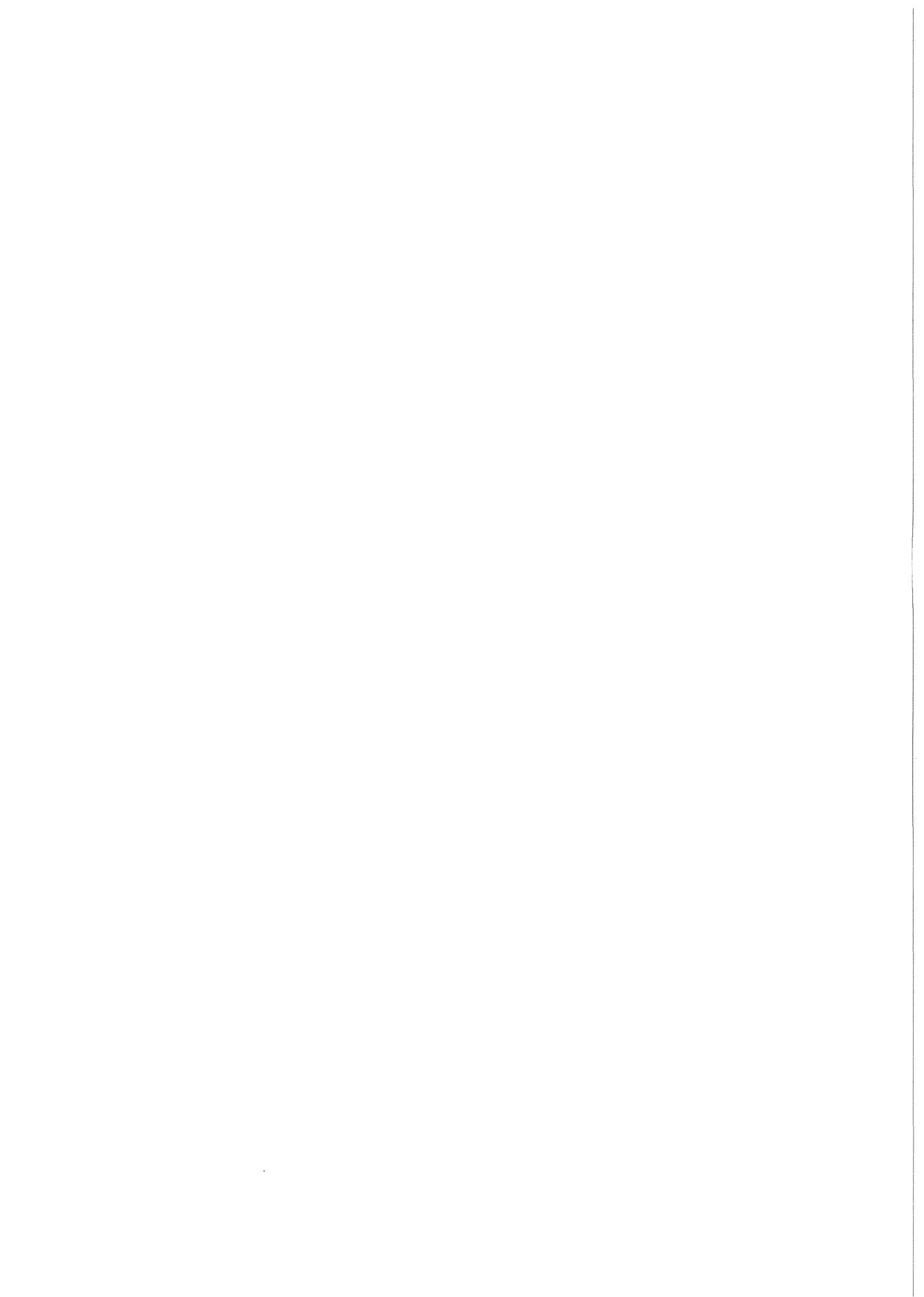


KfK 4284
Juli 1987

On the Derivation of Thermodynamic Restrictions for Materials with Internal State Variables

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Kernforschungszentrum Karlsruhe GmbH
Postfach 3640, 7500 Karlsruhe 1

ISSN 0303-4003

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Summary

Thermodynamic restrictions for the constitutive relations of an internal variable model are derived by evaluating the Clausius-Duhem entropy inequality with two different approaches. The classical Coleman-Noll argumentation of Rational Thermodynamics applied by Coleman and Gurtin to an internal variable model is summarized. This approach requires an arbitrary modulation of body forces and heat supply in the interior of the body which is subject to criticism. The second approach applied in this presentation is patterned after a concept of Müller and Liu, originally developed within the context of a different entropy inequality and different classes of constitutive models. For the internal variable model the second approach requires only the modulation of initial values on the boundary of the body.

In the course of the development of the second approach certain differences to the argumentation of Müller and Liu become evident and are pointed out. Finally, the results demonstrate that the first and second approach give the same thermodynamic restrictions for the internal variable model. The derived residual entropy inequality requires further analysis.

Zur Ableitung konstitutiver Restriktionen für Materialien mit internen Variablen

Zusammenfassung

Unter Verwendung zweier verschiedener Vorgehensweisen werden thermodynamische Restriktionen für die konstitutiven Gleichungen eines Internen Variablen-Modells durch Auswertung der Clausius-Duhem Entropieungleichung abgeleitet. Die klassische Coleman-Noll'sche Argumentation der Rationalen Thermodynamik, wie sie von Coleman und Gurtin für ein Internes Variablen Modell angewandt wurde, wird zusammenfassend dargestellt. Diese Vorgehensweise erfordert die beliebige Einstellbarkeit der Volumenkräfte und Wärmequellen bzw. -senken im Innern des Körpers; diese Methode ist nicht unumstritten. Die zweite Vorgehensweise, die in dieser Studie angewandt wird, orientiert sich an einem Konzept von Müller und Liu, ursprünglich entwickelt im Zusammenhang mit einer anderen Entropieungleichung und anderen Klassen konstitutiver Modelle. Für das Interne Variablen-Modell erfordert die zweite Vorgehensweise nur die beliebige Einstellbarkeit von Anfangswerten auf der Oberfläche des Körpers.

Im Rahmen der Entwicklung der zweiten Vorgehensweise treten bestimmte Unterschiede zur Argumentationsweise von Müller und Liu auf; darauf wird erläuternd hingewiesen. Schließlich zeigen die Ergebnisse, daß die erste und die zweite Vorgehensweise dieselben thermodynamischen Restriktionen für das Interne Variablen-Modell liefern. Die abgeleitete Restentropieungleichung erfordert noch eine weitere Auswertung.

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1. Introduction

Within the context of the R & D activity "Metallic Materials and Structures under Complex Loading" it is planned to perform a systematic analysis of different constitutive models with internal variables on the basis of continuum thermodynamics. These internal variable models serve to describe the elastic-plastic response of metals under complex stress or deformation histories.

It is well known that continuum thermodynamics imposes restrictions on the constitutive equations. However, frequently the constitutive relations have been and are developed on a purely mechanical basis. But it is obvious that a thermo-mechanical theory embracing mechanical and thermodynamic principles has a richer physical content. Therefore, a purely mechanical constitutive theory should be interpretable at least as a special case of the more embracing thermo-mechanical theory. Part of the thermodynamical restrictions are also reflected in such special situations, for example when only isothermal processes are considered.

The thermodynamic restrictions of the constitutive equations derive from an evaluation of an entropy principle together with the appropriate balance equations of the continuum and the assumed constitutive relations. Beside the restrictions associated with an entropy principle there are conditions due to material objectivity and the symmetry properties of the material.

Whereas the validity of the balance equations is generally not questioned the entropy principle or the entropy production inequality has raised many controversies which persist at the present time [1-5]. Very often the entropy principle is taken to be the Clausius-Duhem inequality given by

$$\Gamma := \frac{D}{Dt} \int_V s \eta dV - \oint_0 \frac{q_k n_k}{T} dO - \int_V \frac{s r}{T} dV \geq 0 \quad (1.1)$$

entropy flux by heat conduction through the surface

entropy supply by external heat sources or sinks

Γ integral production of entropy

η specific entropy

q_k components of heat flux vector

r external heat supply (sources or sinks)

- T absolute temperature
 ρ density
 V volume of the body
 O surface area of the body
 n_k components of the external unit normal vector on O

Subscripts take the values $k = 1, 2, 3$ and the usual summation convention applies to repeated subscripts. It appears that this inequality (1.1) including heat sources and sinks at first has been set up by Truesdell and Toupin [6]. Equ. (1.1) is motivated from the second law of thermostatics of homogeneous processes.

Application of the divergence theorem to the surface integral in (1.1) yields*

$$\int_V \left\{ \rho \dot{\eta} + \left(\frac{q_k}{T} \right)_{,k} - \frac{s_r}{T} \right\} dV \geq 0$$

and since this is assumed to be valid for any volume V one obtains the local Clausius-Duhem inequality:

$$\rho \dot{\eta} + \left(\frac{q_k}{T} \right)_{,k} - \frac{s_r}{T} = \rho \dot{\eta} + \frac{q_{k,k}}{T} - \frac{1}{T^2} q_k T_{,k} - \frac{s_r}{T} \geq 0 \quad (1.2)$$

In 1963 Coleman and Noll [7] described a logical context for this inequality which allowed to draw conclusions from this inequality. This context has three ingredients as follows [8]:

- (1) A mathematical description of the physical system and a definition of a thermodynamic process for the system. Such a process is defined to be time-dependent set of configurations, force systems, and temperature, integral energy, entropy, heat supply and heat flux compatible with the balance of linear momentum and moment of momentum and the energy balance equation. Thus, some of the quantities describe the possible internal evolution of the system, while others describe the possible actions of the environment on the system.

* The dot ($\dot{\quad}$) represents the material time derivative and the comma ($\quad_{,k}$) denotes the partial derivative with respect to the material coordinate x^k .

- (2) Constitutive assumptions describing the material behaviour of the above physical system. Such assumptions are equations relating the various quantities that make up the internal portion of a thermodynamic process. A thermodynamic process that satisfies the constitutive equations is said to be admissible.
- (3) A definition of the production of entropy for every thermodynamic process of every system of the type under consideration. This was taken to be the left hand side of (1.1).

Once these ingredients are prescribed a "dissipation postulate (second law)" is required to hold:

"For all admissible thermodynamic processes and for every part of the body, the entropy production must be non-negative."

The decisive word of this postulate are the quantifiers "all" and "every". The quantifier "every" allows to transform the integral Clausius-Duhem inequality (1.1) into its local form (1.2) as derived above. The quantifier "all" makes the postulate a restrictive condition on the constitutive assumptions. Indeed, if the constitutive relations are laid down at will and without restrictions, the specific entropy production cannot be expected to be non-negative for all admissible processes. Thus, the dissipation postulate is not a restriction on the kind of process that can occur but a restriction on the material behavior (for more details see section 2).

The concept of Coleman and Noll, applied by many others and promoted by Truesdell [10], has been criticized for several reasons, e.g.:

- (a) Entropy and absolute temperature are well defined, derived quantities only in thermostatics (equilibrium states). Their transfer to the thermodynamics of irreversible processes involves hypothetical generalizations [1, 2, 11, 12].
- (b) Closely connected with (a) is the question which inequality should replace the Clausius-Duhem inequality [2, 11, 12].
- (c) Some authors (e.g. [13]) reject the requirement that the entropy inequality should be satisfied identically for all admissible processes such that it represents a restriction on the constitutive equations. Instead it is interpreted as a constraint on processes. This interpretation appears to be unacceptable (see section (2)) if sufficiently smooth processes or unique constitutive relations are considered. However, when discontinuous processes are envisaged [14 - 16] or when the material behaviour is not represented by the same set of constitutive relations in the whole range of interest [14, 15], the entropy inequality plays a dual role: A restriction on the constitutive relations and on the possible motions and temperatures, i.e. processes.

(d) The Coleman-Noll argumentation considers a large variety of admissible thermodynamic processes. From a physical standpoint an admissible process is controlled by prescribing the distribution and history of the body force and heat supply as well as initial and boundary conditions. In the approach of Coleman and Noll the body force and heat supply are required to be assignable in any way but initial and boundary conditions need not to be considered explicitly (see section 2). Woods [18 -20] has criticized this aspect among others: It requires a fictitious body force and a fictitious heat supply unconnected with any genuine physical sources of these quantities. These distributions could be supplied only by some imponderable medium permeating the body ("phlogiston axiom"). However, these external fields lie beyond control at interior points of the body. Green [21] did respond to the criticism in [18] but obviously without much success (compare [19, 20]).

In 1967 the Coleman-Noll approach was used by Coleman and Gurtin [22] to develop thermodynamic restriction for the constitutive equations of nonlinear materials with internal variables whose temporal evolution is governed by ordinary differential equations. Later this development was the basis for material models describing elastic-plastic behaviour (e.g. [23, 24]).

Also in this study it is the purpose to derive the thermodynamic restrictions for the constitutive relations of an internal variable model using the Clausius-Duhem entropy inequality and the dissipation postulate but accounting for the criticism of the "phlogiston axiom". This new approach is based on an idea of Müller [25 - 28] where body forces and heat supply are not allowed to be assignable in any way but where the arbitrariness of initial conditions induce a sufficiently large variety of admissible thermodynamic processes. Müller developed his approach in connection with an entropy inequality more general than (1.2) and for other classes of materials. Thus his results cannot simply be transferred to the present problem.

In section 2 the classical Coleman-Noll argumentation is described for the purpose of illustration. In section 3 the new approach is developed in a stepwise manner starting from a simple one-dimensional problem - the rigid heat conductor without internal variables - to the three-dimensional problem including the full set of constitutive relations. This stepwise procedure is recommended because of the mathematical peculiarities of the derivations. The study closes with a discussion of the results.

2. Description of the Classical Methodology of Rational Thermodynamics for Materials with Internal State Variables

The following discussion is restricted to the thermodynamics of infinitesimal deformations of solid bodies. Cartesian coordinates are used throughout and index notation is applied.

The local forms of the balance equations of linear momentum, moment of momentum and energy are as follows*

Linear momentum

$$\rho \ddot{u}_e - t_{ke,k} = \rho b_e \quad (2.1)$$

Moment of momentum

$$t_{ke} = t_{ek} \quad (2.2)$$

Energy

$$\rho \dot{e} - t_{ke} \dot{e}_{ke} + q_{k,k} = \rho r \quad (2.3)$$

Strain - displacement relations

$$e_{ke} = \frac{1}{2} (u_{k,e} + u_{e,k}) \quad (2.4)$$

where the yet undefined quantities are

u_k components of the displacement vector

e_{ke} components of the infinitesimal strain tensor

* Actually the balance equations are formulated as integral balance equations for a finite portion of the body. The derivation of the differential balance equations from the integral balance equations is a subtle process and involves a locality postulate.

- t_{kl} components of the stress tensor
- b_k components of the specific body force
- E specific internal energy .

For infinitesimal deformations the mass balance equation need not to be considered.

Obviously, the balance of moment of momentum leads to an algebraic condition, the symmetry of the stress tensor. This symmetry condition is interpreted as a restriction on the constitutive equations for the stresses. The two other balance equations represent a set of four partial differential equations, which govern the thermomechanical process.

It is evident that these equations must be supplemented by further equations to close the system. These equations are the constitutive relations. For an internal variable model they are assumed to be given by

$$\left. \begin{aligned} t_{kl} &= \hat{t}_{kl}(e_{mn}, T, g_k, \alpha_y) = \hat{t}_{lk} \\ g_k &= \hat{g}_k(e_{mn}, T, g_k, \alpha_y) \\ E &= \hat{E}(e_{mn}, T, g_k, \alpha_y) \\ \eta &= \hat{\eta}(e_{mn}, T, g_k, \alpha_y) \end{aligned} \right\} (2.5)$$

and ordinary differential equations represent the evolution equations for the internal variables α_y

$$\dot{\alpha}_y = f_y(e_{mn}, T, g_k, \alpha_y), \quad y = 1, 2, \dots, n. \quad (2.6)$$

The quantity T denotes the absolute temperature and the vector g_k is the temperature gradient

$$g_k := T_{,k} = \frac{\partial T}{\partial x^k}. \quad (2.7)$$

The above relations represent an application of the "rule of equipresence". This rule* asserts [22], that a quantity present as an independent variable in one

* Some authors have raised this to the status of an axiom but this is certainly unacceptable.

constitutive equation of a material should also be so present in all, unless its presence contradicts some general law of physics or the assumed symmetry of the material. Thus, this rule is basically an anti-discriminatory postulate [3]. However, for special materials and/or approximate theories dependence on one or the other variable may even disappear.

The constitutive equations (2.5) and (2.6) given above implicitly contain the assumption that the constitutive functions \hat{e}_k , \hat{q}_k , \hat{e} , $\hat{\eta}$ and \hat{f}_y do not depend on the thermodynamic process, i.e. their forms are not affected by the present state characterized by the set

$$\Pi := \{e_{mn} = e_{nm}, T, g_k, \alpha_y\} \quad (2.8)$$

or by the temporal or spatial derivatives of these variables. Thus, it is assumed that for every process the response of the material is always represented by the same set of constitutive functions. It should be pointed out that this assumption is not always acceptable when modelling realistic material behavior; then extra considerations are necessary [14, 15].

This system of equations together with a prescribed body force and heat supply as well as initial and boundary conditions completely define the problem. It is obvious that the local entropy balance equation so far does not play any role; nevertheless this inequality is required to be satisfied.

On the first sight this may be achieved in two ways:

- The entropy inequality is a restriction on the admissible thermodynamic process, i.e. on the solution of the above system of equations for a given set of the body force, heat supply, and initial and boundary conditions.

For instance, the solution $u_k(x_m, t)$, $T(x_m, t)$ and $\alpha_y(x_m, t)$ and the dependent variables, especially $g_k(x_m, t)$ and $\eta(x_m, t)$, are inserted in the entropy inequality. Within a certain time interval $t_0 \leq t \leq t_1$, some solutions may be consistent with the inequality (1.2), i.e.

$$T \left(\rho \dot{\eta} + \left(\frac{q_k}{T} \right)_k \right) \geq \rho r$$

and are thus physically acceptable. However, in general it is not to be expected that the above solution obeys this condition.

In reality a process is determined by prescribing the body force, heat supply as well as initial and boundary conditions. Thus, failure to satisfy the entropy inequality would mean that these quantities are restricted by the entropy inequality.

- However, this view is hardly acceptable. In continuum thermodynamics the external agencies are not part of the solution but are presumed to be given by some extra considerations. The body forces and the heat supply as well as the actions on the boundary of the body represent the influence of the environment on the body whereas the initial conditions at some initial time reflect the history of the body up to this time. Thus, continuum theories and any other theory consider only a section of the material world and only part of the evolution of the body. It is certainly true that these external agencies are also subjected to physical laws but these are not necessarily part of the continuum theory. Thus, when analyzing the mathematical and physical consistency of a continuum theory in general, it is quite natural to consider the external agencies and initial conditions as arbitrary. Consequently, the entropy inequality should be satisfied irrespective of the choice of the external agency and initial conditions, i.e. for all processes compatible with the balance equations and assumed constitutive relations. Evidently, this includes processes due to external agencies which cannot be realized. This is the interpretation of Coleman and Noll [7] and others laid down in the "dissipation postulate" (see page 3).

This interpretation and an approach developed by Coleman and Noll allows a systematic evaluation of the entropy inequality to derive logical consequences from this postulate for the constitutive relations. In effect, these consequences will restrict the constitutive functions in their dependence on certain independent variables and will reduce the number of constitutive functions which are in accordance with the thermodynamic principle.

Following Coleman and Noll [7] and Coleman and Gurtin [22] the approach is as follows. For some set of body forces and heat supply as well as initial and boundary conditions the relevant field functions u_k , T and α_γ are determined by solving the initial-boundary value problem. This procedure for obtaining an admissible thermodynamic process may be reversed. Assume that at an initial time the initial values of the internal variables are given by

$$(\alpha_\gamma)_{t=t_0} = \alpha_\gamma^0, \quad \gamma = 1, 2, \dots, n. \quad (2.9)$$

Further, consider a displacement field $u_k(x_m, t)$ and a temperature field $T(x_m, t)$. The quantities

$$\alpha_\gamma, e_{kl} = \frac{1}{2}(u_{k,l} + u_{l,k}), T, g_k = \frac{\partial T}{\partial x_k} \quad (2.10)$$

are functions of x_m and t and are assumed to be smooth enough to ensure the existence of a unique solution $\alpha_\gamma(x_m, t)$ of the evolution equation (2.6). Thus, prescribing $u_k(x_m, t)$, $T(x_m, t)$ and the initial values $\alpha_\gamma(x_m)$, the independent variables

$$\Pi = \{e_{kl}, T, g_k, \alpha_\gamma\} \quad (2.11)$$

are known at any time and every point in the body. From the set (2.11) via the constitutive relations (2.5) and (2.6) one can calculate the dependent variables

$$t_{kl}, q_k, \epsilon, \eta \quad (2.12)$$

as functions of x_m and t . Then the associated body force and heat supply is uniquely obtained from the balance equations. Furthermore, the initial and boundary conditions in the body and on the surface of the body may be determined from the values of the field functions at the initial time and on the surface.

The latter quantities, i.e. body force, heat supply etc., may now be prescribed. The associated initial-boundary value problem yields exactly those field function $u_k(x_m, t)$, $T(x_m, t)$ and $\alpha_\gamma(x_m)$ which were the starting point, if the initial-boundary value problem admits a unique solution. This uniqueness condition is implied in the further analysis.

Consequently, the following alternative for the evaluation of the dissipation postulate exists:

- (1) Evaluation for all (i.e. arbitrary) body forces, heat supplies, and all initial and boundary conditions; these quantities are actually determining an admissible thermodynamic process.
- (2) Evaluation for all (i.e. arbitrary) sufficiently smooth set of functions $u_k(x_m, t)$, $T(x_m, t)$ and initial values $\alpha_\gamma(x_m)$.

Coleman and Noll [7] and Coleman and Gurtin [22] have taken the second alternative as a basis for the evaluation of the Clausius-Duhem entropy in-

equality. This procedure will be described in the following.

The elimination of the heat supply from the entropy inequality (1.2) using the local energy balance equation

$$\rho r = \rho \dot{e} - t_{kl} \dot{e}_{kl} + q_{k,k}$$

gives

$$\begin{aligned} \rho \dot{\eta} - \frac{\rho \dot{e}}{T} + \frac{t_{kl} \dot{e}_{kl}}{T} - \frac{q_{k,k}}{T} + \left(\frac{q_k}{T} \right)_{,k} \\ = \rho \dot{\eta} - \frac{\rho \dot{e}}{T} + \frac{t_{kl} \dot{e}_{kl}}{T} - \frac{q_k q_k}{T^2} \geq 0 \end{aligned} \quad (2.13)$$

where the definition equ. (2.7) is observed. With the constitutive relations (2.5) one has

$$\left. \begin{aligned} \dot{e} &= \frac{\partial \hat{e}}{\partial e_{mn}} \dot{e}_{mn} + \frac{\partial \hat{e}}{\partial T} \dot{T} + \frac{\partial \hat{e}}{\partial g_m} \dot{g}_m + \frac{\partial \hat{e}}{\partial \alpha_\gamma} \dot{\alpha}_\gamma \\ \dot{\eta} &= \frac{\partial \hat{\eta}}{\partial e_{mn}} \dot{e}_{mn} + \frac{\partial \hat{\eta}}{\partial T} \dot{T} + \frac{\partial \hat{\eta}}{\partial g_m} \dot{g}_m + \frac{\partial \hat{\eta}}{\partial \alpha_\gamma} \dot{\alpha}_\gamma \end{aligned} \right\} (2.14)$$

Inserting this in (2.13) and rearranging according to the rates of the independent variables one obtains

$$\begin{aligned} \left[\rho \frac{\partial \hat{\eta}}{\partial e_{mn}} - \frac{1}{T} \rho \frac{\partial \hat{e}}{\partial e_{mn}} + \frac{1}{T} \hat{t}_{mn} \right] \dot{e}_{mn} \\ + \left[\rho \frac{\partial \hat{\eta}}{\partial T} - \frac{1}{T} \rho \frac{\partial \hat{e}}{\partial T} \right] \dot{T} \\ + \left[\rho \frac{\partial \hat{\eta}}{\partial g_m} - \frac{1}{T} \rho \frac{\partial \hat{e}}{\partial g_m} \right] \dot{g}_m + \dots \end{aligned} \quad (2.15)$$

$$\dots + \left[\rho \frac{\partial \hat{\eta}}{\partial \alpha_\gamma} - \frac{1}{T} \rho \frac{\partial \hat{E}}{\partial \alpha_\gamma} \right] \dot{\alpha}_\gamma - \frac{\hat{q}_k \dot{q}_k}{T^2} \geq 0$$

where the evolution equation (2.6) is accounted for.

For an arbitrary admissible thermodynamic process, characterized by an arbitrary choice of the smooth functions $u_k(x_m, t)$, $T(x_m, t)$ and $\alpha_\gamma(x_m)$, the elements of the two sets

$$\overline{\mathcal{T}} = \{ e_{mn} = e_{nm}, T, g_m = \bar{t}_{,m}, \alpha_\gamma \} \quad (2.16)$$

$$\overline{\mathcal{R}} = \{ \dot{e}_{mn} = \dot{e}_{nm}, \dot{T}, \dot{g}_m = \dot{\bar{t}}_{,m} \} \quad (2.17)$$

may take locally (i.e. for a material point) arbitrary values independent of each other at any time. For example, there may be two admissible processes leading locally to the same set $\overline{\mathcal{T}}$ but having different rates $\overline{\mathcal{R}}_1$ and $\overline{\mathcal{R}}_2$. If the constitutive functions $\hat{\eta}$, \hat{E} , $\hat{t}_{kl} = \hat{t}_{lk}$ and \hat{q}_k could indeed be chosen at will without restrictions, then the inequality (2.15) would represent a constraint on the two sets $\overline{\mathcal{T}}$ and $\overline{\mathcal{R}}$, i.e. on the thermodynamic process (compare Paglietti [13]). This is not acceptable and therefore the inequality should identically be satisfied in the constitutive functions for all processes, i.e. for all sets $\overline{\mathcal{T}}$ and $\overline{\mathcal{R}}$.

It is important to note, that the rates \dot{e}_{mn} etc. occur only linearly in the inequality. Since the set $\overline{\mathcal{R}}$ is independent of $\overline{\mathcal{T}}$ and arbitrary, the coefficients of the rates $\overline{\mathcal{R}}$ in equ. (2.15) must vanish identically for all sets $\overline{\mathcal{T}}$, since otherwise a violation of the inequality would be possible. This yields the following constitutive restrictions

$$\left. \rho \frac{1}{2} \left(\frac{\partial \hat{\eta}}{\partial e_{mn}} + \frac{\partial \hat{\eta}}{\partial e_{nm}} \right) - \frac{1}{T} \rho \frac{1}{2} \left(\frac{\partial \hat{E}}{\partial e_{mn}} + \frac{\partial \hat{E}}{\partial e_{nm}} \right) + \frac{1}{T} \hat{t}_{mn} = 0 \right\}$$

$$\left. \begin{aligned} \frac{\partial \hat{\eta}}{\partial T} - \frac{1}{T} \frac{\partial \hat{E}}{\partial T} &= 0 \\ \frac{\partial \hat{\eta}}{\partial g_m} - \frac{1}{T} \frac{\partial \hat{E}}{\partial g_m} &= 0 \end{aligned} \right\} (2.18)$$

and the residual entropy inequality

$$\rho \left(\frac{\partial \hat{\eta}}{\partial \alpha_\gamma} - \frac{1}{T} \frac{\partial \hat{E}}{\partial \alpha_\gamma} \right) \dot{\alpha}_\gamma - \frac{\hat{g}_k \dot{g}_k}{T^2} \geq 0. \quad (2.19)$$

The first equation is obtained by observing that only six components of the strain rate tensor \dot{e}_{mn} can be varied independently and that \dot{e}_{mn} is symmetric.

This result can be put in a more compact form by introducing the free energy function (Helmholtz function)

$$\hat{\psi} := \hat{E} - T \hat{\eta} \quad (2.20)$$

where $\hat{\psi}$ is a function of the variables $\hat{\pi}$. Thus

$$\left. \begin{aligned} \frac{\partial \hat{E}}{\partial e_{mn}} &= \frac{\partial \hat{\psi}}{\partial e_{mn}} + T \frac{\partial \hat{\eta}}{\partial e_{mn}} \\ \frac{\partial \hat{E}}{\partial T} &= \frac{\partial \hat{\psi}}{\partial T} + \hat{\eta} + T \frac{\partial \hat{\eta}}{\partial T} \\ \frac{\partial \hat{E}}{\partial \alpha_\gamma} &= \frac{\partial \hat{\psi}}{\partial \alpha_\gamma} + T \frac{\partial \hat{\eta}}{\partial \alpha_\gamma} \end{aligned} \right\} (2.21)$$

Introducing this in (2.18) gives finally

$$\rho \frac{1}{2} \left(\frac{\partial \hat{\psi}}{\partial e_{mn}} + \frac{\partial \hat{\psi}}{\partial e_{nm}} \right) = \hat{t}_{mn}$$

$$\left. \begin{aligned} \frac{\partial \hat{\psi}}{\partial T} &= -\hat{\eta} \\ \frac{\partial \hat{\psi}}{\partial g_m} &= 0 \end{aligned} \right\} (2.22)$$

and the residual entropy inequality

$$\left. \begin{aligned} -s \frac{\partial \hat{\psi}}{\partial \alpha_y} \hat{f}_y - \frac{\hat{q}_k \hat{q}_k}{T^2} &\geq 0 \\ \text{or} \\ s \frac{\partial \hat{\psi}}{\partial \alpha_y} \hat{f}_y + \frac{\hat{q}_k \hat{q}_k}{T^2} &\leq 0 \end{aligned} \right\} (2.23)$$

With (2.20) and (2.22)₂ one notes that also

$$\hat{\epsilon} = \hat{\psi} - T \frac{\partial \hat{\psi}}{\partial T} . \quad (2.24)$$

One concludes that the free energy $\hat{\psi}$ is independent of the temperature gradient g_m and so are $\hat{\eta}$, $\hat{\epsilon}$ and \hat{t}_{kl} . Equ. (2.22) and (2.24) show that the constitutive equations for the stress, entropy and internal energy follow from the free energy function and cannot be chosen independently. These results are well known.

It is obvious that the evaluation of the Clausius-Duhem entropy inequality does not end here: The residual entropy inequality imposes restrictions on the evolution functions \hat{f}_y and the heat flux vector \hat{q}_k and likely there exists a relation between $\partial \hat{\psi} / \partial \alpha_y$ and \hat{f}_y . This requires further analysis which is not part of this study.

3. An Alternative Derivation of Constitutive Restrictions

3.1 General Remarks

It has already been noted in section 1 and it is demonstrated in section 2 that the Coleman-Noll argumentation is based, among others, on the assumption that body forces and heat supply are at our disposal and thus may be modulated at will. This has been heavily criticized by Woods for physical reasons (see section 1).

It is felt that the arbitrary choice of initial and boundary conditions is sufficiently rich to induce a large variety of processes in the body even for a fixed, prescribed body force and heat supply. In the following analysis it will be shown how the Clausius-Duhem entropy inequality is to be evaluated to give constitutive restrictions if only the initial and boundary conditions are allowed to take arbitrary values. However, it should be observed that these conditions must be consistent with the partial differential equations to give a unique solution.

This approach is based on the work of Müller [25-28] and Liu [29] who applied a similar argument to an extended form of the Clausius-Duhem entropy inequality and to a rather different set of constitutive relations; Müller assumes that the entropy flux is not given by q_h/T but by a constitutive equations in its own right. Also the concept of absolute temperature is dismissed. The independent variables in the constitutive relations are e.g. the deformation gradient (or strain), the (empirical) temperature, the temperature gradient and additionally the rate of temperature. Within this frame an admissible thermodynamic process may be characterized by a pure initial value problem. If the initial values and the constitutive functions are analytic* then using the Cauchy-Kowalewski theorem [30-31] it can be shown that a unique analytic solution exists.

Since some of these basic assumptions are not relevant for the problem tackled in the present study one cannot simply refer to the results of Müller and Liu; a step by step approach is necessary.

3.2 The Rigid Heat Conductor without Internal Variables

To simplify the discussion a rigid heat conductor without internal variables is

* A real function $f(x_s)$ of several variables $x_s, s = 0, 1, \dots, n$ is called analytic in the neighbourhood of a point \tilde{x}_s if $f(x_s)$ can be represented there by a convergent power series.

considered first. In the general three-dimensional case the governing equations are

Assumed constitutive relations*

$$\left. \begin{aligned} \epsilon &= \hat{\epsilon}(T, g_m, x_k) \\ \eta &= \hat{\eta}(T, g_m, x_k) \\ g_k &= \hat{g}_k(T, g_m, x_k) \end{aligned} \right\} (3.1)$$

where

$$g_m := \frac{\partial T}{\partial x_m} = T_{,m} \quad (3.2)$$

Balance of energy

$$\rho \frac{\partial \hat{\epsilon}}{\partial T} \dot{T} + \rho \frac{\partial \hat{\epsilon}}{\partial g_m} \dot{g}_m + \frac{\partial \hat{g}_k}{\partial T} g_k + \frac{\partial \hat{g}_k}{\partial g_m} g_{m,k} + \frac{\partial \hat{g}_k}{\partial x_k} - \rho r = 0 \quad (3.3)$$

and the Clausius-Duhem entropy inequality

$$\begin{aligned} &\rho \frac{\partial \hat{\eta}}{\partial T} \dot{T} + \rho \frac{\partial \hat{\eta}}{\partial g_m} \dot{g}_m + \frac{1}{T} \left(\frac{\partial \hat{g}_k}{\partial T} g_k + \frac{\partial \hat{g}_k}{\partial g_m} g_{m,k} + \frac{\partial \hat{g}_k}{\partial x_k} \right) \\ &- \frac{1}{T^2} g_k g_k - \frac{\rho r}{T} \geq 0 \end{aligned} \quad (3.4)$$

* The assumed explicit dependence on the material coordinates x_k allows for inhomogeneous material response.

It is fairly simple to show that the evaluation of the entropy inequality on the basis of the Coleman-Noll argument yields the following restrictions on the constitutive relations (compare with (2.22)): With

$$\hat{\psi} := \hat{\epsilon} - T \hat{\eta} \quad (3.5)$$

one obtains

$$\left. \begin{aligned} \frac{\partial \hat{\psi}}{\partial T} &= - \hat{\eta} \\ \frac{\partial \hat{\psi}}{\partial g_m} &= 0 \\ \hat{\epsilon} &= \hat{\psi} - T \frac{\partial \hat{\psi}}{\partial T} \end{aligned} \right\} (3.6)$$

and the residual inequality

$$\frac{1}{T^2} \hat{q}_k q_k \leq 0. \quad (3.7)$$

It is obvious that the free energy and thus the entropy and the internal energy are independent of the temperature gradient.

In the following it is intended to proof that the same restrictions are obtained by allowing the initial- and boundary conditions to assume arbitrary values but without modulation of the heat supply; thus \mathcal{T} is fixed in the further analysis. For the sake of simplicity a one-dimensional homogeneous heat conductor is treated first.

3.2.1 The One-Dimensional Rigid Heat Conductor

3.2.1.1 The Initial-Boundary Value Problem and the Initial Temperature Rate

The assumed constitutive relations for the homogeneous heat conductor are

$$\epsilon = \hat{\epsilon}(T, q)$$

$$\eta = \hat{\eta}(T, q)$$

$$q = \hat{q}(T, q)$$

} (3.8)

with

$$q := \frac{\partial T}{\partial x} .$$

(3.9)

The balance of energy reads

$$\rho \frac{\partial \hat{\epsilon}}{\partial T} \dot{T} + \rho \frac{\partial \hat{\epsilon}}{\partial q} \dot{q} + \frac{\partial \hat{q}}{\partial T} q + \frac{\partial \hat{q}}{\partial q} \frac{\partial q}{\partial x} - \rho r = 0 \quad (3.10)$$

or with (3.9)

$$a \frac{\partial^2 T}{\partial x^2} + b \frac{\partial^2 T}{\partial x \partial t} + d = 0 \quad (3.11)$$

where a , b and d are functions of T , $\partial T / \partial x$ and $\partial T / \partial t$:

$$a = \frac{\partial \hat{q}}{\partial q}$$

$$b = \rho \frac{\partial \hat{\epsilon}}{\partial q}$$

$$d = \rho \frac{\partial \hat{\epsilon}}{\partial T} \dot{T} + \frac{\partial \hat{q}}{\partial T} q - \rho r$$

} (3.12)

This is a special form* of the general quasilinear P.D.E. of second order

$$a \frac{\partial^2 T}{\partial x^2} + b \frac{\partial^2 T}{\partial x \partial t} + c \frac{\partial^2 T}{\partial t^2} + d = 0 \quad (3.13)$$

whose characteristic condition is given by

$$\Delta = \begin{vmatrix} a & b & c \\ x' & t' & 0 \\ 0 & x' & t' \end{vmatrix} = a \cdot (t')^2 - b x' t' + c \cdot (x')^2 \quad (3.14)$$

$$x' = \frac{dx}{d\lambda} \quad , \quad t' = \frac{dt}{d\lambda} \quad ; \quad (3.15)$$

here λ is a parameter along a characteristic curve given by the parameter representation

$$x = x(\lambda) \quad , \quad t = t(\lambda) \quad . \quad (3.16)$$

With

$$\frac{t'}{x'} = \frac{dt}{dx} \quad (3.17)$$

the characteristic condition reads

$$a \left(\frac{dt}{dx} \right)^2 - b \frac{dt}{dx} + c = 0 \quad (3.18)$$

* It is noted that by introducing a suitable coordinate transformation $\xi = \hat{\xi}(x, t)$
 $\tau = \hat{\tau}(x, t)$ one may transform (3.11) to obtain a quasilinear P.D.E. of the general form
 (3.13).

and thus

$$\frac{dt}{dx} = \frac{b}{2a} \pm \frac{1}{2a} \sqrt{b^2 - 4ac}. \quad (3.19)$$

If two real solutions exist, i.e. if

$$b^2 - 4ac > 0, \quad (3.20)$$

then the P.D.E. is of hyperbolic type. Since $c \neq 0$, two real characteristic curves exist given by

$$\left(\frac{dt}{dx}\right)_1 = 0, \quad \left(\frac{dt}{dx}\right)_2 = \frac{b}{a}. \quad (3.21)$$

Thus, the first set of characteristic curves are parallels to the x-axes in the (x,t)-plane and the second set are curved lines which are not predetermined but depend on the solution $T(x,t)$.

Usually two types of initial value problems may be prescribed for a hyperbolic P.D.E. [30-33]:

(a) Cauchy problems

A Cauchy problem for a general hyperbolic P.D.E. is characterized by prescribing T and $\partial T / \partial n$ along on open non-characteristic curve Γ^* in the (x,t)-plane; here $(\partial / \partial n)$ is the derivative along the normal of Γ .

(b) Darboux problems (characteristic initial value problems)

A characteristic initial value problem is defined by prescribing T along two intersecting characteristics.

From the theory of P.D.E. it is known that these problems admit a unique solution [30].

For the hyperbolic heat conduction problem equ. (3.11) neither (a) nor (b) appears to be physically reasonable: For physical reasons part of the initial condition is characterized by prescribing T along the x-axes at $t=0$, e.g.

$$T(x,0) = T_0(x), \quad 0 \leq x.$$

* This curve is not allowed to intersect twice any characteristic

However, the x -axis is a characteristic curve and therefore the Cauchy problem is not applicable here.

On the other hand, additional prescription of the temperature along the characteristic (3.21)₂ is conceptually not impossible but physically rather complex.

A more reasonable situation is an initial-boundary value problem, e.g. the initial condition is assumed as above and the temperature is given as a function of time at $x=0$. Thus

$$\left. \begin{aligned} T(x, 0) &= \bar{T}(x) & 0 \leq x & & \text{initial condition} \\ T(0, t) &= \tilde{T}(t) & 0 \leq t & & \text{boundary condition} \end{aligned} \right\} (3.22)$$

with

$$\bar{T}(0) = \tilde{T}(0). \quad (3.23)$$

This situation is related to a Goursat problem [32]. In the further analysis existence of a solution of the above initial-boundary value problem is implied.

In the following a procedure is indicated which allows to calculate the initial temperature rate

$$y(x) := \left(\frac{\partial T}{\partial t} \right)_{t=0} \quad (3.24)$$

at any point in the regime $0 \leq x$ on the basis of the differential equation (3.10) and the initial and boundary conditions (3.22). Further, it is indicated that higher derivatives $(\partial^2 T / \partial t^2)_{t=0}$, $(\partial^3 T / \partial t^3)_{t=0}$ etc. may be obtained too.

Observing the definition (3.24) and the initial condition (3.22)₁ the energy balance equation (3.10) at $t=0$ reduces to the following linear ordinary differential equation for the temperature rate $y(x)$

$$A \frac{dy}{dx} + B y = C, \quad 0 \leq x \quad (3.25)$$

where A, B, C are given functions of x :

$$\begin{aligned}
 A &= \rho \left(\frac{\partial \hat{E}}{\partial q} \right)_{t=0} \\
 B &= \rho \left(\frac{\partial \hat{E}}{\partial T} \right)_{t=0} \\
 C &= (\rho \tau)_{t=0} - \left(\frac{\partial \hat{q}}{\partial T} \frac{\partial T}{\partial x} + \frac{\partial \hat{q}}{\partial q} \frac{\partial q}{\partial x} \right)_{t=0}
 \end{aligned}
 \left. \begin{array}{l}
 \text{functions of} \\
 T_0, dT_0/dx \\
 \\
 \text{functions of} \\
 x, T_0, dT_0/dx, \\
 d^2T_0/dx^2
 \end{array} \right\} (3.26)$$

In general terms the solution of (3.25) may be written as

$$y(x) = \exp\left(-\int_0^x \beta d\xi\right) \left[\alpha + \int_0^x \gamma \exp\left(\int_0^\xi \beta d\tau\right) d\xi \right] \quad (3.27)$$

with

$$\beta := \frac{B}{A}, \quad \gamma := \frac{C}{A} \quad (3.28)$$

and where α is an integration constant. Therefore a unique solution for $y(x)$ is obtained if the temperature rate $y(x)$ is prescribed at a single position $x = x_0$. This requirement is derived from the boundary condition at $x_0 = 0$:

$$\left(\frac{y}{x} \right)_{x=x_0=0} = \left(\frac{dT}{dt} \right)_{t=0} \quad (3.29)$$

Consequently

$$\alpha = \left(\frac{dT}{dt} \right)_{t=0} \quad (3.30)$$

The higher time derivatives of the temperature at $t=0$ are determined as follows. The partial derivatives of the energy balance equation (3.10) with respect to time reads

$$\rho \frac{\partial \hat{E}}{\partial T} \ddot{T} + \rho \frac{\partial \hat{E}}{\partial q} \ddot{q} = \ddot{C}' \quad (3.31)$$

where

$$\begin{aligned}
 \tilde{C}' = & \mathcal{F} \dot{T} - \left(\frac{\partial \mathcal{F}}{\partial T} \dot{q} + \frac{\partial \mathcal{F}}{\partial q} \dot{q}_{,x} \right) \\
 & - \mathcal{F} \left(\frac{\partial^2 \mathcal{E}}{\partial T^2} \dot{T} + \frac{\partial^2 \mathcal{E}}{\partial T \partial \mathcal{F}} \dot{q} \right) \dot{T} \\
 & - \mathcal{F} \left(\frac{\partial^2 \mathcal{E}}{\partial \mathcal{F} \partial T} \dot{T} + \frac{\partial^2 \mathcal{E}}{\partial \mathcal{F}^2} \dot{q} \right) \dot{q} \\
 & - \left(\frac{\partial^2 \mathcal{F}}{\partial T^2} \dot{T} + \frac{\partial^2 \mathcal{F}}{\partial T \partial q} \dot{q} \right) \mathcal{F} - \left(\frac{\partial^2 \mathcal{F}}{\partial \mathcal{F} \partial T} \dot{T} + \frac{\partial^2 \mathcal{F}}{\partial \mathcal{F}^2} \dot{q} \right) \mathcal{F}_{,x}.
 \end{aligned} \tag{3.32}$$

Introducing the definition

$$\mathcal{Y}'(x) := \left(\frac{\partial^2 T}{\partial t^2} \right)_{t=0}, \tag{3.33}$$

equation (3.31) at $t=0$ simplifies to an ordinary differential equation which has the same structure as equation (3.25):

$$A \frac{d\mathcal{Y}'}{dx} + B \mathcal{Y}' = C' \tag{3.34}$$

where A and B are defined as above and

$$C' = (\tilde{C}')_{t=0}. \tag{3.35}$$

Note that again A, B and C' are known functions which can be determined from the initial and boundary conditions and the solution equ. (3.27). The general solution of (3.34) has the same form as (3.27) except that \mathcal{Y} has to be exchanged by

$$\mathcal{Y}' = \frac{C'}{A} \tag{3.36}$$

and the integration constant is α' . But α' is obtained from the boundary condition (3.22)₂ by differentiation

$$(\mathcal{Y}')_{x=0} = \left(\frac{d^2 \tilde{T}}{dt^2} \right)_{t=0}. \tag{3.37}$$

In an analogous way the time derivatives of the temperature at $t=0$ may be determined up to any order. Thus, it is evident that the initial and boundary conditions (3.22) as well as the differential equation (3.10) are sufficient to determine the first, the second and all higher time derivatives of the temperature at $t=0$ for every point in the regime $0 \leq x^*$. This process of successive determination of the initial derivatives can be continued without limitation if the differential equation and initial and boundary conditions are analytic. Therefore, if the solution $T(x,t)$ can be expanded in a convergent Taylor series at $t=0$ for every point $0 \leq x^*$, the series coefficients are uniquely determined and thus the solution $T(x,t)$ is unique.

3.2.1.2 Evaluation of the Clausius-Duhem Entropy Inequality

In the one-dimensional case the entropy inequality (3.4) reduces to

$$\rho \frac{\partial \eta}{\partial T} \dot{T} + \rho \frac{\partial \eta}{\partial g} \dot{g} + \frac{1}{T} \left(\frac{\partial \eta}{\partial T} g + \frac{\partial \eta}{\partial g} g_{,x} \right) - \frac{1}{T^2} g g - \frac{sr}{T} \geq 0. \quad (3.38)$$

An admissible thermodynamic process is equivalent to a solution of the initial-boundary value problem for the temperature. However, such a solution is not at hand. But in the neighbourhood of the initial time $t=0$ complete information about $T(x,t)$ is available, if $T(x,t)$ can be represented by a convergent Taylor series close to $t=0$ at any point $0 \leq x^*$. Therefore, the entropy inequality is evaluated at $t=0$ for any material point $0 \leq x^*$.

If the constitutive equations (3.8) are assumed to be known then the entropy inequality at some material point $x^* = \check{x}$ may be viewed as an inequality relating the quantities

$$\Pi = \left\{ T, g = \frac{\partial T}{\partial x} \right\}_{x^* = \check{x}} \quad (3.39)$$

and

$$\mathcal{R} = \left\{ \dot{T} = \frac{\partial T}{\partial t}, \quad \dot{g} = \frac{\partial^2 T}{\partial x \partial t}, \quad g_{,x} = \frac{\partial^2 T}{\partial x^2} \right\}_{x=\tilde{x}} \quad (3.40)$$

as well as the prescribed heat supply r . Similarly the local energy balance equation (3.10) at $x=\tilde{x}$ is considered as an equation relating the sets \mathcal{R} and \mathcal{T} as well as r . It is important to note that the elements of \mathcal{R} occur linearly in the entropy inequality and in the energy balance equation. But the elements of \mathcal{T} are non-linearly involved in both relations. At $t=0$ the quantities \mathcal{R} and \mathcal{T} assume the following values:

$$\mathcal{R}_0 = \left\{ \begin{aligned} (\dot{T})_0 &= \dot{y}(x) \\ (\dot{g})_0 &= \frac{d\dot{y}(x)}{dx} \\ (g_{,x})_0 &= \frac{d^2 T_0(x)}{dx^2} \end{aligned} \right\} \quad \mathcal{T}_0 = \left\{ \begin{aligned} (T)_0 &= T_0(x) \\ (g)_0 &= \frac{dT_0(x)}{dx} \end{aligned} \right\}. \quad (3.41)$$

Recalling now that the initial temperature distribution $T_0(x)$ may be chosen at will, one concludes that at a point $x=\tilde{x}$ the quantities

$$\mathcal{U}_0 = \left\{ T_0(\tilde{x}), \quad \left(\frac{dT_0(x)}{dx} \right)_{\tilde{x}}, \quad \left(\frac{d^2 T_0(x)}{dx^2} \right)_{\tilde{x}} \right\} \quad (3.42)$$

may take arbitrary values locally. However, the initial temperature rate \dot{y} and its derivative $d\dot{y}/dx$ are not independent locally but are related to each other and to the set \mathcal{U}_0 via the local energy balance equation at $t=0$, i.e. equ. (3.25). Similarly the temperature rate \dot{T} and its derivative $\dot{g} = \partial \dot{T} / \partial x$ are related by equ. (3.10) at later times. This interdependence of \dot{T} and \dot{g} due to the energy balance equation may be accounted for by expressing \dot{g} in terms of \dot{T} , or \dot{T} in terms of \dot{g} , as well as the other elements of the sets \mathcal{R} and \mathcal{T} and the heat supply r . Here \dot{T} is expressed in terms of \dot{g} . This is motivated by the fact that in the two- and three-dimensional heat conduction problem the temperature

rate is related to more than just one of its spatial gradients via the energy balance equation; thus, \dot{T} may be expressed by its gradients but not conversely.

Consequently, equation (3.10) yields

$$\dot{T} = \frac{1}{s \frac{\partial \epsilon}{\partial T}} \left\{ s r - s \frac{\partial \epsilon}{\partial g} \dot{g} - \frac{\partial q}{\partial T} q - \frac{\partial q}{\partial g} q_{,x} \right\}. \quad (3.43)$$

Inserting this result into the entropy inequality (3.38) and rearranging gives

$$\begin{aligned} & \left(s \frac{\partial \eta}{\partial g} - s \frac{\partial \eta / \partial T}{\partial \epsilon / \partial T} \frac{\partial \epsilon}{\partial g} \right) \dot{g} \\ & + \left(\frac{1}{T} - \frac{\partial \eta / \partial T}{\partial \epsilon / \partial T} \right) \frac{\partial q}{\partial g} q_{,x} \\ & + \left(\frac{1}{T} - \frac{\partial \eta / \partial T}{\partial \epsilon / \partial T} \right) \frac{\partial q}{\partial T} q \\ & - \left(\frac{1}{T} - \frac{\partial \eta / \partial T}{\partial \epsilon / \partial T} \right) s r - \frac{1}{T^2} q q \geq 0. \end{aligned} \quad (3.44)$$

Especially at $t=0$ this reduces to

$$\begin{aligned} & s \left(\frac{\partial \eta}{\partial g} - \frac{\partial \eta / \partial T}{\partial \epsilon / \partial T} \frac{\partial \epsilon}{\partial g} \right)_{t=0} \frac{d\gamma}{dx} \\ & + \left(\frac{1}{T} - \frac{\partial \eta / \partial T}{\partial \epsilon / \partial T} \right)_{t=0} \left(\frac{\partial q}{\partial g} \right)_{t=0} \frac{d^2 T_0}{dx^2} \\ & + \left(\frac{1}{T} - \frac{\partial \eta / \partial T}{\partial \epsilon / \partial T} \right)_{t=0} \left(\frac{\partial q}{\partial T} q \right)_{t=0} \\ & - s \left(\frac{1}{T} - \frac{\partial \eta / \partial T}{\partial \epsilon / \partial T} \right)_{t=0} (r)_{t=0} - \left(\frac{q q}{T^2} \right)_{t=0} \geq 0 \end{aligned} \quad (3.45)$$

where $\frac{dy}{dx}$ may be obtained from the solution (3.27) or the differential equation (3.25); one obtains

$$\frac{dy}{dx} = \gamma - \beta \dot{\gamma}. \quad (3.46)$$

It should be observed that except $(\pi)_{t=0}$ all terms in brackets in equ. (3.45) are functions of only T_0 and dT_0/dx . The same is true for the functions β and γ . Thus, dy/dx and d^2T_0/dx^2 occur linearly in the entropy inequality.

If one chooses $x = \bar{x} = 0$ then (3.46) reduces to the simple relation

$$\left(\frac{dy}{dx}\right)_{x=0} = \left(\gamma(T_0, \frac{dT_0}{dx})\right)_{x=0} - \left(\beta(T_0, \frac{dT_0}{dx})\right)_{x=0} (\dot{\bar{T}})_{t=0}. \quad (3.47)$$

Thus, for a fixed prescribed initial temperature distribution $T_0(x)$ the derivative dy/dx at $x=0$ may take any value since the boundary value $\bar{T}(t)$ at $x=0$ and hence $\dot{\bar{T}}$ may be manipulated at will and independently of $T_0(x)$, except for (3.23).

Consequently, in the entropy inequality (3.45) taken at $x=0$ the quantities

$$\left\{ \frac{dy}{dx}, \frac{d^2T_0}{dx^2} \right\} \quad \text{at } x=0 \quad (3.48)$$

and

$$\mathbb{T}_0 = \left\{ T_0, \frac{dT_0}{dx} \right\} \quad \text{at } x=0 \quad (3.49)$$

may take any value independently of each other.

Since the quantities (3.48) are linearly involved in (3.45) and the entropy inequality should not be violated for any choice of (3.48), the coefficients of dy/dx and d^2T_0/dx^2 must vanish, i.e.

$$\left. \begin{aligned} \left(\frac{\partial \hat{\eta}}{\partial \dot{\gamma}} - \frac{\partial \hat{\eta}/\partial T}{\partial \hat{E}/\partial T} \frac{\partial \hat{E}}{\partial \dot{\gamma}} \right)_{\substack{t=0 \\ x=0}} &= 0 \\ \left(\frac{1}{T} - \frac{\partial \hat{\eta}/\partial T}{\partial \hat{E}/\partial T} \right)_{\substack{t=0 \\ x=0}} \left(\frac{\partial \dot{\gamma}}{\partial \dot{\gamma}} \right)_{\substack{t=0 \\ x=0}} &= 0. \end{aligned} \right\} \quad (3.50)$$

Since it is assumed that

$$\frac{\partial \hat{\eta}}{\partial g} \neq 0 \quad (3.51)$$

equ. (3.50)₂ yields

$$\left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right)_{\substack{t=0 \\ x=0}} = 0. \quad (3.52)$$

Therefore (3.50)₁ simplifies to

$$\left(\frac{\partial \hat{\eta}}{\partial g} - \frac{1}{T} \frac{\partial \hat{E}}{\partial g} \right)_{\substack{t=0 \\ x=0}} = 0. \quad (3.53)$$

If one assumes that the two constitutive functions \hat{E} and $\hat{\eta}$ could be chosen at will, then (3.52) and (3.53) would represent two conditions on T_0 and dT_0/dx at $x=0$. However, this is in contrast to the basic assumption that the initial condition T_0 as well as dT_0/dx could be chosen at will locally. Therefore, the two conditions (3.52) and (3.53) are to be interpreted as restrictions on the constitutive functions \hat{E} and $\hat{\eta}$: They are required to satisfy (3.52) and (3.53) identically.

Introducing the free energy function

$$\hat{\psi} = \hat{E} - T\hat{\eta} = \hat{\psi}(T, g) \quad (3.54)$$

such that

$$\left. \begin{aligned} \frac{\partial \hat{\psi}}{\partial T} &= \frac{\partial \hat{E}}{\partial T} - T \frac{\partial \hat{\eta}}{\partial T} - \hat{\eta} \\ \frac{\partial \hat{\psi}}{\partial g} &= \frac{\partial \hat{E}}{\partial g} - T \frac{\partial \hat{\eta}}{\partial g} \end{aligned} \right\} (3.55)$$

then (3.53) yields

$$\left(\frac{\partial \hat{\psi}}{\partial g} \right)_{\substack{t=0 \\ x=0}} = 0. \quad (3.56)$$

and from (3.52) one obtains

$$\left(\frac{\partial \hat{\psi}}{\partial T} + \hat{\eta} \right)_{\substack{t=0 \\ x=0}} = 0. \quad (3.57)$$

Equ. (3.56) and (3.57) are restrictions on the functions $\hat{\psi}$ and $\hat{\eta}$ at $t=0$ and $x=0$. Since the constitutive functions are not assumed to depend on time and position explicitly, these restrictions are generally valid, i.e.

$$\frac{\partial \hat{\psi}}{\partial g} = 0, \quad \frac{\partial \hat{\psi}}{\partial T} = -\hat{\eta} \quad (3.58)$$

and the internal energy is restricted by

$$\hat{E} = \hat{\psi} + T \frac{\partial \hat{\psi}}{\partial T}. \quad (3.59)$$

With the result (3.52) two other terms in the entropy inequality (3.45) vanish identically, especially the term involving the heat supply, and (3.45) reduces to the residual entropy inequality

$$-(qg)_{\substack{t=0 \\ x=0}} \geq 0$$

and generally

$$-qg \geq 0. \quad (3.60)$$

The results (3.58) and (3.59) show that the free energy, entropy and internal energy do not depend on the temperature gradient. As a consequence the function b in the energy balance equation (3.11) vanishes identically. Thus, equation (3.11) is required to be parabolic with a single characteristic curve (compare (3.14) and (3.15))

$$\frac{dt}{dx} = t' = 0$$

passing through a point in the (x, t) -plane.

Further, the differential equation (3.25) for the initial temperature rate $y(x)$ degenerates to a linear algebraic equation for y , since according to (3.26)₁

$$A \equiv 0.$$

Therefore, the prescription of the temperature history at a point $x = \tilde{x} = 0$ is not required any more to obtain a unique solution of (3.25). Also for a solution of (3.11) the boundary condition (3.22) is not required if initial condition (3.22)₁ is given.

3.2.2 The Two- and Three-Dimensional Heat Conductor

3.2.2.1 The Initial-Boundary Value Problem for the Two-Dimensional Case and the Initial Temperature Rate

The constitutive relations for an inhomogeneous heat conductor are assumed to be given by

$$\left. \begin{aligned} \epsilon &= \hat{\epsilon}(T, q_\beta, x_\gamma) \\ \eta &= \hat{\eta}(T, q_\beta, x_\gamma) \\ q_\alpha &= \hat{q}_\alpha(T, q_\beta, x_\gamma), \quad \alpha, \beta, \gamma = 1, 2 \end{aligned} \right\} (3.61)$$

where

$$q_\beta := \frac{\partial T}{\partial x_\beta}. \quad (3.62)$$

The energy balance equation reads

$$\rho \frac{\partial \hat{\epsilon}}{\partial T} \dot{T} + \rho \frac{\partial \hat{\epsilon}}{\partial q_\beta} \dot{q}_\beta + \frac{\partial \hat{q}_\beta}{\partial T} q_\beta + \frac{\partial \hat{q}_\alpha}{\partial q_\beta} q_{\beta, \alpha} + \frac{\partial \hat{q}_\alpha}{\partial x_\alpha} - \rho r = 0 \quad (3.63)$$

Analogous to the discussion in section 3.2.1.1 an initial-boundary value problem is considered. The initial temperature is prescribed in a simply connected region \mathcal{B} of the (x_1, x_2) -plane:

$$T(x_\alpha, 0) = \bar{T}(x_\alpha) \quad \text{in } \mathcal{B}. \quad (3.64)$$

Along its open boundary \mathcal{R}_0 , defined by the parameter representation

$$x_\alpha = x_\alpha^*(\xi), \quad \alpha = 1, 2 \quad (3.65)$$

the temperature is assumed to be a given function of time, i.e.

$$T(x_\alpha^*, t) = \tilde{T}(f, t) \quad (3.66)$$

such that

$$\tilde{T}(f, 0) = T_0(x_\alpha^*). \quad (3.67)$$

From (3.64) the initial temperature gradient is found to be

$$(g_\alpha)_{t=0} = \frac{\partial T_0}{\partial x_\alpha}.$$

Introducing the abbreviation (3.24) for the initial temperature rate $(\dot{T})_{t=0}$ the energy balance at $t=0$ is written as

$$A_\alpha \gamma_{,\alpha} + B \gamma = C \quad (3.68)$$

with

$$\left. \begin{aligned} A_\alpha &= s \left(\frac{\partial \hat{E}}{\partial g_\alpha} \right)_{t=0} \\ B &= s \left(\frac{\partial \hat{E}}{\partial T} \right)_{t=0} \\ C &= s(r)_{t=0} - \left(\frac{\partial \hat{q}_\mu}{\partial T} g_\alpha + \frac{\partial \hat{q}_\alpha}{\partial g_\beta} g_{\beta,\alpha} + \frac{\partial \hat{q}_\alpha}{\partial x_\alpha} \right)_{t=0}. \end{aligned} \right\} (3.69)$$

Since the constitutive functions (3.61) depend* only on the temperature and its gradients, the right hand side of (3.69) is determined by the initial condition (3.64).

Equation (3.68) represents a linear first order P.D.E. for the initial temperature rate γ with two independent variables x_1 and x_2 . In contrast to the one-dimensional case an integral representation of the solution is not readily obtained. The functions $A_\alpha, \alpha=1,2$ and $(C-B\gamma)$ define a field of vectors in the

* The dependence on the material point is of no consequence in this context.

(x_1, x_2, y) -space, i.e. the characteristic directions which are tangential to the integral surface $y(x_1, x_2)$ - the solution of the linear P.D.E. (3.68) [30, 33]. With the field of directions, characterized by the direction numbers $(A_1, A_2, C - By)$ a family of characteristic curves is associated, which at each point are tangent to the direction field. Thus, for any characteristic curve the relation

$$\frac{dx_1}{A_1} = \frac{dx_2}{A_2} = \frac{dy}{C - By} \quad (3.70)$$

holds [33]. If s is a parameter along a characteristic curve (e.g. the arc length) and denoting the ratio (3.70) by ds , the condition (3.70) defining the characteristic curves is equivalent to the characteristic system of ordinary differential equations given by

$$\frac{dx_\alpha}{ds} = A_\alpha, \quad \alpha = 1, 2, \quad \frac{dy}{ds} = C - By; \quad (3.71)$$

A_1, A_2, B and C do not explicitly depend on s . According to the theory of systems of O.D.E.'s of 1. order a solution of (3.71) is uniquely determined by prescribed initial values

$$x_1 = x_1^*, \quad x_2 = x_2^*, \quad y = y^* \quad \text{for } s = 0. \quad (3.72)$$

It is noted that the first two equations of (3.71) can be solved independently of the third since A_1 and A_2 do not depend on y . The solution $x_1(s), x_2(s)$ and $y(s)$ represents a spatial curve - a characteristic curve - in the three-dimensional space with coordinates x_1, x_2, y .

It may be proved [30, p. 51] that every integral surface $y(x_1, x_2)$, i.e. solution of (3.69), is generated by a one-parametric set of characteristic curves (Fig. 1) and vice versa. To obtain such a surface it suffices to prescribe the initial value y^* not only at one point in the (x_1, x_2) -plane but along some curve, e.g. the boundary \mathcal{R} given by the parameter representation (3.65). With (3.66) the initial value y^* along the boundary \mathcal{R} is given by

$$y^*(\xi) = \left(\frac{\partial \tilde{T}}{\partial t}(\xi, t) \right)_{t=0} \quad (3.73)$$

on \mathcal{R} : $x_\alpha = x_\alpha^*(\xi), \quad \alpha = 1, 2$

This set of data generates a spatial curve \mathcal{R} in the (x_1, x_2, y) -space (Fig. 1).

The integral surface which goes through \mathcal{R} is constructed as follows. At every point P along the spatial curve \mathcal{R} the characteristic curve \mathcal{C} passing through P is determined by solving the characteristic equations (3.68). Thus a one-parametric set of characteristic curves

$$x_1(s, \xi), \quad x_2(s, \xi), \quad y(s, \xi) \tag{3.74}$$

is obtained. These curves generate a surface $y(x_1, x_2)$ if the first two functions allow to represent the two parameters (s, ξ) in terms of x_1 and x_2 . This is assured at least in the neighbourhood of \mathcal{R} if the differentials ds and $d\xi$ may be expressed in terms of dx_1 and dx_2 . The total differentials of the first two functions (3.74) are given by

$$\left. \begin{aligned} dx_1 &= \frac{\partial x_1}{\partial s} ds + \frac{\partial x_1}{\partial \xi} d\xi \\ dx_2 &= \frac{\partial x_2}{\partial s} ds + \frac{\partial x_2}{\partial \xi} d\xi, \end{aligned} \right\} \tag{3.75}$$

ds and $d\xi$ are uniquely expressed in terms of dx_1 and dx_2 if the coefficient determinant of the linear system of equations (3.75) is nonsingular

$$\Delta := \frac{\partial x_1}{\partial s} \frac{\partial x_2}{\partial \xi} - \frac{\partial x_2}{\partial s} \frac{\partial x_1}{\partial \xi} \neq 0.$$

On the boundary curve \mathcal{R} this condition reduces to

$$\Delta = \overset{*}{A}_1 \frac{dx_2^*}{d\xi} - \overset{*}{A}_2 \frac{dx_1^*}{ds} \neq 0 \tag{3.76}$$

if the characteristic equations (3.71) and the parameter representation of \mathcal{R} equ. (3.65) are observed.

This condition may also be obtained in a somewhat less abstract way.

Assuming that the function $y(s, \xi)$ may be expressed also as a function of x_1 and x_2 one gets (coordinate transformation)

$$\left. \frac{\partial y}{\partial s} = \frac{\partial y}{\partial x_1} \frac{\partial x_1}{\partial s} + \frac{\partial y}{\partial x_2} \frac{\partial x_2}{\partial s} \right\} \tag{3.77}$$

$$\frac{\partial \gamma}{\partial \xi} = \frac{\partial \gamma}{\partial x_1} \frac{\partial x_1}{\partial \xi} + \frac{\partial \gamma}{\partial x_2} \frac{\partial x_2}{\partial \xi} .$$

At the boundary curve equ. (3.77) reduces to

$$\begin{aligned} C^* - B^* \gamma^* &= \left(\frac{\partial \gamma}{\partial x_1} \right)^* A_1^* + \left(\frac{\partial \gamma}{\partial x_2} \right)^* A_2^* \\ \frac{d\gamma^*}{d\xi} &= \left(\frac{\partial \gamma}{\partial x_1} \right)^* \frac{dx_1^*}{d\xi} + \left(\frac{\partial \gamma}{\partial x_2} \right)^* \frac{dx_2^*}{d\xi} ; \end{aligned} \quad (3.78)$$

here A_1^*, A_2^*, B^* and C^* are obtained from (3.69) along the boundary. Equ. (3.78) is a set of linear equations for the two gradients

$$\left(\frac{\partial \gamma}{\partial x_1} \right)^* , \left(\frac{\partial \gamma}{\partial x_2} \right)^* \quad (3.79)$$

which determine the orientation of a surface element of the integral surface along the boundary. If the coefficient determinant is non-vanishing, i.e.

$$\Delta := A_1^* \frac{dx_2^*}{d\xi} - A_2^* \frac{dx_1^*}{d\xi} \neq 0 , \quad (3.80)$$

the gradients (3.79) are uniquely determined at any point along \mathcal{R} in terms of local properties of the initial values γ^* and $d\gamma^*/d\xi$ as well as properties of the boundary curve. Thus, if condition (3.80) is satisfied, the form of the boundary \mathcal{R} , the functions A_1, B, C and $\bar{T}_0(x), \bar{T}(t)$ and their derivatives allow to construct a surface element of the integral surface $\gamma(x_1, x_2)$ at a point along \mathcal{R} .

If the determinant Δ vanishes for every point along the boundary then \mathcal{R} is a characteristic curve and a unique solution $\gamma(x_1, x_2)$ for the initial value (3.73) does not exist [30, p. 54]. Consequently, the condition (3.80) is assumed to be satisfied in the further analysis.

Analogous to section 3.2.1.1 the higher order time derivatives of the temperature at $t=0$, e.g.

$$\gamma'(x_{\alpha}) := \left(\frac{\partial^2 T}{\partial t^2} \right)_{t=0} ,$$

may be obtained by differentiation of the appropriate equations. This is not studied here.

3.2.2.2 The Initial-Boundary Value Problem for the Three-Dimensional Case and the Initial Temperature Rate

The results presented for the two-dimensional case are extended to the three-dimensional one. Here one has to observe that the subscripts in equ. (3.61) to (3.63) take the values $k=1,2,3$. Further, the initial condition for the temperature in a region \mathcal{B} of the (x_1, x_2, x_3) -space is

$$T(x_k, t) = \bar{T}_0(x_k) \quad \text{in } \mathcal{B} \quad \text{at } t=0. \quad (3.81)$$

The boundary condition on the open boundary surface \mathcal{R}_0 , which is defined by the parameter representation*

$$x_k = x_k^*(\xi, \tau), \quad k=1,2,3, \quad (3.82)$$

where ξ and τ are surface coordinates on \mathcal{R}_0 , is given by

$$T(x_k^*, t) = \tilde{T}(\xi, \tau, t) \quad \text{on } \mathcal{R}_0 \quad \text{for all } t. \quad (3.83)$$

The function \tilde{T} is prescribed. On the surface \mathcal{R}_0 the given function $\bar{T}_0(x_k)$ is related to $\tilde{T}(\xi, \tau, t)$ by

$$\bar{T}_0(x_k^*) = \tilde{T}(\xi, \tau, 0). \quad (3.84)$$

The governing partial differential equation for the initial temperature rate

$$Y(x_k) := \left(\frac{\partial T}{\partial t} \right)_{t=0} \quad (3.85)$$

* Different points on \mathcal{R}_0 correspond to different pairs (ξ, τ)

is

$$A_k y_{,k} + B y = C \quad (3.86)$$

where the functions A_k $k=1,2,3$, B and C have the same structure as (3.67) but the subscripts take the values 1 to 3. The quantities A_k and $C - B y$ define a field of vectors in the four-dimensional (x_1, x_2, x_3, y) -space, i.e. the characteristic directions. The associated characteristic "curves" in the (x_1, x_2, x_3, y) -space are defined by the characteristic system of O.D.E.'s

$$\frac{dx_k}{ds} = A_k \quad k=1,2,3 \quad \frac{dy}{ds} = C - B y . \quad (3.87)$$

The projections of these curves in the three-dimensional (x_1, x_2, x_3) -space are given by the solution of the first three differential equations (3.87). Since the functions A_k do not depend on y , the characteristic projections may be determined independently of y . For prescribed initial values (e.g. on \mathcal{R}_0)

$$x_k = x_k^* = x_k^*(\xi, \tau) \quad \text{for} \quad s=0 \quad (3.88)$$

a characteristic projection represents a spatial curve in the (x_1, x_2, x_3) -space. The solution y of the third characteristic equation (3.87) for a prescribed initial value

$$y = y^* \quad \text{for} \quad s=0 \quad (3.89)$$

is considered as a "density" distribution along the characteristic projection. In the present context the solution of (3.87)₄ subject to (3.89) is the initial temperature rate distribution along the characteristic projection in the (x_1, x_2, x_3) -space.

The solutions of the characteristic equations (3.87) are defined without specific reference to the first order P.D.E. (3.86). But analogous to the two-dimensional case (section 3.2.2.1) the following relations apply[30]: Every solution of the P.D.E. (3.86) can be represented by a two-parametric set of characteristic projections and their density distributions and every such set represents a solution of (3.86). Further, if a projected characteristic curve and its density distribution satisfies the P.D.E. (3.86) at one point, then it is a solution of (3.86) at all other points along the projection.

A solution of the P.D.E. (3.86) is constructed as follows. From the boundary condition (3.83) for the temperature on the surface \mathcal{R} appropriate initial values \tilde{y}^* on \mathcal{R}_0 are obtained by setting

$$\tilde{y}^* = \tilde{y}^*(\xi, \tau) = \left(\frac{\partial}{\partial t} \tilde{T}(\xi, \tau, t) \right)_{t=0}. \quad (3.90)$$

To every point of \mathcal{R} a single characteristic projection is associated and these curves in the (x_1, x_2, x_3) -space are not intersecting. The solution of the characteristic equations (3.87) with initial values (3.88) and (3.90) yields the characteristic projections

$$x_k^v = \hat{x}_k^v(s, \xi, \tau) \quad k = 1, 2, 3 \quad (3.91)$$

and the density distribution

$$y = \hat{y}(s, \xi, \tau) \quad (3.92)$$

with

$$\left. \begin{aligned} \hat{x}_k^v(0, \xi, \tau) &= x_k^v(\xi, \tau), \quad k = 1, 2, 3 \\ \hat{y}(0, \xi, \tau) &= \tilde{y}^*(\xi, \tau) \end{aligned} \right\} (3.93)$$

The functions \hat{x}_k^v and \hat{y} are unique and are continuously differentiable functions of their arguments. Differentiation of (3.91) yields

$$dx_k^v = \frac{\partial \hat{x}_k^v}{\partial s} ds + \frac{\partial \hat{x}_k^v}{\partial \xi} d\xi + \frac{\partial \hat{x}_k^v}{\partial \tau} d\tau. \quad (3.94)$$

In the neighbourhood of \mathcal{R}_0 (i.e. $s \rightarrow 0$) equ. (3.94) reduces to

$$dx_k^v = A_k^* ds + \frac{\partial x_k^v}{\partial \xi} d\xi + \frac{\partial x_k^v}{\partial \tau} d\tau, \quad k=1,2,3 \quad (3.95)$$

when the characteristic equations (3.87)₁₋₃ and the initial values (3.93)₁₋₃ are observed. This is a linear relation between the differentials dx_k^v and $ds, d\xi, d\tau$

which may be solved for the second set of differentials if the coefficient determinant

$$\Delta := \begin{vmatrix} A_1^* & \frac{\partial x_1^*}{\partial \xi} & \frac{\partial x_1^*}{\partial \tau} \\ A_2^* & \frac{\partial x_2^*}{\partial \xi} & \frac{\partial x_2^*}{\partial \tau} \\ A_3^* & \frac{\partial x_3^*}{\partial \xi} & \frac{\partial x_3^*}{\partial \tau} \end{vmatrix} \quad (3.96)$$

is non-vanishing:

$$\Delta \neq 0. \quad (3.97)$$

Equ. (3.97) assures that relations (3.91) may be solved for \mathcal{S} , ξ and τ in the neighbourhood of \mathcal{P} . Then a unique representation of the density distribution (3.92) exists in terms of the coordinates x_k^* at least close to the surface \mathcal{P} . If (3.97) is satisfied the surface \mathcal{P} is called "non-characteristic".

The condition (3.97) with (3.96) is the appropriate extension of (3.80). In the following condition (3.97) is implied.

3.2.2.3 Evaluation of the Clausius-Duhem Entropy Inequality for the Three-Dimensional Case

The discussion follows similar lines as in section 3.2.1.2. The dissipation postulate requires that every admissible thermodynamic process obeys the local Clausius-Duhem inequality (3.4) for all times and for all material points in the body. The general solution of the initial-boundary value problem for the temperature, characterizing a general admissible process, is not readily available. However, at time $t = 0$ the initial temperature distribution is assumed to be known and, according to section 3.2.2.2, the initial temperature rate $\dot{\gamma}$ (and also higher derivatives $(\ddot{\gamma})_{t=0}$ etc.) can be determined. Thus in the neighbourhood of $t = 0$ and

close to the boundary surface \mathcal{R} the temperature field $T(x_k, t)$ may be constructed in terms of initial and boundary values*. Therefore, the entropy inequality (3.4) is evaluated at $t = 0$ and for a material point close to or on the boundary surface \mathcal{R} .

Assuming the constitutive equations (3.1) to be given then the entropy inequality (3.4) at some fixed material point $x_k = \tilde{x}_k$ is a condition relating the derivatives

$$\mathcal{R} = \left\{ \dot{T} = \frac{\partial T}{\partial t}, \dot{g}_k = \frac{\partial^2 T}{\partial x_k^2 \partial t}, g_{k,m} = \frac{\partial^2 T}{\partial x_k^2 \partial x_m^2} \right\}_{x_k = \tilde{x}_k} \quad (3.98)$$

and

$$\mathcal{T} = \left\{ T, g_k = \frac{\partial T}{\partial x_k} \right\}_{x_k = \tilde{x}_k} \quad (3.99)$$

as well as the heat supply r , which is prescribed. Also the local energy balance equation (3.3) is relating the sets \mathcal{R} and \mathcal{T} as well as r . One notes that the elements of \mathcal{R} are linearly involved in the entropy inequality and in the energy balance. On the other hand \mathcal{T} is nonlinearly involved in both relations. At $t = 0$ the sets \mathcal{R} and \mathcal{T} take the following values:

$$\mathcal{R}_0 = \left\{ \begin{aligned} (\dot{T})_0 &= \dot{y} \\ (\dot{g}_k)_0 &= \frac{\partial \dot{y}}{\partial x_k} \\ (g_{k,m})_0 &= \frac{\partial^2 \dot{y}}{\partial x_k^2 \partial x_m^2} \end{aligned} \right\}, \quad \mathcal{T}_0 = \left\{ \begin{aligned} (T)_0 &= \bar{T}_0 \\ (g_k)_0 &= \frac{\partial \bar{T}_0}{\partial x_k} \end{aligned} \right\}. \quad (3.100)$$

* It should be observed, that this actually requires a prove that the solution $T(x_k, t)$ can be represented by a convergent Taylor series in the above regime. Such a prove seems not readily derivable.

Since the initial temperature distribution $T_0(x_k)$ may be chosen at will, the quantities

$$\mathcal{U}_0 = \left\{ T_0, \frac{\partial T_0}{\partial x_k}, \frac{\partial^2 T_0}{\partial x_k \partial x_m} \right\} \quad (3.101)$$

assume arbitrary values locally. On the other hand, the first two elements of \mathcal{R}_0 , i.e. the initial temperature rate $\dot{\gamma}$ and its spatial derivatives $\partial \dot{\gamma} / \partial x_k$, are not independent locally. They are related to each other and to the set \mathcal{U}_0 by the local energy balance equations at $t=0$. This interdependence applies also for the temperature rate \dot{T} and its spatial derivatives $\dot{g}_k = \partial \dot{T} / \partial t \partial x_k$ at some later time $t > 0$. This is accounted for by expressing \dot{T} in terms of \dot{g}_k and other elements of \mathcal{R} and \mathcal{T} .

The local energy balance (3.3) at some time $t > 0$ and any material point $x_k = \tilde{x}_k$ yields

$$\dot{T} = \frac{1}{\rho} \frac{1}{\partial \hat{E} / \partial T} \left[\rho r - \rho \frac{\partial \hat{E}}{\partial g_m} \dot{g}_m - \frac{\partial \hat{q}_k}{\partial T} g_k - \frac{\partial \hat{q}_k}{\partial g_m} g_{m,k} - \frac{\partial \hat{q}_k}{\partial x_k} \right] \quad (3.102)$$

With (3.102) the temperature rate \dot{T} is eliminated from the entropy inequality which takes the form

$$\begin{aligned} & \left(\rho \frac{\partial \hat{\eta}}{\partial g_m} - \rho \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \frac{\partial \hat{E}}{\partial g_m} \right) \dot{g}_m \\ & + \left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right) \frac{\partial \hat{q}_k}{\partial g_m} g_{m,k} \\ & + \left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right) \frac{\partial \hat{q}_k}{\partial T} g_k \\ & + \left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right) \frac{\partial \hat{q}_k}{\partial x_k} \\ & - \left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right) \rho r - \frac{1}{T^2} \hat{q}_k g_k \geq 0. \end{aligned} \quad (3.103)$$

At $t = 0$ this reduces to

$$\begin{aligned}
 & s \left(\frac{\partial \hat{\eta}}{\partial \hat{g}_m} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \frac{\partial \hat{E}}{\partial \hat{g}_m} \right)_{t=0} \frac{\partial \hat{y}}{\partial x_m} \\
 & + \left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right)_{t=0} \left(\frac{\partial \hat{q}_k}{\partial \hat{g}_m} + \frac{\partial \hat{q}_m}{\partial \hat{g}_k} \right)_{t=0} \frac{1}{2} \frac{\partial^2 T_0}{\partial x_m \partial x_k} \\
 & + \left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right)_{t=0} \left(\frac{\partial \hat{q}_k}{\partial T} \hat{g}_k \right)_{t=0} \\
 & + \left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right)_{t=0} \left(\frac{\partial \hat{q}_k}{\partial x_k} \right)_{t=0} \\
 & - \left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right)_{t=0} (s\tau)_{t=0} - \left(\frac{1}{T^2} \hat{q}_k \hat{q}_k \right)_{t=0} \geq 0.
 \end{aligned} \tag{3.104}$$

The formulation of the second term of (3.104) accounts for the symmetry of the second derivative $\partial T_0 / \partial x_m \partial x_k$.

It is noted that all terms in brackets* are functions of T_0 and $\partial T_0 / \partial x_e$ which are nonlinearly involved and which may take arbitrary values locally. Also the second derivative $\partial T_0 / \partial x_m \partial x_k$, representing six independent quantities, is arbitrary locally and is linearly involved in (3.104). The initial temperature rate \hat{y} , whose spatial derivatives appear linearly in (3.104), is the solution of the linear P.D.E. (3.86). It is possible to formulate the general integral of (3.86) analogous to (3.27) (see ref. [31]) and to obtain $\partial \hat{y} / \partial x_m$ by differentiation. However, if attention is restricted to material points on the boundary surface \mathcal{R}_0 the derivatives $\partial \hat{y} / \partial x_m$ are easily expressed in terms of initial values on \mathcal{R}_0 . With the results of section 3.2.2.2 a unique solution $\hat{y}(x_e)$ of the P.D.E. (3.86) exists. The introduction of the characteristic equations (3.87) and their solutions (3.91) and (3.92) allows to differentiate the function $\hat{y}(\hat{x}_k)$ with respect to s , i.e. the parameter along the characteristic curves, as well as ξ and τ , i.e. the surface coordinates of \mathcal{R}_0 . This yields

* Except the term $(s\tau)_{t=0}$

$$\left. \begin{aligned}
 \frac{\partial y}{\partial s} &= \frac{\partial y}{\partial \hat{x}_1} \frac{\partial \hat{x}_1}{\partial s} + \frac{\partial y}{\partial \hat{x}_2} \frac{\partial \hat{x}_2}{\partial s} + \frac{\partial y}{\partial \hat{x}_3} \frac{\partial \hat{x}_3}{\partial s} \\
 \frac{\partial y}{\partial \xi} &= \frac{\partial y}{\partial \hat{x}_1} \frac{\partial \hat{x}_1}{\partial \xi} + \frac{\partial y}{\partial \hat{x}_2} \frac{\partial \hat{x}_2}{\partial \xi} + \frac{\partial y}{\partial \hat{x}_3} \frac{\partial \hat{x}_3}{\partial \xi} \\
 \frac{\partial y}{\partial \tau} &= \frac{\partial y}{\partial \hat{x}_1} \frac{\partial \hat{x}_1}{\partial \tau} + \frac{\partial y}{\partial \hat{x}_2} \frac{\partial \hat{x}_2}{\partial \tau} + \frac{\partial y}{\partial \hat{x}_3} \frac{\partial \hat{x}_3}{\partial \tau} .
 \end{aligned} \right\} (3.105)$$

Considering only material points on the boundary surface \mathcal{R}_0 (i.e. $s=0$) one obtains

$$y = y^*(\xi, \tau), \quad \frac{\partial y}{\partial s} = C^* - B^* y^*, \quad \frac{\partial y}{\partial \xi} = \frac{\partial y^*}{\partial \xi}, \quad \frac{\partial y}{\partial \tau} = \frac{\partial y^*}{\partial \tau}$$

$$\frac{\partial \hat{x}_1}{\partial s} = A_1^*, \quad \frac{\partial \hat{x}_2}{\partial \xi} = \frac{\partial \hat{x}_2^*}{\partial \xi}, \quad \frac{\partial \hat{x}_3}{\partial \tau} = \frac{\partial \hat{x}_3^*}{\partial \tau}$$

and (3.105) reduces to

$$\left. \begin{aligned}
 C^* - B^* y^* &= \left(\frac{\partial y}{\partial \hat{x}_1} \right)_{\mathcal{R}_0} A_1^* + \left(\frac{\partial y}{\partial \hat{x}_2} \right)_{\mathcal{R}_0} A_2^* + \left(\frac{\partial y}{\partial \hat{x}_3} \right)_{\mathcal{R}_0} A_3^* \\
 \frac{\partial y^*}{\partial \xi} &= \left(\frac{\partial y}{\partial \hat{x}_1} \right)_{\mathcal{R}_0} \frac{\partial \hat{x}_1^*}{\partial \xi} + \left(\frac{\partial y}{\partial \hat{x}_2} \right)_{\mathcal{R}_0} \frac{\partial \hat{x}_2^*}{\partial \xi} + \left(\frac{\partial y}{\partial \hat{x}_3} \right)_{\mathcal{R}_0} \frac{\partial \hat{x}_3^*}{\partial \xi} \\
 \frac{\partial y^*}{\partial \tau} &= \left(\frac{\partial y}{\partial \hat{x}_1} \right)_{\mathcal{R}_0} \frac{\partial \hat{x}_1^*}{\partial \tau} + \left(\frac{\partial y}{\partial \hat{x}_2} \right)_{\mathcal{R}_0} \frac{\partial \hat{x}_2^*}{\partial \tau} + \left(\frac{\partial y}{\partial \hat{x}_3} \right)_{\mathcal{R}_0} \frac{\partial \hat{x}_3^*}{\partial \tau}
 \end{aligned} \right\} (3.106)$$

These are three linear equations for the three unknown derivatives $\partial y / \partial \hat{x}_k$ on \mathcal{R}_0 . A unique solution exists since the coefficient determinant is Δ , which is assumed to be non-vanishing (equ. (3.97)). Thus, the derivatives $\partial y / \partial \hat{x}_k$ at a point on \mathcal{R}_0 are uniquely determined by

$$A_k^* \quad k=1,2,3, \quad B^*, \quad C^*$$

determined by the choice of $x_k, T_0, \partial T_0 / \partial x_k$ on R_0 .

$$\frac{\partial x_k^*}{\partial \xi}, \quad \frac{\partial x_k^*}{\partial \tau} \quad k=1,2,3$$

determined by the choice of R_0

$$y^*, \quad \frac{\partial y^*}{\partial \xi}, \quad \frac{\partial y^*}{\partial \tau}$$

determined by the choice of $\left(\frac{\partial \tilde{T}(x,t,t)}{\partial t}\right)_{t=0}$ on R_0 et al.

It is important to note that the quantities $(\partial y / \partial x_k)_{R_0}$ at a point on R_0 are linearly depending on the initial temperature rate and its surface derivatives $\partial y^* / \partial \xi, \partial y^* / \partial \tau$. The latter quantities may take locally arbitrary values independently of each other. Consequently, this property is completely transferred to $(\partial y / \partial x_k)_{R_0}$.

With these results the inequality (3.104) is evaluated for a material point on the boundary surface R_0 . Since

$$\partial y / \partial x_m \quad \text{and} \quad \partial^2 T_0 / \partial x_m \partial x_k = \partial^2 T_0 / \partial x_k \partial x_m$$

may take arbitrary values on R_0 and are linearly involved in (3.104) their coefficients must vanish:

$$\left. \begin{aligned} & \left(\frac{\partial \hat{\eta}}{\partial g_m} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \frac{\partial \hat{E}}{\partial g_m} \right)_{t=0, R_0} = 0 \\ & \left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right)_{t=0, R_0} \left(\frac{\partial \hat{q}_k}{\partial g_m} + \frac{\partial \hat{q}_m}{\partial g_k} \right)_{t=0, R_0} \frac{1}{2} = 0 \end{aligned} \right\} (3.107)$$

Further, it is assumed* that

$$\left(\frac{\partial \hat{q}_k}{\partial g_m} + \frac{\partial \hat{q}_m}{\partial g_k} \right)_{t=0} \neq 0 \quad (3.108)$$

at least for some k and m . Thus, (3.107)₂ yields

$$\left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right)_{t=0} = 0 \quad (3.109)$$

for all admissible thermodynamic processes. This is a restriction on the constitutive functions $\hat{\eta}$ and \hat{E} ; otherwise eq. (3.109) would represent a relation between T_0 and its derivative $\partial T_0 / \partial x_k$ at a point on \mathcal{R} , but this in contrast to the basic assumption. Therefore, (3.107)₂ simplifies to read

$$\left(\frac{\partial \hat{\eta}}{\partial g_m} - \frac{1}{T} \frac{\partial \hat{E}}{\partial g_m} \right)_{t=0} = 0 \quad (3.110)$$

which is another restriction on \hat{E} and $\hat{\eta}$. With the result (3.109) three other terms in the inequality drop out, especially the one involving the heat supply. Eq. (3.104) reduces to the residual entropy inequality

$$-\left(\frac{1}{T_0} q_k g_m \right)_{t=0} \geq 0 \quad \text{or} \quad (q_k g_m)_{t=0} \leq 0. \quad (3.111)$$

With the free energy function

$$\hat{\psi} = \hat{E} - T \hat{\eta} = \hat{\psi}(T, g_m) \quad (3.112)$$

such that

$$\frac{\partial \hat{\psi}}{\partial T} = \frac{\partial \hat{E}}{\partial T} - T \frac{\partial \hat{\eta}}{\partial T} - \hat{\eta} \quad (3.113)$$

* It is a simple matter to show that only the symmetric part of $\partial q_k / \partial g_m$ gives a contribution to the energy balance equation (3.3). Thus, not all elements of the symmetric part should be vanishing identically.

$$\frac{\partial \hat{\psi}}{\partial g_m} = \frac{\partial \hat{\epsilon}}{\partial g_m} - T \frac{\partial \hat{\eta}}{\partial g_m}$$

one obtains from (3.110)

$$\left(\frac{\partial \hat{\psi}}{\partial g_m} \right)_{t=0}^{\mathcal{R}_0} = 0 \quad (3.114)$$

and (3.109) yields

$$\left(\frac{\partial \hat{\psi}}{\partial T} + \hat{\eta} \right)_{t=0}^{\mathcal{R}_0} = 0. \quad (3.115)$$

These two restrictions apply to the time $t = 0$ and any material point on \mathcal{R}_0 . Since the constitutive functions (3.1) do not explicitly depend on \mathcal{t} , the choice of the initial time is irrelevant. Further, the constitutive functions may depend explicitly on the material coordinate \mathcal{X}_R (if inhomogenous material response is assumed), and the conditions (3.114) and (3.115) are derived only for material points on the boundary surface \mathcal{R}_0 . Nevertheless, the position of \mathcal{R}_0 may be chosen fairly arbitrary except that it should be non-characteristic. Thus, the constitutive restrictions apply to any time and any point in the rigid heat conductor. Hence,

$$\left. \begin{aligned} \frac{\partial \hat{\psi}}{\partial g_m} &= 0 \\ \frac{\partial \hat{\psi}}{\partial T} &= -\hat{\eta} \end{aligned} \right\} (3.116)$$

and with (3.112)

$$\hat{\epsilon} = \hat{\psi} - T \frac{\partial \hat{\psi}}{\partial T} \quad (3.117)$$

for any point in the body.

The results show that $\hat{\psi}$, $\hat{\epsilon}$ and $\hat{\eta}$ do not depend on the temperature gradient and entropy is given by (3.116)₂.

3.3 The Three-Dimensional Deformable Heat Conductor with Internal Variables

3.3.1 The Initial-Boundary Value Problem and Initial Derivatives

For an internal variable model the constitutive equations are given by (2.5) and (2.6). If inhomogeneous material behaviour is assumed, the relations are extended to read

$$\left. \begin{aligned} t_{ke} &= \hat{t}_{ke}(e_{mn}, T, g_k, \alpha_\gamma, x_j) = \hat{t}_{ek} \\ g_k &= \hat{g}_k(\dots) \\ \epsilon &= \hat{\epsilon}(\dots) \\ \eta &= \hat{\eta}(\dots) \end{aligned} \right\} (3.118)$$

and

$$\dot{\alpha}_\gamma = f_\gamma(\dots), \quad \gamma = 1, 2, \dots, n$$

With these relations the balance of linear momentum equ. (2.1) yields after differentiation

$$\begin{aligned} \rho \ddot{u}_e &= \rho b_e + \left[\frac{\partial \hat{t}_{ke}}{\partial e_{mn}} e_{mn,k} + \frac{\partial \hat{t}_{ke}}{\partial T} g_k \right. \\ &\quad \left. + \frac{\partial \hat{t}_{ke}}{\partial g_m} g_{m,k} + \frac{\partial \hat{t}_{ke}}{\partial \alpha_\gamma} \alpha_{\gamma,k} + \frac{\partial \hat{t}_{ke}}{\partial x_k} \right] \end{aligned} \quad (3.119)$$

and the energy balance reads

$$\begin{aligned}
 & \left(\rho \frac{\partial \hat{E}}{\partial e_{mn}} - \hat{t}_{mn} \right) \dot{e}_{mn} + \rho \frac{\partial \hat{E}}{\partial T} \dot{T} + \rho \frac{\partial \hat{E}}{\partial g_k} \dot{g}_k + \rho \frac{\partial \hat{E}}{\partial \alpha_j} \dot{\alpha}_j \\
 & + \frac{\partial \hat{q}_k}{\partial e_{mn}} e_{mn,k} + \frac{\partial \hat{q}_k}{\partial T} T_k + \frac{\partial \hat{q}_k}{\partial g_m} g_{m,k} + \frac{\partial \hat{q}_k}{\partial \alpha_j} \alpha_{j,k} \\
 & + \frac{\partial \hat{q}_k}{\partial x_k} - \rho r = 0.
 \end{aligned} \tag{3.120}$$

These four equations are the governing P.D.E. for the four primary unknown functions, i.e. the three displacement components u_k and the temperature T .

The following initial conditions are to be prescribed in a certain region B of the body

initial displacement	$u_k(x_m, 0) = u_{0k}(x_m)$	}	(3.121)
initial velocity	$\dot{u}_k(x_m, 0) = v_{0k}(x_m)$		
initial temperature distribution	$T(x_m, 0) = T_0(x_m)$		
initial distribution of the internal variables	$\alpha_j(x_m, 0) = \alpha_{0j}(x_m)$		

From these initial conditions the initial values of the strains, strain rates, temperature gradient as well as the gradient of the internal variables are easily obtained:

initial strains	$e_{0kl} = \frac{1}{2} (u_{0k,l} + u_{0l,k})$	}	(3.122)
initial strain rates	$\dot{e}_{0kl} = \frac{1}{2} (v_{0k,l} + v_{0l,k})$		
initial temperature gradient	$T_{0,k} = T_{0,k}$		
initial gradient of internal variables	$\alpha_{0j,k} = \partial \alpha_j / \partial x_k$		

Further, higher order derivatives are obtained too:

$$\begin{aligned}
 \text{initial gradients of strains } e_{mn,k} &= \frac{\partial e_{mn}}{\partial x_k} \\
 &= \frac{1}{2} \left(\frac{\partial^2 u_m}{\partial x_n \partial x_k} + \frac{\partial^2 u_n}{\partial x_m \partial x_k} \right) \\
 \text{initial gradients of } & \\
 \text{temperatur gradients } g_{m,k} &= \frac{\partial g_{0m}}{\partial x_k} = \frac{\partial^2 T_0}{\partial x_m \partial x_k}
 \end{aligned}
 \quad \left. \vphantom{\begin{aligned} e_{mn,k} \\ g_{m,k} \end{aligned}} \right\} (3.123)$$

Assuming that the constitutive equations and the initial values (3.121) as well as their appropriate derivatives (3.122) and (3.123) are given, the balance of linear momentum allows* to calculate the initial acceleration \ddot{u}_e at every point in \mathcal{B} .

The situation is somewhat different with the local balance of energy. Equ. (3.120) represents a linear P.D.E. of 1. order for the initial temperature rate

$$\gamma := \left(\frac{\partial T}{\partial t} \right)_{t=0} \quad (3.124)$$

and it has the same structure as in section 3.2.2.2, i.e.

$$A_k \gamma_{,k} + B \gamma = C \quad (3.125)$$

where

$$\begin{aligned}
 A_k &= s \left(\frac{\partial \hat{E}}{\partial g_k} \right)_{t=0} \\
 B &= s \left(\frac{\partial \hat{E}}{\partial T} \right)_{t=0} \\
 C &= s(\sigma)_{t=0} - \left(\frac{\partial \hat{q}_k}{\partial e_{mn}} e_{mn,k} + \frac{\partial \hat{q}_k}{\partial T} g_k + \frac{\partial \hat{q}_k}{\partial g_m} g_{m,k} \right. \\
 &\quad \left. + \frac{\partial \hat{q}_k}{\partial d_{j,k}} d_{j,k} + \frac{\partial \hat{q}_k}{\partial x_k} \right)_{t=0}
 \end{aligned}
 \quad \left. \vphantom{\begin{aligned} A_k \\ B \\ C \end{aligned}} \right\} (3.126)$$

— ...

* The volume force b_e is taken to be prescribed.

$$\dots - \left(\rho \frac{\partial \hat{E}}{\partial e_{mn}} - \hat{t}_{mn} \right) \hat{e}_{mn} - \rho \left(\frac{\partial \hat{E}}{\partial \alpha_\gamma} \hat{f}_\gamma \right)_{t=0} .$$

With the initial values (3.121) to (3.123) the functions (3.126) are fully determined and independent of \mathcal{R} .

From the results of section 3.2.2.2 it is evident that the linear P.D.E. (3.125) has a unique solution $\mathcal{Y}(x_k^*)$ if the initial temperature rate is prescribed along an open non-characteristic boundary surface \mathcal{R}_0 , i.e.

$$\mathcal{Y}(x_k^*) = \mathcal{Y}^*(\xi, \tau) = \left(\frac{\partial \tilde{T}(\xi, \tau, t)}{\partial t} \right)_{t=0} \quad (3.127)$$

where $\tilde{T}(\xi, \tau, t)$ is given along \mathcal{R}_0 and ξ, τ are surface coordinates on \mathcal{R}_0 . \mathcal{R}_0 is defined by the parameter representation

$$x_k^* = x_k^*(\xi, \tau) \quad k = 1, 2, 3. \quad (3.128)$$

The condition, that \mathcal{R}_0 is non-characteristic, is given by equ. (3.97), i.e.

$$\Delta = \begin{vmatrix} A_1^* & \frac{\partial x_1^*}{\partial \xi} & \frac{\partial x_1^*}{\partial \tau} \\ A_2^* & \frac{\partial x_2^*}{\partial \xi} & \frac{\partial x_2^*}{\partial \tau} \\ A_3^* & \frac{\partial x_3^*}{\partial \xi} & \frac{\partial x_3^*}{\partial \tau} \end{vmatrix} \neq 0 \quad (3.129)$$

where A_k^* represents the values of (3.126)₁ on \mathcal{R}_0 .

From the discussion in section 3.2.2.2 it is clear that higher order time derivatives of the temperature and displacement at $t = 0$ can be obtained if necessary. This requires time differentiation of the balance equations and the boundary condition on \mathcal{R}_0 . Further, mechanical boundary conditions need not be explicitly considered, if the requirements in appendix 1 are satisfied.

3.3.2 Evaluation of the Clausius-Duhem Entropy Inequality

Inserting the constitutive relations (3.118) into the entropy inequality (1.2) and performing the appropriate derivations yields

$$\begin{aligned}
 & \rho \frac{\partial \hat{\eta}}{\partial e_{mn}} \dot{e}_{mn} + \rho \frac{\partial \hat{\eta}}{\partial T} \dot{T} + \rho \frac{\partial \hat{\eta}}{\partial g_{mn}} \dot{g}_{mn} + \rho \frac{\partial \hat{\eta}}{\partial \alpha_y} \dot{\alpha}_y \\
 & + \frac{1}{T} \left[\frac{\partial \hat{q}_k}{\partial e_{mn}} e_{mn,k} + \frac{\partial \hat{q}_k}{\partial T} T_k + \frac{\partial \hat{q}_k}{\partial g_{mn}} g_{mn,k} + \frac{\partial \hat{q}_k}{\partial \alpha_y} \alpha_{y,k} + \frac{\partial \hat{q}_k}{\partial x_k} \right] \\
 & - \frac{1}{T^2} q_k T_k - \frac{1}{T} \rho r \geq 0.
 \end{aligned} \tag{3.130}$$

With the same argumentation as in section 3.2.2.2 this inequality should be satisfied identically for all admissible thermomechanical processes at $t = 0$ and on the boundary surface \mathcal{R} . It is noted that the entropy inequality relates the quantities

$$\mathcal{T} = \{ e_{mn}, T, g_k, \alpha_y \} \tag{3.131}$$

and

$$\mathcal{R} = \{ \dot{e}_{mn}, e_{mn,k}, \dot{T}, \dot{g}_k, g_{k,m}, \alpha_{y,k} \} \tag{3.132}$$

as well as the prescribed heat supply r . The set \mathcal{T} collects the independent arguments in the constitutive relations and the set \mathcal{R} represents their first temporal and spatial derivatives. The time derivative $\dot{\alpha}_y$ is not contained in \mathcal{R} since it is fully determined by the set \mathcal{T} via the evolution equation (3.118)₅.

Furthermore, the local energy balance equation (3.120) is relating \mathcal{R} , \mathcal{T} and r too. \mathcal{R} is linearly involved here and in the entropy inequality, but \mathcal{T} is nonlinearly involved. At $t = 0$ the sets \mathcal{R} and \mathcal{T} take the following values:

$$\mathbb{R}_0 = \left\{ \begin{array}{l} (\dot{e}_{mn})_0 = \dot{e}_{0mn} \\ (e_{mn,k})_0 = \partial_0 e_{mn} / \partial x_k \\ (\dot{T})_0 = \dot{\gamma} \\ (\dot{g}_k)_0 = \partial \dot{\gamma} / \partial x_k \\ (g_{k,m})_0 = \partial^2 T_0 / \partial x_k \partial x_m \\ (\alpha_{\gamma,k})_0 = \alpha_{0\gamma,k} \end{array} \right\}, \quad \mathbb{T}_0 = \left\{ \begin{array}{l} (e_{mn})_0 = e_{0mn} \\ (T)_0 = T_0 \\ (g_k)_0 = \partial T_0 / \partial x_k \\ (\alpha_{\gamma})_0 = \alpha_{0\gamma} \end{array} \right\}. \quad (3.133)$$

Since the initial distributions of the displacements, the velocities, the temperature and the internal variables in region \mathcal{B} may be chosen at will, the quantities

$$\psi_0 = \left\{ e_{0mn}, \partial_0 e_{mn} / \partial x_k, \dot{e}_{0mn}, T_0, \partial T_0 / \partial x_k, \partial^2 T_0 / \partial x_k \partial x_m, \alpha_{0\gamma}, \partial \alpha_{0\gamma} / \partial x_k \right\} \quad (3.134)$$

assume arbitrary values locally at a material point. However, the two residual elements of the set \mathbb{R}_0 , i.e. $\dot{\gamma}$ and $\partial \dot{\gamma} / \partial x_k$, as well as the local value of the acceleration $(\ddot{u}_e)_0$ are not independent. If at $t=0$ the set ψ_0 is prescribed, then the acceleration is completely determined by the set ψ_0 for a given body force $(b)_0$ via the local balance of linear momentum. This interrelation needs not to be accounted for when evaluating the entropy inequality since the acceleration $(\ddot{u}_e)_0$ does not explicitly appear in this inequality. On the other hand, the initial temperature rate $\dot{\gamma}$ and its spatial derivatives $\partial \dot{\gamma} / \partial x_k$ are related to each other and to the set ψ_0 via the local energy balance at $t=0$. This latter interrelation is taken into account by solving the energy balance equation for the initial temperature rate $\dot{\gamma}$ and inserting the result in the entropy inequality at $t=0$. This yields

$$\left(\rho \frac{\partial \hat{\eta}}{\partial e_{mn}} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \left[\rho \frac{\partial \hat{E}}{\partial e_{mn}} - \hat{t}_{mn} \right] \right)_{t=0} \dot{e}_{0mn} + \dots$$

$$\begin{aligned}
 & \dots + \left(s \frac{\partial \hat{\eta}}{\partial g_m} - s \frac{\partial \hat{\eta}/\partial \tau}{\partial \hat{E}/\partial \tau} \frac{\partial \hat{E}}{\partial g_m} \right)_{t=0} \frac{\partial y}{\partial x_m} \\
 & + \left(\frac{1}{T} - \frac{\partial \hat{\eta}/\partial \tau}{\partial \hat{E}/\partial \tau} \right)_{t=0} \left(\frac{\partial \hat{q}_k}{\partial e_{mn}} \right)_{t=0} \frac{\partial e_{mn}}{\partial x_k} \\
 & + \left(\frac{1}{T} - \frac{\partial \hat{\eta}/\partial \tau}{\partial \hat{E}/\partial \tau} \right)_{t=0} \left(\frac{\partial \hat{q}_k}{\partial g_m} \right)_{t=0} \frac{\partial^2 T_0}{\partial x_m \partial x_k} \\
 & + \left(\frac{1}{T} - \frac{\partial \hat{\eta}/\partial \tau}{\partial \hat{E}/\partial \tau} \right)_{t=0} \left(\frac{\partial \hat{q}_k}{\partial \alpha_\gamma} \right)_{t=0} \frac{\partial \alpha_\gamma}{\partial x_k} \\
 & + \left(\frac{1}{T} - \frac{\partial \hat{\eta}/\partial \tau}{\partial \hat{E}/\partial \tau} \right)_{t=0} \left(\frac{\partial \hat{q}_k}{\partial \tau} g_k \right)_{t=0} \\
 & + \left(\frac{1}{T} - \frac{\partial \hat{\eta}/\partial \tau}{\partial \hat{E}/\partial \tau} \right)_{t=0} \left(\frac{\partial \hat{q}_k}{\partial x_k} \right)_{t=0} \\
 & - \left(\frac{1}{T} - \frac{\partial \hat{\eta}/\partial \tau}{\partial \hat{E}/\partial \tau} \right)_{t=0} (s r)_{t=0} - \left(\frac{1}{T^2} \hat{q}_k g_k \right)_{t=0} \\
 & + \left(s \frac{\partial \hat{\eta}}{\partial \alpha_\gamma} - \frac{\partial \hat{\eta}/\partial \tau}{\partial \hat{E}/\partial \tau} \frac{\partial \hat{E}}{\partial \alpha_\gamma} \right)_{t=0} \left(\hat{f}_\gamma \right)_{t=0} \geq 0
 \end{aligned} \tag{3.135}$$

Attention is now restricted to material points on the non-characteristic boundary surface \mathcal{R}_0 . Following the derivation in section 3.2.2.3 it may be shown that the derivatives $\partial y / \partial x_k$ at a point on \mathcal{R}_0 (i.e. $(\partial y / \partial x_k)_{\mathcal{R}_0}$) are uniquely determined by

$$\left. \begin{aligned}
 & A_k^* \quad k=1,2,3, \quad B^*, \quad C^* \\
 & \frac{\partial x_k^*}{\partial \xi}, \quad \frac{\partial x_k^*}{\partial \tau} \quad k=1,2,3 \\
 & \hat{y}^*, \quad \frac{\partial \hat{y}^*}{\partial \xi}, \quad \frac{\partial \hat{y}^*}{\partial \tau}
 \end{aligned} \right\} \tag{3.136}$$

where the values A_k^* , B^* , C^* are obtained from (3.126) for points on \mathcal{R}_0 . The derivatives $(\partial y / \partial x_k)_{\mathcal{R}_0}$ depend linearly on the initial temperature rate and its surface derivatives on \mathcal{R}_0 , i.e. y^* , $\partial y^* / \partial y$, $\partial y^* / \partial x$, which may take locally arbitrary values independently of each other. Therefore the three values $(\partial y^* / \partial x_k)_{\mathcal{R}_0}$ may be chosen at will. Consequently, the initial values on \mathcal{R}_0

$$\left. \begin{aligned} \dot{e}_{mn} &= \dot{e}_{nm}, \quad \partial y / \partial x_m, \quad \partial e_{mn} / \partial x_k = \partial e_{nm} / \partial x_k \\ \partial^2 T_0 / \partial x_k \partial x_m &= \partial^2 T_0 / \partial x_m \partial x_k, \quad \partial \alpha_y / \partial x_k \end{aligned} \right\} (3.137)$$

occur linearly in the entropy inequality and are allowed to take any values; here their appropriate symmetry properties, as indicated, must be observed. Since the entropy inequality should not be violated for any admissible thermodynamic process, i.e. any set of values (3.137), their corresponding coefficients should vanish:

$$\left. \begin{aligned} &\left\{ s \frac{1}{2} \left(\frac{\partial \hat{\eta}}{\partial e_{mn}} + \frac{\partial \hat{\eta}}{\partial e_{nm}} \right) - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \left[s \frac{1}{2} \left(\frac{\partial \hat{E}}{\partial e_{mn}} + \frac{\partial \hat{E}}{\partial e_{nm}} \right) - \hat{t}_{mn} \right] \right\}_{t=0} = 0 \\ &\left(\frac{\partial \hat{\eta}}{\partial g_m} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \frac{\partial \hat{E}}{\partial g_m} \right)_{t=0} = 0 \\ &\left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right)_{t=0} \left(\frac{\partial \hat{q}_k}{\partial e_{mn}} + \frac{\partial \hat{q}_k}{\partial e_{nm}} \right)_{t=0} \frac{1}{2} = 0 \\ &\left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right)_{t=0} \left(\frac{\partial \hat{q}_k}{\partial g_m} + \frac{\partial \hat{q}_k}{\partial g_n} \right)_{t=0} \frac{1}{2} = 0 \\ &\left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right)_{t=0} \left(\frac{\partial \hat{q}_k}{\partial \alpha_y} \right)_{t=0} = 0 \end{aligned} \right\} (3.138)$$

Similarly to equ. (3.108) it is required that

$$\left(\frac{\partial q_k}{\partial g_m} + \frac{\partial q_m}{\partial g_k} \right)_{t=0} \neq 0 \quad \text{at least for some } k \text{ and } m. \quad (3.139)$$

Thus, (3.138)₄ yields

$$\left(\frac{1}{T} - \frac{\partial \hat{\eta} / \partial T}{\partial \hat{E} / \partial T} \right)_{t=0} = 0 \quad (3.140)$$

so that (3.138)₃ and (3.138)₅ are satisfied too. With (3.140) equ. (3.138)₁ and (3.138)₂ reduce to

$$\left. \begin{aligned} & \left\{ \rho \frac{1}{2} \left(\frac{\partial \hat{\eta}}{\partial e_{mn}} + \frac{\partial \hat{\eta}}{\partial e_{nm}} \right) - \frac{1}{T} \left[\rho \frac{1}{2} \left(\frac{\partial \hat{E}}{\partial e_{mn}} + \frac{\partial \hat{E}}{\partial e_{nm}} \right) - \hat{t}_{mn} \right] \right\}_{t=0} = 0 \\ & \left(\frac{\partial \hat{\eta}}{\partial g_m} - \frac{1}{T} \frac{\partial \hat{E}}{\partial g_m} \right)_{t=0} = 0. \end{aligned} \right\} (3.141)$$

Observing (3.140) several other terms drop out in the entropy inequality which reduces to

$$\left\{ \rho \left(\frac{\partial \hat{\eta}}{\partial \alpha_\gamma} - \frac{1}{T} \frac{\partial \hat{E}}{\partial \alpha_\gamma} \right) f_\gamma - \frac{1}{T^2} q_k g_k \right\}_{t=0} \geq 0 \quad (3.142)$$

The introduction of the free energy function $\hat{\psi}$

$$\hat{\psi} = \hat{E} - T \hat{\eta} = \hat{\psi}(e_{mn}, T, g_m, \alpha_\gamma, x_k) \quad (3.143)$$

allows to write the above results in a lucid form:

$$\left. \begin{aligned} \text{equ. (3.141)}_1 & \Rightarrow \rho \frac{1}{2} \left(\frac{\partial \hat{\psi}}{\partial e_{mn}} + \frac{\partial \hat{\psi}}{\partial e_{nm}} \right) = \hat{t}_{mn} \\ \text{equ. (3.140)} & \Rightarrow \frac{\partial \hat{\psi}}{\partial T} = -\hat{\eta} \end{aligned} \right\} (3.144)$$

$$\text{equ. (3.141)}_2 \Rightarrow \frac{\partial \hat{\psi}}{\partial \hat{g}_m} = 0$$

$$\text{inequ. (3.142)} \Rightarrow \rho \frac{\partial \hat{\psi}}{\partial \alpha_j} \hat{f}_j + \frac{1}{T_0} \hat{q}_k \hat{g}_k \leq 0 .$$

Actually, these conditions are derived only for material points on the boundary surface \mathcal{R} and at $t = 0$. Since the constitutive equations do not explicitly depend on t , the choice of the initial time is irrelevant. Further, the position of \mathcal{R} may be chosen fairly arbitrarily except that it should be non-characteristic. Thus, the above restrictions (3.144) apply to any time and any point in the body.

Finally, the comparison with the results (2.22) and (2.23) obtained with the conventional method shows complete agreement.

3.3.3 Exploitation of the Clausius-Duhem Entropy Inequality with Lagrange Multipliers

The derivation of constitutive restrictions from the entropy inequality in section 3.3.2 shows strong similarities with the evaluation of a variational principle subjected to auxiliary conditions (constraints). The satisfaction of the entropy inequality for all "variations" of the set \mathcal{R} , which is linearly involved, is similar to a variational statement. The energy balance equation represents a condition relating the elements of \mathcal{R} , which are again linearly involved, such that they are not independent; this relation represents a constraint on \mathcal{R} .

In the calculus of variations the method of Lagrange multipliers is used to free the variations from constraints. Thus, it is reasonable to investigate whether this method can be used when exploiting the entropy inequality. This investigation has been done by Liu [29] in the context of a more general entropy inequality and different constitutive relations than discussed in this study. From section 3.3.2 it is clear that the evaluation of the Clausius-Duhem entropy inequality (on \mathcal{R} at $t = 0$) with respect to various choices of the set \mathcal{R} , constrained by the energy balance equation, is a purely algebraic problem. This is also so for more general situations. Thus, Liu has proved* that the following three algebraic statements are equivalent [27-29]:

* A more readable prove is given by Müller [27, 28].

(a) The inequality

$$a_{\gamma} X_{\gamma} + \beta \geq 0 \quad (3.145)$$

holds for all $X_{\gamma}, \gamma=1,2,\dots,n$ which satisfy the equations (constraints)

$$A_{\Delta\gamma} X_{\gamma} + B_{\Delta} = 0, \quad \Delta=1,2,\dots,p \quad \text{with } n > p \quad (3.146)$$

(b) There exist quantities Λ_{Δ} (independent of X_{γ}) such that for all X_{γ} (not subjected to any constraint conditions) the inequality

$$a_{\gamma} X_{\gamma} + \beta - \Lambda_{\Delta} (A_{\Delta\gamma} X_{\gamma} + B_{\Delta}) \geq 0 \quad (3.147)$$

holds.

(c) There exist quantities Λ_{Δ} such that

$$\begin{aligned} a_{\gamma} &= \Lambda_{\Delta} A_{\Delta\gamma}, \quad \gamma = 1, 2, \dots, n \\ \beta - \Lambda_{\Delta} B_{\Delta} &\geq 0 \end{aligned} \quad (3.148)$$

The equation (3.145) represents the entropy inequality at $t=0$ and on \mathcal{R}_0 , the equations (3.146) correspond to the constraining balance equations and the Λ_{Δ} 's are the Lagrange multipliers; the quantities X_{γ} are to be varied, i.e. they are those derivatives of the displacement and temperature fields as well as other fields which appear linearly in the entropy inequality and which are determined by initial values on the surface \mathcal{R}_0 . Thus, the first statement (a) obviously reflects the original problem.

In the following the Lagrange multiplier method, i.e. statement (b), is applied to the basic equations of section 3.3.2 for the purpose of demonstration.

The set \mathcal{X} collects the following quantities

$$\mathcal{X} = \{X_{\gamma}\} = \left\{ \mathcal{R}, \ddot{u}_1, \ddot{u}_2, \ddot{u}_3 \right\}_{t=0}^{\mathcal{R}_0}; \quad (3.149)$$

thus, X_{γ} consists of the initial values of the set \mathcal{R} and of the three components of the acceleration all taken at a point of \mathcal{R}_0 . Without defining the quantities $a_{\gamma}, \beta, A_{\Delta\gamma}$ and B_{Δ} , which requires extensive renumbering, the entropy inequality (3.130) is extended by introducing four Lagrange multipliers, i.e.

Λ_ϵ associated to the energy balance equation

Λ_{ν_i} associated to the three balance equation for the linear momentum,
 $i = 1, 2, 3$

such that the χ_y are unconstrained. Thus, the unconstrained entropy inequality (3.147) takes the following form

$$\begin{aligned}
 & s \frac{\partial \hat{\eta}}{\partial e_{mn}} \dot{e}_{mn} + s \frac{\partial \hat{\eta}}{\partial T} \dot{T} + s \frac{\partial \hat{\eta}}{\partial g_m} \dot{g}_m + s \frac{\partial \hat{\eta}}{\partial \alpha_y} \dot{\chi}_y \\
 & + \frac{1}{T} \left[\frac{\partial \hat{q}_k}{\partial e_{mn}} e_{mn,k} + \frac{\partial \hat{q}_k}{\partial T} g_k + \frac{\partial \hat{q}_k}{\partial g_m} g_{m,k} + \frac{\partial \hat{q}_k}{\partial \alpha_y} \alpha_{y,k} + \frac{\partial \hat{q}_k}{\partial \chi_k} \right] \\
 & - \frac{1}{T^2} \hat{q}_k g_k - \frac{1}{T} s r \\
 & + \Lambda_\epsilon \left[\left(s \frac{\partial \hat{E}}{\partial e_{mn}} - \hat{t}_{mn} \right) \dot{e}_{mn} + s \frac{\partial \hat{E}}{\partial T} \dot{T} + s \frac{\partial \hat{E}}{\partial g_k} \dot{g}_k + s \frac{\partial \hat{E}}{\partial \alpha_y} \dot{\chi}_y \right. \\
 & \quad \left. + \frac{\partial \hat{q}_k}{\partial e_{mn}} e_{mn,k} + \frac{\partial \hat{q}_k}{\partial T} g_k + \frac{\partial \hat{q}_k}{\partial g_m} g_{m,k} + \frac{\partial \hat{q}_k}{\partial \alpha_y} \alpha_{y,k} + \frac{\partial \hat{q}_k}{\partial \chi_k} \right. \\
 & \quad \left. - s r \right] \\
 & + \Lambda_{\nu_i} \left[s \ddot{u}_i - \frac{\partial \hat{t}_{ke}}{\partial e_{mn}} e_{mn,k} - \frac{\partial \hat{t}_{ke}}{\partial T} g_k - \frac{\partial \hat{t}_{ke}}{\partial g_m} g_{m,k} \right. \\
 & \quad \left. - \frac{\partial \hat{t}_{ke}}{\partial \alpha_y} \alpha_{y,k} - \frac{\partial \hat{t}_{ke}}{\partial \chi_k} - s b_e \right] \geq 0. \tag{3.150}
 \end{aligned}$$

Rearranging with respect to the elements of the set \mathcal{X} one obtains

$$\left[s \frac{\partial \hat{\eta}}{\partial e_{mn}} + \Lambda_\epsilon \left(s \frac{\partial \hat{E}}{\partial e_{mn}} - \hat{t}_{mn} \right) \right] \dot{e}_{mn} + \dots$$

$$\begin{aligned}
 & \dots + \left[\left(\frac{1}{T} + \Lambda_\epsilon \right) \frac{\partial \hat{q}_k}{\partial e_{mn}} - \Lambda_{v_e} \frac{\partial \hat{t}_{kl}}{\partial e_{mn}} \right] \underline{e_{mn, k}} \\
 & + \left[s \frac{\partial \hat{\eta}}{\partial T} + \Lambda_\epsilon s \frac{\partial \hat{E}}{\partial T} \right] \underline{\dot{T}} \\
 & + \left[s \frac{\partial \hat{\eta}}{\partial g_m} + \Lambda_\epsilon s \frac{\partial \hat{E}}{\partial g_m} \right] \underline{\dot{g}_m} \\
 & + \left[\left(\frac{1}{T} + \Lambda_\epsilon \right) \frac{\partial \hat{q}_k}{\partial g_m} - \Lambda_{v_e} \frac{\partial \hat{t}_{kl}}{\partial g_m} \right] \underline{g_{m, k}} \\
 & + \left[\left(\frac{1}{T} + \Lambda_\epsilon \right) \frac{\partial \hat{q}_k}{\partial \alpha_y} - \Lambda_{v_e} \frac{\partial \hat{t}_{kl}}{\partial \alpha_y} \right] \underline{\alpha_{y, k}} \\
 & + \Lambda_{v_e} s \underline{\ddot{u}_e} \\
 & + \left(s \frac{\partial \hat{\eta}}{\partial \alpha_y} + \Lambda_\epsilon s \frac{\partial \hat{E}}{\partial \alpha_y} \right) \underline{\hat{f}_y} + \left(\frac{1}{T} + \Lambda_\epsilon \right) \left(\frac{\partial \hat{q}_k}{\partial T} g_k + \frac{\partial \hat{q}_k}{\partial x_k} - s r \right) \\
 & - \Lambda_{v_e} \left(\frac{\partial \hat{t}_{kl}}{\partial T} g_k + \frac{\partial \hat{t}_{kl}}{\partial x_k} \right) - \frac{1}{T_e} \hat{q}_k g_k \geq 0. \quad (3.151)
 \end{aligned}$$

Here it is understood that the unconstrained entropy inequality (3.151) is evaluated at a point of the non-characteristic boundary surface \mathcal{B} at time $t = 0$. However, any special notation, e.g. using the subscript 0, is suppressed. The quantities denoted by the wavy line are the elements of the set \mathcal{X} and are linearly involved without constraints. However, certain symmetry properties must be observed, i.e.

$$\dot{e}_{mn} = \dot{e}_{nm}, \quad \underline{e_{mn, k}} = \underline{e_{nm, k}}, \quad \underline{g_{m, k}} = \underline{g_{k, m}} \quad (3.152)$$

Variation of the accelerations yields

$$\Lambda_{\dot{v}_\epsilon} = 0. \quad (3.153)$$

Since the requirement (3.139) also applies here, the variation of the second spatial derivative of the temperature $g_{m,k}$ together with (3.152) gives

$$\frac{1}{T} + \Lambda_\epsilon = 0 \quad \text{or} \quad \Lambda_\epsilon = -\frac{1}{T}. \quad (3.154)$$

Consequently, several other terms in the inequality drop out. Finally, the variations of the initial strain rate \dot{e}_{mn} , temperature rate \dot{T} and its first spatial gradient \dot{g}_m yield, observing (3.152),

$$\left. \begin{aligned} \frac{1}{2} \rho \left(\frac{\partial \hat{\eta}}{\partial e_{mn}} + \frac{\partial \hat{\eta}}{\partial e_{nm}} \right) - \frac{1}{T} \left[\frac{1}{2} \rho \left(\frac{\partial \hat{E}}{\partial e_{mn}} + \frac{\partial \hat{E}}{\partial e_{nm}} \right) - \dot{t}_{mn} \right] &= 0 \\ \rho \frac{\partial \hat{\eta}}{\partial T} - \frac{1}{T} \rho \frac{\partial \hat{E}}{\partial T} &= 0 \\ \rho \frac{\partial \hat{\eta}}{\partial g_m} - \frac{1}{T} \rho \frac{\partial \hat{E}}{\partial g_m} &= 0 \end{aligned} \right\} (3.155)$$

and the residual entropy inequality

$$\rho \left(\frac{\partial \hat{\eta}}{\partial \alpha_\gamma} - \frac{1}{T} \frac{\partial \hat{E}}{\partial \alpha_\gamma} \right) \dot{\alpha}_\gamma - \frac{1}{T^2} \hat{g}_k \dot{g}_k \geq 0 \quad (3.156)$$

to be taken on \mathcal{B} and at $t=0$. Comparison with the result equ. (3.140) to (3.142) of the previous derivation shows complete agreement.

4. Discussion and Conclusions

The results of section 3, especially the constitutive restrictions (3.144) for a deformable heat conductor with internal variables, demonstrate that the dissipation postulate in connection with the variability of the initial values on the boundary of the body leads to the same constitutive restrictions as the classical Coleman-Noll argumentation. Here it should be kept in mind that the classical Clausius-Duhem entropy inequality was used and deformations were assumed to be infinitesimal.

The approach taken in section 3 follows arguments of Müller [25-28] and Liu [29] and here Wood's "phlogiston objection" [18-20] does not apply: Body forces and heat supply are kept fixed, only the initial values (equ. (3.137)) on the boundary are required to be arbitrary locally to satisfy identically the entropy inequality on the non-characteristic boundary surface of the body at the initial time $t = 0$.

It is evident that the influence of the environment on a body can be modulated much easier on the surface of the body than in its interior. Nevertheless, this modulation on the boundary of the body may be criticized along similar lines as Wood's phlogiston objection because initial and boundary conditions cannot be varied arbitrarily in the natural world. However, it appears to be reasonable to require the continuum theory, which models only a part of the real world, to be mathematically and physically consistent whatever the effects of the environment on the body.

The comparison of the mathematical development presented in this study with those of Müller [25-28] and Liu [29] deserves some comments. As already mentioned (section 3.1) Müller proposed and used a more advanced entropy inequality than assumed in this report. Further, the constitutive classes treated in [25-28] are different from the one analysed in this report. Among others, the constitutive assumptions in [25-28] are characterized by the fact that all constitutive functions involve not only the spatial derivative of the (empirical) temperature but also its temporal derivative as an independent (state) variable. As a consequence, the energy balance equation contains linearly the 2nd order time derivative of the temperature as the highest time derivative. Further, the prescription of suitable initial conditions at every point of the body in the (x_1, x_2, x_3) -space yields a non-characteristic Cauchy problem. Thus, the initial conditions suffice to determine all derivatives of the field functions at a point with respect to the initial time $t = 0$. Assuming the constitutive functions and the initial data to be real analytic functions, the Cauchy-Kowalewski theorem [30] may be

applied in the work of Müller and Liu to prove existence and uniqueness of the initial value problem. Thus, any choice of the initial data determine a unique admissible thermodynamic process.

The situation is different for the case treated in this report. This is primarily due to the fact that the constitutive functions are not assumed to depend on the temperature rate. Consequently the prescription of suitable initial conditions at every point in the (x_1, x_2, x_3) -space is not sufficient for a unique solution since the (x_1, x_2, x_3) -space represents a characteristic three-dimensional manifold. Therefore, it is required in addition, that the history of the temperature is prescribed for $t = 0$ on a material surface of the body. This boundary surface has to be non-characteristic with respect to the P.D.E. governing the initial temperature rate in the body, i.e. the energy balance equation at $t = 0$.

For the initial-boundary value problem the Cauchy-Kowalewski theorem is not applicable and it appears that a general existence theorem is not available [30-35]. However, it is shown in this study, explicitly for the one-dimensional case, that the boundary and initial data allow to determine uniquely the initial ($t = 0$) temporal, spatial and mixed derivatives of any order of the field functions at any point on the non-characteristic boundary surface and in the interior of the body provided the data and the differential equations are continuous differentiable* up to any order. Thus, if the initial-boundary value problem admits a solution and if this solution can be expanded in a convergent Taylor series at a point of the body and at the initial time, then this solution is unique locally. The non-availability of an existence theorem requires to suppose that there exists an admissible thermodynamic process which assumes the initial data in the body and the data on its boundary surface such that the sets \mathcal{R} and \mathcal{T} (equ. (3.133)) on \mathcal{R} may be considered** as a representative of an admissible thermodynamic process. But it should be noted that the formal exploitation of the Clausius-Duhem entropy inequality is not affected by this assumption since all relevant quantities contained in the sets \mathcal{R} and \mathcal{T} are uniquely determined by the differential equations and the initial data on the non-characteristic boundary surface.

* This is the case when the data and the P.D.E. are real analytic.

** Note that \mathcal{R} is constrained by the energy balance equation.

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Appendix 1 (see page 48)

It is important to note that from a physical point of view the initial conditions (3.126) and the prescription of the temperature history \tilde{T} on the open boundary \mathcal{R} is not sufficient to define the complete thermomechanical process in the body for all $t \geq 0$. On the boundary \mathcal{R} (and possibly other boundaries) the non-thermal mechanical actions of the environment on the body should be specified too, e.g. the displacement or stress boundary conditions. To exclude the possibility of discontinuous process (solutions) it is implicitly required that the mechanical boundary conditions at $t = 0$ are compatible with the initial values on the boundary. For example, if the displacement history on the boundary \mathcal{R} is given, this function and its first time-derivative is required to take the values of the functions (3.121)_{1,2}; furthermore, the second time-derivative has to be compatible with the initial acceleration obtained from the balance of linear momentum (3.119) at $t = 0$.

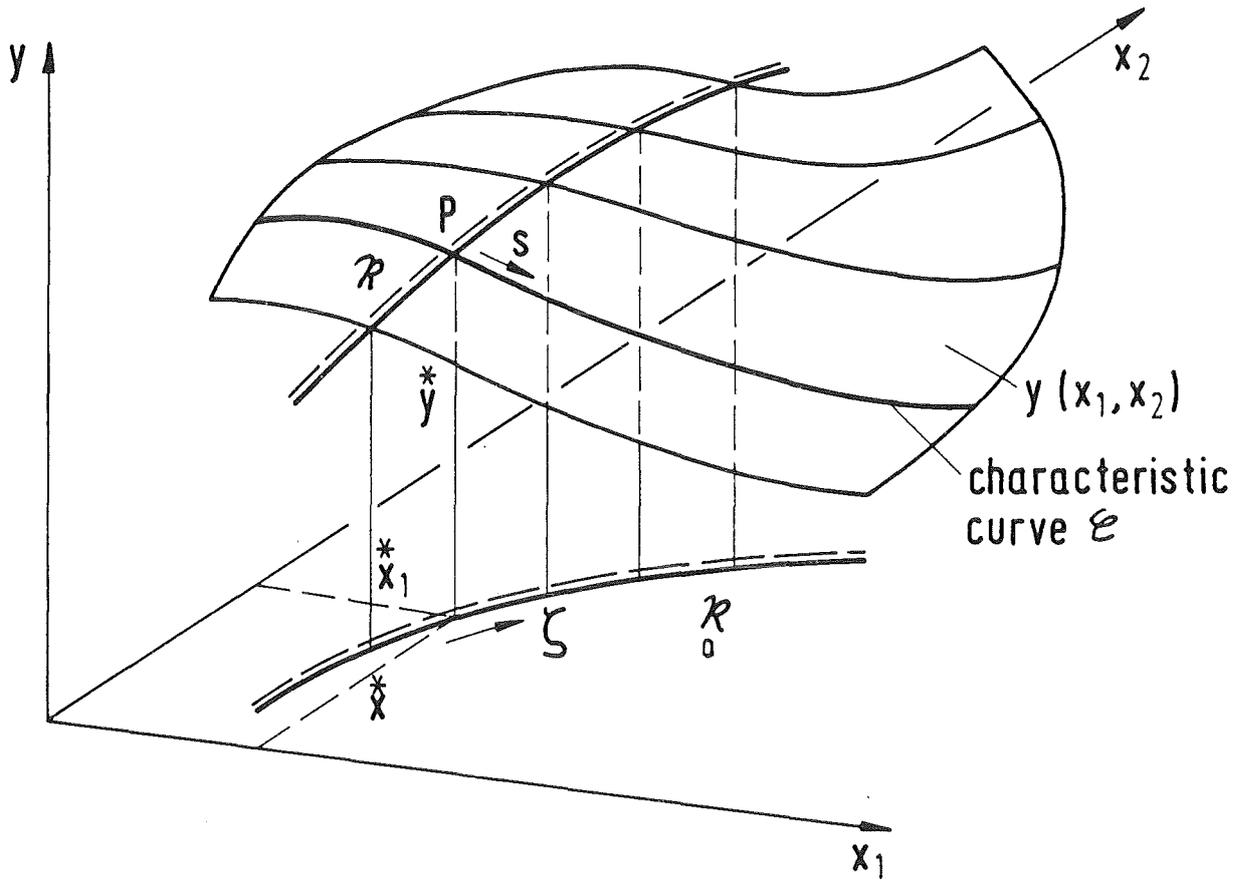


Fig. 1: Integral surface and characteristic curves of a Cauchy problem for a linear first order P.E.D.