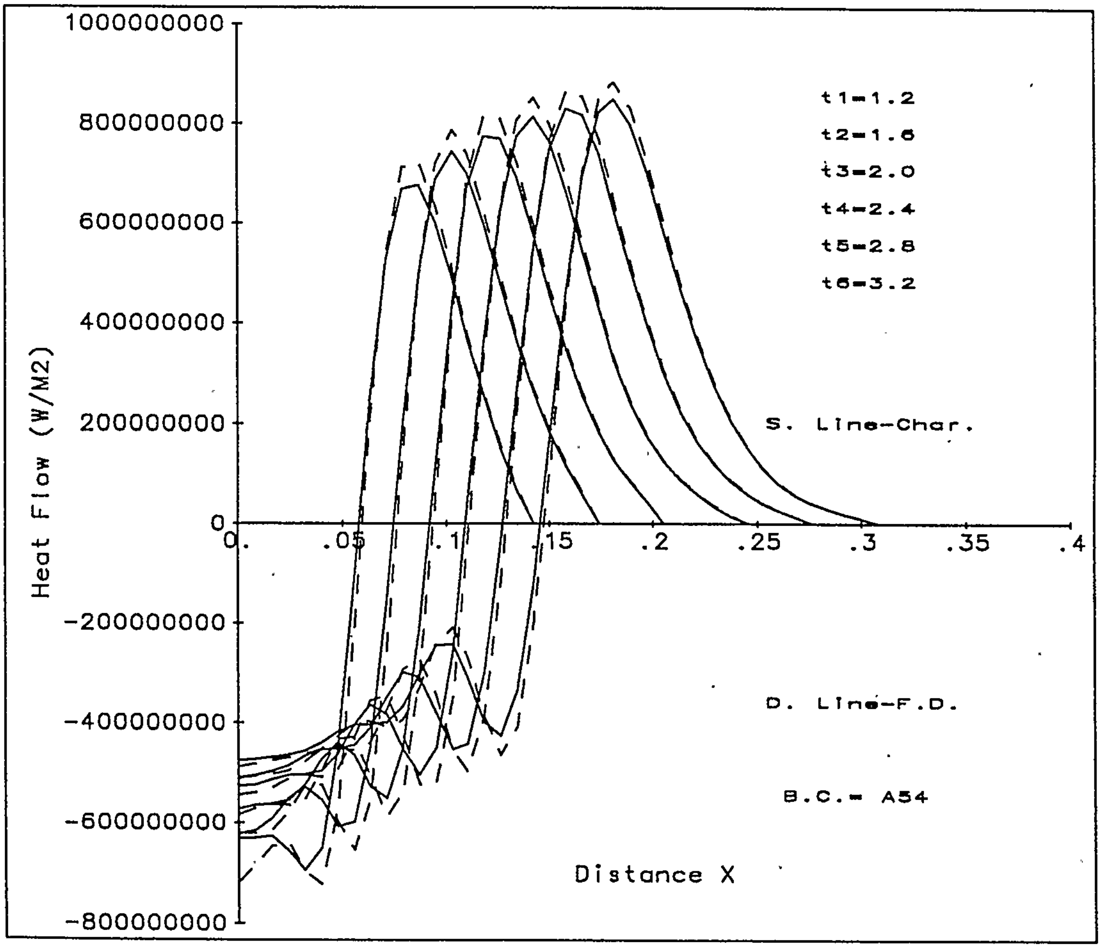

Fig. 6.34 Heat flow distribution along x-axis due to stress step input alone (σ_0=340 MPA)

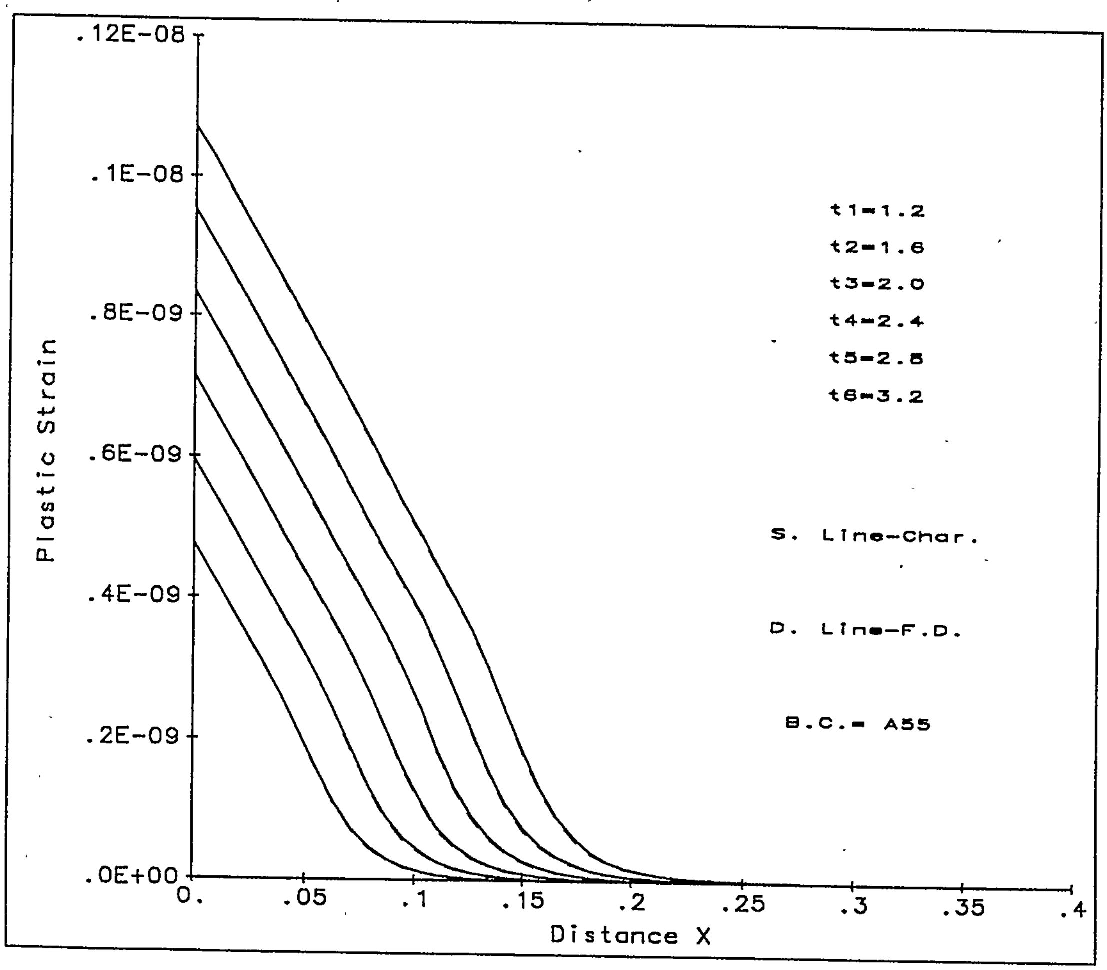

Fig. 6.35 Plastic strain distribution along x-axis due to stress step input alone (σ_0=340 MPA)

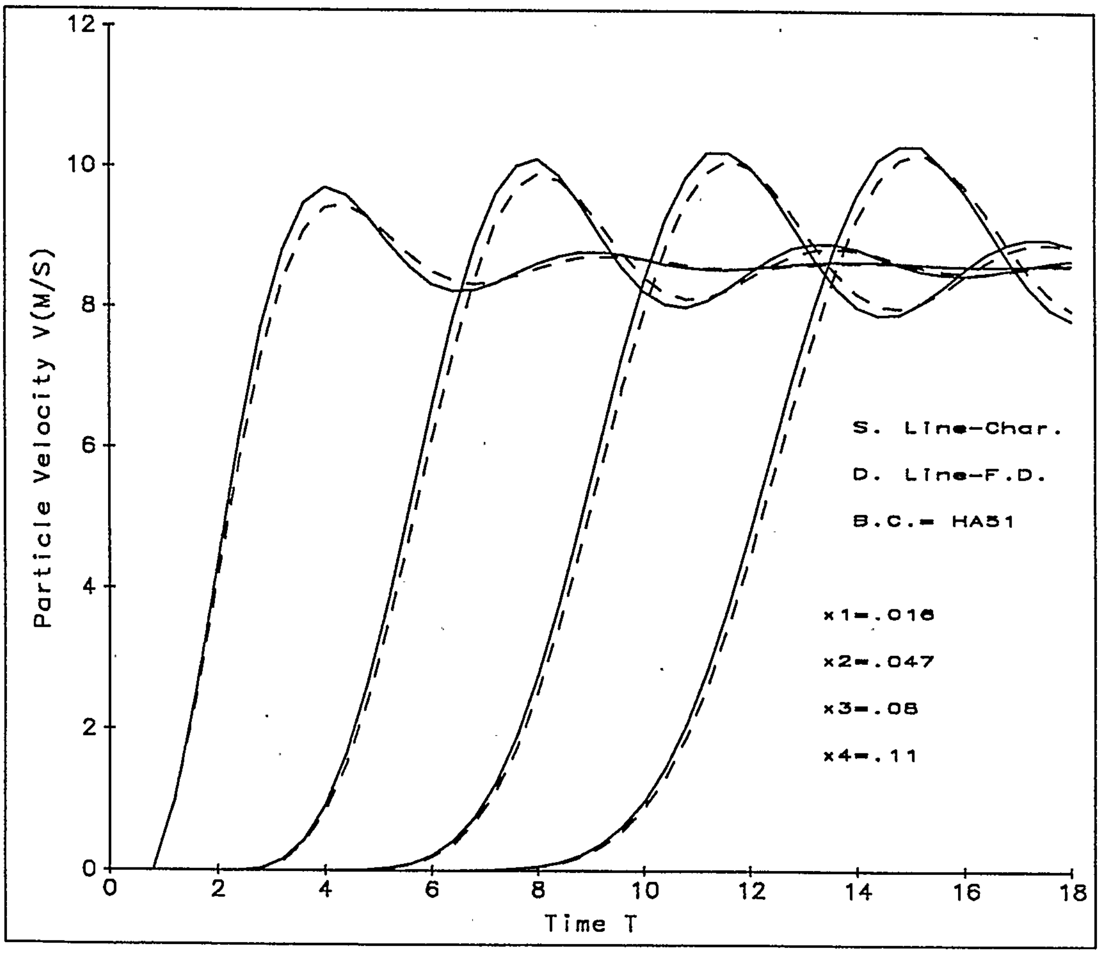

Fig. 6.36 Velocity response at certain positions due to stress step input alone (σ_0=340 MPA)

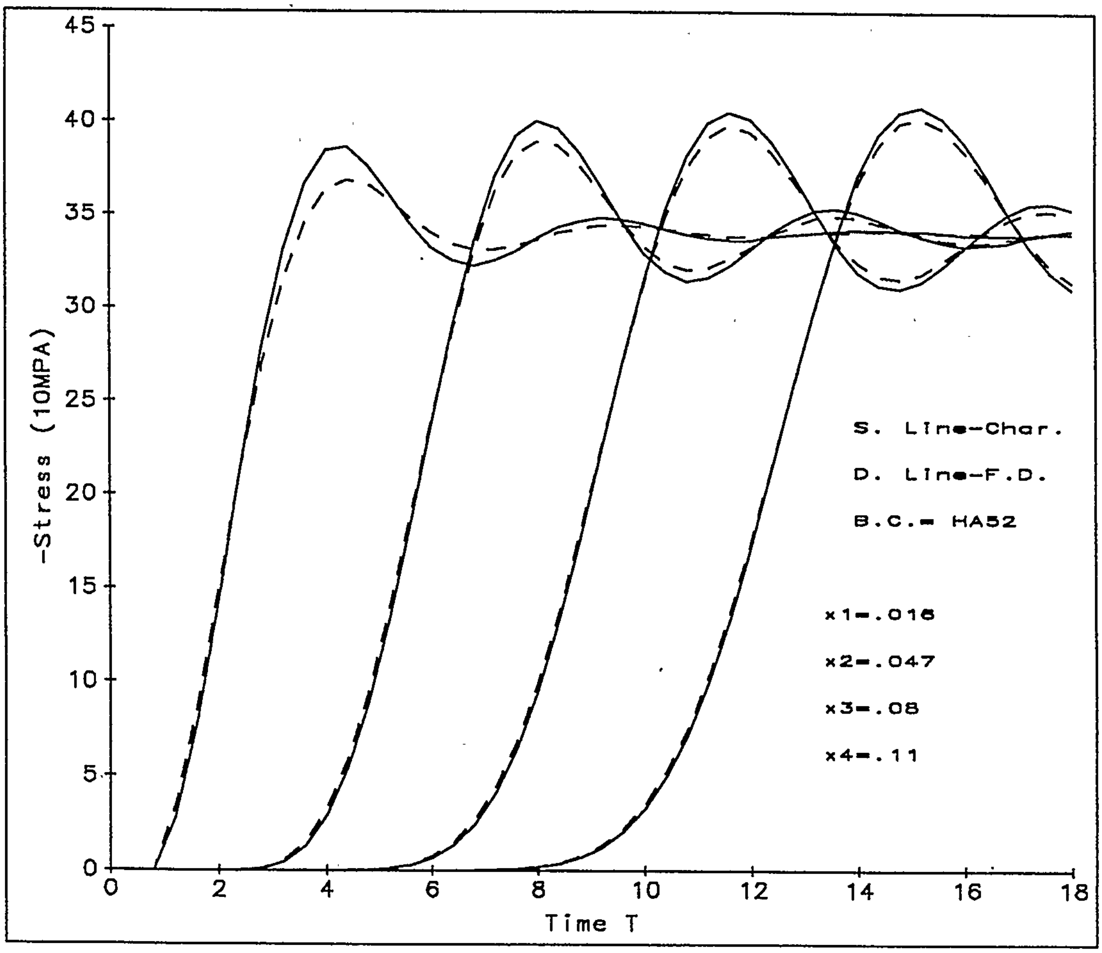

Fig. 6.37 Stress response at certain positions due to stress step input alone (σ_0=340 MPA)

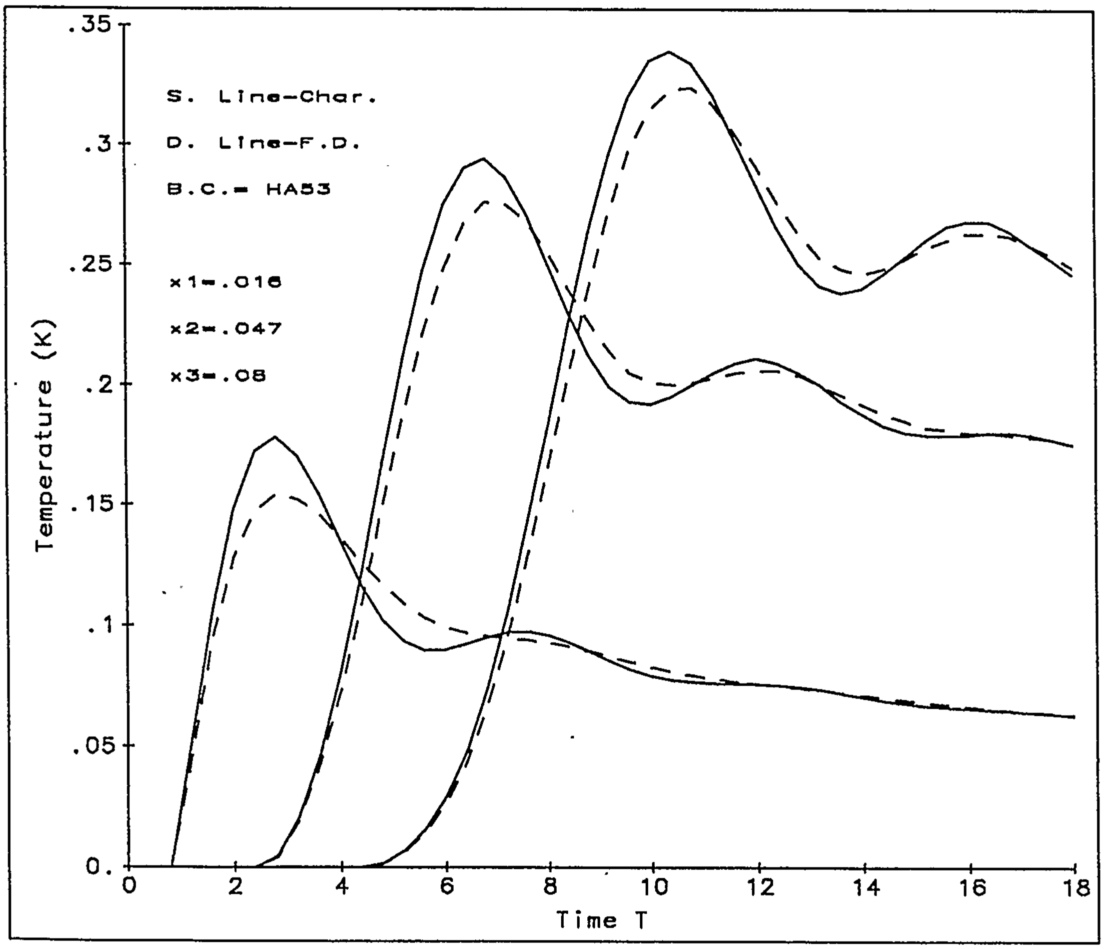

Fig. 6.38 Temperature response at certain positions due to stress step input alone (σ_0=340 MPA)

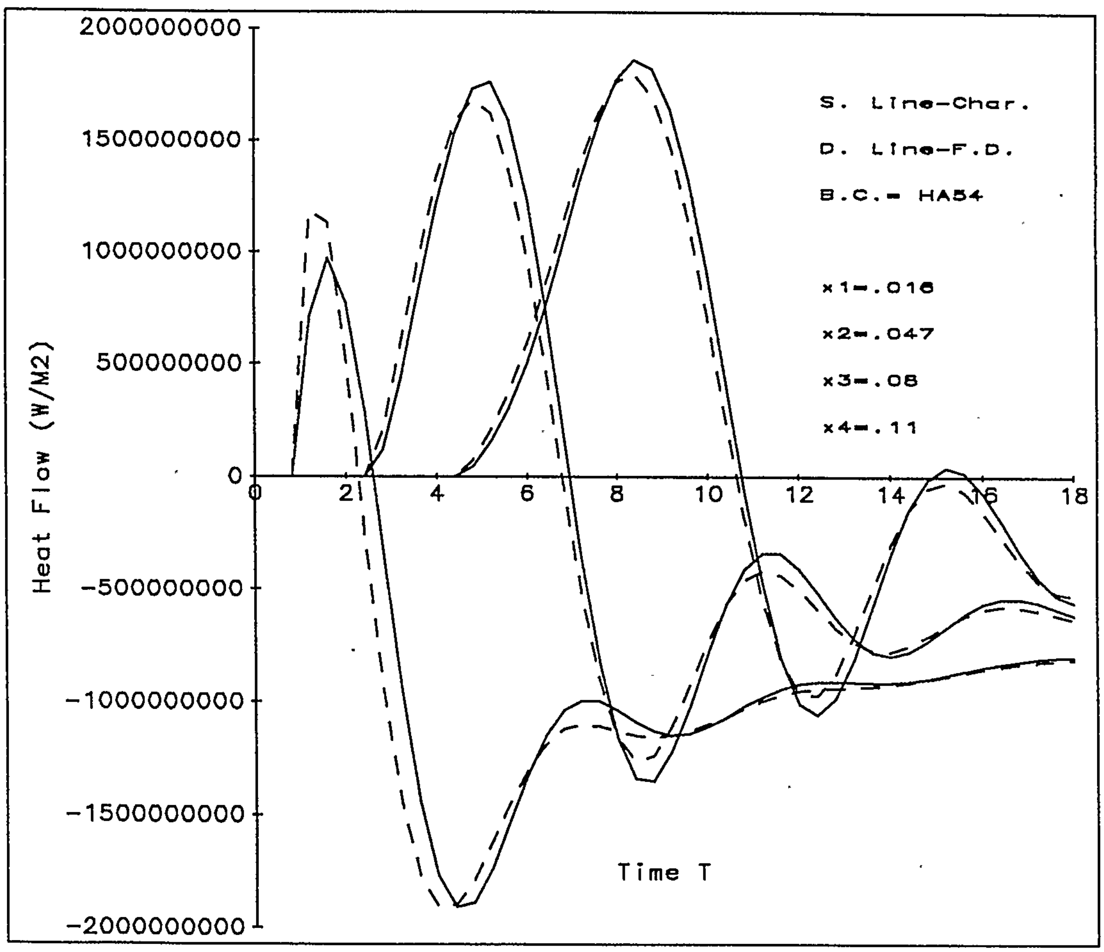

Fig. 6.39 Heat flow response at certain positions due to stress step input alone (σ_0=340 MPA)

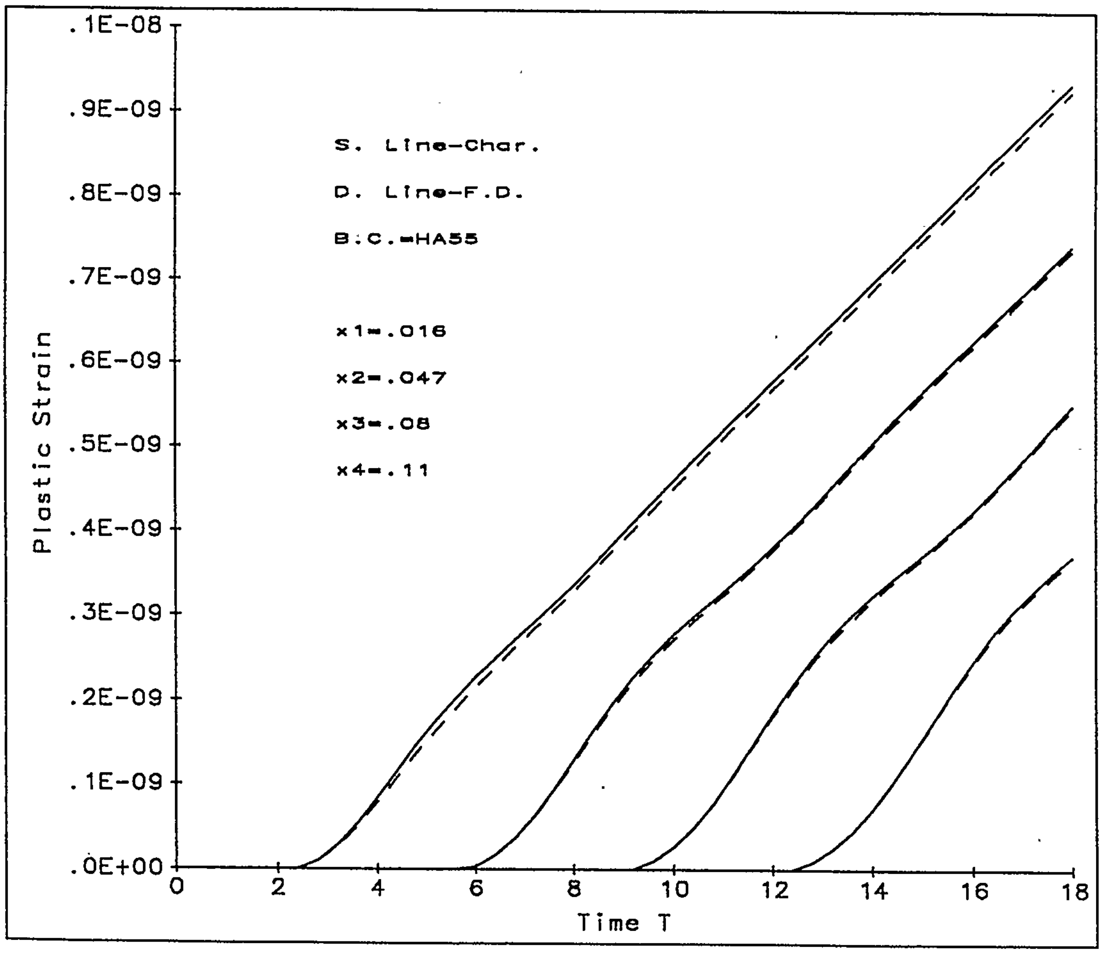

Fig. 6.40 Plastic strain response at certain positions due to stress step input alone (σ_0=340 MPA)

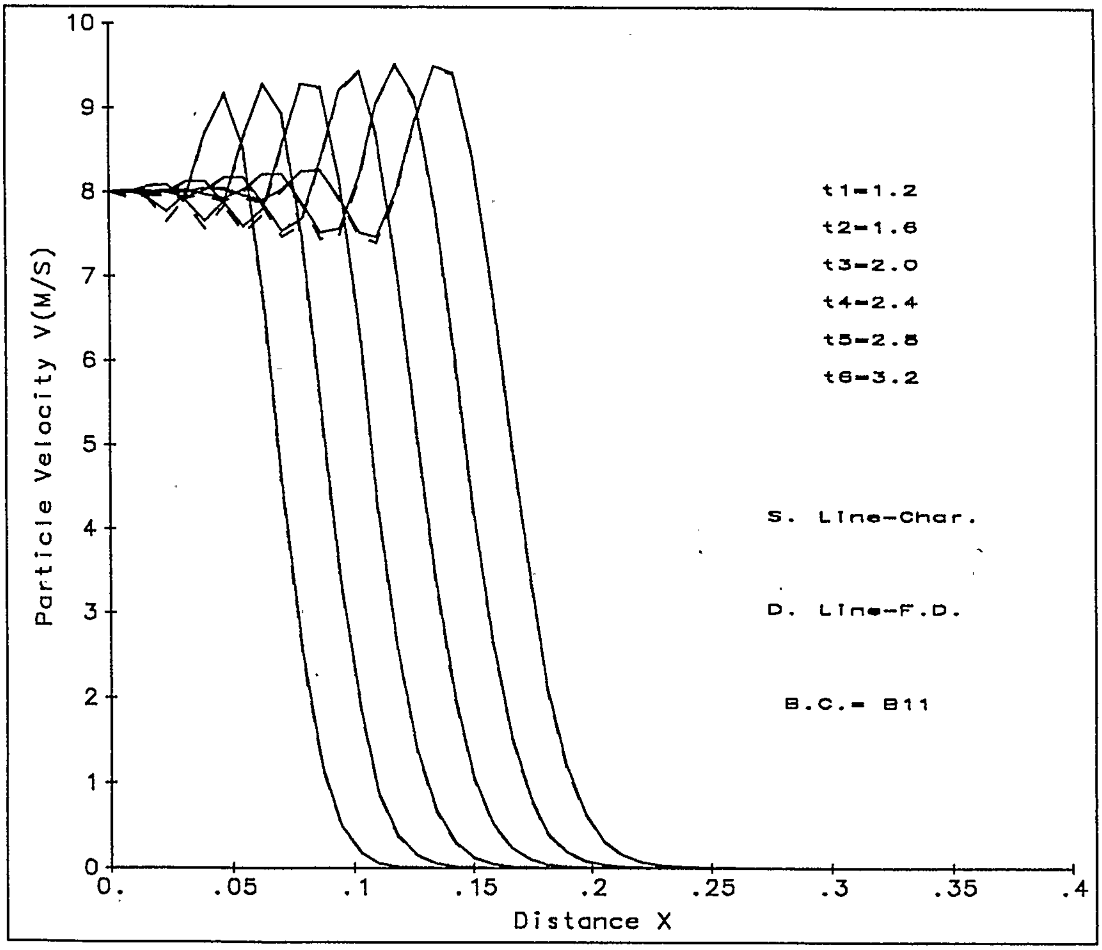

Fig. 6.41 Velocity distribution along x-axis due to velocity and temperature step inputs (V_0=8 M/S,θ_0=5K)

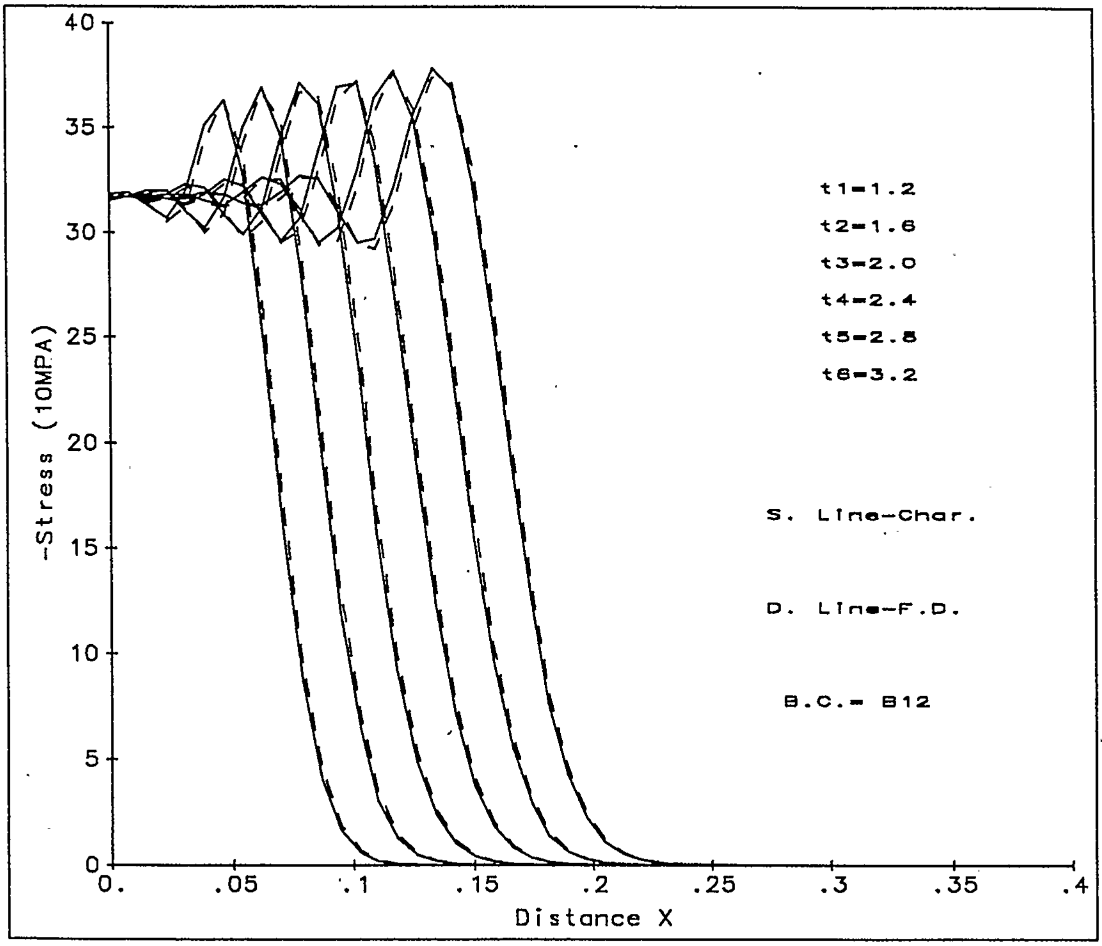

Fig. 6.42 Stress distribution along x-axis due to velocity and temperature step inputs (V_0=8 M/S,θ_0=5K)

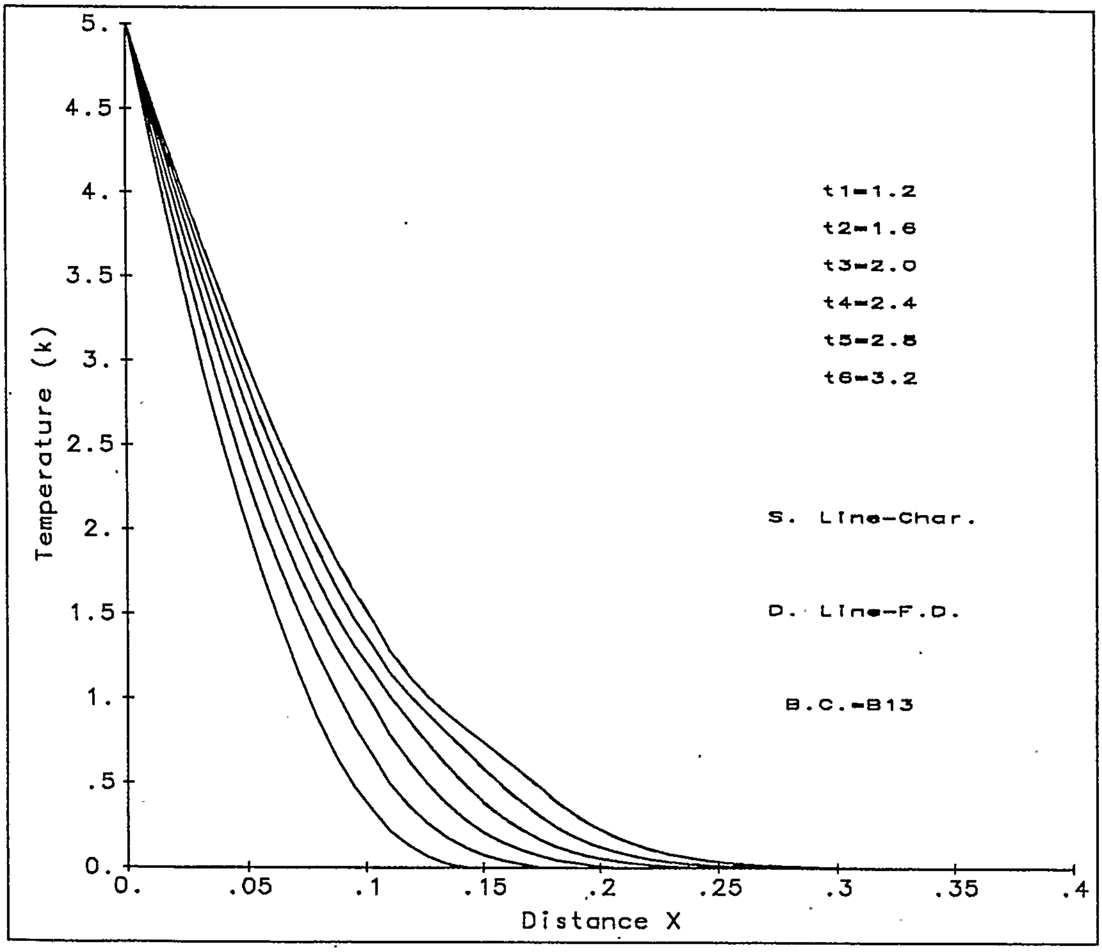

Fig. 6:43 Temperature distribution along x-axis due to velocity and temperature step inputs (V_0=8 M/S,θ_0=5K)

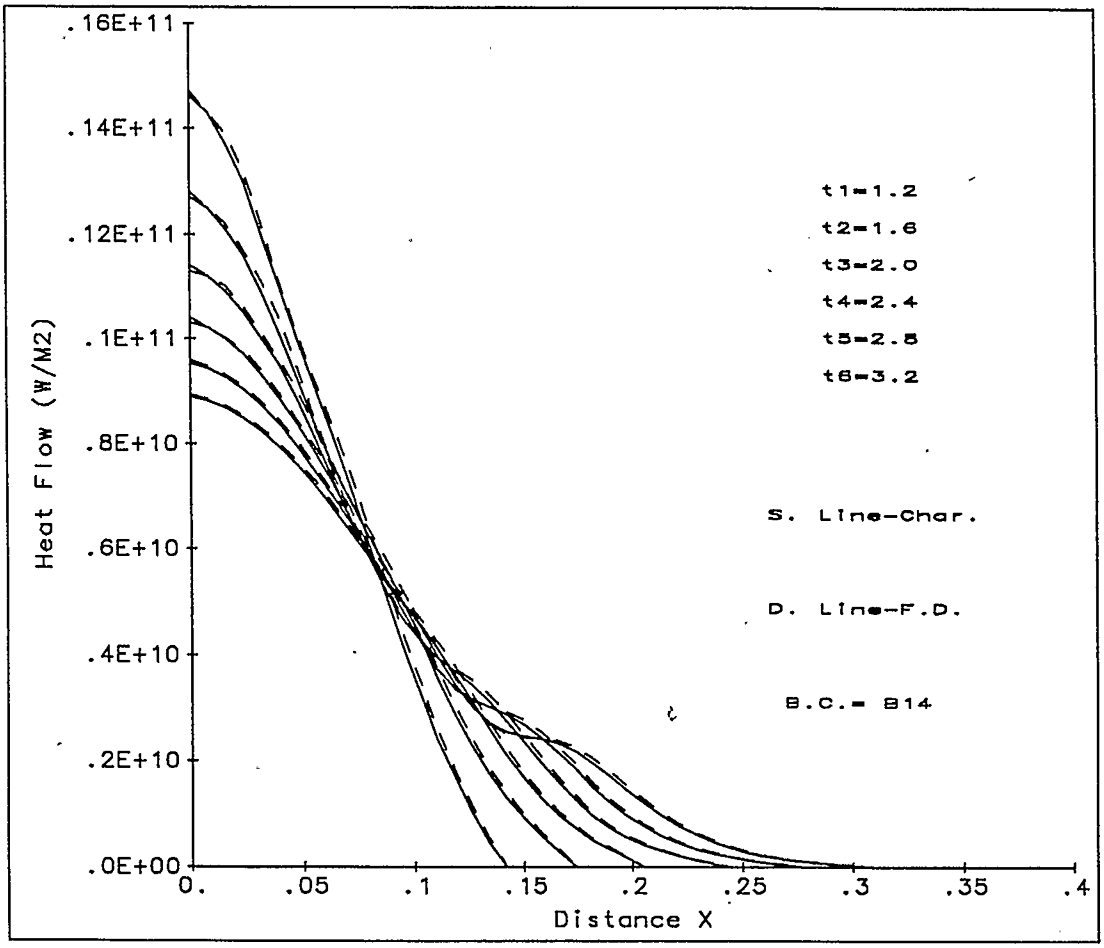

Fig. 6.44 Heat flow distribution along x-axis due to velocity and temperature step inputs (V_0=8 M/S,θ_0=5K)

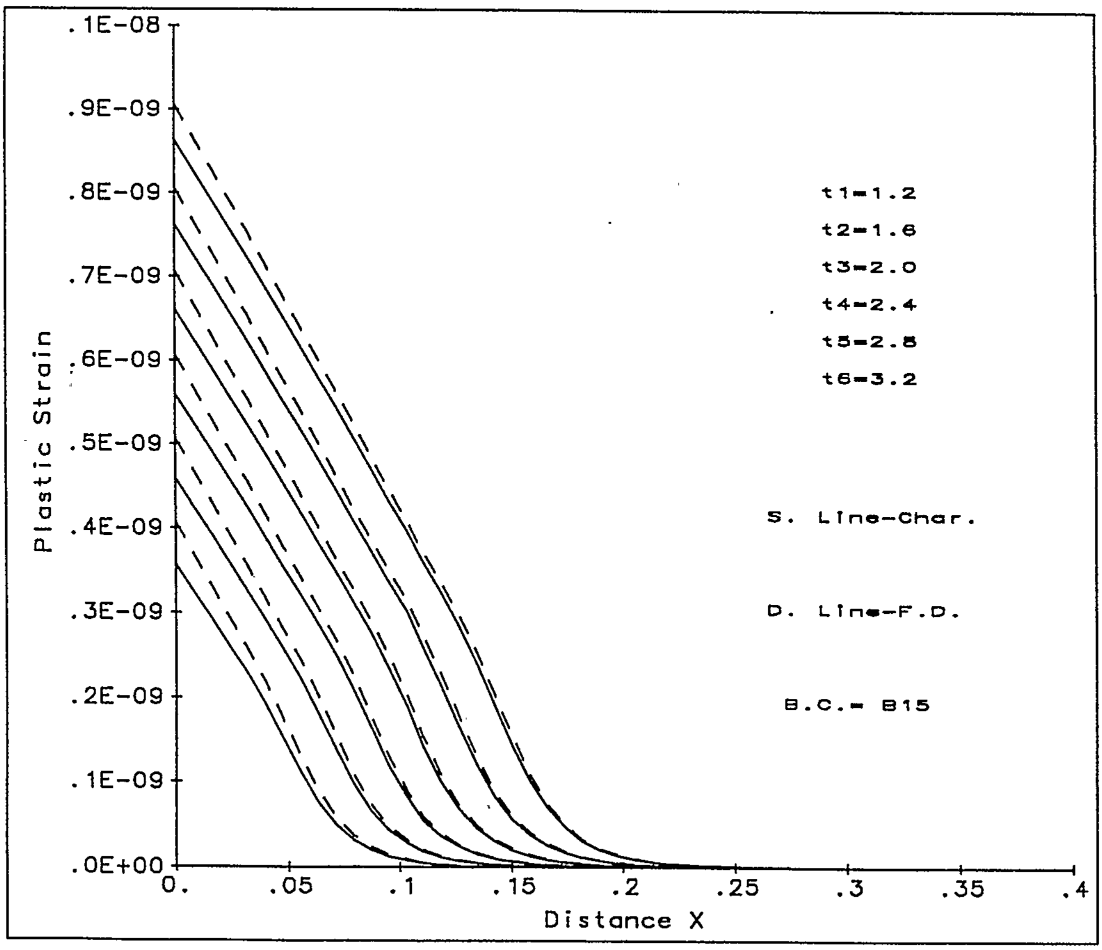

Fig. 6.45 Plastic strain distribution along x- axis due to velocity and temperature step inputs (V_0=8 M/S,θ_0=5K)

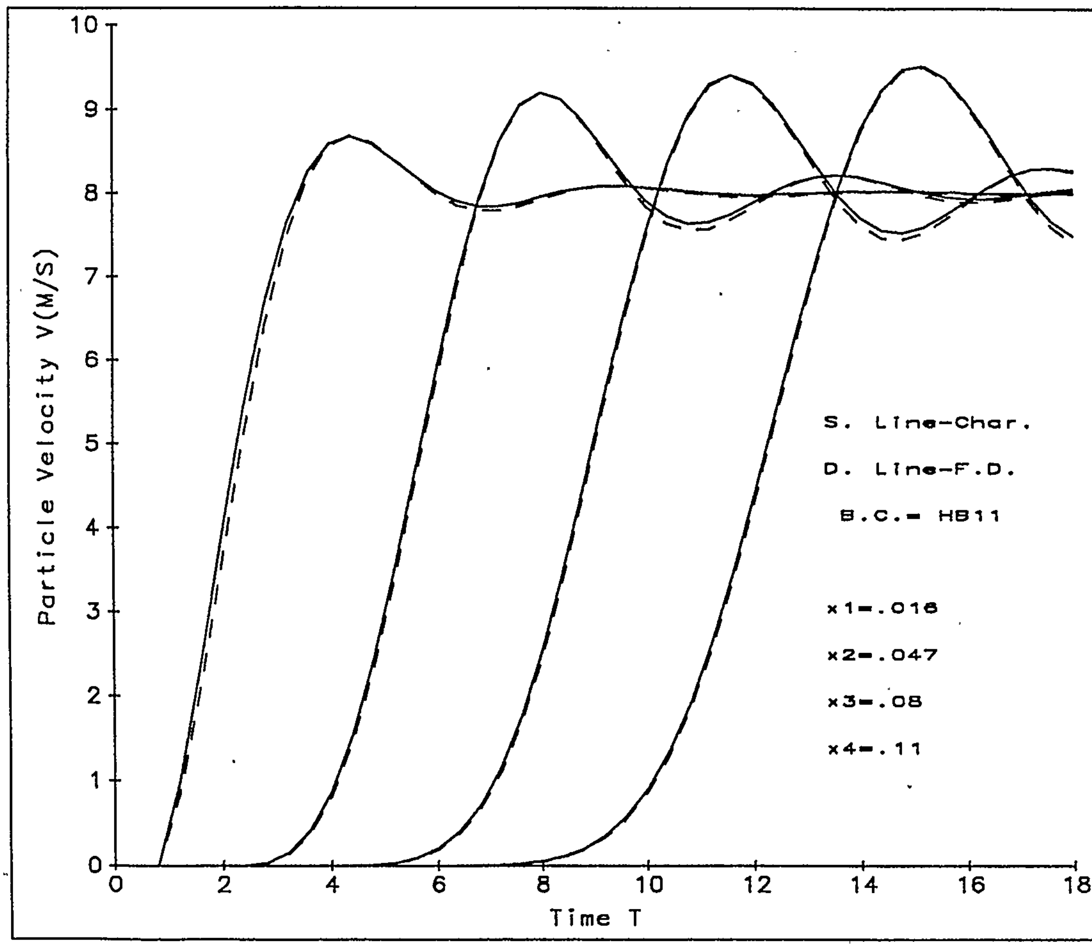

Fig. 6.46 Velocity response at certain positions due to velocity and temperature step inputs (V_0=8 M/S,θ_0=5K)

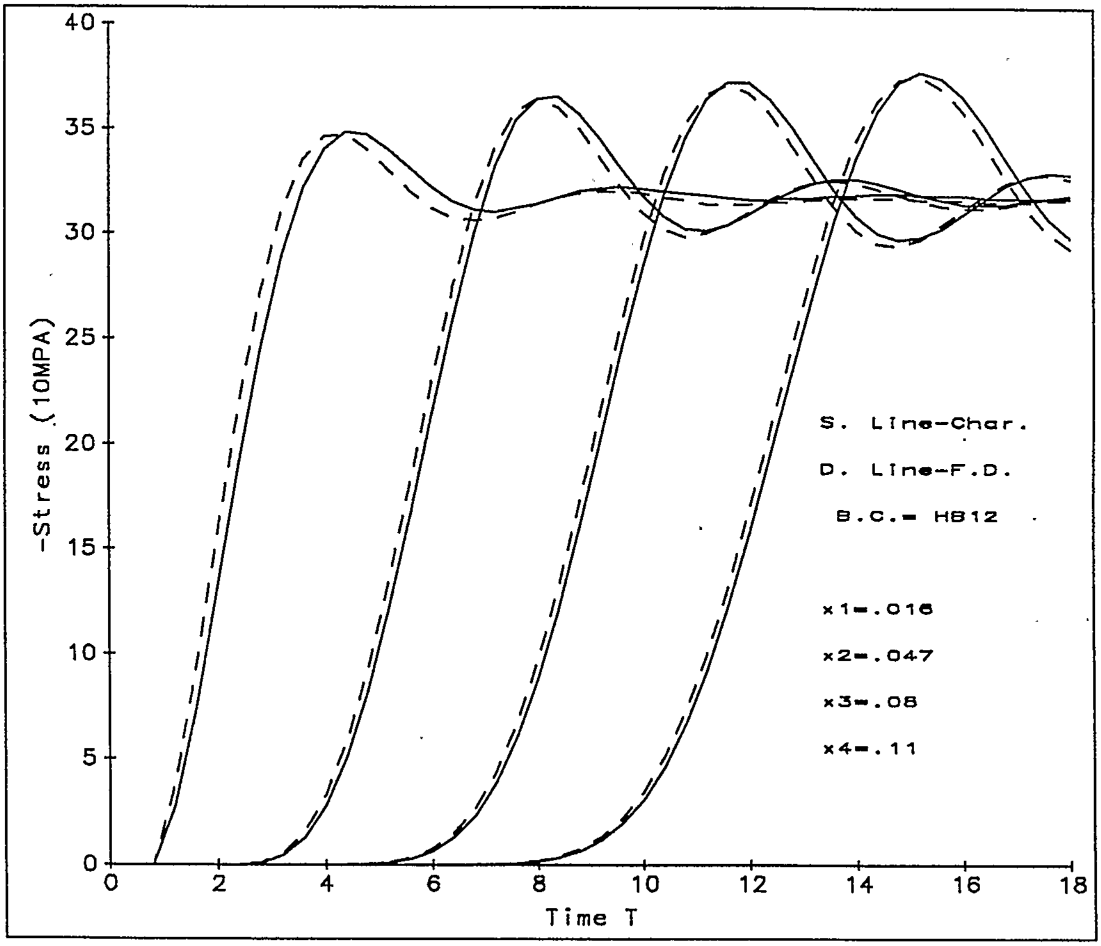

Fig. 6.47 Stress response at certain positions due to velocity and temperature step inputs (V_0=8 M/S,θ_0=5K)

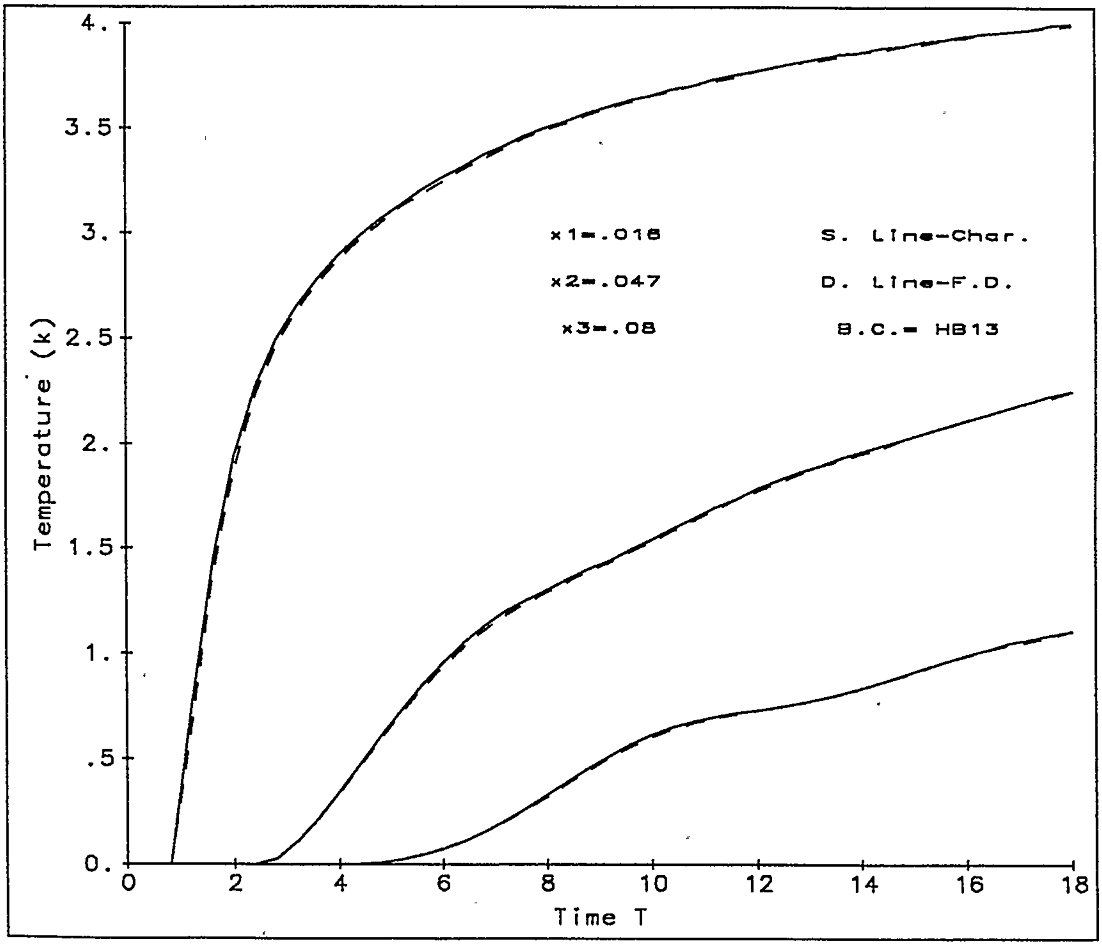

Fig. 6.48 Temperature response at certain positions due to velocity and temperature step inputs (V_0=8 M/S,θ_0=5K)

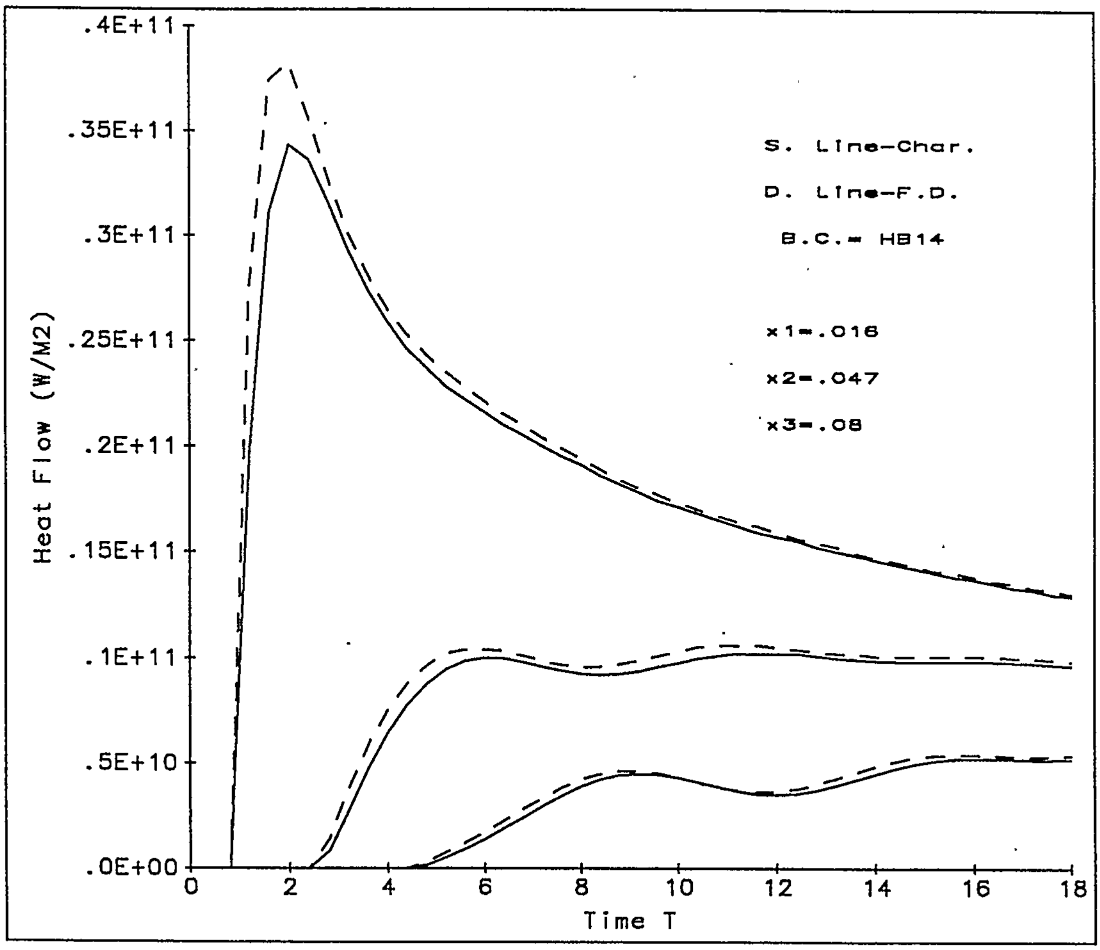

Fig. 6.49 Heat flow response at certain positions due to velocity and temperature step inputs (V_0=8 M/S,θ_0=5K)

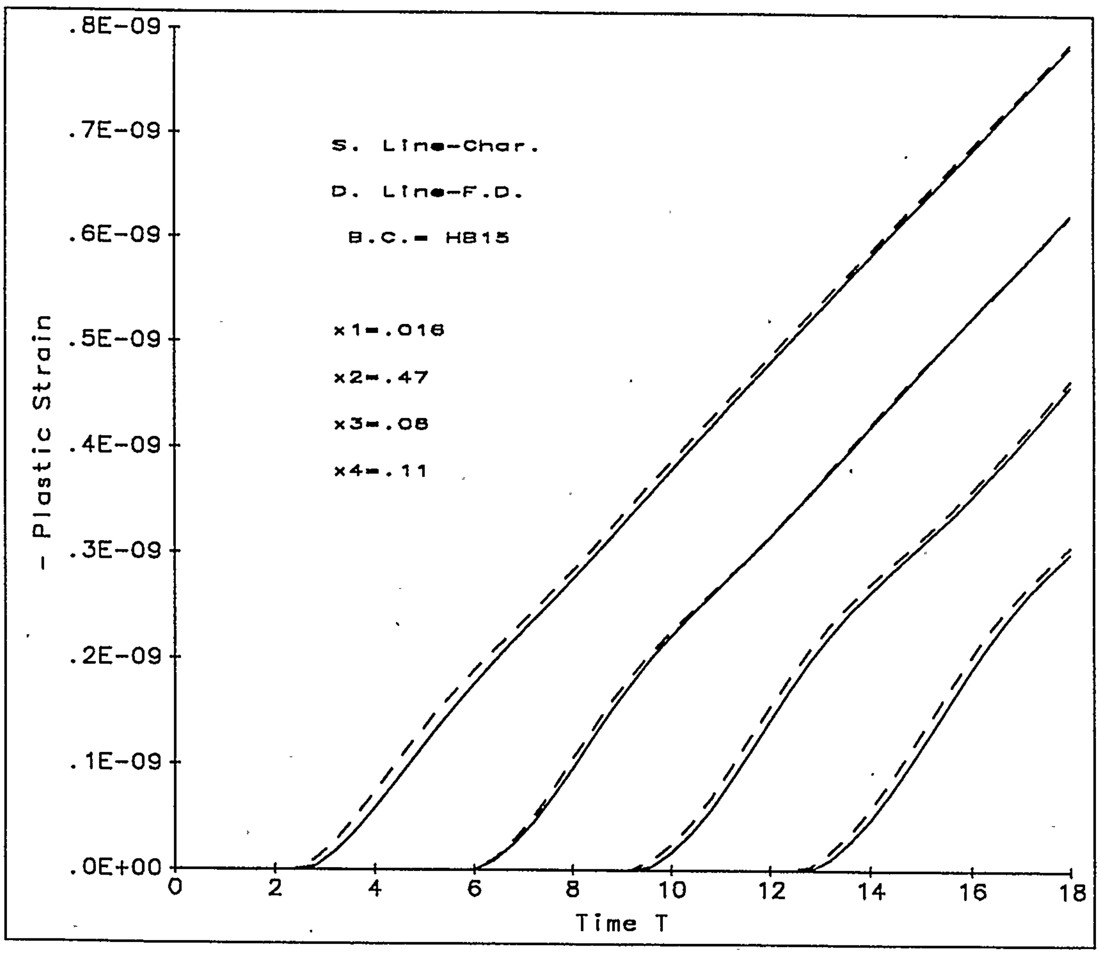

Fig. 6.50 Plastic strain response at certain positions due to velocity and temperature step inputs (V_0=8 M/S,θ_0=5K) .

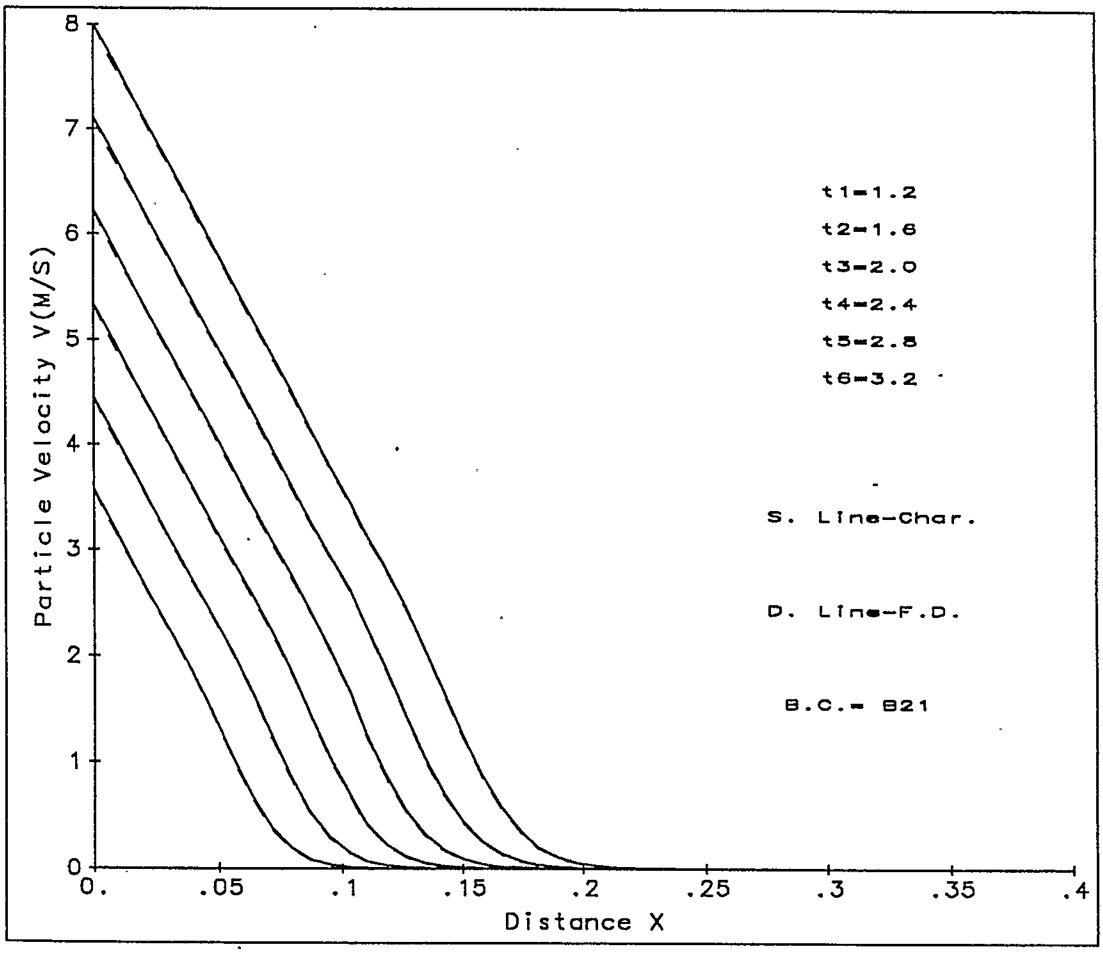

Fig. 6.51 Velocity distribution along x-axis due to velocity and temperature ramp inputs (V_0=8 M/S,θ_0=5K)

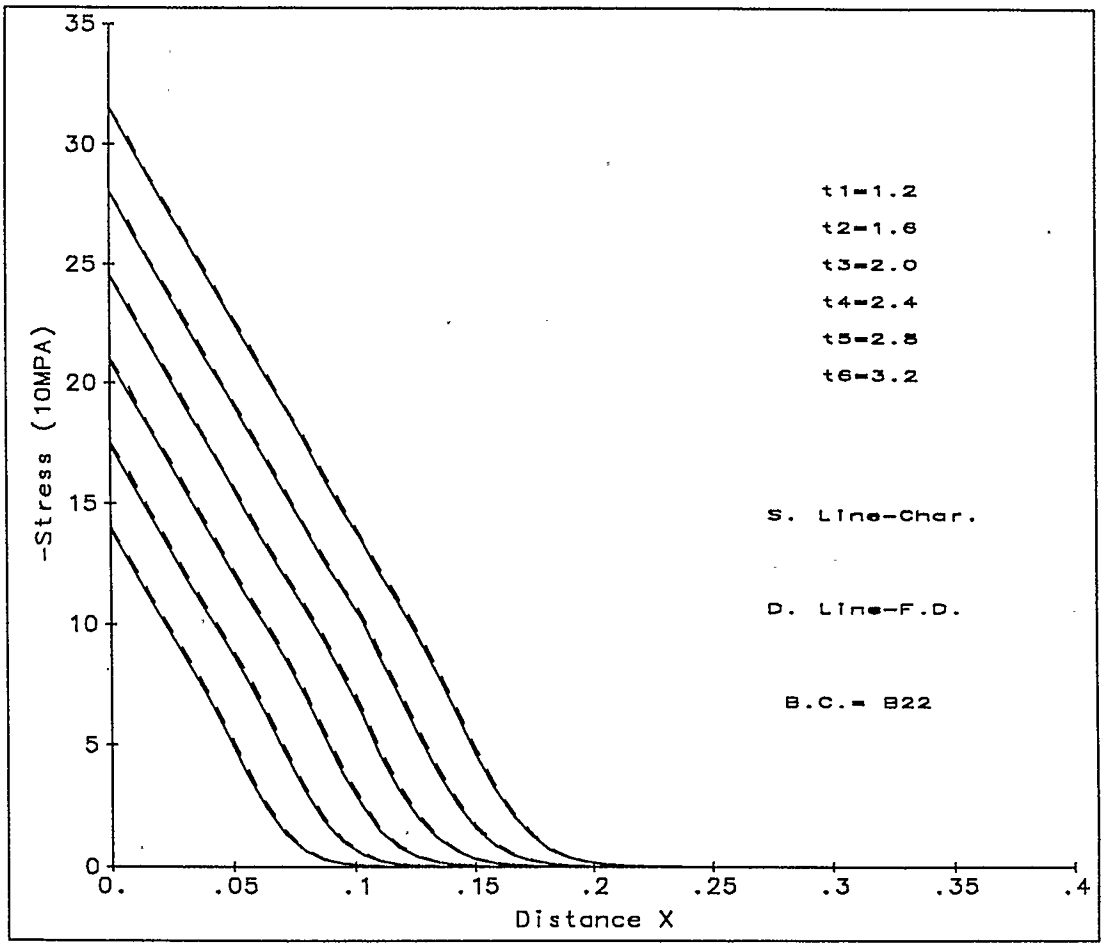

Fig. 6.52 Stress distribution along x-axis due to velocity and temperature ramp inputs (V_0=8 M/S,θ_0=5K)

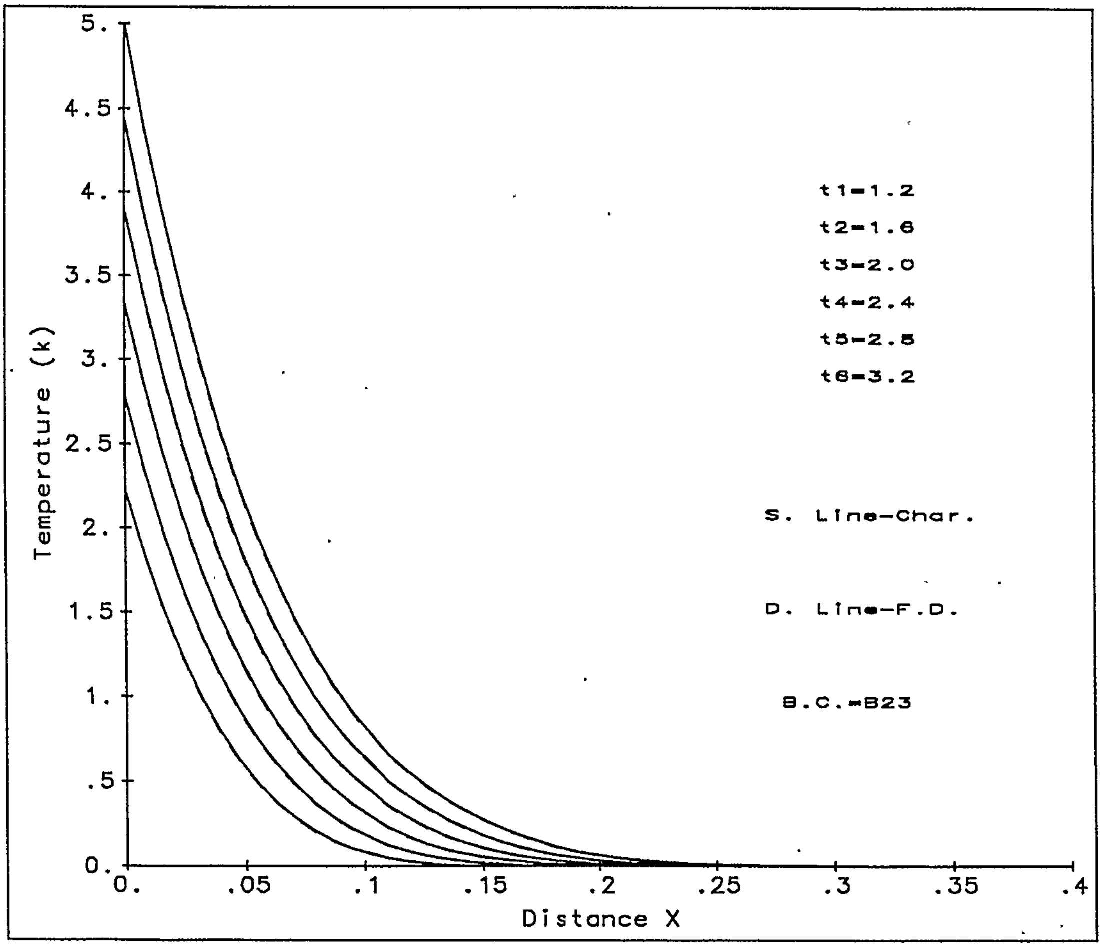

Fig. 6.53 Temperature distribution along x-axis due to velocity and temperature ramp inputs (V_0=8 M/S,θ_0=5K)

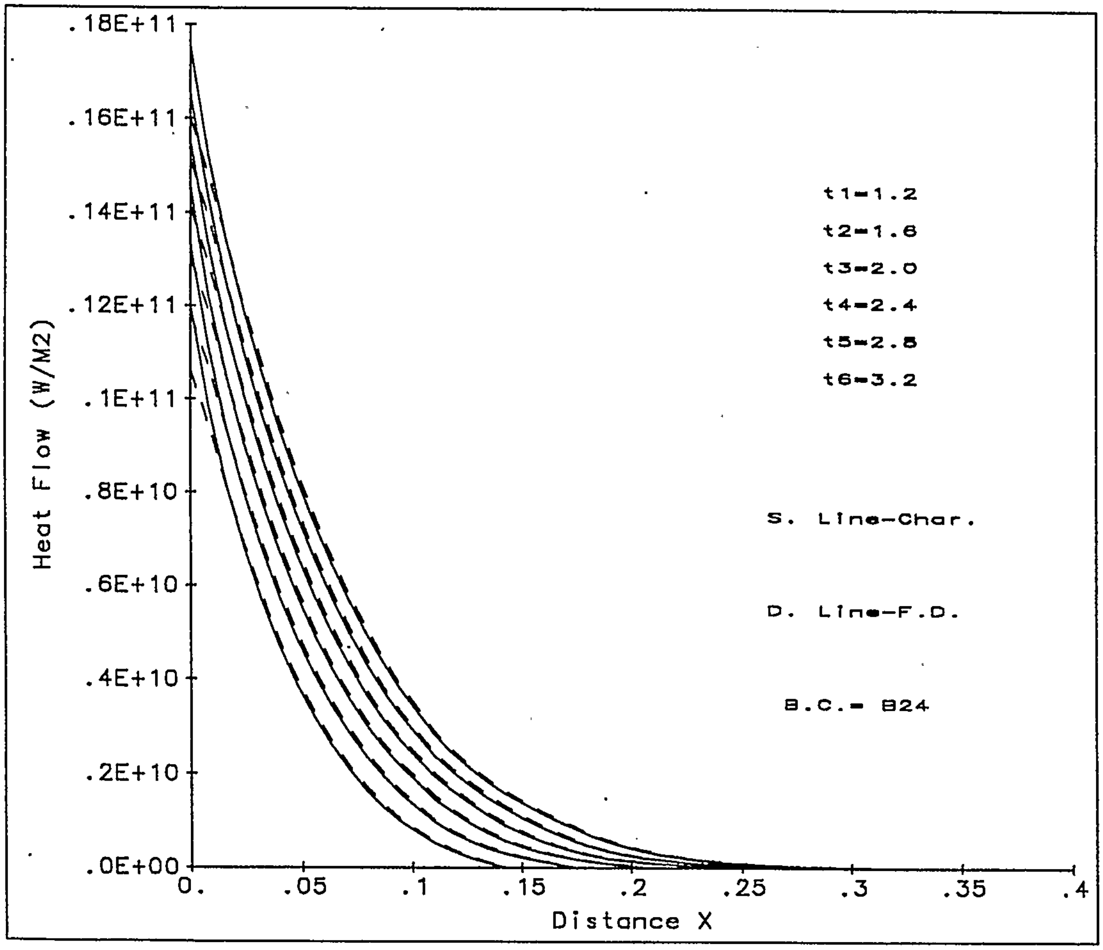

Fig. 6.54 Heat flow distribution along x-axis due to velocity and temperature ramp inputs (V_0=8 M/S,θ_0=5K)

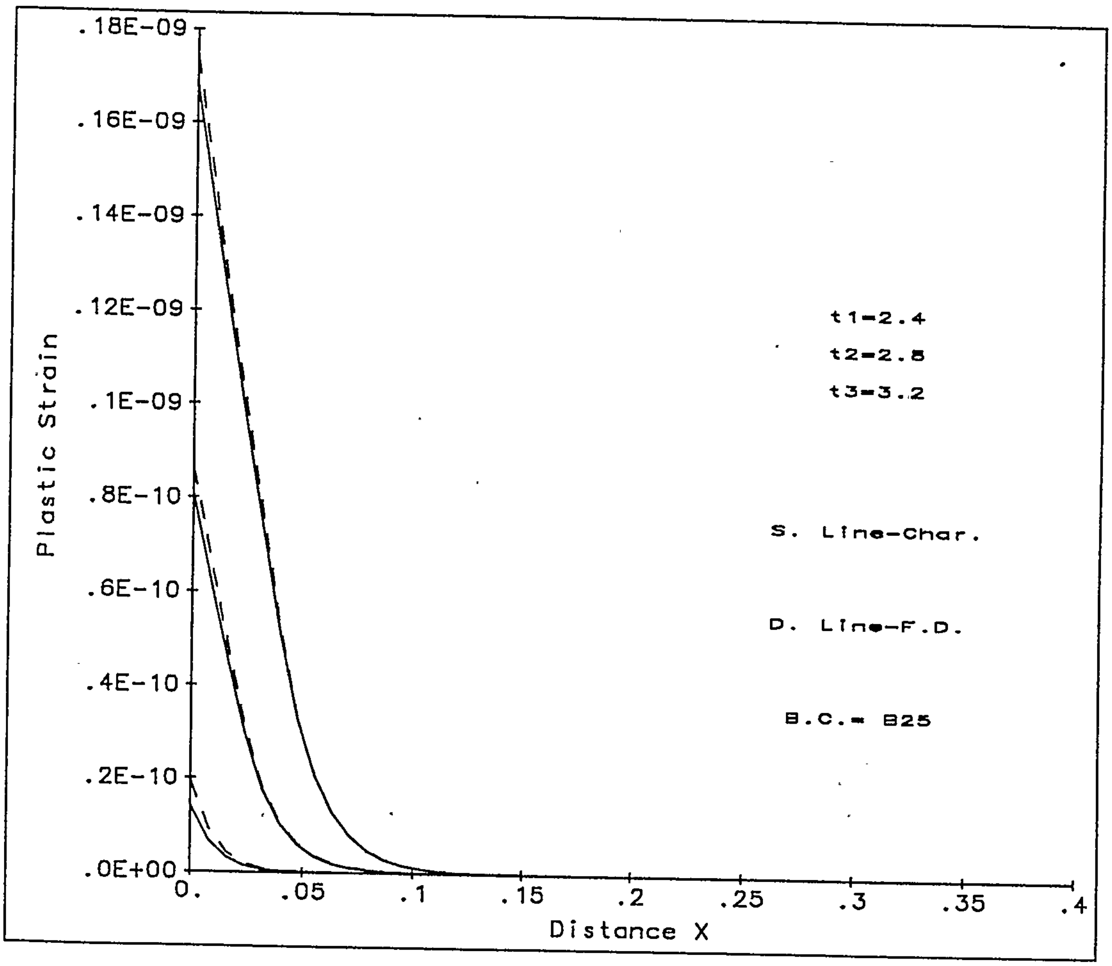

Fig. 6.55 Plastic strain distribution along x-axis due to velocity and temperature ramp inputs (V_0=8 M/S,θ_0=5K)

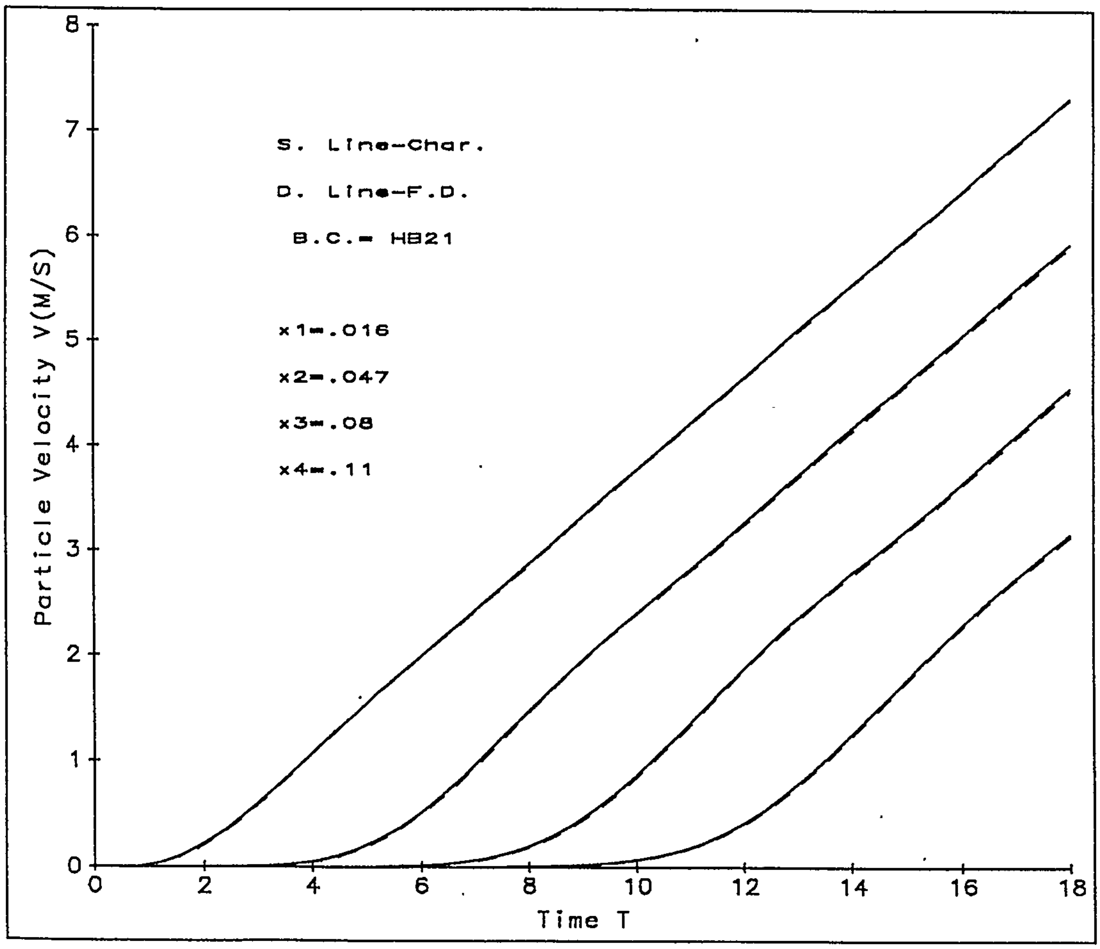

Fig. 6.56 Velocity response at certain positions due to velocity and temperature ramp inputs (V_0=8 M/S,θ_0=5K)

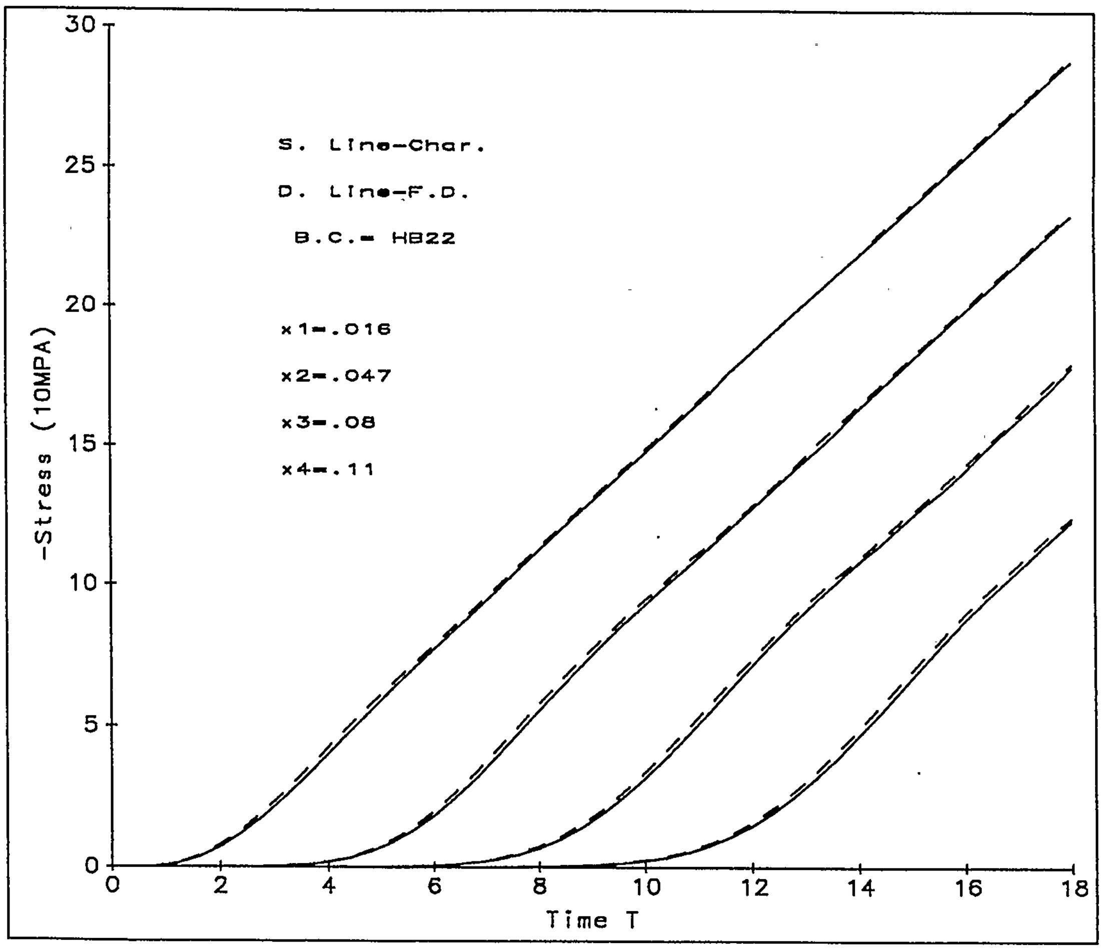

Fig. 6.57 Stress response at certain positions due to velocity and temperature ramp inputs (V_0=8 M/S,θ_0= K)

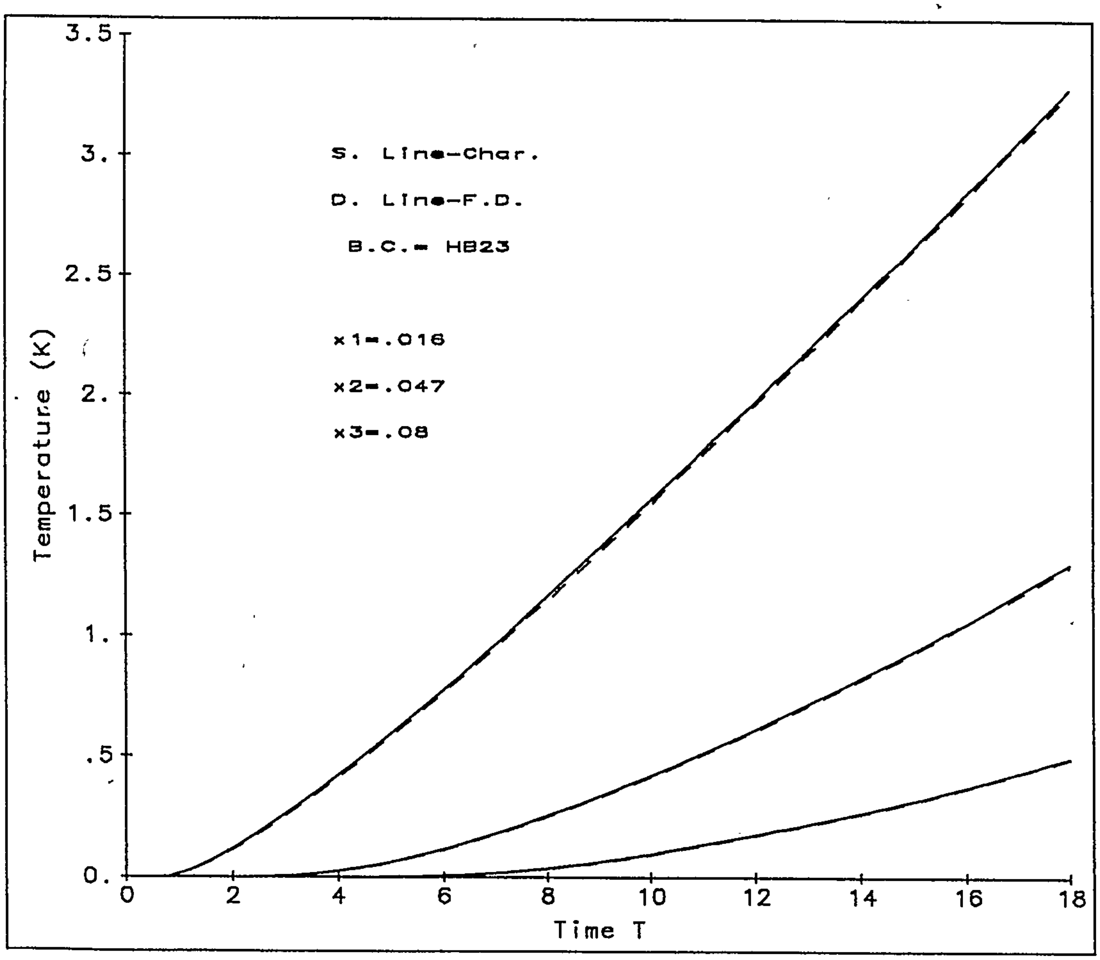

Fig. 6.58 Temperature response at certain positions due to velocity and temperature ramp inputs (V_0=8 M/S,θ_0=5K)

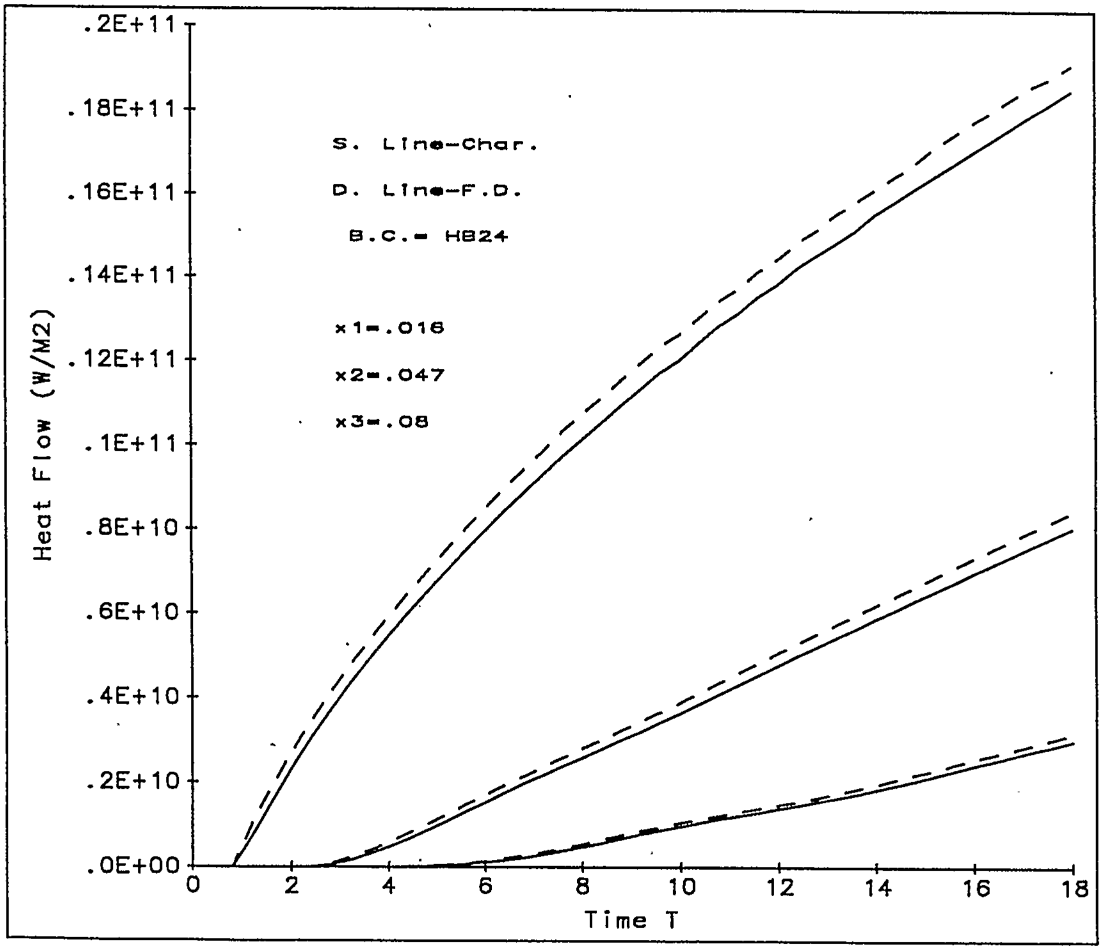

Fig. 6.59 Heat flow response at certain positions due to velocity and temperature ramp inputs (V_0=8 M/S,θ_0=5K)

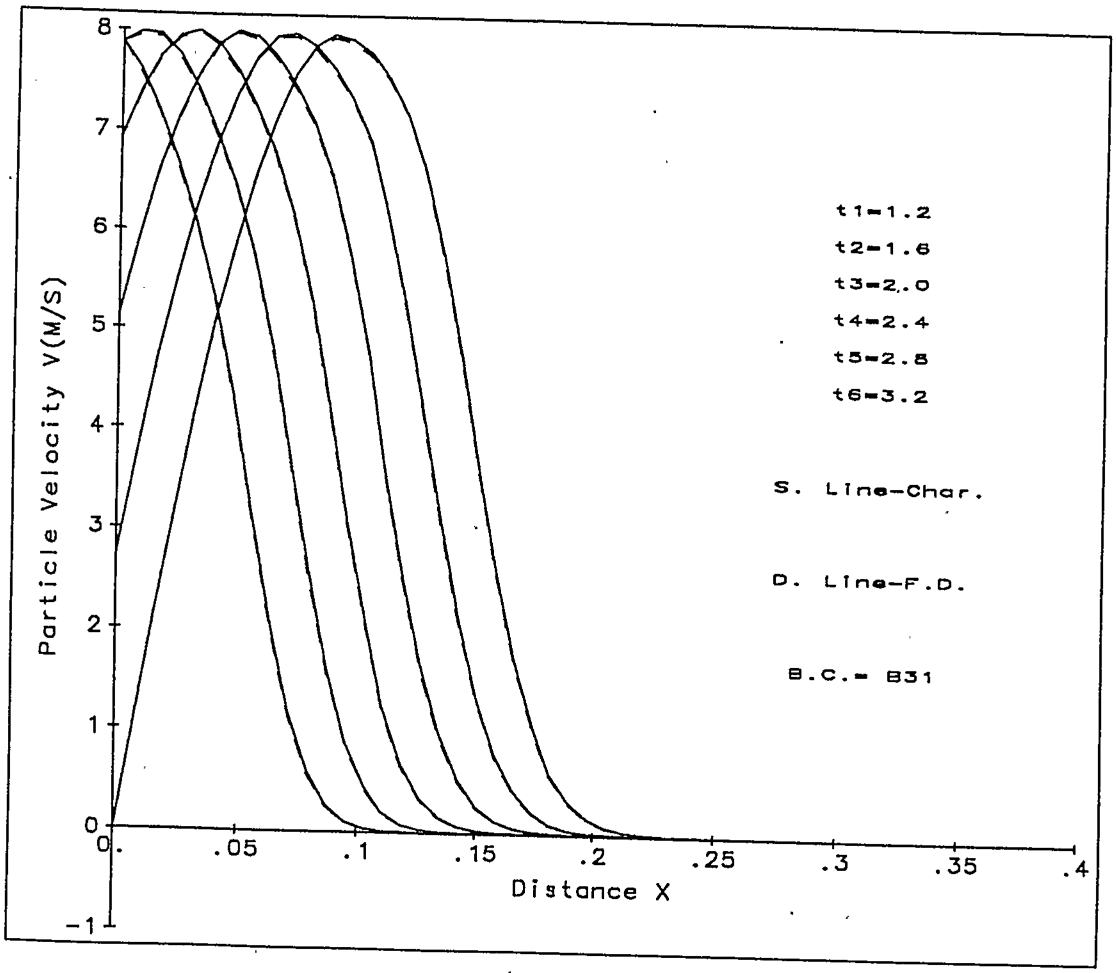

Fig. 6.61 Velocity distribution along x-axis due to velocity and temperature sinusoid inputs (V_0=8 M/S,θ_0=5K)

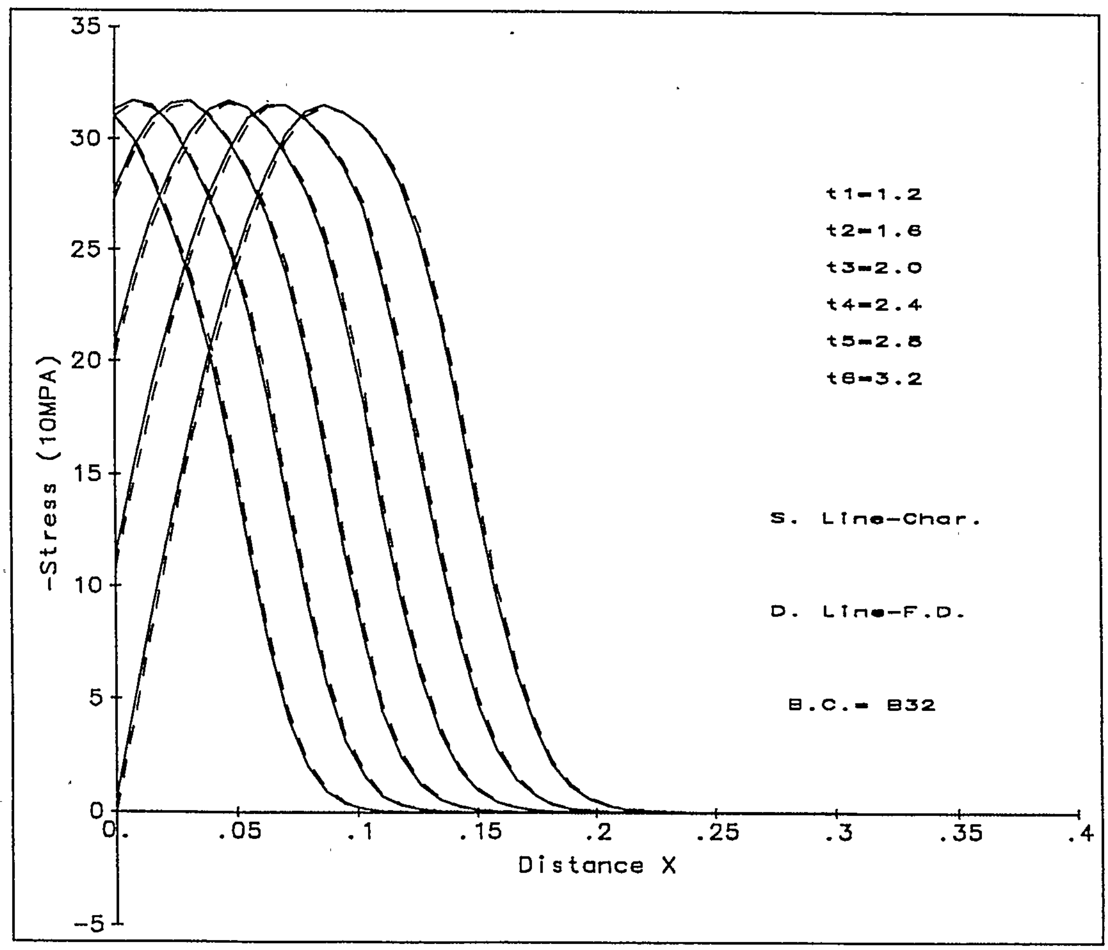

Fig. 6.62 Stress distribution along x-axis due to velocity and temperature sinusoid inputs (V_0=8 M/S,θ_0=5K).

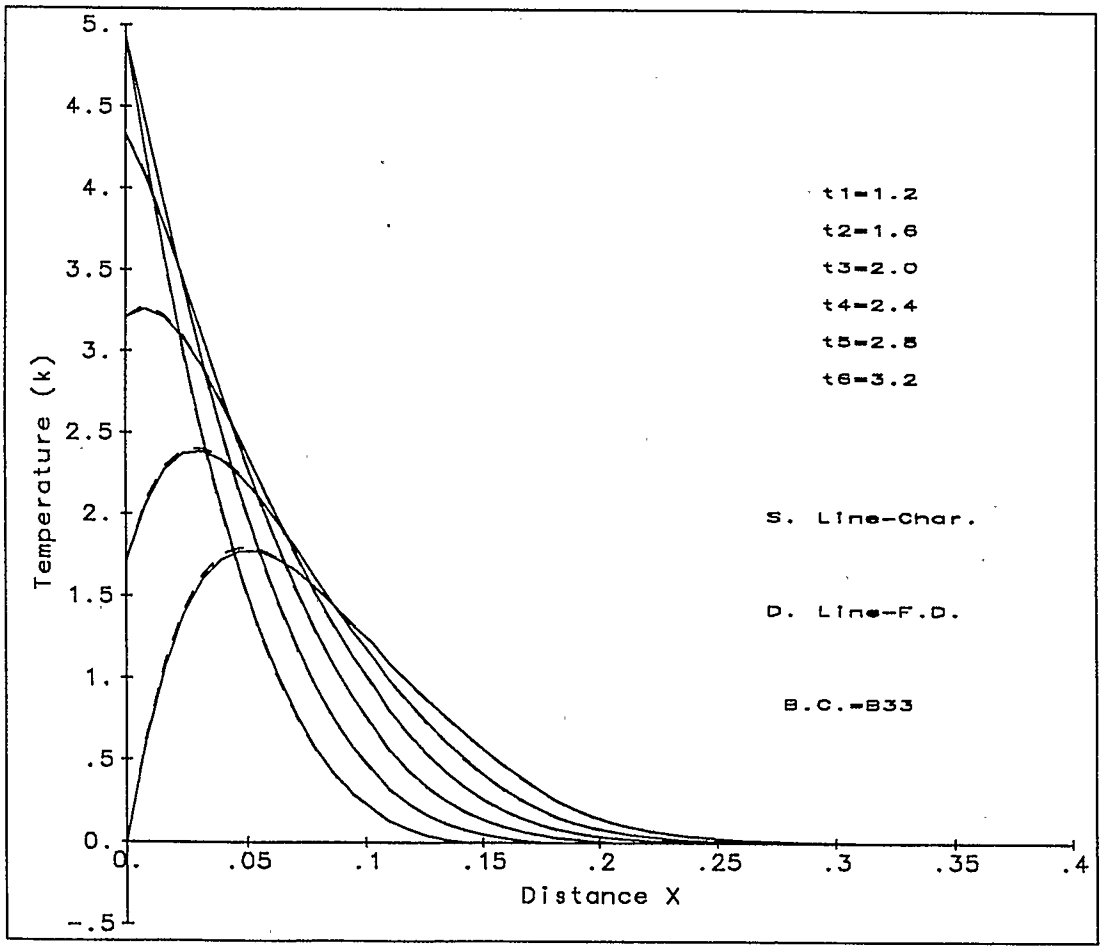

Fig. 6.63 Temperature distribution along x-axis due to velocity and temperature sinusoid inputs (V_0=8 M/S,θ_0=5K).

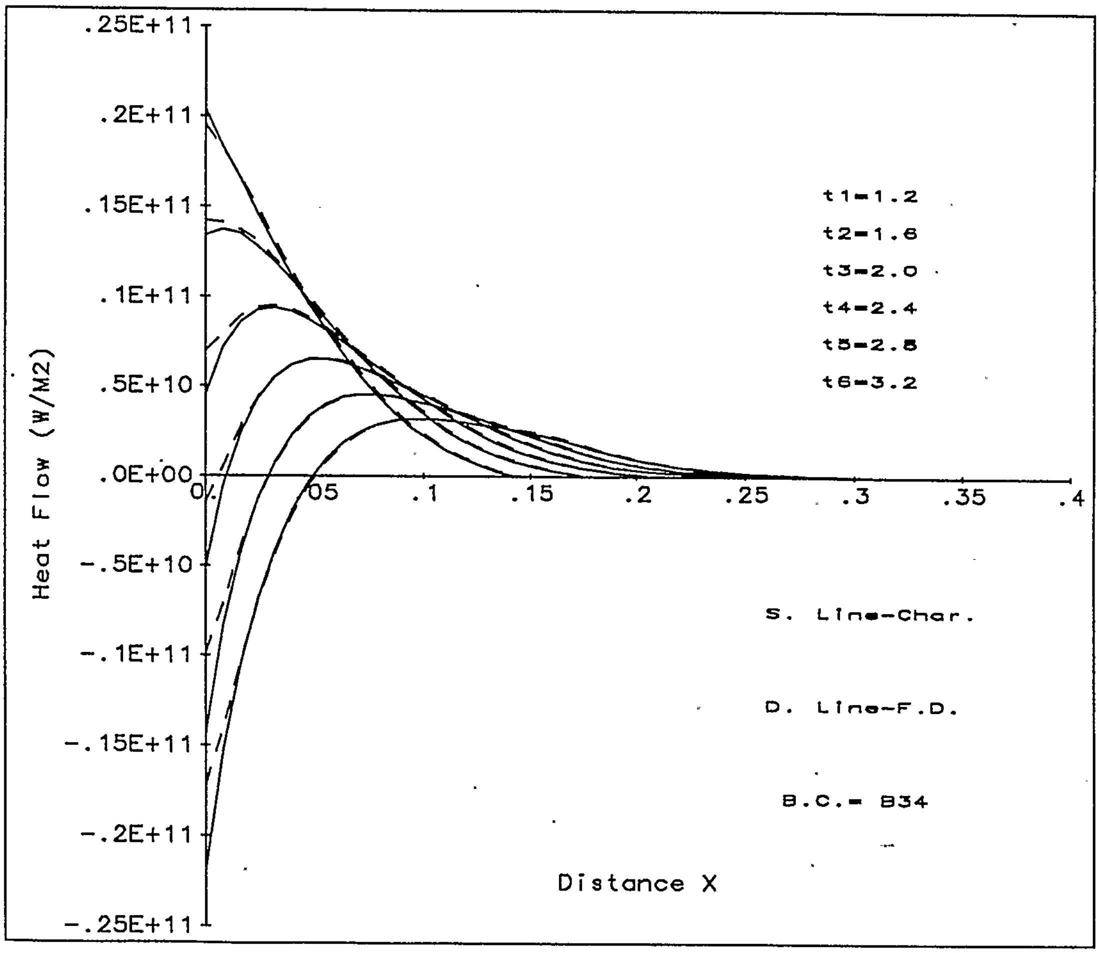

Fig. 6.64 Heat flow distribution along x-axis due to velocity and temperature sinusoid inputs (V_0=8 M/S,θ_0=5K)

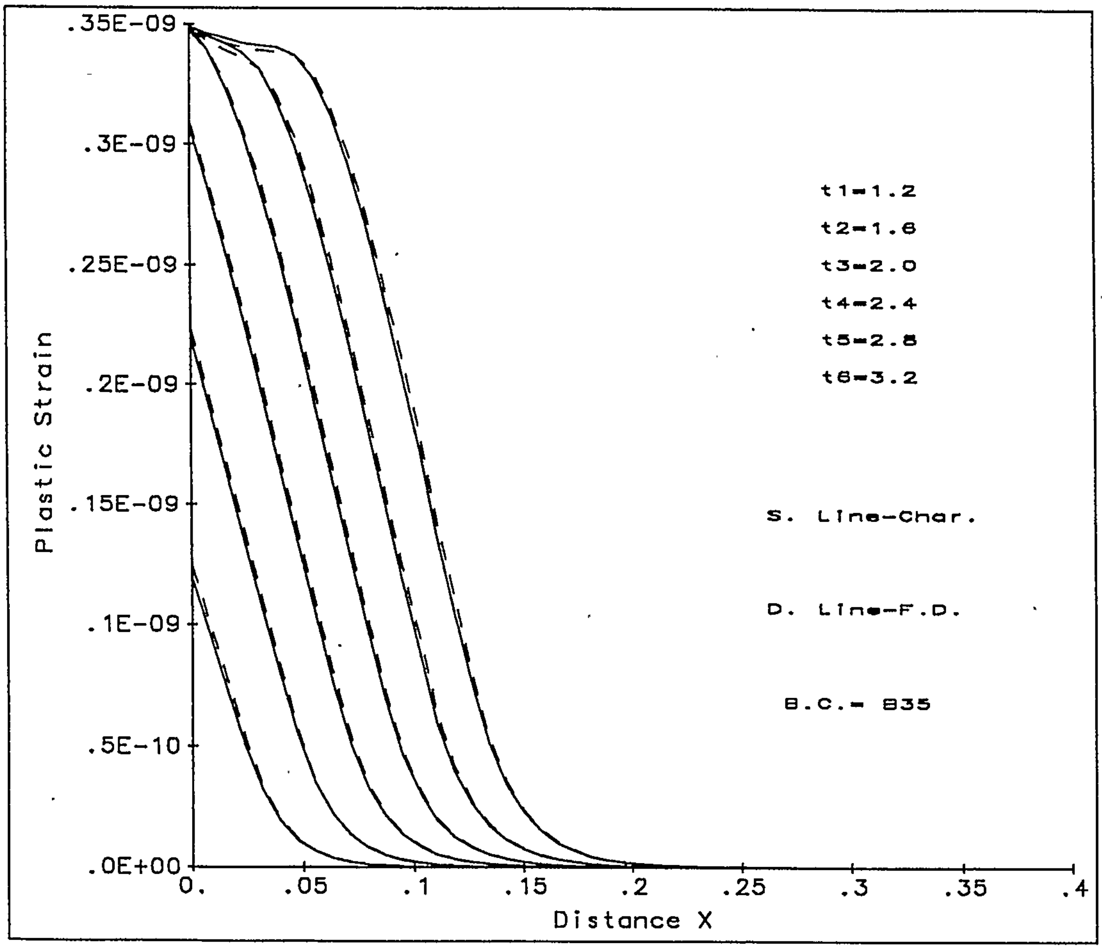

Fig. 6.65 Plastic strain distribution along x-axis due to velocity and temperature sinusoid inputs (V_0=8 M/S,θ_0=5K)

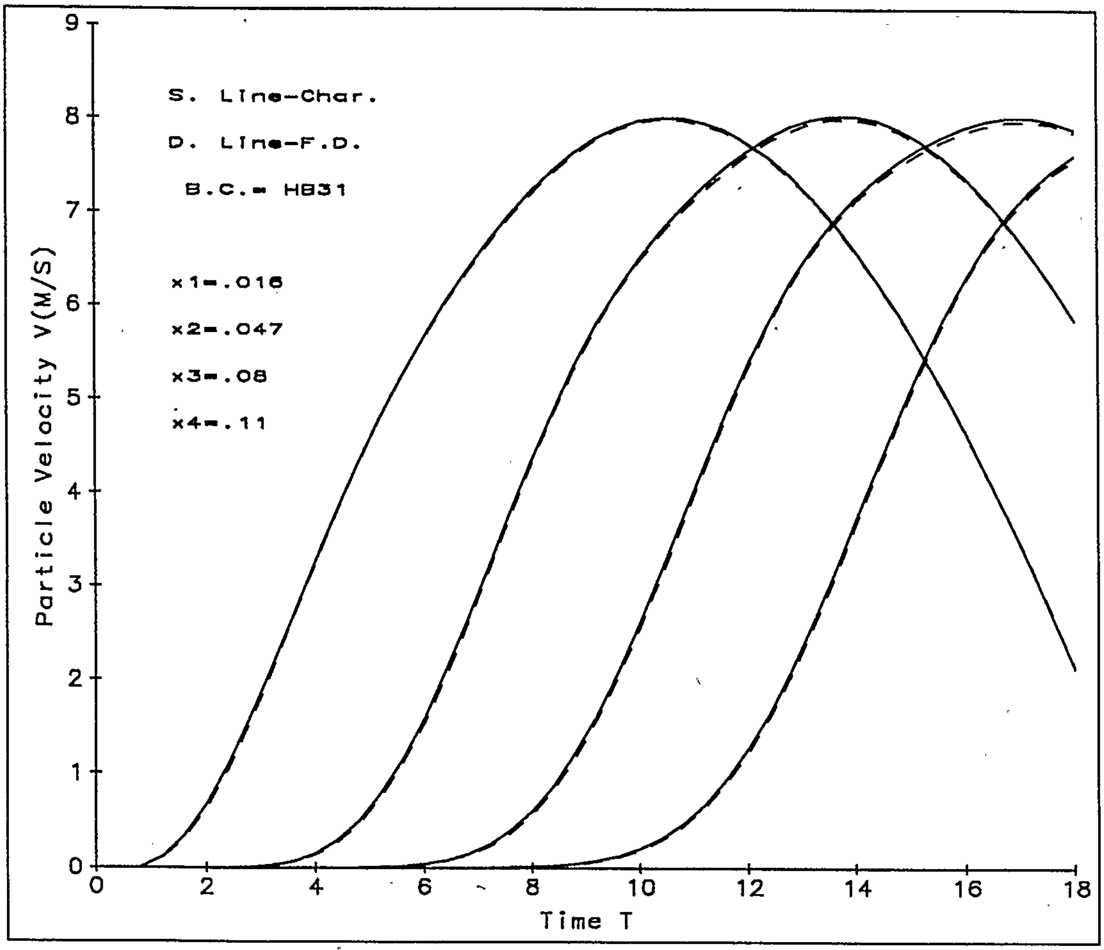

Fig. 6.66 Velocity response at certain positions due to velocity and temperature sinusoid inputs (V_0=8 M/S,θ_0=5K)

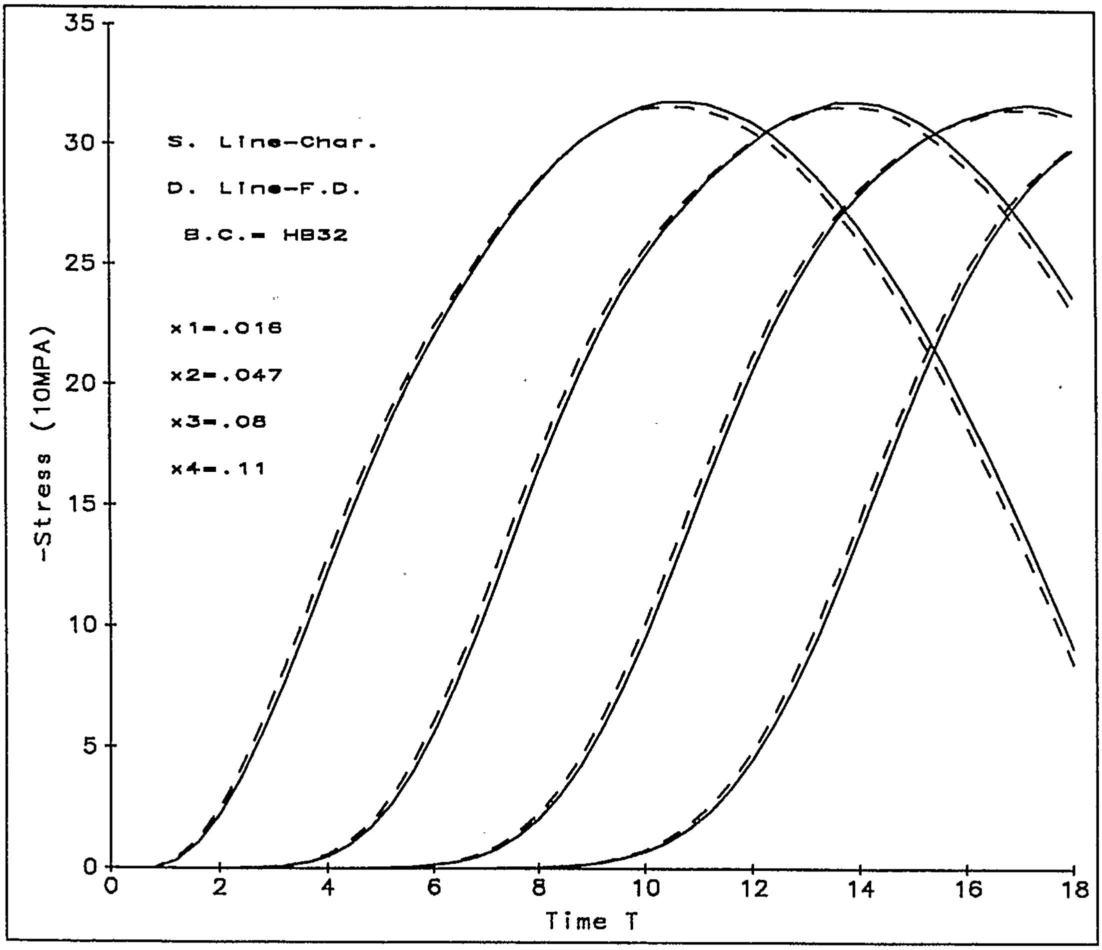

Fig. 6.67 Stress response at certain positions due to velocity and temperature sinusoid inputs (V_0=8 M/S,θ_0=5K)

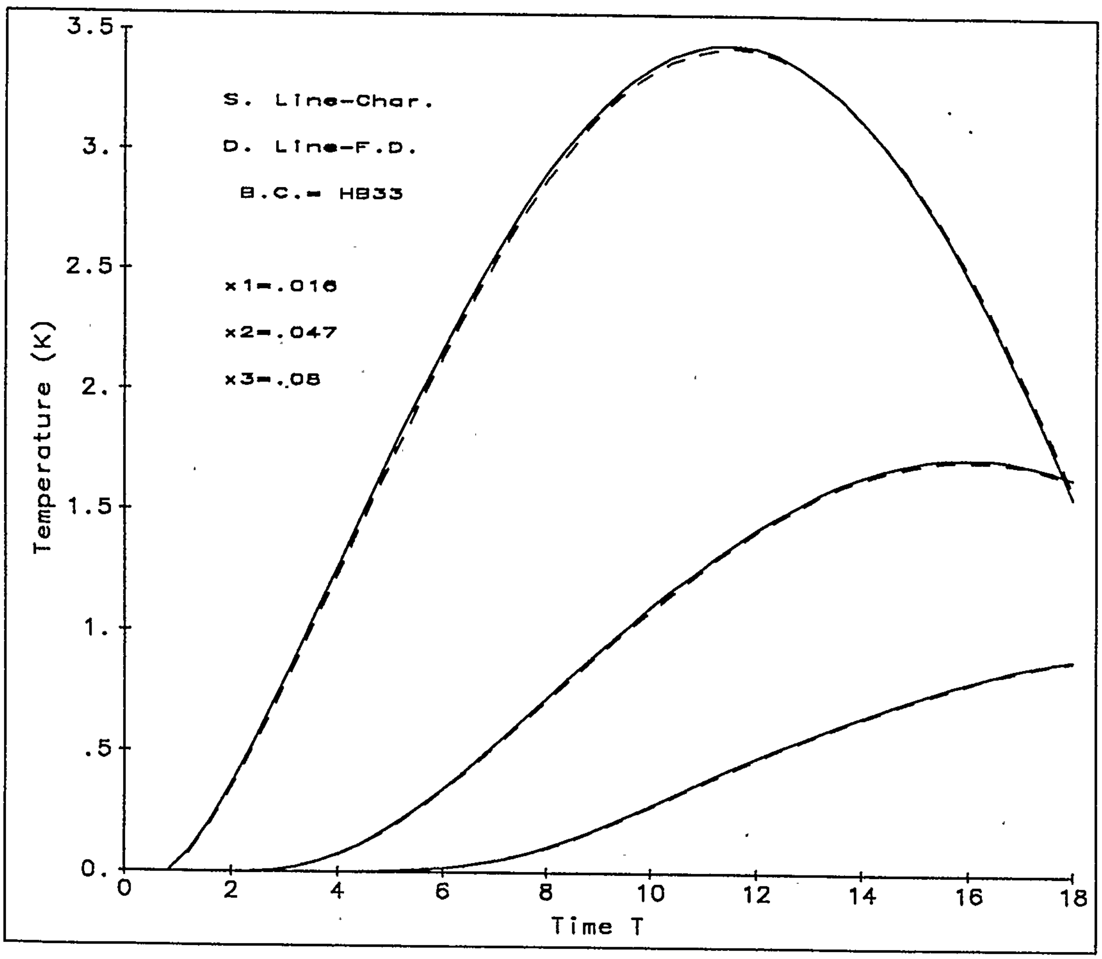

Fig. 6.68 Temperature response at certain positions due to velocity and temperature sinusoid inputs (V_0=8 M/S,θ_0=5K)

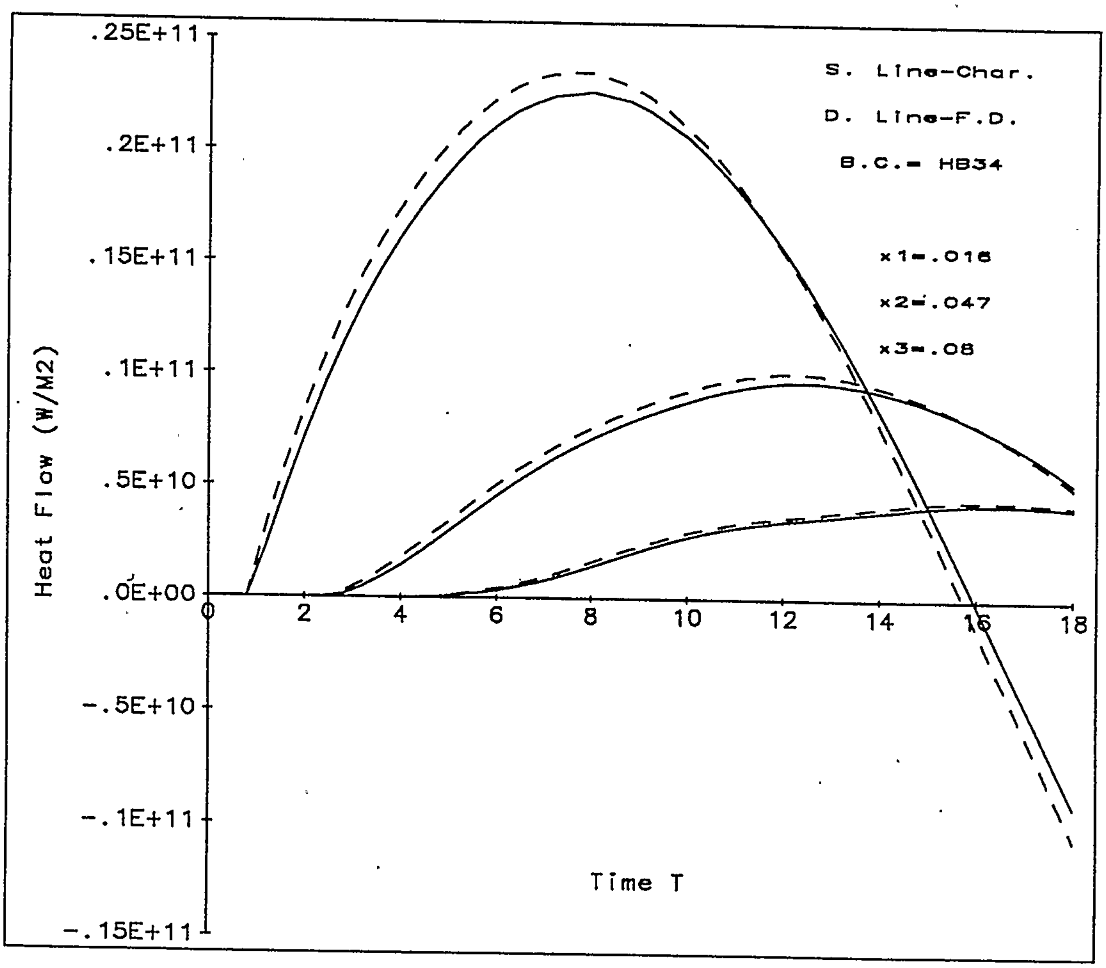

Fig. 6.69 Heat flow response at certain positions due to velocity and temperature sinusoid inputs (V_0=8 M/S,θ_0=5K)

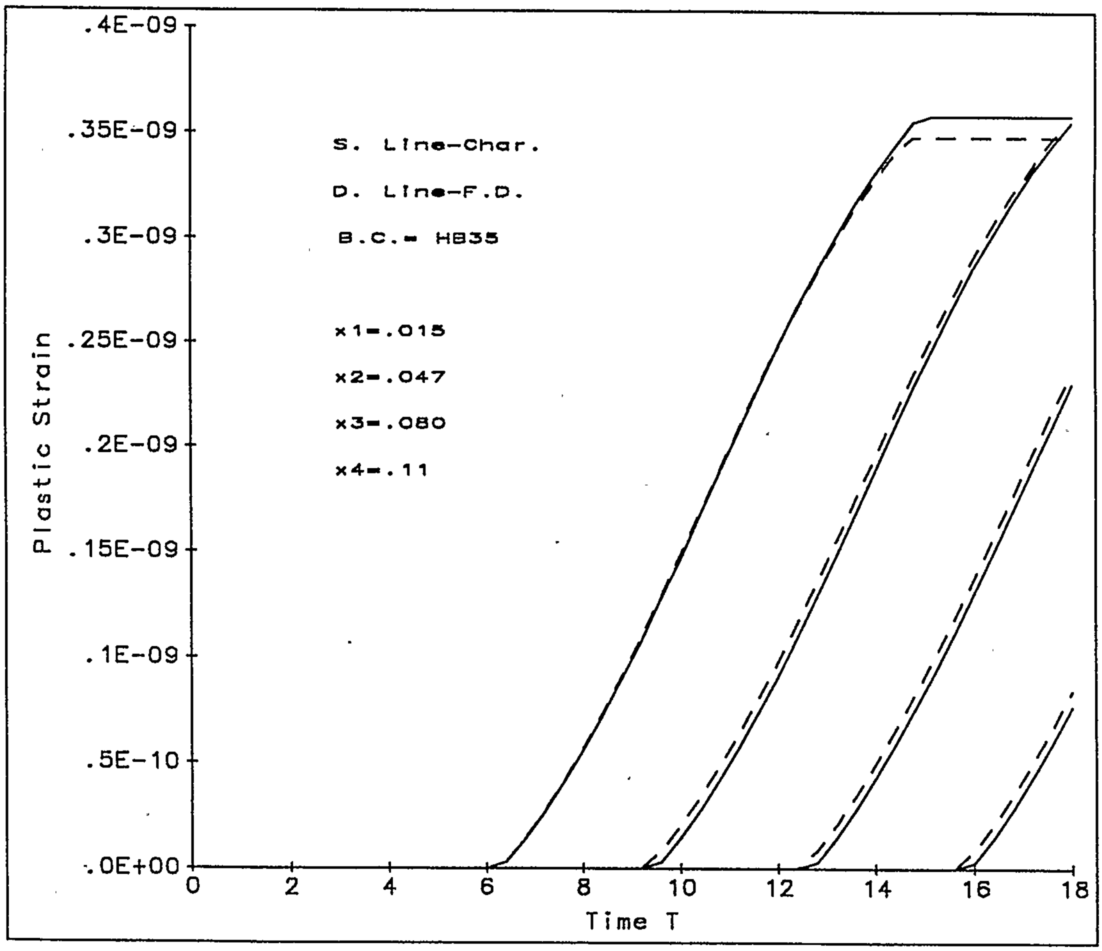

Fig. 6.70 Plastic strain response at certain positions due to velocity and temperature sinusoid inputs (V_0=8 M/S,θ_0=5K)

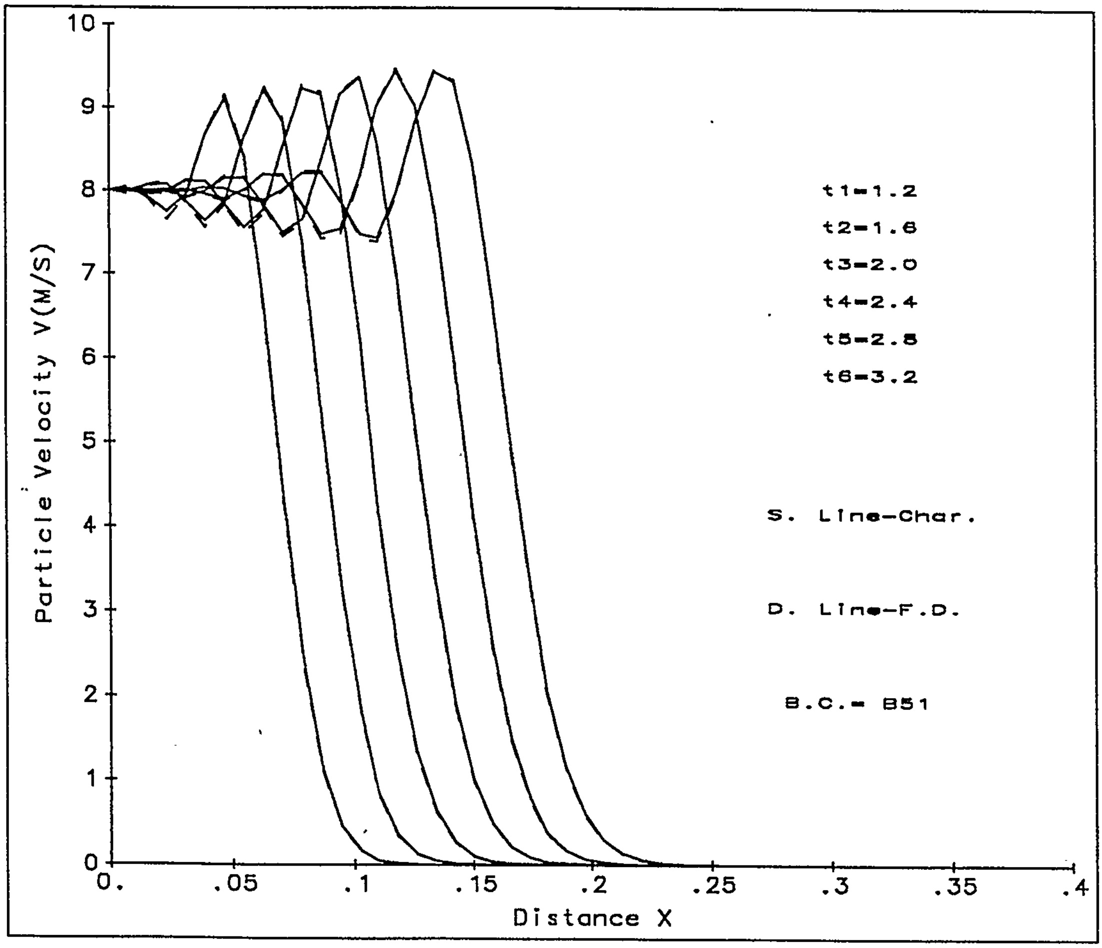

Fig. 6.71 Velocity distribution along x-axis at different times due to a velocity step input alone (V_0=8 M/S)

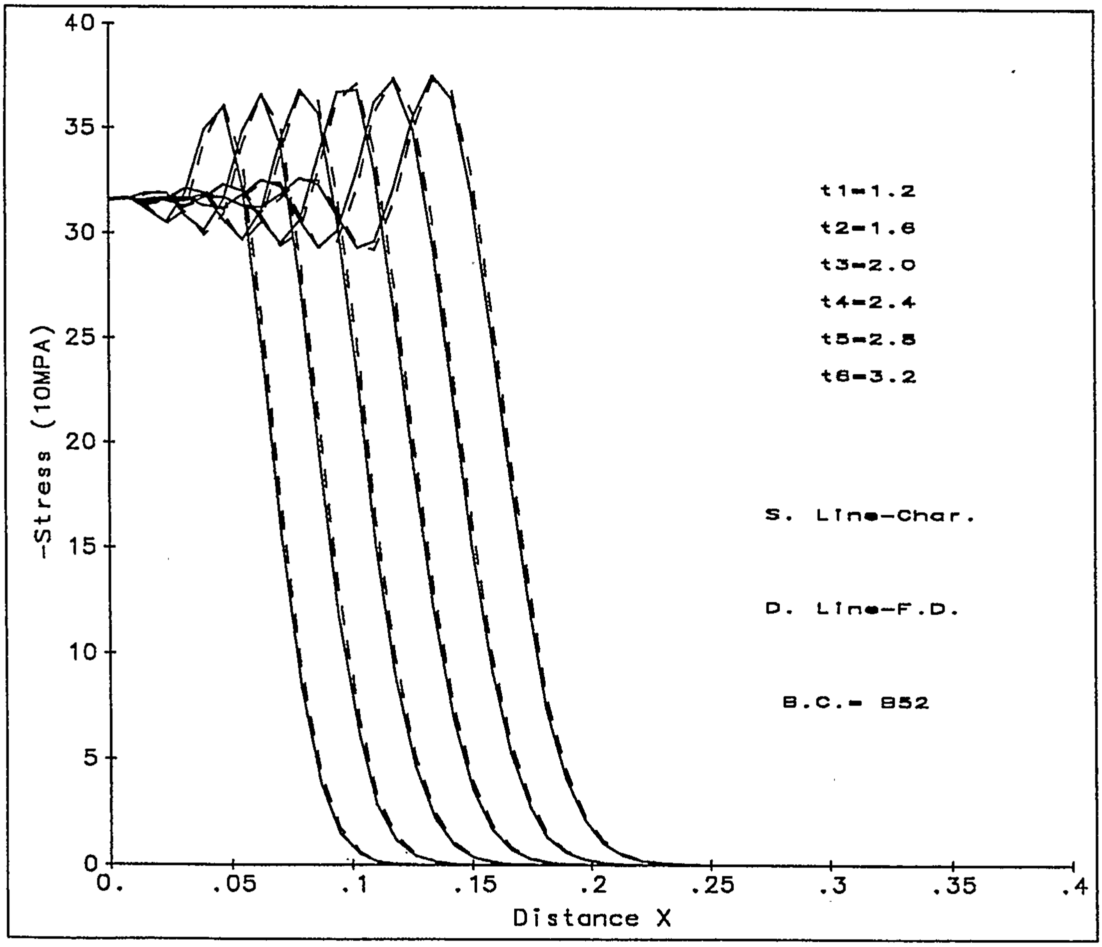

Fig. 6.72 Stress distribution along x-axis at different times due to a velocity step input alone (V_0=8 M/S)

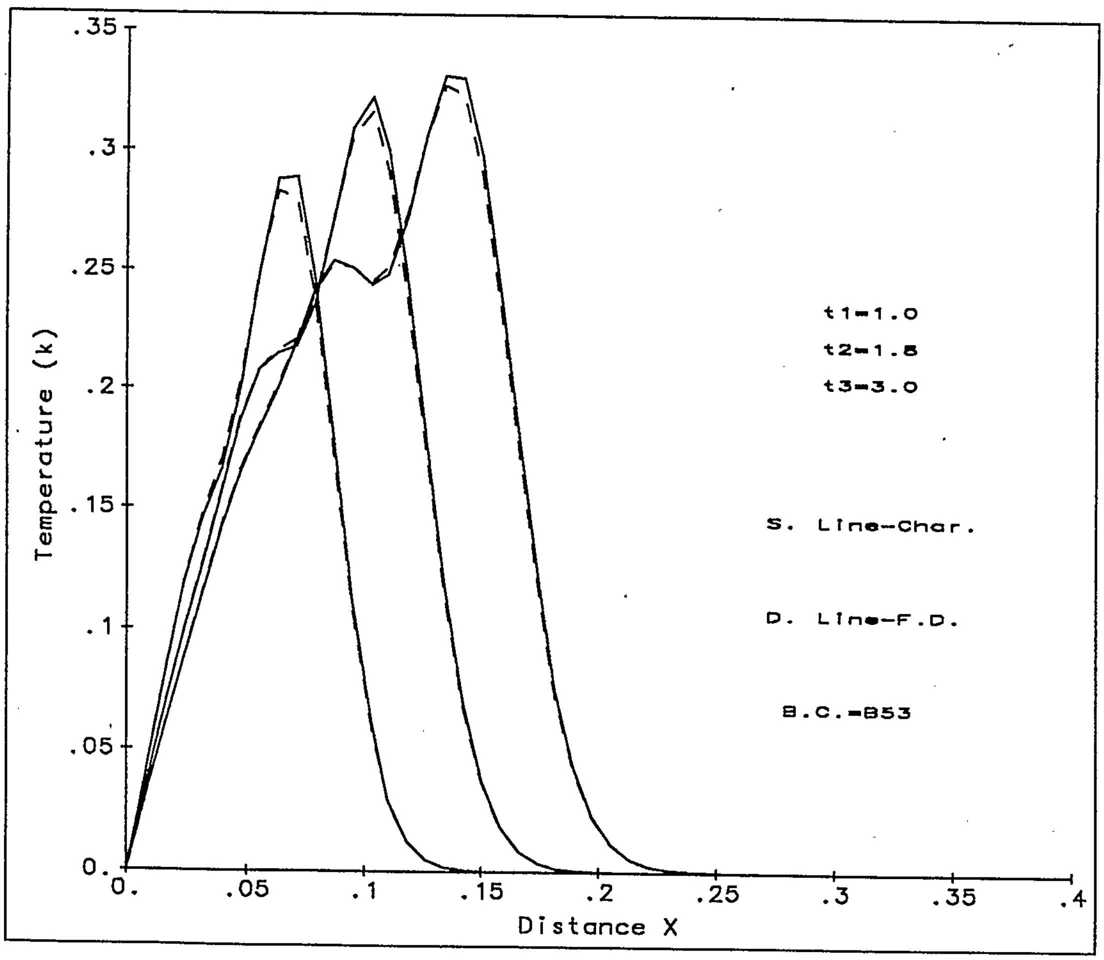

Fig. 6.73 Temperature distribution along x-axis at different times due to a velocity step input alone (V_0=8 M/S)

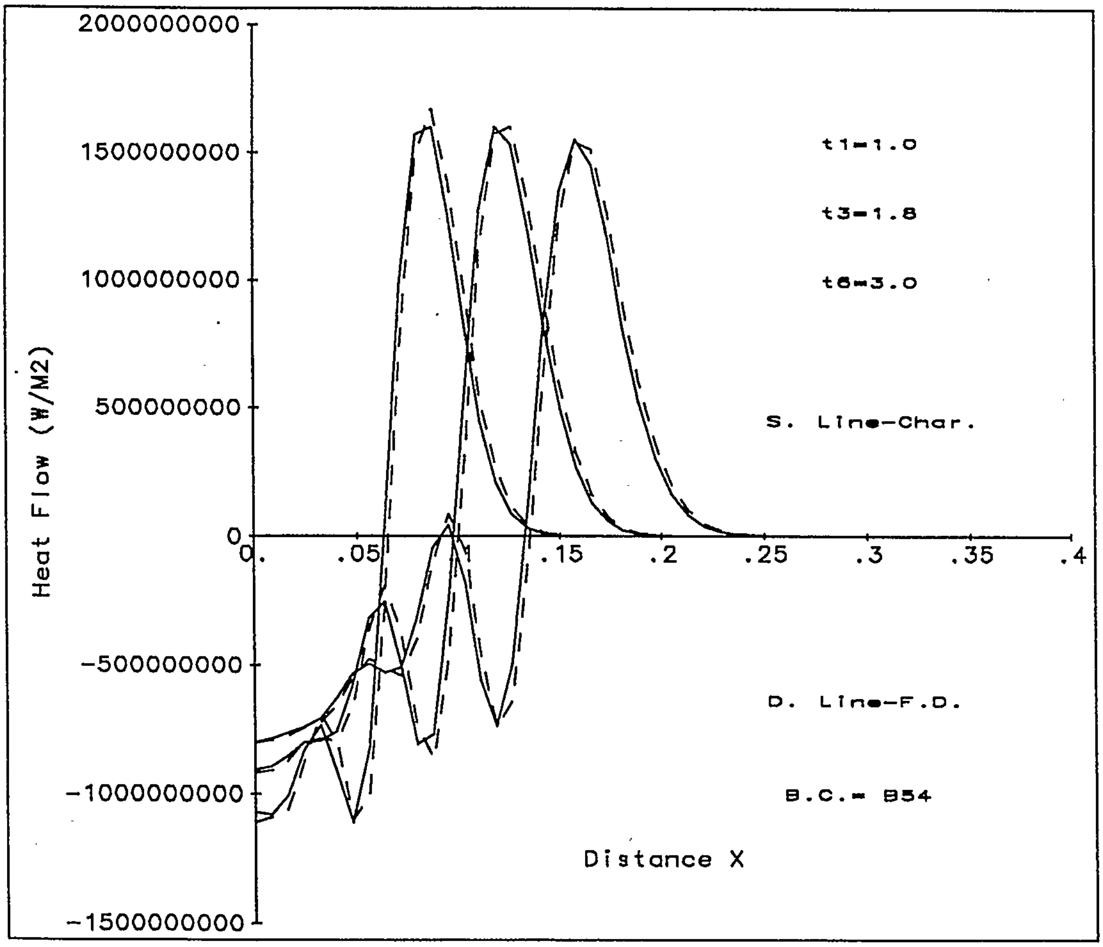

Fig. 6.74 Heat flow distribution along x-axis at different times due to a velocity step input alone (V_0=8 M/S)

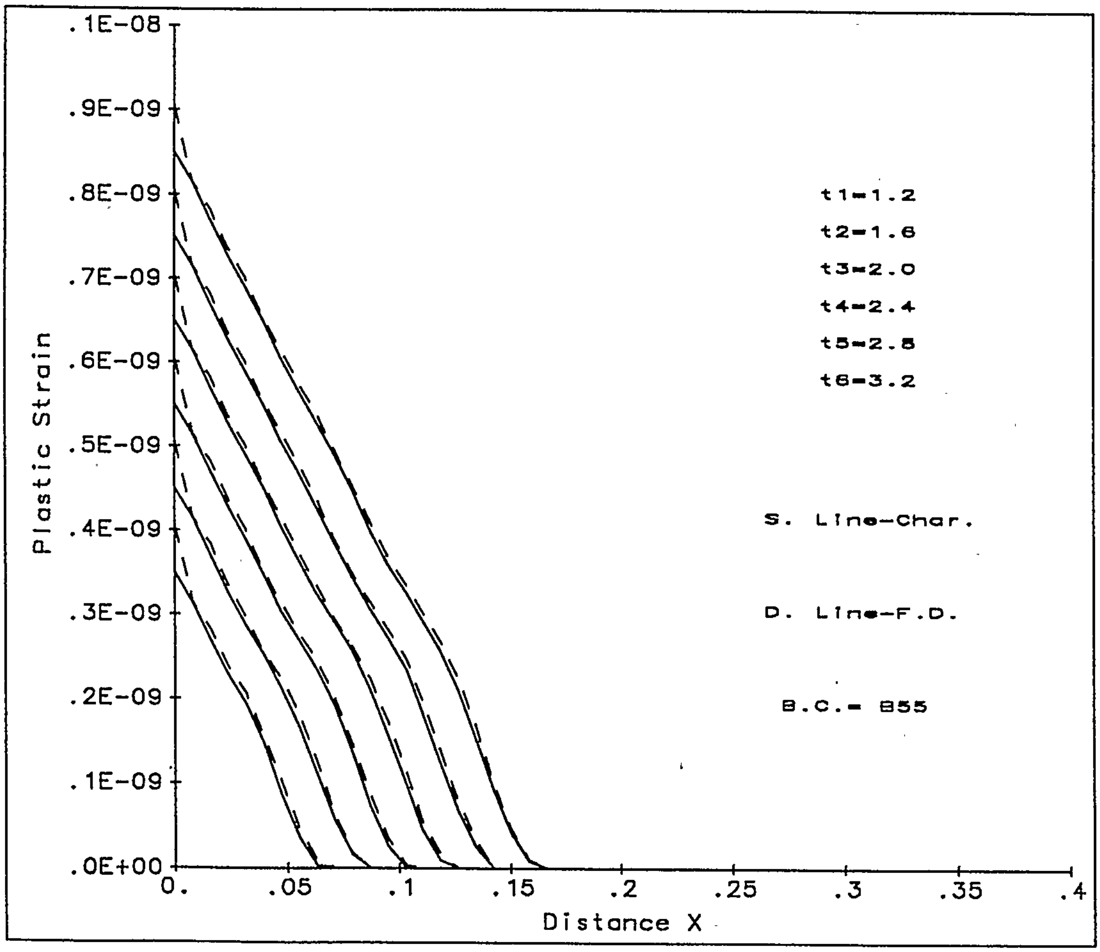

Fig. 6.75 Plastic strain distribution along x-axis at different times due to a velocity step input alone (V_0=8 M/S)

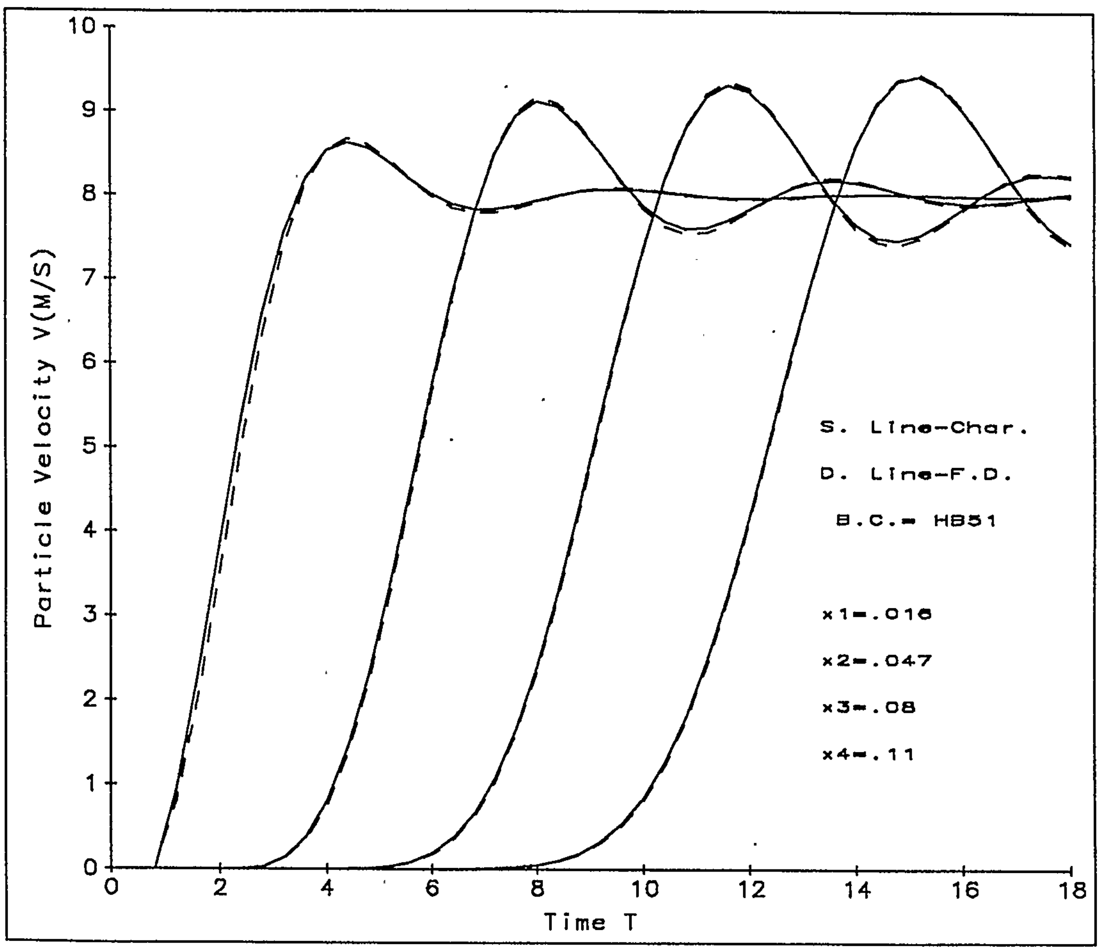

Fig. 6.76 Velocity response at certain positions due to a velocity step input alone (V_0=8 M/S)

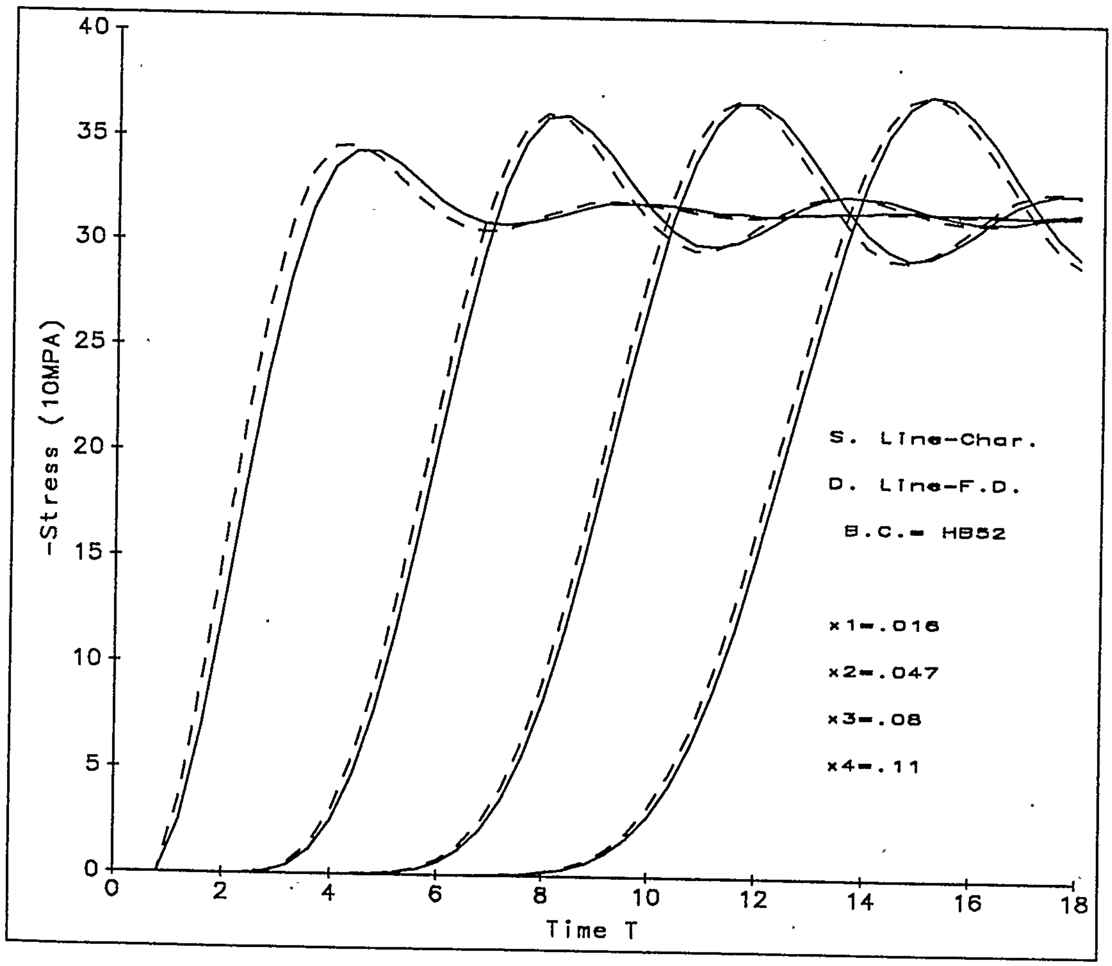

Fig. 6.77 Stress response at certain positions due to a velocity step input alone (V_0=8 M/S)

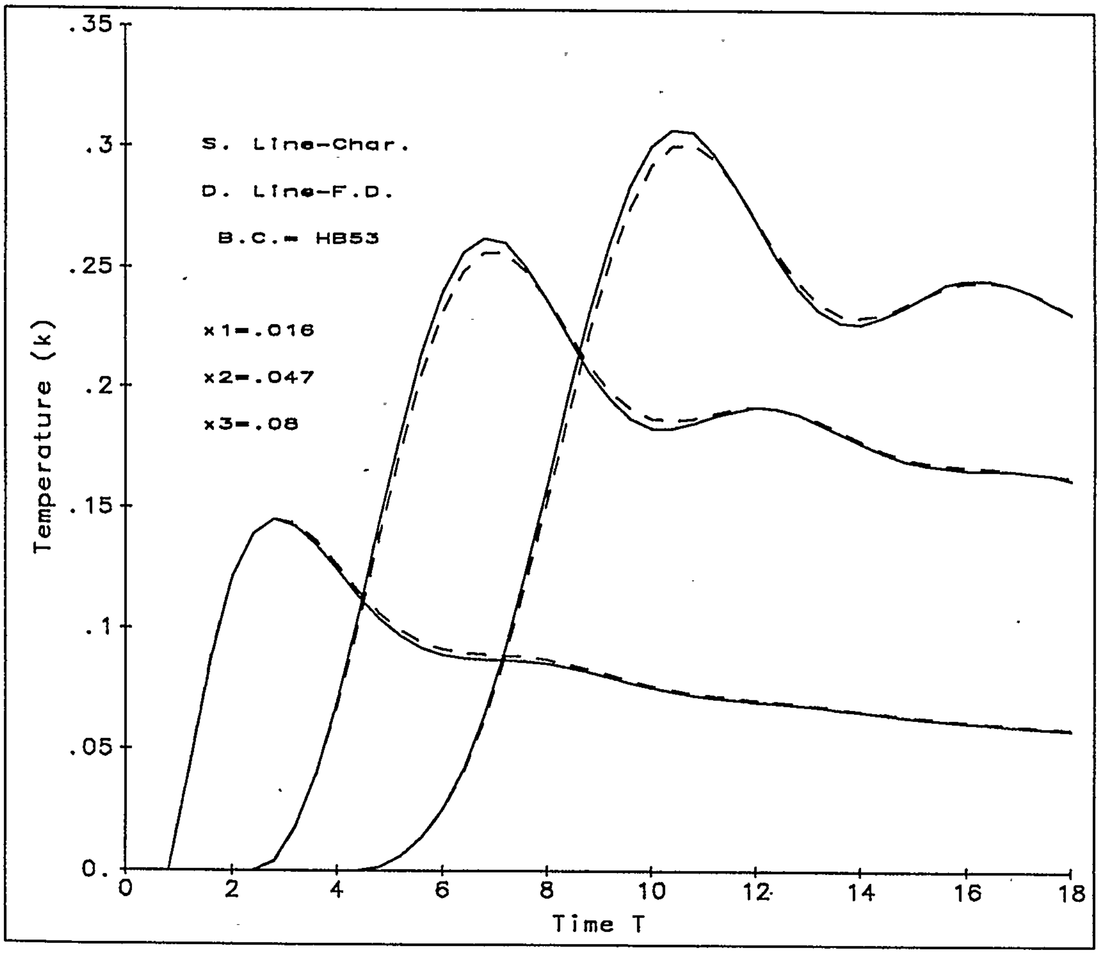

Fig. 6.78 Temperature response at certain positions due to a velocity step input alone (V_0=8 M/S)

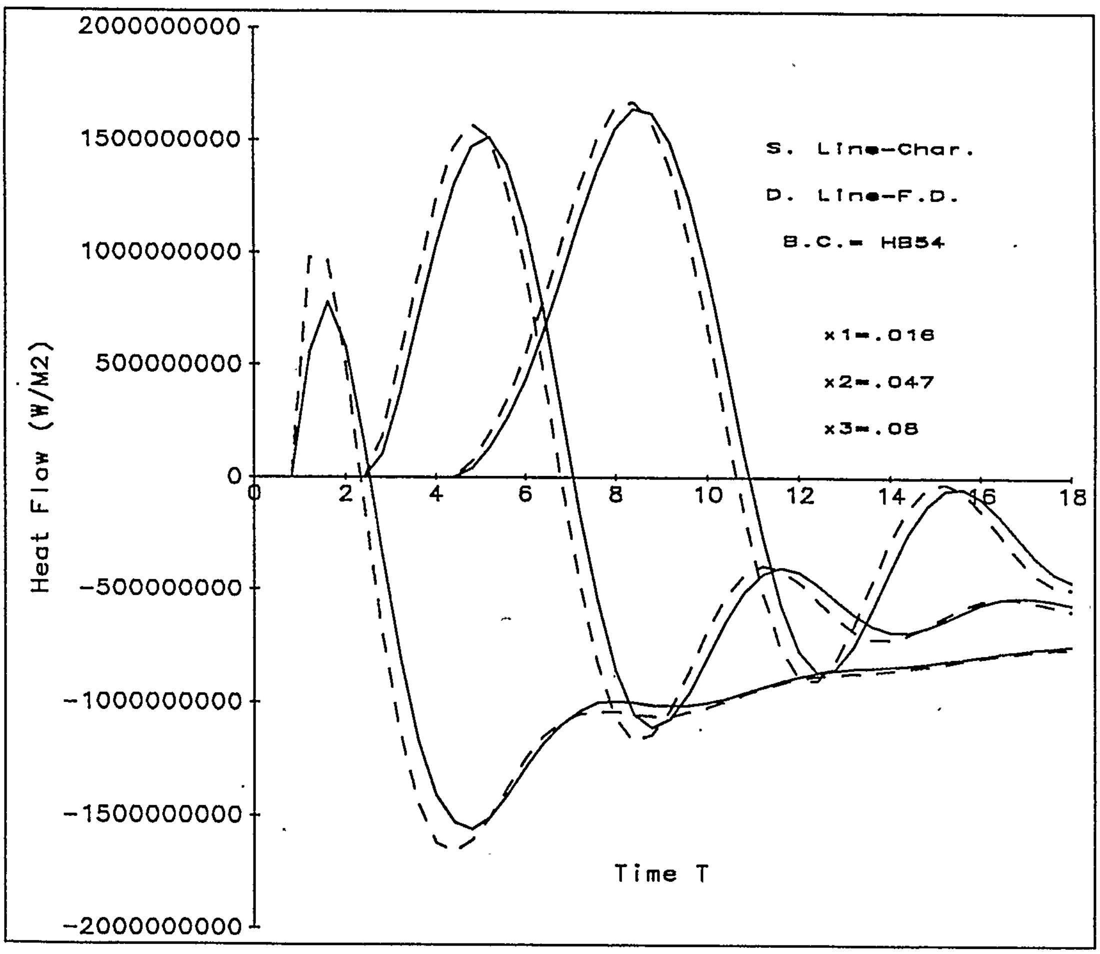

Fig. 6.79 Heat flow response at certain positions due to a velocity step input alone (V_0=8 M/S)

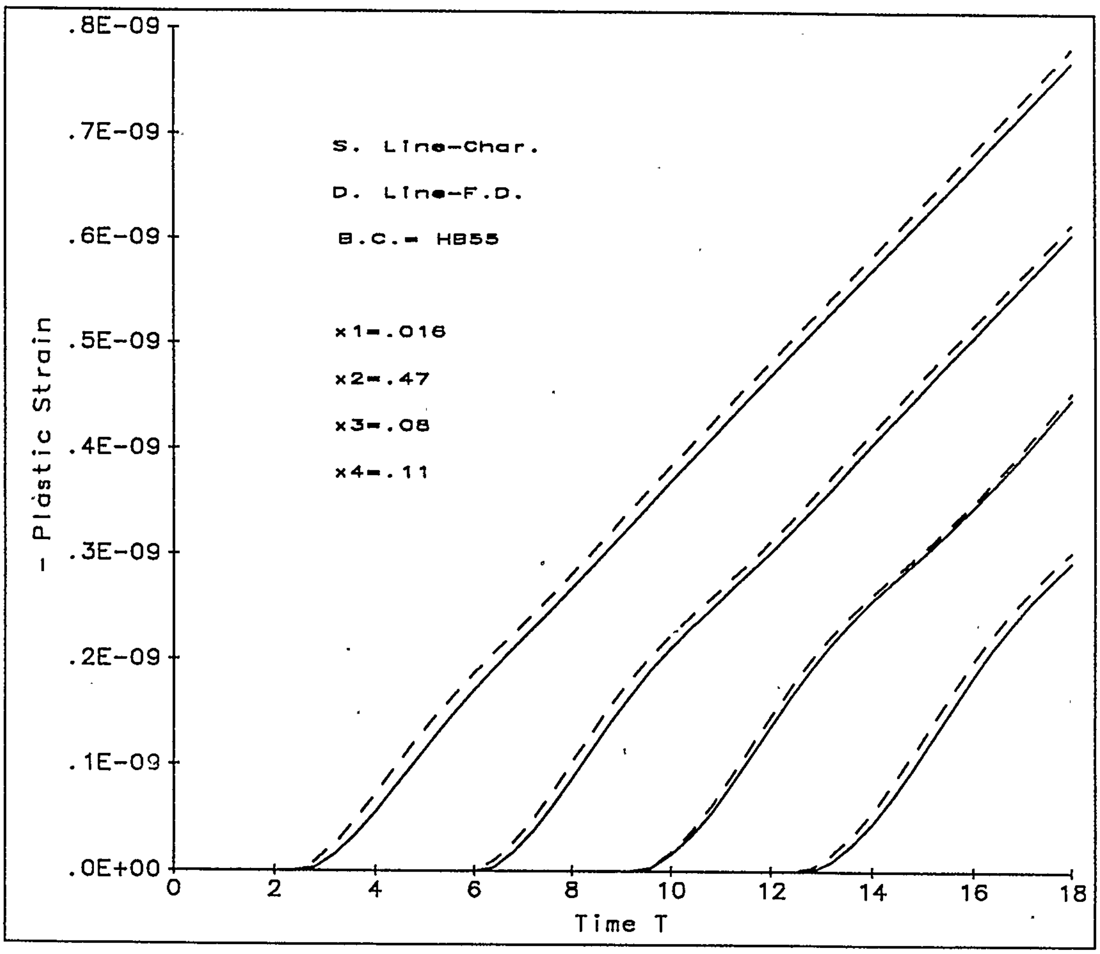

Fig. 6.80 Plastic strain response at certain positions due to a velocity step input alone (V_0=8 M/S)

takes about 6 units of time, and at x_4=0.11, it takes more than 7 units for the velocity to reach its maximum value. Similar feature can be seen in Fig.6.7 and Fig.6.37 for stress, Fig.6.9 for heat flow, Fig.6.38 for temperature *etc.* This "dulling" phenomenon is due to the fact that in our system the front and trailing edges of the waves are propagated by different velocities. As time increases, the distance between the front and the trailing edges increases correspondingly. The increased abscissa decreases the slope.

Although the velocity and stress inputs are decreasing functions of time in boundary conditions coded by A3 and B3, which correspond to Fig.6.21 to Fig.6.30 and Fig.6.61 to Fig.6.70, respectively, at any point x=constant the plastic strain once established never goes down. This tallies with the assertion that the evolution of internal state variables is irreversible. Fig.6.30 and Fig.6.70 clearly show the feature.

Cattaneo's hyperbolic equation of heat conduction has been employed in the analysis of the thermomechanical coupled system. The relaxation time included in the equation is decisive for selecting the time step of integration algorithm. No matter whether characteristics or the two-sub-step finite deference method is used, the time step utilized can never be greater than the relaxation time in order to obtain a convergent solution. By the achievement of modern computer science, even if super computer is used, it is still impossible to get the results corresponding to a really long time. Our observations are drawn from the profiles sketched with the certain calculated data; yet, it brings us a distinct picture.

6.4 Discussion

When an elastic long rod is impacted at one end, the particle velocity and elastic strain are propagated in the form of a shock wave. There is a discontinuity or jump formed at the wavefront. However, for thermoplastic wave propagation the situation is different. The numerical results presented in the preceding section have shown that the discontinuity only exists at the end of the rod. As the waves are propagated along the rod, the sharpness of the discontinuity becomes vanishingly small. It suggests there is no shock wave propagated in the rod.

Orisamolu [4.6] has numerically studied the wave propagation problem associated with thermoplasticity, in which Cattaneo's hyperbolic heat conduction equation and a plastic constitutive relation associated with internal state variables are employed. In spite of the assertion on jump conditions at wave fronts, some of his numerical results show the feature similar to an acceleration wave. When the end of rod is subject e d to a step input of stress or velocity and temperature change, the sharpness of the step decreases as the waves propagate along the rod. This feature is indicated by Fig.6.9a, Fig.6.9b, Fig.6.13a, Fig.6.17a, Fig.6.17b, Fig.6.19a, Fig.6.19b *et cetera* [4.6].

Cristescu and Suliciu have presented some numerical results of plastic wave propagation in Chapter IV, Section 4, [4.1], where a rate-independent constitutive equation is employed. The results suggest that when the end of the rod is impacted, discontinuity of strain shows up clearly at the positions near the end. However, as the distance of the point from the end becomes larger, the discontinuity vanishes.

In Chapter VII, [4.1], the existence of real acceleration waves has been discussed. It is shown when Cattaneo's hyperbolic heat conduction equation and a plastic constitutive equation with internal state variables are employed, quasi-linear thermoplastic equation system with real eigenvalues leads to the existence of acceleration waves inside the body. That conclusion is congruent with the numerical results obtained in this research.

6.5 Conclusions

In this research, a constitutive theory of thermoplasticity is developed based on the free energy function and the dissipation function. At first, the physical aspects and the constitutive features of the two leading functions are examined and clarified. It is found that the free energy is a decreasing function of the internal state variables; and it is also found that for a plastically incompressible material there is no explicit coupling between the temperature change and plastic deformation for evaluation of the energy. A relation between the two leading functions is established. This expression can be employed to directly derive the plastic constitutive equations. Contribution of the strain hardening parameter to the free energy has been taken into account, and the dissipative feature of softening of this parameter is considered by a particularly assigned function which is able to relate the experimental results to the constitutive equations.

Based upon the examination of the leading functions, a model system of constitutive equations has been established. The system includes the evolution of entropy, law of heat conduction and plastic constitutive equations.

From the numerical results the following conclusions can be obtained:

i. Both the characteristics and two-sub-step finite difference methods are applicable to generate a convergent result for the problem of plastic wave propagation, if the time-step is correctly selected.

ii. Generally speaking, the method of characteristics is more strict, and gives a sharper solution in most cases, therefore, is more suitable and dependable for solving hyperbolic partial differential equations. However, compared with the other, it is more involved and more computer-time consuming. Roughly, it is 20 to 40 times more time consuming than the two-sub-step finite difference method.

iii. The results show that after being propagated in the plastic medium, the discontinuity of step input is "dulled" so smoothly that the values of the dependent variables are continuous at the front of the waves. But it can be seen from the related figures that their derivatives are still discontinues. By the definition those kinds of waves are classified as acceleration waves. In other words, the thermo-mechanical coupled waves propagated in plastic media are of acceleration type.

iv. The discontinuity associated with step input is propagated between the front and the trailing edges of the waves. As time increases, the distance between the two edges increases correspondingly, and the the discontinuity becomes vanishingly small.

v. The mechanical waves (stress, velocity, plastic strain) and the thermal waves (temperature increment, heat flow) are coupled and propagate between the leading and trailing edges with the same velocity.

Consistency is an important feature of the newly established constitutive relations. Thermoplastic analysis based on fundamental laws associated with numerical calculation which clarify some basic facts of plastic wave propagation problems have not been hitherto reported in the literature. I hope this research would make a further step in the developing efforts of the related areas.

6.6 Recommendation for Further Research

From the development presented in Chapter 3 it is seen that there are three factors which are decisive for the plastic constitutive equations. The first one is the strain hardening parameter which is related to cold work and contributes to the free energy function. The second is the time-dependent term of plastic strain which is closely related to the dissipation function; and the third the softening rule of the strain hardening parameter, which constitutes another part of dissipative power. Different kinds of materials correspond to different combinations of these factors, which are characterized by corresponding material properties. Experimental research efforts are recommended to identify the these material properties for various engineering materials.

Since the 60's of this century a great number of experiments have been done on determining material behaviors at elevated temperature to meet the growing industrial needs. Because most of the works are empirically based, the essential features of thermoplasticity are seldom taken into account. After so many years of continuous development it is the time to relate the theory of thermoplasticity to the experimental results of metallic materials at elevated temperature.

At the same time, material science is expected to make more research efforts towards the relation of strain hardening and micro structure movement at different temperature levels. A better understanding of micro scale movement is of vital importance for further development of thermoplasticity of metallic materials.

REFERENCES

1.1 Clifton, R. J., "Plastic Waves: Theory and Experiment", In: *Mechanics Today,* Vol. 1, Nemat-Nasser, S. (Ed.), pp. 103-167, Pergamon Press, New York (1974).

1.2 Taylor, G. I., "The Plastic Wave in a Wire Extended by an Impact Load", *British Ministry of Home Security, Civil Defense Research Committee Report RC 329* (1942).

1.3 Bell, J. F., "Propagation of Plastic Waves in Pre-Stressed Bars", *Technical Report No.5*, Department of Mechanical Engineering, The Johns Hopkins University, Baltimore (1951).

1.4 Klopp, R. W., Clifton, R. J. and Shawki, T. G., "Pressure-Shear Impact and the Dynamic Viscoplastic Response of Metals", *Mechanics of Materials,* Vol. 4, pp. 375-385 (1985).

1.5 Achenbach, J. D., *Wave Propagation in Elastic Solids,* North-Holland, Amsterdam (1973).

1.6 Von Karman, Th. and Duwez, P., "The propagation of Plastic Deformation in Solids", *Journal of Applied Physics,* Vol..21, pp. 987-994 (1950).

1.7 Drucker, D. C., "The Continuum Theory of Plasticity on the Macroscale and Microscale", *ASTM Journal of Materials,* Vol.1, pp. 873-910 (1966).

1.8 Riff, .R and Simitses, G. J., "Thermo-Elasto-Viscoplastic Analysis of Problems in Extension and Shear", *Computers & Structures,* Vol. 29, pp. 293-300 (1988).

1.9 Kosinski, W., " Thermal Waves in Inelastic Bodies", *Archives of Mechanics,* Vol. 27, pp. 733-748 (1975).

1.10 White, M. R. and Griffis, L. V., "The Propagation of Plasticity in Uniaxial Compression". *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 15, pp. 256-260 (1948).

1.11 Drucker, D. C., "Conventional and Unconventional Plastic Response and Representation", *Applied Mechanics Reviews,* Vol. 41 , PP. 151-167 (1988).

1.12 Drucker, D. C., "On Past Developments, Current Activities and Future Directions in Plasticity", *Res Mechanica,* Vol. 21, pp. 393-400 (1987).

1.13 Bever, M. B., Holt, D. L. and Titchener, A. L., "The Stored Energy of Cold Work", In: *Progress in Materials Science,* Chalmers, B., Christian, J. W., and Massalski, T. B.(Eds.) Vol.17, Pergamon Press, New York (1973).

1.14 Kim, Y. H., "Analysis of Deformation-Induced Heating in Tensile Testing Using a Finite Element Method", Ph.D. Thesis, The Ohio State University (1987).

1.15 Clifton, R. J., "Dynamic Plasticity", *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 50, pp. 941-952 (1983).

1.16 Raniecki, B., "The Influence of Dynamical Thermal Expansion on the Propagation of Plane Elastic-Plastic Stress waves", *Quarterly of Applied Mathematics,* Vol.29, pp. 277-290 (1971).

1.17 Rice, J. R., "Continuum Mechanics and Thermodynamics of Plasticity in Relation to Microscale Deformation Mechanics", In: *Constitutive Equations in Plasticity,* Argon, A. S.(Ed.), MIT Press, Cambridge (1975).

1.18 Campbell, J. D., "Dynamic Plasticity: Macroscopic and Microscopic Aspects", *Materials Science and Engineering,* Vol. 12, pp. 3-21 (1973).

1.19 Graff, K. F., *Wave Motion in Elastic Solids,* Ohio State University Press, Columbus (1975).

1.20 Lee, L. H. N., "Dynamic Plasticity", *Nuclear Engineering and Design,* Vol. 27, pp. 386-397 (1974).

1.21 Cristescu, N., "Dynamic Plasticity", *Applied Mechanics Reviews,* Vol. 21, pp. 659-668 (1968).

1.22 Rakhmatulin, K. A., "Propagation of a Wave of Unloading", *PMM,* Vol.9, pp.91-100 (1945).

1.23 Cristescu, N., *Dynamic Plasticity,* North-Holland, Amsterdam (1967).

1.24 Hill,R., *The Mathematical Theory of Plasticity,* Oxford University Press, London (1950).

1.25 Hopkins, H. G., "Dynamic Inelastic Deformation of Metals", *Applied Mechanics reviews,* Vol. 14, pp. 417-431 (1961).

1.26 Bodner, S. R. and Aboudi, J., "Stress Wave Propagation in Rods of Elastic-Viscoplastic Materials", *International Journal of Solids and Structures,* Vol. 19, pp. 305-314 (1983).

1.27 Data, H., "Propagation of Plastic Wave in a Long Rod with Consideration of Temperature Rise", *Proceedings of the International Conference on Computational Mechanics,* Yagawa, G. and Atluri, S. N.(Eds.), Vol. 2, Springer-Verlag, Tokyo (1986).

1.28 Markenscoff, X. and Clifton, R. J., "Radiation from Expanding Circular Dislocation Loops and Elastic Precursor Decay", *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 49, pp. 792-796 (1982).

1.29 Hirose, A. and Lonngren, K. E., *Introduction to Wave Phenomena,* John Wiley & Sons, New York (1985).

1.30 Lee, E. H., "Some Recently Developed Aspects of Plastic Wave Analysis", In: *Wave Propagation in Solids,* Miklowith, J.(Ed.), ASME, (1969).

1.31 Francis, P. H., "Elastoplastic Wave Propagation in a RAte-Sensitive Finite Rod Having a Thermal Gradient", *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 91, pp. 315-323 (1970).

1.32 Nowacki, W. K., *Stress Waves in Non-Elastic Solids,* Pergamon Press, Oxford (1978).

1.33 Titchener, A. L. and Bever, M. B., "The Stored Energy of Cold Work", In: *Progress in Metal Physics,* Chalmers, B. and King, R.(Eds.), Vol. 7, pp. 247-338, Pergamon Press, New York (1958).

1.34 Aifantis, E. C., "The Physics of Plastic Deformation", *Intrnational Journal of Plasticity,* Vol. 3, pp. 211-247 (1987).

1.35 Clifton, R. J., "Stress Wave Experiments in Plasticity:, *International Journal of Plasticity*, Vol. 1, pp. 289-302 (1985).

1.36 Zukas, J. A., Nicholas, T., Swift, H. F. and Curran, D. R., *Impact Dynamics,* John Wiley & Sons, New York (1982).

1.37 Farre, W. S. and Taylor, G. I., "The Heat Developed During Plastic Extension of Metals", *Proceeding of Royal Society* (London), Series A, Vol. 107, pp. 422-451 (1925).

1.38 Prager, W., *Introduction to Plasticity,* Addison-Wesley, Reading, Massachusetts (1959).

1.39 Mendelson, A., *Plasticity: Theory and Application,* Robert, E. Krieger Publishing Company, New York (1968).

1.40 Kolsky, H., "An Introduction of the Mechanical Properties of Materials at Very High Rate of Loading", *Proceeding of the Physical Society,* Section B, Vol. 62, pp. 676-700 (1949).

1.41 Gyarmati, I., *Non-equilibrium Thermodynamics,* Springer-Verlag (1970).

1.42 Kukudjanov, V. N., "On Wave Propagation in a Coupled Thermo-Elastic-Plastic Medium", *Archives of Mechanics,* Vol. 29, pp. 325-338 (1977).

1.43 Francis, P. H. and Lindholm, U. S., "The Effect of Temperature Gradients on the Propagation of Elastoplastic Waves", *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 90, pp. 441-448 (1968).

1.44 Fung, Y, C., *Foundations of Solid Mechanics,* Prentice-Hall, Englewood Cliffs, New Jersey (1965).

1.45 Prigogine, I., *Introduction to Thermodynamics of Irreversible Process,* 2nd ed. Interscience Pub. Wiley, New York (1961).

1.46 Gilman, J. J., *Micromechanics of Flow in Solids*, McGraw-Hill, New York (1969).

1.47 Eringen, A. C., *Mechanics of Continua*, John Wiley & Sons, New York (1967).

2.1 Ghoneim, H. and Matsuoka,S.,"Thermoviscoplasticity by Finite Element: Tensile and Compression Test", *International Journal of Solids and Structures,* Vol. 23, pp. 1133-1143 (1987).

2.2 Kröner, E., "Dislocation: A New Concept in the Continuum Theory of Plasticity", *Journal of Mathematics and Physics,* Vol. 42, pp. 27-37 (1962).

2.3 Chen, P. J., *Selected Topics in Wave Propagation,* Noordhoff International Publishing, Leyden (1976).

2.4 Ponter, A. R. S., Bataille, J. and Kestin, J., "A Thermodynamic Model for the Time Dependent Plastic Deformation of Solids", *Journal de Mecanique,* Vol. 18, pp. 511-539 (1979).

2.5 Coleman, B.D. and Gurtin, M. E., "Thermodynamics with Internal State Variables", *Journal of Chemical Physics,* Vol.47, pp. 597-613 (1967).

2.6 Coleman, B. D., "Thermodynamics of Materials with Memory", *Archives for Rational Mechanics and Analysis,* Vol. 17, pp. 1-46 (1964).

2.7 Kluitenberg, G. A., "Plasticity and Nonequilibrium Thermodynamics", In: *The Constitutive Law in Thermoplasticity*, Lehmann, Th.(Ed.), Springer-Verlag, New York (1984).

2.8 Hart, W., "Constitutive Relations for the Nonelastic Deformation of Matals", *Transactions of the ASME, Journal of Engineering Materials and Technology,* Vol. 98, pp. 193-202 (1976).

2.9 Lehmann, Th., "Some Thermodynamic Considerations of Phenomenological Theory of Non-Isothermal Elastic-Plastic Deformations", *Archives of Mechanics,* Vol. 24, pp. 975-989 (1972).

2.10 Cernocky, E. P. and Krempl, E., "A Theory of Thermoviscoplasticity Based on Infinitesimal Total Strain", *International Journal of Solids and Structures,* Vol. 16, pp. 723-741 (1980).

2.11 Ziegler, H. and Wehrli, C., "The Derivation of Constitutive Relations from the Free Energy and the Dissipation Function", *Advances in Applied Mechanics,* Vol. 25, pp. 183-228 (1987).

2.12 Kratochvil, J. and Dillon, O. W., "Thermodynamics of Elastic-Plastic Materials as a Theory with Internal State Variables", *Journal of Applied Physics,* Vol. 40, pp. 3207-3218 (1969).

2.13 Marzer, A. and Bodner, S. R., "Analytical Formulation of a Rate and Temperature Dependent Stress-Strain Relation", *Transactions of the ASME, Journal of Engineering Materials and Technology,* Vol. 101, pp. 254-257 (1979).

2.14 Lubliner, J., "On the Thermodynamic Foundations of Non- Linear Solid Mechanics", *International Journal of Non-Linear Mechanics,* Vol. 7, pp. 237-254 (1972).

2.15 Rice, J. R., "Inelastic Constitutive Relations for Solids: An Internal-Variable Theory and its Application to Metal Plasticity", *Journal of the Mechanics and Physics of Solids,* Vol.19, pp.433-455 (1971).

2.16 Schapery, R. A., "Application of Thermodynamics to Thermomechanical, Fracture, and Birefringent Phenomena in Viscoelastic Media", *Journal of Applied Physics,* Vol. 35, pp. 1451-1465 (1964).

2.17 Swearengen, J. C. and Holbrrok, J. H., "Internal Variable Models for Rate-Dependent Plasticity: Analysis of Theory and Experiment", *Res Mechanica,* Vol. 13, pp. 93-128 (1958).

2.18 Gurtin, M. E., Williams, W. O. and Suliciu, I., "On Rate-Type Constitutive Equations and the Energy of Viscoelastic and Viscoplastic Materials", *International Journal of Solids and Structures,* Vol. 16, pp. 607-617 (1980).

2.19 Kraotchvil, J. and Dillon, O. W., "Thermodynamics of Crystalline Elastic-Viscoplastic Materials", *Journal of Applied Physics,* Vol. 41, pp. 1470-1479 (1970).

2.20 Kraotchvil, J., "Meaning of Internal Variables In Plasticity", *International Journal of Engineering Science,* Vol.16, pp.403-413 (1978).

2.21 Bamman, D. J. and Aifantis, E. C., "On a Proposal for a Continuum with Microstructure", *Acta Mechanica,* Vol. 45, pp. 91-121 (1982).

2.22 Lubliner, J., "A Thermodynamic Yield Criterion in Viscoplasticity", *Acta Mechanica,* Vol. 30, pp. 165-174 (1978).

2.23 Lehmann, Th., "On the Concept of Stress-Strain Relation in Plasticity", *Acta Mechanica,* Vol.42, pp. 263-275 (1982).

2.24 Anand, L., "Constitutive Equations for Hot-Working of Metals", *International Journal of Plasticity,* Vol.1, pp. 213-231 (1985).

2.25 Nunziato, J. W. and Drumheller, D. S., "Thermodynamics of Maxwellian Materials", *International Journal of Solids and Structures,* Vol. 14, pp. 545-558 (1978).

2.26 Lubliner, J., "On Fading Memory In Materials of Evolutionary Type", *Acta Mechanica,* Vol.8, pp. 75-81 (1969).

2.27 Allen, D. H., A Thermodynamic Framework for Comparison of Current Thermoviscoplastic Constitutive Models for Metals at Elevated Temperature", *Proceedings of the First International Conference on Constitutive Laws for Engineering Materials: THeory and Application,* Desai C. S. and Gallgher, R. H. (Eds.), pp. 61-69, John Wiley & Sons, New York (1984).

2.28 Biot, M. A., "Variational Principles in Irreversible Thermodynamics with Application to Viscoelasticity", *Physical Review,* Vol. 97, pp. 1463-1469 (1955).

2.29 Lavenda, B. H., *Thermodynamics of Irreversible Processes,* John Wiley & Sons, New York (1978).

2.30 Bampi, F. and Morro, A., "Non-Equilibrium Thermodynamics: A Hidden Variable Approach", In: *Recent Developments in Nonequilibrium Thermodynamics,* Casas-Vázquez, J., Jou, D., and Lebon, G. (Eds.), pp. 211-232, Springer-Verlag (1984).

2.31 Eringen, A. C., *Mechanics of Continua,* John Wiley & Sons, New York (1967).

2.32 Ziegler, H., "An Attempt to Generalize Onsager's Principle, and its Significance for Rheological Problems", *Zeitschrift für Angwandte Mathematik und Physik,* Vol. 9b, pp. 748-763 (1958).

2.33 Eckart, C., "The Thermodynamics of Irreversible Processes,IV, The Theory of Elasticity and Anelasticity", *Physical Review,* Vol. 73, pp. 373-382 (1948).

2.34 Perzyna, P. and Wojno, W., "Thermodynamics of a Rate Sensitive Material", *Archives of Mechanics,* Vol. 5, pp. 499-511 (1968).

2.35 Riff, R., Carlson, R. L. and Simitses, G. J., "Thermodynamically Consistent Constitutive Equations for Nonisothermal Large-Strain, Elastoplastic, Creep Behavior", *AIAA Journal,* Vol.25, pp. 114-122 (1987).

2.36 Perzyna, P., "Thermodynamics of Rheological Materials with Internal Changes", *Journal de Mecanique,* Vol.10, pp. 391-408 (1971).

2.37 Bell, J. F., "Propagation of Plastic Waves in Pre-stressed bar", Dept. of Mech. Engng. *Technical Report No.5,* The Johns Hopkins University, Baltimore (1951).

2.38 Sternglass, E. J.and Stuart, D. A., "An Experimental Study of the Propagation of Transient Longitudinal Deformation in Elastoplastic Media", *Journal of Applied Mechanics,* Vol. 20, pp. 427-434 (1953).

2.39 Clifton, R. J.,"Dynamic Deformation of Elastic-Plastic Solids Under Conditions of Plane Strain", Ph. D. thesis, Dept. of Civil Engng, Carnegie-Mellon University of Pittsburgh (1963).

2.40 Hunter, S. C. and Johnson, I. A., "The Propagation of Small Amplitude Elastic-Plastic Waves in Pre-Stressed Cylindrical Bars", In: *Stress Waves in Anelastic Solids*, Kolsky, H. and Prager, W.(Eds.) pp. 149-165 (1964).

2.41 Sokolovsky, V. V., "Propagation of Elastic Visco-Plastic Waves in Bars", *P. M. M.* Vol. pp. 261-280 (1948).

2.42 Malvern, L. E., "Plastic Wave Propagation in a Bar of Material Exhibiting a Strain-Rate Effect", *Quarterly of Applied Mathematics*, Vol. 8, pp. 405-411 (1951).

2.43 Lee, E. H.,"Wave Propagation in Inelastic Materials", In:IUTAM Collog. *Deformation and Flow of Solids,* (1956).

2.44 Marvern, L. E., "Longitudinal Waves of Plastic Deformation in a Bar of Material Exhibiting a Starain-Rate Effect", *Journal of Applied Mechanics,* Vol. 18, pp. 203-208 (1951).

2.45 Wood, E. R. and Phillips A., "On the Theory of Plastic Wave Propagation", *Journal of Mechanics and Physics of Solids,* Vol.15, pp. 241-154 (1967).

2.46 Efron, L. and Malvern, L. E., "Electromagnetic Velocity-Transducer Studies of Plastic Waves in Aluminum Bars", *Experimental Mechanics* , Vol. 9, pp. 255-262 (1969).

2.47 Cristescu, N., "A Procedure for Determining the Constitutive Equations for Materials Exhibiting both Time-dependent and Time-independent Plasticity", *International Journal of Solids and Structures*, Vol.8, pp. 511-531 (1972).

2.48 Craggs, J. W., "Propagation of Infinitesimal Plane Waves in Elastic-Plastic Materials", *Journal of Mechanics and Physics of Solids*, Vol. 5, pp. 115-124 (1957).

2.49 Hill, R., "Acceleration Waves in Solids", *Journal of Mechanics and Pysics of Solids,* Vol. 10, pp. 1-16 (1962).

2.50 Christensen, R. M., *Theory of Viscoelasticity,* Academic Press, Inc. New York (1971).

3.1 Besdo, T., "Total Lagrangean Strain-Space-Representation of the Elasto-Plasticity of Metals", *Proceedings of the Second International Conference on Constitutive Laws for Engineering Materials: Theory and Application,* Desai, C.S. *et al.*(Eds.),pp. 1357-1364 Elsevier Science Publishing, New York (1987).

3.2 Bodner, S. R., Partom, I. and Partom, Y., " Uniaxial Cyclic Loading of Elastic-Voscoplastic Materials", *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 46, pp. 805-810 (1979).

3.3 Bever, M. B., Holt, D. L. and Titchener, A. L.,"The Stored Energy of Cold Work", In: *Progress in Materials Science,* Chalmers, B., Christian, J. W. and Massalski, T. B. (Eds.), Vol. 17, Pergamon Press, New York (1973).

3.4 Benallal, A. and Cheikh, A. B., "Modelling of Anisothermal Effects in Elasto-Viscoplasticity", *Proceedings of the IUTAM Jean Mandel Memorial Symposium on Thermomechanical Couplings in Solids,* Bui, H. D. and Nguyen, Q. S.(Eds.), pp. 403-409, North-Holland, Amsterdam (1987).

3.5 Riff, R. and Simitses, G. J., "Thrmo-Elasto-Viscoplastic Analysis of Problems in Extension and Shear", *Computer & Structures,* Vol.29, pp. 293-300 (1988).

3.6 Kim, S. J. and Oden, J. T., "Finite Element Analysis of a Class of Problems in Finite Elastoplasticity Based on the Thermodynamical Theory of Materials of Type N", *Computer Methods in Applied Mechanics and Engineering,* Vol. 53, pp. 277-302 (1985).

3.7 Klopp, R. W., Clifton, R. J. and Shawki, T. G., "Pressure-Shear Impact and Dynamic Viscoplastic Response of Metals", *Mechanics of Materials,* Vol. 4, pp. 375-385 (1985).

3.8 Sherief, H. H. and Dhaliwal, R. S., "Generalized One-Dimensional Thermal-Shock Problem for Small Times", *Journal of Thermal Stresses,* Vol. 4, pp.407-420 (1981).

3.9 Chrysochoos, A., "The Heat Evolved During an Elastic-Plastic Transformation at Finite Strain", *Proceeding of the IUTAM Jean Mandel Memorial Symposium on Thermomechanical Coupling in Solids,* Bui, H. D. and Nguyen, Q. S.(Eds.), pp. 79-84, North-Holland, Amsterdam (1987).

3.10 Lord, H. W. and Shulman, Y., "A Generalized Dynamical Theory of Thermoelasticity", *Journal of the Mechanics and Physics of Solids,* Vol. 15, pp. 299-309 (1967).

3.11 Benallal, A. and Marquis, D., "Constitutive Equations for Nonproportional Cyclic Elasto-Viscoplasticity", *Transactions of the ASME, Journal of Engineering Materials and Technology,* Vol.109, pp. 326-336 (1987).

3.12 Achenbach, J. D., "The Influence of Heat Conduction on Propagation Stress Jumps", *Journal of the Mechanics and Physics of Solids,* VOl. 16, pp. 273-282 (1968).

3.13 Beghi, M. G., Bottani, C. E. and Caglioti, G., "Irreversible Thermodynamics of Metals Under Stress", *Res Mechanica,* Vol. 19, pp. 365-379 (1986).

3.14 Kratochvil, J. and Dillon, O. W., "Thermodynamics of Cristalline Elastic-Viscoplastic Materials", *Journal of Applied Physics,* Vol. 41, pp. 1470-1479 (1970).

3.15 Kratochvil, J. and Dillon, O. W., "Thermodynamics of Elastic-Plastic Materials as a Theory with Internal State Variables", *Journal of Applied Physics,* Vol. 40, pp. 3207-3218 (1969).

3.16 Hsu, T. R., *The Finite Element Method in Thermomechanics,* Chapter 9, Allen & Unwin, Winchester (1986).

3.17 Ziegler, H. and Wehrli, C., "The Derivation of Constitutive Relations from the Free Energy and the Dissipation Function", *Advances in Applied Mechanics,* Vol. 25, pp.183-238 (1987).

3.18 Bodner, S. R. and Parton, Y.,"Constitutive Equations for Elastic-Viscoplastic Strain-Hardening Materials", *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 42, pp. 385-389 (1975).

3.19 Boit, M. A., "Theory of Stress-Strain Relations in Anisotropic Viscoelasticity and Relaxation Phenomena", *Journal of Applied Physics,* Vol. 25, pp. 1385-1391 (1954).

3.20 Lehmann, Th., "On a Generalized Constitutive Law for Finite Deformation in Thermo-Plasticity and Thermo-Viscoplasticity", *Proceedings of the Second International Conference on Constitutive Laws for Engineering Materials: Theory and Application*, Desai, C. S. *et al* (Eds.), pp. 173-184, Elsevier Science Publishing Co.. New York (1987).

3.21 Allen, D. H., "Predicted Axial Temperature Gradient in a Viscoplastic Uniaxial Bar Due to Thermomechanical Coupling", *International Journal for Numerical Methods in Engineering,* Vol. 23, pp. 903-917 (1986).

3.22 Green, A. E. and Naghdi, P. M., "On Thermodynamic Restrictions in the Theory of Elastic-Plastic Materials", *Acta Mechanica,* Vol.30, pp. 157-162 (1978).

3.23 Perrone, N. and Bhadra, P., "A Simplified Method to Account for Plastic Rate Sensitivity with Large Deformations", *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 46, pp. 811-816 (1979).

3.24 Drucker, D. C.,"From Limited Experimental Information to Appropriately Idealized Stress-Strain Relations", In: *Mechanics of Engineering Materials,* Desai, C. S. and Gallagher, R. H.(Eds.), John Wiley & Sons, Chichester, pp. 231-251 (1984).

3.25 Chang, W. P. and Cozzarell, F. A., "On the Thermodynamics of Nonlinear Single Integral Representations for Thermovisco-elastic Materials with Application on One-Dimensional Wave Propagation", *Acta Mechanica,* Vol. 25, pp. 187-206 (1977).

3.26 Ghoneim, H., Matsuoka, S. and Chen, Y., "Viscoplastic Modelling with Strain Rate History Dependency", *Transactions of the ASME, Journal of Applied Mechanics,* Vol.50, pp. 465-468 (1983).

3.27 Bohatier, C. and Chento, J., "Finite Element Formulations for Non-Steady-State Large Viscoplastic Deformations", *International Journal of Numerical Methods in Engineering,* Vol. 21, pp. 1697-1708 (1985).

3.28 Bruhus, O. T. and Müller, R., "Some Remarks on the Application of Two-Surface Model in Plasticity", *Acta Mechanica,* Vol. 53, pp. 81-104 (1984).

3.29 Mroz, Z. and Trampczunski, W. A., "On the Creep-Hardening Rule for Metals with a Memory for Maximal Prestress", *International Journal of solids and Structures,* Vol.20, pp. 467-486 (1984).

3.30 Ting, T. C. T., "Plastic Wave Propagation in Linearly Work-Hardening Materials", *Transactions of the ASME,Journal of Applied Mechanics,* Vol. 40, pp. 1045-1049 (1973).

3.31 Palgen, L. and Drucker, D. C., "The Structure of Stress- Strain Relations in Finite Elasto-Plasticity", *International Journal of Solids and Structures,* Vol. 19, pp. 519-531 (1983).

3.32 Onsager, L., "Reciprocal Relations in Irreversible Processes I", *Physical Review,* Vol. 37, pp. 405-426 (1931).

3.33 Onsager, L., "Reciprocal Relations in Irreversible Processes II", *Physical Review,* Vol. 38, pp. 2265-2279 (1931).

3.34 Ziegler, H., *An Introduction to Thermomechanics*, 2nd ed. North-Holland, Amsterdam (1983).

3.35 Cowper, G. R. and Symonds, P. S., "Strain-Hardening and Starin-Rate Effects in the Impact Loading of Cantilever Beams", ONR Contract Nonr-562(10), NR-064-406, Grad. Div. of Appl. Math., Bron Univ., *Tech.Rept.* No.28 (1957).

3.36 Bodner, S. R. and Symonds, P. S., "Experimental and Theoretical Investigation of Plastic Deformation of Cantilever Beams Subjected to Impulsive Loading", *ASME Journal of Applied Mechanics* Vol.29, pp. 719-728 (1962).

4.1 Cristescu, N. and Suliciu, I., *Viscoplasticity,* Martinus Nijhoff Publishers, The Hague, Boston, London (1982).

4.2 Malvern, L. E., *Introduction to the Mechanics of a Continuous Medium,* Prentice-Hall, Inc., Englewood Cliffs, New Jersey (1969).

4.3 Gilat, A. and Clifton, R. J., "Pressure-Shear Waves in 6061-T6 Aluminum Alpha-Titanium", *Journal of the Mechanics and Physics of Solids*, Vol. 33, pp. 263-284 (1985).

4.4 Goel, R. P. and Malvern, L. E., "Elastic-Plastic Plane Waves with Combined Compressive and Two Shear Stresses in a Half Space", *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 38, pp. 895-898 (1971).

4.5 Ohno, N. and Kachi, Y., "A Constitutive Model of Cyclic Plasticity for Nonlinear Hardening Materials", *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 53, pp. 395-403 (1986).

4.6 Orisamolu, I. R., "Continuum Thermodynamics Formulation and Numerical Simulation of the Propagation of Coupled Thermomechanical Waves in Inelastic Solids", Ph.D. Thesis, Department of Mechanical Engineering, The University of Calgary, Calgary (1988).

4.7 Jeffrey, A. and Taniuti, T., *Nonlinear Wave Propagation with Applications to Physics and Magnetohydrodynamics,* Academic Press, New York (1964).

4.8 Kosinski, W., "One-Dimensional Shock Waves in Solids with Internal State Variables", *Archives of Mechanics,* Vol. 27, pp. 445-458 (1975).

4.9 Achenbach, J. D., *Wave Propagation in Elastic-Solids,* North-Holland, Amsterdam (1973).

4.10 Aifantics, E. C., "Remarks on Media with Microstructure", *Mechanics Research Communications,* Vol.5, pp. 139-145 (1978).

4.11 Clifton, R. J., "Stress Wave Experiments in Plasticity", *International Journal of Plasticity,* Vol. 1, pp. 289-302 (1985).

4.12 Bailey, P. B. and Chen, P. J., "Shocks and Induced Discontinuities in Materials with Internal State Variables-Applications to Finite Linear Viscoelasticity", *Acta Mechanica,* Vol. 60, pp. 251-164 (1986).

4.13 Eringen, A. C. and Suhubi, E. S., *Elastodynamics,* Vol. 1, Finite Motions, Academic Press, New York (1974).

4.14 Chen, P. J., *Selected Topics in Wave Propagation,* Noordhoff international Publishing, Leyden (1976).

4.15 Hashiguchi, K., "Constitutive Equations of Elastoplastic Materials with Anisotropic Hardening and Elastic-Plastic Transition", *Transactions of the ASME, Journal of Applied Mechanics,* Vol.48, pp. 297-301 (1981).

4.16 Chaboche, J. L. and Rousselier, G., "On the Plastic and Viscoplastic Constitutive Equations-PartI: Rules Developed with Internal Variable Concept; PartII: Application of Internal Variable Concepts to the 316 Stainless Steel", *ASME Journal of Pressure Vessel Technology,* Vol. 105, pp. 153-164 (1983).

4.17 Carroll, M. M., "A Rate-Independent Constitutive Theory for Finite Inelastic Deformation", *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 54, pp. 15-21 (1987).

4.18 Asaro, R. J., "Crystal Plasticity", *ASME Journal of Applied Mechanics (50 the Anniversary Issue),* Vol.50, pp. 921-934 (1983).

4.19 Casey, J. and Naghdi, P. M., "Further Constitutive Results in Finite Plasticity", *Quarterly Journal of Mechanics and Applied Mathematics,* Vol. 37, pp. 231-259 (1984).

4.20 Naghdi, P. M., "Constitutive Restrictions for Idealized Elastic-Viscoplastic Materials", *Transactions of the ASME, Journal of Applied Mechanics,* Vol. 51, pp. 93-101 (1984).

4.21 Rubin, M. B., "An Elastic-Viscoplastic Model for Metals Subjected to High Compression", *ASME Journal of Applied Mechanics,* Vol. 54, pp. 532-538 (1987).

4.22 Rubin, M. B., "An Elastic-Viscoplastic Model for Large Deformation", *International Journal of Engineering Science,* Vol.24, pp. 1083-1095 (1986).

5.1 Lapidus, L. and Rinder, G. D., *Numerical Solution of Partial Differential Equations in Science and Engineering,* John Wiley & Sons, New York (1982).

5.2 Marcowitz, Th. M. U., *Numerical Solution of Partial Differential Equations,* Springer-Verlag, New York, Heidelberg, Berlin (1980).

5.3 Van Der Hovwen, P. J., *Finite Difference Methods for Solving Partial Differential Equations,* Mathematisch Centrum, Amsterdam (1968).

5.4 Osher, S., "Hyperbolic Equations in Regions with Characteristic Boundaries or with Corners", In: *Numerical Solution of Partial Differential Equations-III SYNSPADE 1975,* Hubbard, B. (Ed.), pp. 413-441 (1976).

5.5 Lister, M., "The numerical Solution of Hyperbolic Partial Differential Equations by the Method of Characteristics", In: *Mathematical Methods for Digital Computers,*Ralston, A. and Wilf, H. S.(Eds.) pp. 165-179, John Wiley & Sons, New York (1960).

5.6 MacCormack, R. W., "The Effect of Viscosity in Hyper-velocity Impact Cratering", *AIAA Paper* No. 69-354 (1969).

5.7 MacCormack, R. W., "Numerical Solution of the Interaction of a Shock Wave with a Laminar Boundary Layer", *Proceedings of the Second International Conference on Numerical Methods in Fluid Dynamics,* Maurice, H. (Ed.), pp. 151-163, Springer-Verlag, Berlin (1971).

5.8 Lorimer, S. A., "A Numerical Study of Some Linear and Nonlinear Elastodynamic Problems", Ph. D. Thesis, The University of Alberta, Edmonton (1986).

5.9 Kot, C. A., "An Improved Constant Time Technique for the Method of Characteristics", *Proceedings of the Third International Conference on Numerical Methods in Fluid Mechanics,* Chabannes,H. and Teman, R. (Eds.), Vol. 1, pp. 130-137, Springer-Verlag, Berlin (1973).

5.10 Haddow, J. B.,Lorimer, S. A., and Trait, R. J., "Non-Linear Combined Axial and Torsional Shear Wave Propagation in an Incompressible Hyperelastic Solid", *International Journal of Non-Linear Mechanics,* Vol. 22, pp. 297-306 (1987).

5.11 Von Neumann, J. and Richtmyer, R. D., "A method for the Numerical Calculation of Hydrodynamic Shocks", *Journal of Applied Physics,* Vol.21, pp. 232-237 (1950).

5.12 Courant, R., Isaacson, W. and Rees, M., "On the Solution of Non-Linear Hyperbolic Differential Equations by Finite Differences", *Communications on Pure and Applied Mathematics,* Vol. 5, pp.243-255 (1952).

5.13 Lax, D. P., "Hyperbolic Systems of Conservation Laws and the Mathematical Theory of Shock Waves", *Regional Conference Series 11 in Applied Mathematics* (1973).

5.14 Meis, Th. and Marcowitz, U., *Numerical Solution of Partial Diiferential Equations,* Springer-Verlag, Inc. New York (1981).

5.15 Bush, W., Esser, R., Hackbush, W. and Herrmann, V., "Extrapolation Applied to the Method of Characteristics for a First Order System of Two Differential Equations", *Numerical Mathematics* Vol.24, pp. 331-353 (1975).

5.16 Massau, J., *Memoire on Integration Graphics of Equations with Partial Derivatives,* F. Meyer-Van Loo, Gent, (1899).

APPENDIX A

INVERSION OF MATRIX A_0

Square matrix $A_0=[a^0_{ij}]$ is given in such a way that the elements other than zero are:

$$a^0_{11} = \rho$$

$$a^0_{22} = D_2$$

$$a^0_{23} = D_1$$

$$a^0_{32} = D_5$$

$$a^0_{33} = D_3$$

$$a^0_{44} = \tau_0$$

$$a^0_{52} = a^0_{55} = 1$$

$$a^0_{53} = -D_4$$

It can be easily seen that det $A_0 = \rho\tau_0\, \tilde{D}$, where $\tilde{D} = D_2D_3 - D_4D_5$. If we set

$$A_0^{-1} = [a_{ij}] ,$$

then the elements other than zero are:

$$a_{22} = \frac{D_3}{\tilde{D}}$$

$$a_{23} = -\frac{D_1}{\tilde{D}}$$

$$a_{32} = -\frac{D_5}{\tilde{D}}$$

$$a_{33} = \frac{D_2}{\tilde{D}}$$

$$a_{44} = \frac{1}{\tau_0}$$

$$a_{52} = -\frac{(D_3+D_4D_5)}{\tilde{D}}$$

$$a_{53} = \frac{(D_1+D_2D_4)}{\tilde{D}}$$

$$a_{55} = 1$$

The matrix with these elements is the inverse of A_0.

APPENDIX B

DETERMINATION OF EIGENVECTORS

The basic equations (4.15b) are written in the following form:

$$Y_t + A\,Y_x = C \quad , \tag{B1}$$

where Y_t, Y_x and C are defined in Chapter 4. Matrix A is expressed as follows

$$A = \begin{pmatrix} 0 & -\frac{1}{\rho} & 0 & 0 & 0 \\ -\frac{D_3}{\tilde{D}} & 0 & 0 & -\frac{D_5}{\tilde{D}} & 0 \\ \frac{D_1}{\tilde{D}} & 0 & 0 & \frac{D_2}{\tilde{D}} & 0 \\ 0 & 0 & \frac{k}{\tau_0} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{B2}$$

As soon as the eigenvalues are available, the left eigenvectors can be found by the following equations

$$l^{(i)}\,A = \lambda^{(i)}\,l^{(i)} \quad . \tag{B3}$$

For eigenvalue $\lambda^{(1)} = 0$, we have

$$[\,l_1\ l_2\ l_3\ l_4\ l_5]\,[A_{ij}] = 0\,[\,l_1\ l_2\ l_3\ l_4\ l_5] \quad , \tag{B4}$$

which yields

$$[l] = [0 \quad 0 \quad 0 \quad 0 \quad 1] \; . \tag{B5}$$

For $\lambda^{(2)} = V_2$, we have

$$[\, l_1 \; l_2 \; l_3 \; l_4 \; l_5] \; [A_{ij}] = V_2 [\, l_1 \; l_2 \; l_3 \; l_4 \; l_5] \quad , \tag{B6}$$

which yields

$$[l] = [\, 1 \quad -\frac{1}{\rho V_2} \quad \frac{\rho V_2^2 \tilde{D} - D_3}{\rho V_2 D_1} \quad \frac{\tau_0}{\rho k}(\frac{\rho V_2^2 \tilde{D} - D_3}{D_1}) \quad 0 \,] \, . \tag{B7}$$

Similarly, for $\lambda^{(4)} = -V_2$:

$$[l] = [\, 1 \quad \frac{1}{\rho V_2} \quad -\frac{\rho V_2^2 \tilde{D} - D_3}{\rho V_2 D_1} \quad \frac{\tau_0}{\rho k}(\frac{\rho V_2^2 \tilde{D} - D_3}{D_1}) \quad 0 \,] \, . \tag{B8}$$

For $\lambda^{(5)} = V_3$:

$$[l] = [\, 1 \quad -\frac{1}{\rho V_3} \quad \frac{\rho V_3^2 \tilde{D} - D_3}{\rho V_3 D_1} \quad \frac{\tau_0}{\rho k}(\frac{\rho V_3^2 \tilde{D} - D_3}{D_1}) \quad 0 \,] \, . \tag{B9}$$

For $\lambda^{(6)} = -V_3$:

$$[l] = [\, 1 \quad \frac{1}{\rho V_3} \quad -\frac{\rho V_3^2 \tilde{D} - D_3}{\rho V_3 D_1} \quad \frac{\tau_0}{\rho k}(\frac{\rho V_3^2 \tilde{D} - D_3}{D_1}) \quad 0 \,] \, . \tag{B10}$$