



Application of a continuum theory of multiphase mixtures to snow on the ground
by Edward Eagan Adams

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in
Mechanical Engineering
Montana State University
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Abstract:

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Mathematical modeling of the snow is accomplished using a relatively recent continuum theory for mixtures where the individual constituents are physically separate. The approach considers the volume fraction occupied by each constituent as an additional kinematic variable. Therefore, in addition to the balance equations for mass, linear momentum, angular momentum and energy, usually applied in continuum mechanics, an equation which accounts for changes in the volume fraction, called the balance of equilibrated force, is included. Balance equations for each constituent as well as for the mixture are considered.

The immiscible nature of the constituents allows constitutive equations which depend only on variables pertaining to that constituent. Exchange between constituents is accounted for by interaction terms which enter the theory through the balance equations for the constituents. Forms for these interaction terms are developed which guarantee that the entropy inequality is not violated.

The model is used to examine isothermal and temperature gradient conditions for an ideal homogeneous snowpack and an ideal snowpack with layers of varying density. Values are calculated for variables as they change from the transient to the steady state response. Results, with the exception of the vapor velocity, demonstrate an excellent correlation when compared with known and conjectured physical phenomena associated with snow metamorphism.

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A thesis submitted in partial fulfillment
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APPROVAL

of a thesis submitted by

Edward Eagan Adams

This thesis has been read by each member of the thesis committee and has been found to be satisfactory regarding content, English usage, format, citation, bibliographic style, and consistency, and is ready for submission to the College of Graduate Studies.

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Signature Edward E. Allen

Date 7/31/87

To Bill, who encouraged me to attempt it, and without whom the process never would have begun. To Bob, who taught me how, and in the course of it became a friend. And especially to Cat, for always being there.

VITA

Edward Eagan Adams was born on July 29, 1950 at Mercy Hospital in Rockville Centre, New York, the son of BelleRita and Edward Thomas Adams. He received his secondary education from Saint Agnes Cathedral High School in Rockville Centre, graduating in 1968. Mr. Adams graduated from Mount Saint Mary's College, Emmitsburg, Maryland in 1972, obtaining a Bachelor of Arts degree in English with a Philosophy minor. He received a Bachelor of Science degree in Earth Sciences under the Geophysics option in 1979, and a Master of Science in Engineering Mechanics, with a Mathematics minor in 1982, from Montana State University, Bozeman, Montana.

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ABSTRACT

Snow on the ground is examined as a saturated two phase granular material consisting of small grains of ice and interstitial pores filled by a single vapor. The snow is considered as a continuous mixture comprised of the ice and vapor constituents which are themselves treated as individual but interacting continua.

Snow is of interest, in and of itself as a commonly encountered geologic material. An improved understanding of it, however, is of widespread benefit since it is a thermodynamically active granular material which exists in the natural environment. Processes similar to those involved in snow metamorphism, including phase change, occur in other materials, but usually at more extreme thermodynamic conditions.

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CHAPTER I

INTRODUCTION

Snow

Snow on the ground is considered as a fine grained granular or porous geologic material with an ice matrix (Figure 1). An improved understanding of snow as a material is of widespread interest, since a large portion of the globe is seasonally or permanently covered with it. The effect of snow on life-style and the environment can be enormous.

It is of obvious interest when considering transportation, watershed management, avalanche hazard, recreational opportunities and the like, but it is also of broad scientific interest, since it is a naturally occurring material which exists at conditions and temperatures conducive to phase change, coupled with heat flux, mass flux, and deformational processes. As a material, snow is very thermodynamically active in its natural environment on the earth's surface, and will undergo a variety of metamorphic processes including the sintering or bonding of grains, complete crystallographic changes of the ice phase, and decomposition through melting or sublimation. Heat and mass flux in snow take place through both the solid and vapor or liquid phases in a manner which may include numerous transfer mechanisms. Since these processes occur under normal atmospheric conditions, it is an excellent model medium which may be applied to other granular geologic and engineering materials where

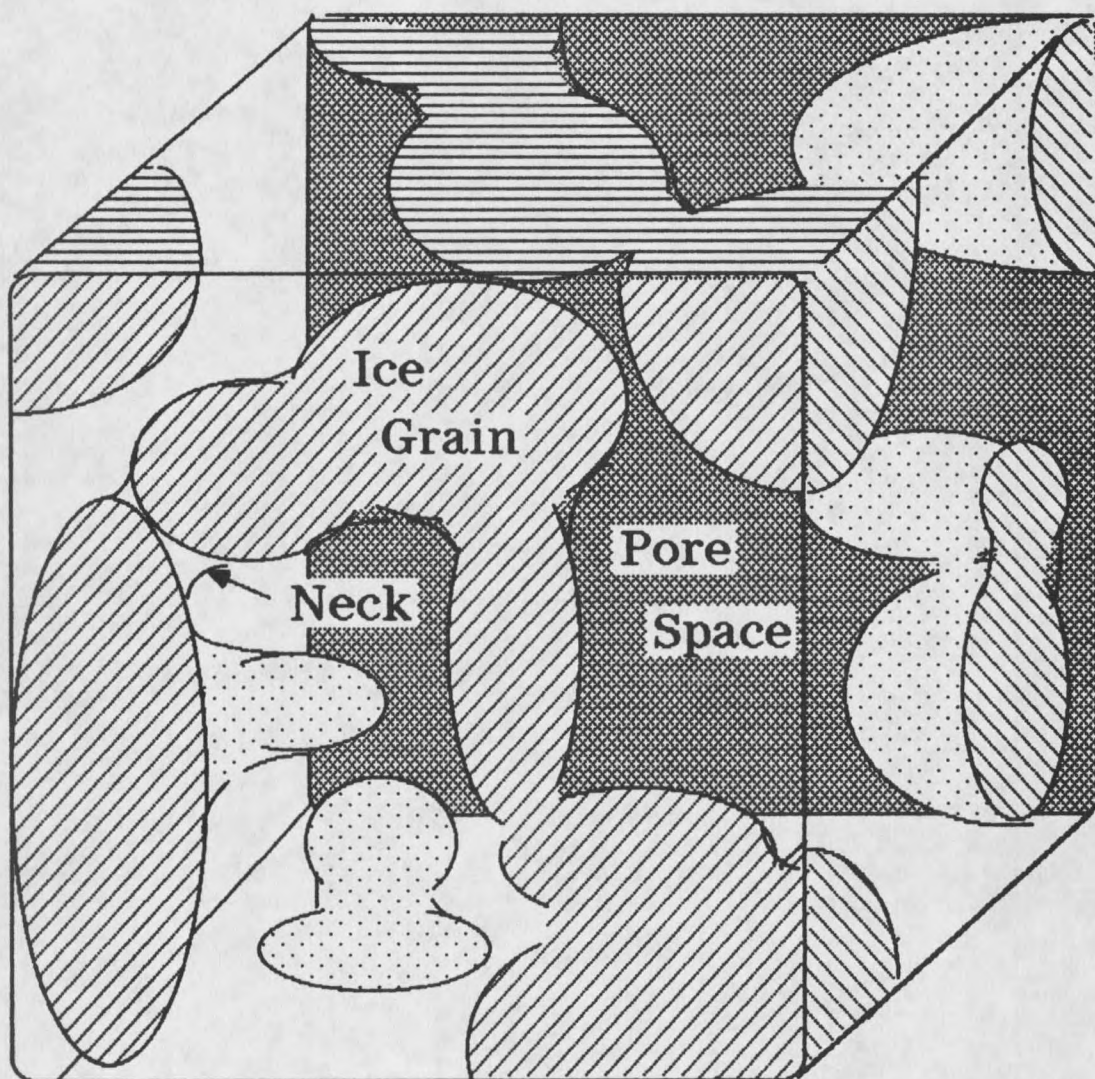


Figure 1. The idealized three dimensional snow on the ground, which is considered as a granular or porous material.

similar processes can take place, but only at more extreme temperatures and pressures.

Metamorphic processes are active in snow from the time of formation in the atmosphere as individual ice crystals, until the ice either evaporates back into the atmosphere or melts as runoff. Atmospheric ice crystals form on condensation nuclei, such as dust, from supercooled water vapor in clouds. Although there are a wide variety of crystal types, the basic crystalline ice structure consists of a basal plane possessing hexagonal symmetry, with an orientation perpendicular to the principal crystallographic axis. Once formed, these intricate crystal forms are in an unstable thermodynamic state and tend to metamorphose toward a more stable configuration after they accumulate as snow on the ground.

In a broad sense there are basically two types of snow on the ground, wet and dry. Snow is considered to be of the wet variety when the interstitial pore spaces between the ice has an obvious liquid water phase present. Wet snow may be liquid-saturated, where the pore is filled with liquid water, or the free water may share the space with a vapor consisting of water vapor and air. In dry snow the liquid phase is not present. The model presented here is concerned with processes which influence dry snow. Dry snow on the ground is generally subcatagorized into two classifications, sometimes based on morphology, but more frequently terms are used which reflect the processes considered to dominate the metamorphic development of the ice forms.

Initially a layer of the fragile atmospherically generated crystals will settle and deteriorate into a more stable configuration, and in the absence

of a large temperature gradient will tend toward a rounded shape. Development of this rounded form is variously termed as destructive metamorphism, equi-temperature metamorphism [LaChapelle, 1969; Sommerfeld, 1969], or the equilibrium growth form [Colbeck, 1981]. The term destructive, which is no longer in widespread use, is based on the "destruction" of the delicate crystals into the rounded form. Equi-temperature implies an isothermal condition, which may be misleading since this situation seldom, if ever, exists in the natural environment for dry snow. Although the process takes place when the temperature gradient may not be the primary driving mechanism of formation, it is not in general an isothermal situation. In fact, some temperature gradient and heat flow between ice grains is necessary for the rounded grains to form at the rates seen in nature [Perla, 1978, from Colbeck, 1981]. Consequently, the terminology "equilibrium growth form" was introduced.

The development of rounded grains will dominate as a growth form in relatively low temperature gradient conditions, when vapor diffusion is the primary means of metamorphism and growth is slow enough so that the rounded equilibrium form is produced. Development of the equilibrium form involves a reduction in surface energy, approaching a minimum. In this process, the presumed controlling mechanism is the difference in vapor pressure at the ice surfaces due to variations in radius of curvature. Mass will migrate from regions of higher vapor pressure (over ice with a smaller radius of curvature), to lower pressure regions. It is this equilibrium growth which is responsible, as an example, for the deterioration of the common six armed, star shaped ice crystal (stellar

dendrite) present in new snow, into the more rounded configuration more typical of an older snow layer (Figure 2).

Due to geothermal heating from below, temperatures at the interface boundary between the ground and the snow usually remain near 0 °C throughout the winter, while the upper snow surface temperature is predominately governed by the ambient atmospheric temperature at the upper snow boundary. When the snow surface temperature is at or above that at the base, melting will occur. If the situation persists free water will eventually bring the snowpack to an isothermal condition typical of a liquid saturated snowpack.

Frequently, however, the surface temperature will be colder than the underlying snow and a temperature gradient is established across the pack. In the presence of sufficiently large temperature gradients (approximately >10 °C/m depending on temperature, pore size, grain size etc.), a striated faceted crystal, known as depth hoar, may develop. This type of development is known as constructive metamorphism, temperature gradient metamorphism [LaChapelle, 1969; Sommerfeld, 1969], or the kinetic growth form [Colbeck, 1981]. Temperature gradient magnitudes of 1 to 10 °C/m are reported to be typical in an alpine snowpack [Yosida, 1963], while gradients of 30 °C/m are reported annually on the Greenland ice sheet [Benson, 1962] and normal gradients of 100 °C/m and as high as 200 °C/m have been reported in central Alaska [Trabant and Benson, 1972].

A pressure gradient associated with thermal gradients will cause a vapor flux from the lower warmer regions toward the upper colder regions. Although conduction of heat is facilitated most readily through the solid

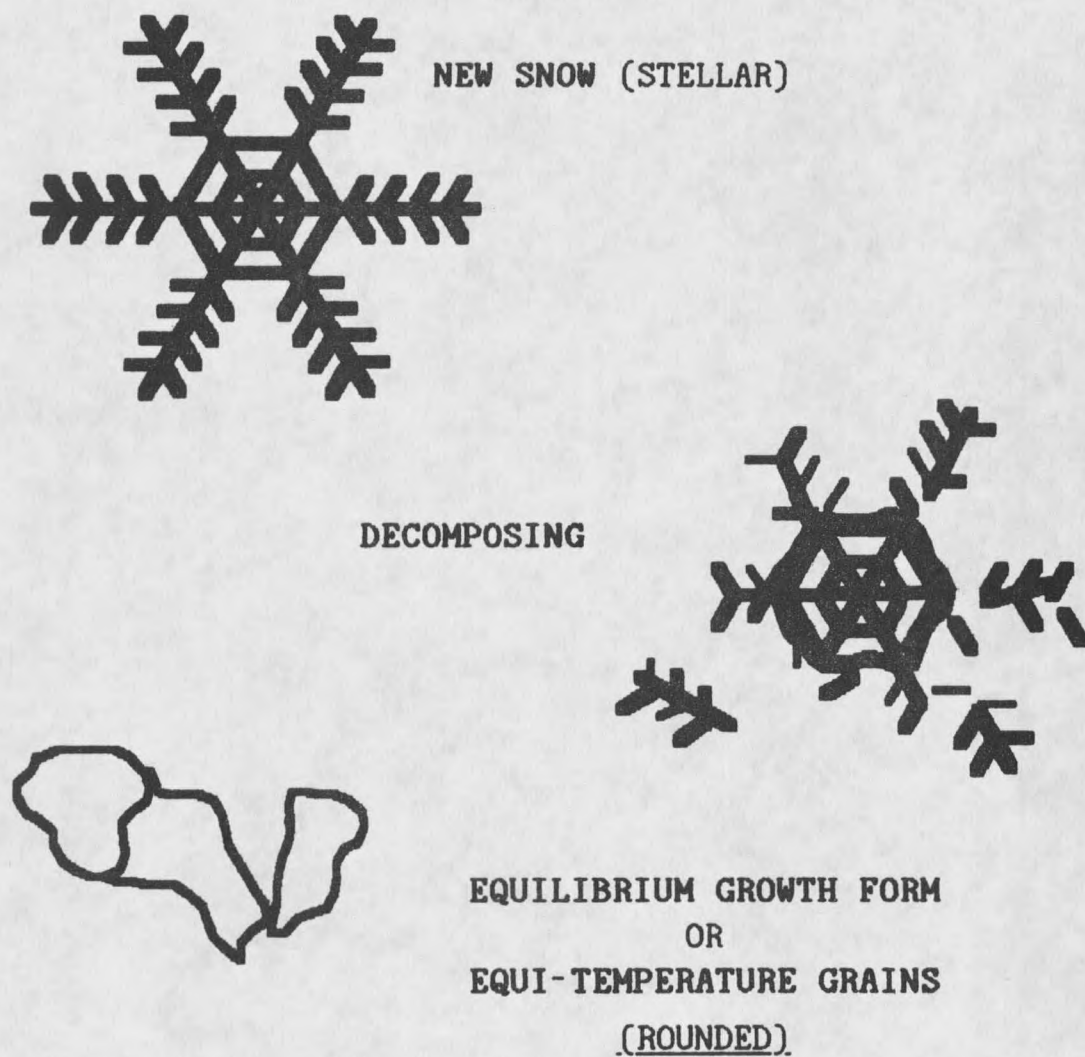


Figure 2. Equilibrium growth or equi-temperature metamorphism, representing the decomposition of unstable crystals into a more stable, rounded configuration.

ice phase, the heat flux will also instigate a mass flux. All of the mass transfer, however, need not take place through the tortuous labyrinth of pores. Mass flux may also proceed through the solid matrix by a "hand to hand" mechanism [Yosida and Kojima, 1950, from Akitaya, 1974], where ice will sublime from the top of a grain (at the bottom of a pore) and the water vapor will be deposited as ice on the bottom of a slightly colder grain above (at the top of the pore) (Figure 3).

A shallow snowpack with differing temperatures at the boundaries will obviously have a larger magnitude of temperature gradient than a thicker pack with the same thermal boundary conditions. As this condition implies, the kinetic growth form of crystal is most pronounced in colder atmospheric environments with shallow snow cover. Low density, poorly bonded snow will also promote faceted crystal growth. Larger pore size associated with lower density snow will allow less restricted vapor movement, encouraging grain growth.

Thermal conductivity in ice is greater than in vapor, so lower density, poorly bonded snow will not facilitate conductive heat flux as readily. Therefore, in a layered stratigraphy typical of a natural snowpack, the magnitude of temperature gradient in lower density, poorly bonded snow will be larger. Thermodynamic processes are generally accelerated at higher temperatures, all else being equal, so growth of depth hoar crystals is most apparent in the lower, warmer, more thermodynamically active regions of the snowpack. Regions of depth hoar crystal development also include small zones above and below crusts [Perla, 1978].

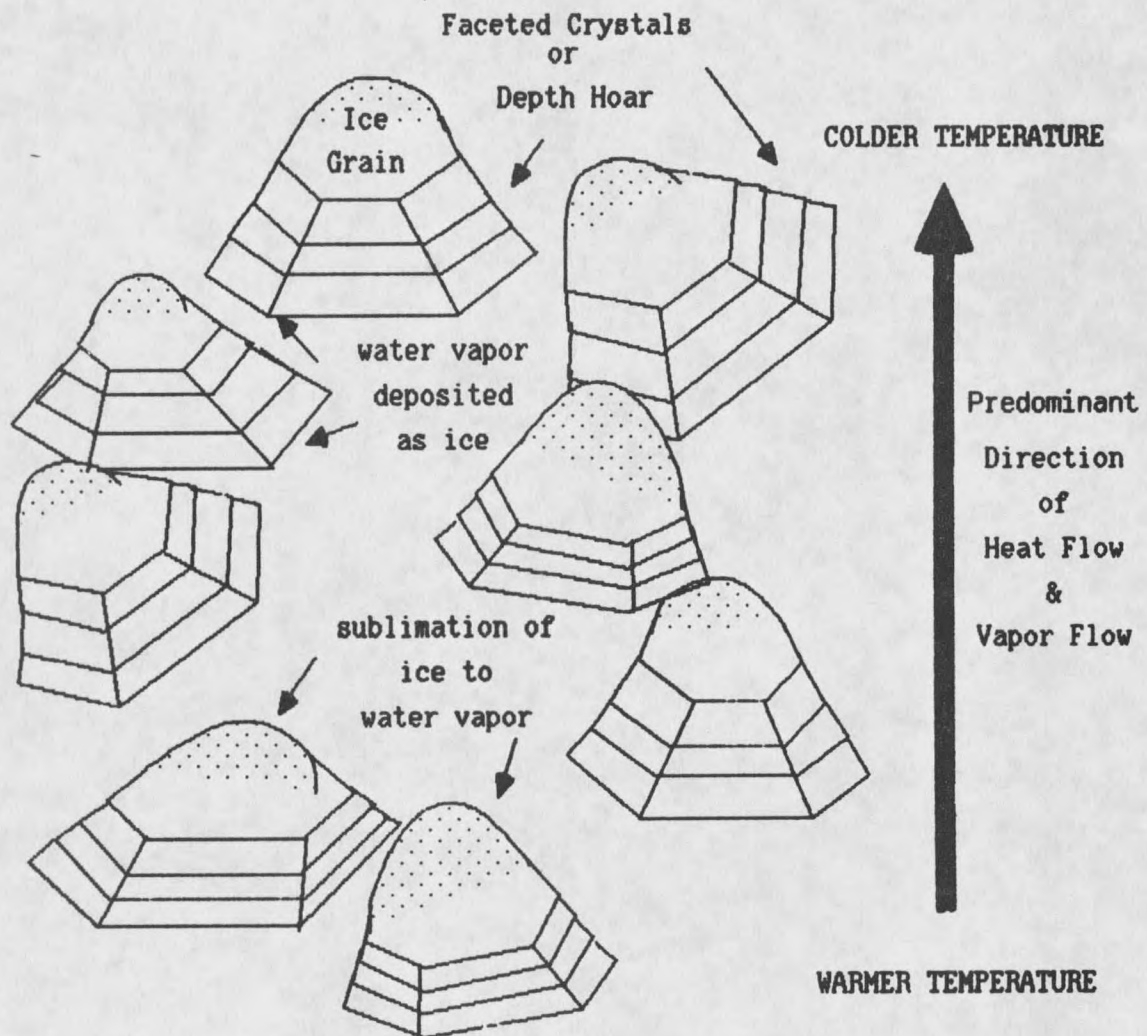


Figure 3. Kinetic growth or temperature gradient metamorphism, showing the direction of vapor flow as well as the orientation of crystal growth.

Importantly, in addition to the form which individual ice grains assume, the overall strength of the snow is affected by the metamorphic process. In the same conditions which dominate the equilibrium growth form, bonds called necks will develop between adjoining ice grains, in a process known as sintering. Presumably, radius of curvature differences will direct the vapor movement toward the lower pressure regions over the concave surfaces which exist when ice grains are brought into contact. It is the deposition of ice at these grain contact points which produce necking. This bonding together of the individual ice grains results in an overall strengthening of the snow. As the process proceeds, necks become larger and the grains lose volume resulting in a fine grained, structurally strong snowpack.

When processes governed by large temperature gradients predominate, a snow layer with little structural integrity develops. This layer consists of large faceted crystals which are poorly bonded together. In snow which has previously been exposed to equilibrium growth form conditions, the rounded grains and necks will disappear, and the noncohesive depth hoar develops. The type of depth hoar discussed here is of the skeleton type, but there also exists a solid type which forms in a lower temperature gradient or at higher snow density [Akitaya, 1974]. This solid type does not show the marked reduction in strength and large crystals typical of the skeleton form although it does have a faceted structure. Fine grained high density snow, greater than 350 kg/m^3 , will result in solid type depth hoar being formed [Marbouty, 1980]. On the subject of structural strength of depth hoar, it is worth noting that of the three stages of crystal development,

anhedral (early development), subhedral (intermediate development), and euhedral (advanced development), the intermediate subhedral stage is the weakest with a local relative maximum temperature gradient at that point [Bradley, Brown and Williams, 1977; Adams and Brown, 1982].

A natural snowpack is usually developed through a series of events and conditions over a period of time and will in general consist of a complex layered stratigraphy. The type of snow precipitated will vary greatly from event to event and will also vary in the course of any particular storm, depending on a myriad of climatic conditions effecting formation and deposition. In addition, as has been mentioned, varying climatic conditions between precipitation events will greatly alter the structure of the snowpack. The upper snow surface may be affected by wind, rain, sun and temperature causing crusts to develop, which are then buried by subsequent snowfall. Wind acting on the surface will fragment ice grains and result in a dense strong smooth layer. Free water formed at the surface from solar insolation, rain or warm atmospheric temperatures may then refreeze forming a stiff layer. Surface hoar which is deposited as a striated faceted crystal directly from the atmospheric vapor onto the snow surface in a manner similar to depth hoar may form a thin weak layer in the pack after it is buried [Lang, Leo and Brown 1984].

Layering will alter the metamorphic processes due to sudden changes in such things as density, permeability, conductivity, and grain and pore size. Metamorphic development of any particular layer is affected by the structure of the entire snowpack. In addition to weaknesses which may develop or persist as a result of the governing thermodynamic conditions,

poor adhesion between layers frequently exist causing structural weaknesses at the interface between layers.

Structural integrity of a snow pack is of significant interest in such areas as over snow vehicle mobility and avalanche hazard evaluation. Failure of a specific zone may be significant. In the case of a vehicle moving over snow it may be significant how deep it will sink and if there is slip between some of the upper layers thereby causing a loss in traction and efficiency. The situation for an avalanche might be quite different since failure at deeper regions will cause a much greater volume of snow to be set into motion. Snow avalanches are extremely difficult to predict, since the medium being dealt with is so complex and thermodynamically active. Most avalanches occur in conjunction with a sudden increase in stress, most frequently caused by deposition of additional snow, or from human involvement such as the the relatively slight additional weight of a skier, climber or vehicle. However, delayed action avalanches also commonly occur, with no apparent warning. It is assumed that the combined processes of metamorphism including deformation due to stress must somehow lead to this final critical instability.

It is apparent that there are many varying conditions and processes which are intricately interwoven and whose interaction must be accounted for in any comprehensive analysis of snow as a material. Snow, and in fact multiphase granular materials in general, have been studied by examining discrete processes which affect its state. The work presented here is an attempt to develop a unified theory for snow in the field. Previous more specific studies such as those involving crystal development may then be

used to assist in the interpretation of quantitative results. The continuum theory of multiphase mixtures is well suited to an application in snow. If the theory can be shown to be even modestly successful, the consequences are quite far reaching, since it demonstrates that this potentially powerful theory, although relatively new and with few applications thus far, can be applied to processes as complex as the one under consideration.

Theory of Multiphase Mixtures

The theory of mixtures deals with the stress, deformation and flow of materials, using the basic, but broad approach of continuum mechanics. Versatility, along with the visual and physical clarity of results is the reason the continuum branch of mechanics is so widely used in engineering applications. In fact, the strongest argument in favor of using the method is the "proof of agreement" with the physical processes which have been successfully modeled.

Analysis of a material as a continuous medium implies a disregard for the molecular structure, but instead envisions a continuous body composed of indefinitely divisible, infinitely small particles or points in space having no volume. This concept of a point is akin to the concept of a limit in differential calculus. Conceptually, the idea of a continuum assumes that in the neighborhood of every particle there is material present.

Basic to the assumptions of continuum mechanics is that all mathematical functions which are employed in a theory are continuous, except perhaps at surfaces or boundaries of regions. There are also some specialized situations where functions may be discontinuous such as the

stress at a wave front; displacements across cracks, where the cracks are not considered as boundaries; etc.

Malvern [1969] divides the study of the theory of continuum mechanics into three distinct parts. These are,

"... (1) **general principles**, assumptions, and consequences applicable to all continuous media, (2) **constitutive equations**, defining the particular idealized material, and (3) **specialized theories** of each individual idealized material built on the foundations of the general principles and constitutive equations of that material to the point where boundary-value problems are formulated and solved for application to specific problems."

Historically, the great majority of continuum models have assumed a single continuous material. Many of these models have been very successful in obtaining the desired information. However, there are large classes of materials for which use of a single material is inappropriate to obtaining some specific information. Fick in 1855 is generally considered to have been the first person to put forth a mathematical theory dealing with the motion of continuous mixtures, in what is now commonly known as "Fick's Law". According to Bedford and Drumheller [1983] it was not until 1957 that the first balance and conservation equations for mixtures as a continuous medium were postulated, by Truesdell [1957].

Consider a continuous body comprised of a number of materials which are intermixed. Let each material itself be considered a continuous body, called a constituent. The entire collection of these constituents taken together is what is known as the mixture. Early work dealing with mixture theory was primarily concerned with mixtures of gases. A basic assumption in this work is that every constituent of the mixture is

considered to be simultaneously present in the same differential region of space. Mixtures satisfying this requirement are referred to as "miscible mixtures". One result of this assumption is that in order to properly retain the generality of the theory, it is expected that any state variables relevant to equations which describe the constitution of an individual material (i.e. the constitutive equations), should incorporate these same variables into all constitutive equations for all constituents of the mixture. The assumption of a mixture composed of constituents which are ideally miscible is the foundation for what is considered the Classical Theory of Mixtures.

It is readily apparent that, while the classical theory is pertinent to a number of applications, the requirement that an element of the mixture contain all of the constituents simultaneously is quite limiting to its scope of applications. Immediately, any mixture which contains immiscible constituents is necessarily excluded from a strict application of the classical theory. Examples of such mixtures are fluid and/or vapor flow in porous or granular material, particle suspensions in fluid or vapor, and bubbly liquids.

Given the basis on which the theory of mixtures has developed, materials such as those just described do not even fit the classical definition of a mixture. However, adaptation to include these types of materials in the classification as a mixture have been successfully accomplished. These theories are to a large extent still in the theoretical development stage, and applications are as yet relatively few. Mixtures of this type are alternatively referred to as immiscible mixtures; mixtures

with structure or microstructure, the implied structure being defined by the interfaces separating constituents; or multiphase mixtures, where discrete phases are involved. In order to describe the multiphased material as a continuous mixture, but also retain the individual integrity of the constituents, regions defining a boundary-value problem must be very large relative to the size of a grain or pore space. An extremely important simplification results from treating the constituents as discrete: the constitutive relations for each constituent are considered independent of the other constituents in the mixture.

Taken from among the theories postulated to deal with immiscible mixtures, one method is to include the fraction of the volume of each constituent relative to the mixture, as an additional kinematic variable. These are called the volume fraction theories. For a collected synopsis of these theories, as well an historical account on developments of mixtures of this type, to 1983, see Bedford and Drumheller [1983]

An approach to dealing with this additional kinematic variable was suggested by Goodman and Cowin [1972], not for a mixture, but for a granular or porous material treated as a single continuum. A model assuming solid grains with vacancies in the interstitial pores is established. As an added kinematical variable, they introduce what is called a volume distribution function, which is representative of that portion of the volume actually occupied by the grains. For example, in the limiting case, where the volume occupied by the pore goes to zero, a solid will remain, in which case the volume distribution will have a value of one. This volume distribution function is equivalent to the volume fraction

when it is introduced into the theory of multiphase mixtures. Since the volume distribution function and the motion are assumed to be kinematically independent, they must be governed by an appropriate number of balance equations. Each volume distribution function, therefore, requires an additional balance equation to those usually applied in continuum mechanics.

Passman [1977] first proposed a theory utilizing the concepts presented by Goodman and Cowin [1972] for a single granular continuum to a multiphase mixture. Each constituent is represented by its volume fraction of the mixture, and the additional balance equation is included for each constituent as well as for the mixture. Nunziato and Walsh [1980] further refined the theory presented by Passman and extended it to include chemical reactions. The development presented in this dissertation treats snow as a multiphase mixture including the mass interaction due to the phase change. This is accomplished by applying the equivalent basic theories of Nunziato and Walsh [1980] and Passman, Nunziato and Walsh [1984] to that specific problem.

CHAPTER II

GENERAL PRINCIPLES FOR A MULTIPHASE MIXTURE

Kinematics

In continuum mechanics a body, β , is composed of a collection of infinitesimal volumes of material referred to as particles, where in a neighborhood of any particle there is material. Referring to a continuous mixture, consider a mixture body, β , which is composed of a number, N , of chemically reacting bodies or constituents, β_a , where $a = 1, 2, \dots, N$.

This presentation uses the fairly common notation that bold faced upper case symbols indicate a tensor and bold faced lower case symbols indicate a vector. Deviations from this convention will be plainly noted in the text.

The region of space occupied by the constituent body at any time, t , is referred to as the constituent configuration. A reference configuration, B_{aR} , is chosen at some time, $t = t_0$. The position of a particle, X_a , of a constituent body at time $t = t_0$ is denoted by a position vector, $\mathbf{X}_a$, measured from a fixed point. Use of a bold faced upper case letter referring to a vector is emphasized here, since this deviates from the standard notation as stated above. More precisely, a particle in the reference configuration has a one to one mapping, which relates a particle, X_a , to its position in the reference configuration,

$$\mathbf{x}_a = \Lambda_a(\mathbf{X}_a). \quad (2.1)$$

This mapping is assumed one to one, and therefore has an inverse relationship,

$$\mathbf{X}_a = \Lambda_a^{-1}(\mathbf{x}_a). \quad (2.2)$$

At each time, t , other than $t = t_0$, there exists a configuration, known as the deformed configuration, B_a . The position of the particle $\mathbf{X}_a$, and therefore the deformed configuration, may change with time. The position vector of the particle in any deformed configuration is denoted by $\mathbf{x}_a$, where

$$\mathbf{x}_a = \Phi_a(\mathbf{X}_a, t). \quad (2.3)$$

Equation 2.3 can be put in terms of the reference configuration, B_{aR} , by using an inverse mapping, Λ^{-1} (equation 2.2). So that

$$\begin{aligned} \mathbf{x}_a &= \Phi_a(\Lambda^{-1}(\mathbf{x}_a), t) \\ &= \chi_a(\mathbf{x}_a, t). \end{aligned} \quad (2.4)$$

Generally speaking, $\mathbf{X}_a$ is referred to as the reference position and $\mathbf{x}_a$ is referred to as the deformed or current position, of the particle $\mathbf{X}_a$.

Using these position vectors, there are a number of ways to describe the motion of a continuum. The type which is employed in this development is the spatial or Eulerian description. This type of description indicates that the independent variables used are the current or instantaneous position, $\mathbf{x}_a$ and time, t . Use of spatial coordinates implies a position in

space and not a specific particle of matter. What it yields is the change of quantities at a fixed position as a function of time.

Particles for each constituent of a mixture do not in general move in unison. Velocities and accelerations for individual constituents must therefore be defined independently. Assuming the motion, χ_a (Equation 2.4), to be sufficiently smooth, denote the velocity of constituent a by,

$$\begin{aligned} \dot{\chi}_a &= \partial[\chi_a(\mathbf{x}_a, t)]/\partial t \\ &= \mathbf{v}_a, \end{aligned} \quad (2.5)$$

and the acceleration by:

$$\begin{aligned} \dot{\mathbf{v}}_a &= \partial \mathbf{v}_a / \partial t \\ &= \partial^2[\chi_a(\mathbf{x}_a, t)]/\partial t^2. \end{aligned} \quad (2.6)$$

The implication in the above equations is that the velocity (Equation 2.5) of a particle is calculated by taking the partial derivative with respect to time, holding $\mathbf{x}_a$ constant; and similarly for the acceleration (Equation 2.6). When the derivative is taken in this manner, it is called the material time derivative. The reverse prime indicates the material time derivative which follows the motion of the a^{th} constituent.

It will prove useful at this point to introduce the deformation gradient tensor, $\mathbf{F}_a$, where

$$\mathbf{F}_a = \nabla \chi_a(\mathbf{x}_a, t). \quad (2.7)$$

Where the del operator, ∇ , indicates that the differentiation is taken with respect to the reference configuration, so this is referring to the gradient

of the deformation with respect to the reference configuration. The deformation gradient (Equation 2.7) maps neighborhoods of the particle positioned at $\mathbf{X}_a$ in the reference configuration, B_{aR} , into neighborhoods of the deformed position $\mathbf{x}_a$ in the deformed configuration B_a .

When the derivative with respect to the spatial coordinates is implied the gradient will be denoted by grad and the divergence by div . If the del operator is used in reference to the spatial system, it will be so indicated.

Next define the velocity gradient as

$$\mathbf{L}_a = \text{grad}(\dot{\mathbf{x}}_a), \quad (2.8)$$

and notice that by the chain rule, using Equations 2.7 and 2.8, that

$$\dot{\mathbf{F}}_a = \mathbf{L}_a \mathbf{F}_a, \quad (2.9)$$

so that

$$\begin{aligned} \dot{\mathbf{F}}_a \mathbf{F}_a^{-1} &= \mathbf{L}_a \\ &= \text{grad}(\dot{\mathbf{x}}_a). \end{aligned} \quad (2.10)$$

In the above, the material time derivative is used, assuming the reference coordinates are known. However, when the spatial description is used this is usually not the case, since a reference position for a particle is usually not known. Let Γ_a be any scalar, vector or tensor valued property of a material, given in terms of the spatial position and time,

$$\Gamma_a = \Gamma_a(\mathbf{x}_a, t).$$

Since, $\mathbf{x}_a$ is a function of time, this must be taken into account. Then the total time derivative, using the chain rule gives,

$$\begin{aligned}\Gamma_a &= \partial \Gamma_a / \partial t \, dt/dt + \text{grad } \Gamma_a \, d\mathbf{x}_a/dt \\ &= \partial \Gamma_a / \partial t + \text{grad } \Gamma_a \, d\mathbf{x}_a/dt.\end{aligned}$$

Substituting the velocity term (Equation 2.5), gives the general form for the material time derivative for any scalar, vector or tensor valued property in spatial coordinates,

$$\Gamma_a = \partial \Gamma_a / \partial t + \text{grad } \Gamma_a \cdot \mathbf{v}_a. \quad (2.11)$$

In this equation, $\partial \Gamma_a / \partial t$ gives the local rate of change in the neighborhood of $\mathbf{x}_a$, and $\text{grad } \Gamma_a \cdot \mathbf{v}_a$ gives the convective rate of change in the neighborhood of a particle. For steady flow the local rate of change will disappear, while in a uniform flow the convective rate will vanish.

The material density of each constituent, γ_a , is defined in the usual way for that particular material, as the mass per unit volume fully occupied by the material. To account for the discrete physical nature of a multiphase mixture, the volume fraction of the a^{th} constituent, v_a , is defined to represent that part per unit volume of the mixture which is filled by constituent a . This implies that a value for the volume fraction is between zero and one, $0 < v_a \leq 1$. In the case where $v_a = 1$, the notion of a multiphase mixture will no longer apply. These are then used to define the partial density of constituent a , ρ_a , as

$$\rho_a = \gamma_a v_a, \quad (2.12)$$

where obviously $\rho_a < \gamma_a$ in the case of a true multiphase mixture.

Up to this point the development of the kinematics has been in terms of the constituents. Next the terms relating to the mixture are given. In the present theory the bulk density for the mixture, ρ , is defined by

$$\rho = \sum \rho_a, \quad (2.13)$$

where $\sum$ indicates summation over all of the constituents which comprise the mixture. This is the notation used throughout the dissertation, unless otherwise noted.

The volume fraction for the mixture, ν , is

$$\nu = \sum \nu_a, \quad (2.14)$$

where $0 < \nu \leq 1$. If $\nu = 1$, the mixture is said to be saturated. When $\nu < 1$, it is unsaturated, indicating that voids exist in the mixture.

Mixture velocity is defined in terms of the constituent velocities as

$$\rho \mathbf{v} = \sum \rho_a \mathbf{v}_a, \quad (2.15)$$

where $\mathbf{v} = \dot{\mathbf{x}}$.

The leading superposed dot implies a time derivative for the mixture, as opposed to the use of the backward prime for time derivatives indicating the constituents. The diffusion velocity for a constituent $\mathbf{u}_a$, which measures its velocity relative to the mixture is

$$\mathbf{u}_a = \mathbf{v}_a - \mathbf{v}. \quad (2.16)$$

It then follows from Equations 2.16, 2.15 and 2.13 that

$$\begin{aligned} \sum \rho_a \mathbf{u}_a &= \sum \rho_a (\mathbf{v}_a - \mathbf{v}) \\ &= \sum \rho_a \mathbf{v}_a - \sum \rho_a \mathbf{v} \end{aligned}$$

$$= \rho \mathbf{v} - \rho \mathbf{v}$$

$$= 0.$$

Similar to the constituents (Equations 2.7 and 2.11), but in terms of $\mathbf{x}$ and t instead of $\mathbf{x}_a$ and t , the velocity gradient for the mixture is,

$$\mathbf{L} = \text{grad } \mathbf{v}, \quad (2.17)$$

and the material time derivative for Γ is,

$$\dot{\Gamma} = \partial \Gamma / \partial t + \text{grad } \Gamma \cdot \mathbf{v}. \quad (2.18)$$

Balance Equations

Generally in continuum mechanics it is assumed that mass, linear momentum, angular momentum, and energy are conserved. The volume fraction theory for multiphase mixtures requires an additional balance equation which accounts for changes in the volume fraction, called the balance of equilibrated force. Two completely equivalent sets of field equations describing these conservation principles are defined for a continuous body, when the functions involved are smooth. Starting from an integral or global form for these balance equations, defined in terms of a region of the continuum, the equivalent differential or local form may be derived for a differential volume element.

In this section the postulated integral forms for the constituents are those given in Passman, Nunziato, and Walsh [1984]. From these, the local balance equations for the constituents are developed and thus shown to be equivalent to the global form. Individual balance equations for each constituent must be related to the other constituents in some manner. This

relationship between constituents is given in the form of interaction terms. These interaction terms, which represent an exchange between constituents, are not present in the usual formulation for a single continuum.

The governing balance equations for the mixture are the same as those given for a single continuous body. Development from the global to local form of the balance equations is not presented for the mixture, since the procedure follows closely that displayed for the constituents (although somewhat less involved), and the equivalence of these equations for a single body has been well established. However, mixture theory requires that summing over all of the constituents for the balance equations must result in the usual balance equations for the mixture. Summing rules sufficient to satisfy this requirement are established.

The global equations given by Passman, Nunziato and Walsh [1984] are consistent with the metaphysical principles laid down by Truesdell [1957; from Passman, Nunziato and Walsh, 1984] and with the general equation of balance as stated by Truesdell [1977]. The general equation of balance for a property Ψ is given as

$$\frac{d}{dt} \left(\int \rho \Psi \, dV \right) - \oint \Upsilon \, dS + \int \rho \xi \, dV = 0,$$

where Υ is a flux term representing the flux of Ψ across the boundary of the region, and ξ is a source term.

Prior to the statement and development of the balance equations, several theorems which are used must be given. The Reynolds transport theorem is

$$\frac{d}{dt} \left(\int \Gamma \rho \, dV \right) = \int \frac{\partial [\Gamma \rho]}{\partial t} \, dV + \oint \Gamma \rho \, \mathbf{v} \cdot \mathbf{n} \, dS. \quad (2.19)$$

where V is volume, Γ is any property of the material, $\mathbf{v}$ is the velocity, $\mathbf{n}$ is the unit normal directed outward from the surface S at a point on the surface dS . The divergence theorem, also referred to as Gauss's theorem or Green's theorem, is used to convert a surface integral to a volume integral. A very general form for this is

$$\oint \mathbf{n} * \Gamma dS = \int \nabla * \Gamma dV, \quad (2.20)$$

[Malvern, 1969], where Γ may be any differentiable scalar vector or tensor defined over the closure of the region of integration and the star product may represent either the dot product or the cross product.

Conservation of Mass for the Constituents

The global form for the mass balance equation describing the principle of conservation of mass for each constituent is given as

$$\int c_a^+ dV = '(\int \rho_a dV), \quad (2.21)$$

where c_a^+ is the mass interaction for the a^{th} constituent.

Applying the Reynolds transport theorem (Equation 2.19) to the term on the right gives,

$$'(\int \rho_a dV) = \int \partial \rho_a / \partial t dV + \oint \rho_a \mathbf{v}_a \cdot \mathbf{n} dS. \quad (2.22)$$

Applying the divergence theorem (Equation 2.20) to convert the surface integral to a volume integral,

$$\oint \rho_a \mathbf{v}_a \cdot \mathbf{n} dS = \int [(\text{grad } \rho_a) \cdot \mathbf{v}_a + \rho_a (\text{div } \mathbf{v}_a)] dV, \quad (2.23)$$

and using the material time derivative (Equation 2.11)

$$\partial \rho_a / \partial t = ' \rho_a - \mathbf{v} \cdot \text{grad } \rho_a. \quad (2.24)$$

This leads from Equation 2.21 by Equations 2.22, 2.23 and 2.24 to the

integral form for the mass balance over the volume,

$$\int [\rho_a - \mathbf{v} \cdot \text{grad } \rho_a + (\text{grad } \rho_a) \cdot \mathbf{v}_a + \rho_a (\text{div } \mathbf{v}_a) - c_a^+] dV = 0$$

or,

$$\int [\rho_a + \rho_a (\text{div } \mathbf{v}_a) - c_a^+] dV = 0 \quad (2.25)$$

which states that the time rate of change of the mass contained within the arbitrary boundary will be the result of the mass flux across the boundary and the mass exchange.

Since the integral is taken over an arbitrary region Equation 2.25 gives a local form for the mass conservation principle, which must be true for each constituent. The Eulerian form for the local balance of mass equation for each constituent is

$$c_a^+ = \rho_a + \rho_a \text{div } \mathbf{v}_a \quad (2.26)$$

Balance of Linear Momentum for the Constituents

The global form for the balance of linear momentum of each constituent is taken as

$$\int \mathbf{m}_a^+ dV = \left(\int \rho_a \mathbf{v}_a dV \right) - \oint \mathbf{T}_a \cdot \mathbf{n} dS - \int \rho_a \mathbf{b}_a dV, \quad (2.27)$$

where $\mathbf{m}_a^+$ is the linear momentum interaction, $\mathbf{T}_a$ is the partial stress tensor and $\mathbf{b}_a$ is the external body force acting on the constituent.

Applying the Reynolds transport theorem (Equation 2.19) to the first term on the right hand side of Equation 2.27 gives

$$\left(\int \rho_a \mathbf{v}_a dV \right) = \int \partial[\rho_a \mathbf{v}_a] / \partial t dV + \oint [\rho_a \mathbf{v}_a] \mathbf{v}_a \cdot \mathbf{n} dS,$$

and the balance of linear momentum becomes

$$\int \mathbf{m}_a^+ dV = \int \partial(\rho_a \mathbf{v}_a)/\partial t dV + \oint (\rho_a \mathbf{v}_a)(\mathbf{v}_a \cdot \mathbf{n}) dS - \oint \mathbf{T}_a \cdot \mathbf{n} dS - \int \rho_a \mathbf{b}_a dV. \quad (2.28)$$

In this $\oint (\rho_a \mathbf{v}_a) \mathbf{v}_a \cdot \mathbf{n} dS$ represents the flux of linear momentum across the boundary. The term $\mathbf{T}_a \cdot \mathbf{n}$ is the part of the total stress vector on the arbitrary boundary which is caused by the a^{th} constituent. Now applying Gauss's theorem (Equation 2.20) to the first surface integral on the right in Equation 2.28 gives

$$\oint (\rho_a \mathbf{v}_a) \mathbf{v}_a \cdot \mathbf{n} dS = \int \text{grad}(\rho_a \mathbf{v}_a) \cdot \mathbf{v}_a + (\rho_a \mathbf{v}_a) \text{div} \mathbf{v}_a dV. \quad (2.29)$$

The div and grad terms must be assumed to be taken from the right, in accordance with the divergence theorem. To clarify this, Gauss's theorem is applied in spatial coordinates using the del operator form and employing index notation. The subscript indicating the constituent will be dropped when the index notation is used. The surface integral in Equation 2.29 is examined again.

$$\begin{aligned} \oint (\rho_a \mathbf{v}_a) \mathbf{v}_a \cdot \mathbf{n} dS &= \oint \rho_a (\mathbf{v}_a \mathbf{v}_a) \cdot \mathbf{n} dS \\ &= \int [\rho_a (\mathbf{v}_a \mathbf{v}_a)] \nabla dV \\ &= \int [(\rho_a \mathbf{v}_a \nabla) \cdot \mathbf{v}_a + \rho_a \mathbf{v}_a (\mathbf{v}_a \cdot \nabla)] dV \\ &= \int [(\rho \mathbf{v}_i \nabla_j) \cdot \mathbf{v}_i + \rho \mathbf{v}_i (\mathbf{v}_j \nabla_j)] dV \\ &= \int [(\rho \partial v_i / \partial x_j) \cdot v_i + \rho v_i (\partial v_j / \partial x_j)] dV \end{aligned}$$

Converting the other surface integral in Equation 2.28 to a volume integral (Equation 2.20) gives

$$\oint \mathbf{T}_a \cdot \mathbf{n} dS = \int \text{div} \mathbf{T}_a dV. \quad (2.30)$$

The divergence is taken from the right, similar to the previous application of Gauss's theorem. Using the index notation for clarification as stated above, gives

$$\begin{aligned}\operatorname{div} \mathbf{T}_a &= T_{ij}(\mathbf{e}_i \mathbf{e}_j) \cdot \partial/\partial x_k \mathbf{e}_k \\ &= \partial T_{ij} / \partial x_k \delta_{jk} \mathbf{e}_i \\ &= \partial T_{ij} / \partial x_j \mathbf{e}_i,\end{aligned}$$

where δ_{jk} is the Kronecker delta and $\mathbf{e}$ are the base vectors,

It should be pointed out that the stress tensor used in this paper is the same as that used in Passman, Nunziato and Walsh [1984] and Truesdell [1969]. The transpose of this stress tensor is sometimes used as well (see for example Malvern [1969]). There the surface traction, $\mathbf{t}$, used in the global form of the balance of linear momentum is given by $\mathbf{t} = \mathbf{n} \cdot \mathbf{T}$, instead of the form used here (Equation 2.27).

Then, collecting terms

$$\begin{aligned}\int [\partial(\rho_a \mathbf{v}_a) / \partial t + \operatorname{div}(\rho_a \mathbf{v}_a) \mathbf{v}_a + (\rho_a \mathbf{v}_a) \operatorname{div} \mathbf{v}_a \\ - \operatorname{div} \mathbf{T}_a - \rho_a \mathbf{b}_a - \mathbf{m}_a^+] dV = 0,\end{aligned}$$

and since the volume is arbitrary a local form is

$$\partial(\rho_a \mathbf{v}_a) / \partial t + \operatorname{grad}(\rho_a \mathbf{v}_a) \mathbf{v}_a + (\rho_a \mathbf{v}_a) \operatorname{div} \mathbf{v}_a - \operatorname{div} \mathbf{T}_a - \rho_a \mathbf{b}_a - \mathbf{m}_a^+ = 0. \quad (2.31)$$

The material time derivative (Equation 2.11) applied to $\rho_a \mathbf{v}_a$ is

$$(\rho_a \mathbf{v}_a)' = \partial(\rho_a \mathbf{v}_a) / \partial t + \mathbf{v}_a \operatorname{grad}(\rho_a \mathbf{v}_a),$$

which allows Equation 2.31 to be rewritten as

$$(\rho_a \mathbf{v}_a) + (\rho_a \mathbf{v}_a) \text{div } \mathbf{v}_a - \text{div } \mathbf{T}_a - \rho_a \mathbf{b}_a - \mathbf{m}_a^+ = 0$$

$$\rho_a \mathbf{v}_a + \rho_a' \mathbf{v}_a + (\rho_a \mathbf{v}_a) \text{div } \mathbf{v}_a - \text{div } \mathbf{T}_a - \rho_a \mathbf{b}_a - \mathbf{m}_a^+ = 0.$$

Substitution for ρ_a from the local form for the mass balance of the constituent (Equation 2.26) yields

$$(c_a^+ - \rho_a \text{div } \mathbf{v}_a) \mathbf{v}_a + \rho_a' \mathbf{v}_a + (\rho_a \mathbf{v}_a) \text{div } \mathbf{v}_a - \text{div } \mathbf{T}_a - \rho_a \mathbf{b}_a - \mathbf{m}_a^+ = 0,$$

so the local form for the constituent balance of linear momentum equation may be written as,

$$\mathbf{m}_a^+ = \rho_a' \mathbf{v}_a - \text{div } \mathbf{T}_a - \rho_a \mathbf{b}_a + c_a^+ \mathbf{v}_a. \quad (2.32)$$

Balance of Angular Momentum of the Constituent

The integral form used for the constituent angular momentum balance equation is

$$\begin{aligned} \int [\mathbf{M}_a^+ + (\mathbf{x}_a \times \mathbf{m}_a^+)] dV \\ = \int (\mathbf{x}_a \times (\rho_a \mathbf{v}_a)) dV - \oint (\mathbf{x}_a \times \mathbf{T}_a \mathbf{n}) dS - \int (\mathbf{x}_a \times \rho_a \mathbf{b}_a) dV, \end{aligned} \quad (2.33)$$

where $\mathbf{M}_a^+$ is the angular momentum interaction of the constituent, and represents a couple effect which may be produced by the interaction of the other constituents with constituent a.

Applying the Reynolds transport theorem (Equation 2.19) to the first term on the right hand side of Equation 2.33 yields

$$\begin{aligned} \int (\mathbf{x}_a \times (\rho_a \mathbf{v}_a)) dV \\ = \int \{ [\partial \mathbf{x}_a / \partial t \times (\rho_a \mathbf{v}_a)] + \mathbf{x}_a \times \partial (\rho_a \mathbf{v}_a) / \partial t \} dV + \oint (\mathbf{x}_a \times (\rho_a \mathbf{v}_a) (\mathbf{v}_a \cdot \mathbf{n})) dS, \end{aligned}$$

then using the material time derivative (Equation 2.14),

$$\begin{aligned}
\left(\int [\mathbf{x}_a \times (\rho_a \mathbf{v}_a)] dV \right) &= \int \{ [\mathbf{x}_a - \mathbf{v}_a \text{grad } \mathbf{x}_a] \times (\rho_a \mathbf{v}_a) + \mathbf{x}_a \times \partial(\rho_a \mathbf{v}_a)/\partial t \} dV \\
&\quad + \oint [\mathbf{x}_a \times (\rho_a \mathbf{v}_a)(\mathbf{v}_a \cdot \mathbf{n})] dS \\
&= \int [\mathbf{v}_a - \mathbf{v}_a \cdot \mathbf{1}] \times (\rho_a \mathbf{v}_a) + \{ \mathbf{x}_a \times \partial(\rho_a \mathbf{v}_a)/\partial t \} dV \\
&\quad + \oint [\mathbf{x}_a \times (\rho_a \mathbf{v}_a)(\mathbf{v}_a \cdot \mathbf{n})] dS \quad (2.34)
\end{aligned}$$

where $\mathbf{1}$ is the identity tensor.

Substitution of Equation 2.34 into equation 2.33 leads to the angular momentum balance for the constituent as

$$\begin{aligned}
\int [\mathbf{M}_a^+ + \mathbf{x}_a \times \mathbf{m}_a^+] dV &= \int [\mathbf{x}_a \times \partial(\rho_a \mathbf{v}_a)/\partial t] dV + \oint [\mathbf{x}_a \times (\rho_a \mathbf{v}_a)(\mathbf{v}_a \cdot \mathbf{n})] dS \\
&\quad - \oint (\mathbf{x}_a \times \mathbf{T}_a \mathbf{n}) dS - \int (\mathbf{x}_a \times \rho_a \mathbf{b}_a) dV, \quad (2.35)
\end{aligned}$$

where $\oint [\mathbf{x}_a \times (\rho_a \mathbf{v}_a)(\mathbf{v}_a \cdot \mathbf{n})] dS$ indicates the flux of the angular momentum across the boundary, and $\oint (\mathbf{x}_a \times \mathbf{T}_a \mathbf{n}) dS$ is the moment of the partial stress vector acting on the surface.

The divergence theorem (Equation 2.20) is applied to the flux of angular momentum term, using indicial notation. The subscript indicating the a^{th} constituent is dropped while the index notation is employed. This gives

$$\begin{aligned}
\oint [\mathbf{x}_a \times (\rho_a \mathbf{v}_a)(\mathbf{v}_a \cdot \mathbf{n})] dS &= \oint [e_{ijk} x_j \rho v_k v_l n_l] dS \\
&= \int \partial [e_{ijk} x_j \rho v_k v_l] / \partial x_l dV \\
&= \int [e_{ijk} \partial x_j / \partial x_l \rho v_k v_l + e_{ijk} x_j \partial(\rho v_k) / \partial x_l v_l + e_{ijk} x_j \rho v_k \partial v_l / \partial x_l] dV \\
&= \int [\text{div } \mathbf{x}_a \mathbf{v}_a \times (\rho_a \mathbf{v}_a) + \mathbf{x}_a \times \mathbf{v}_a \cdot \text{grad } (\rho_a \mathbf{v}_a) + \mathbf{x}_a \times \rho_a \mathbf{v}_a \text{div } \mathbf{v}_a] dV \\
&= \int [\mathbf{x}_a \times \mathbf{v}_a \cdot \text{grad } (\rho_a \mathbf{v}_a) + \mathbf{x}_a \times \rho_a \mathbf{v}_a \text{div } \mathbf{v}_a] dV, \quad (2.36)
\end{aligned}$$

where e_{ijk} is the permutation symbol.

Using the component form for the moment of the partial stress vector acting on the surface, and again dropping the subscript for the constituent while the index notation is employed,

$$\oint (\mathbf{x}_a \times \mathbf{T}_a \mathbf{n}) dS = \oint [e_{ijk} x_j T_{kp} n_p] dS.$$

Now, applying the divergence theorem (Equation 2.20)

$$\begin{aligned} \oint [e_{ijk} x_j T_{kp} n_p] dS &= \int \{ \partial [e_{ijk} x_j T_{kp}] / \partial x_p \} dV \\ &= \int \{ e_{ijk} [\partial x_j / \partial x_p T_{kp} + x_j \partial T_{kp} / \partial x_p] \} dV \\ &= \int \{ e_{ijk} [\delta_{jp} T_{kp} + x_j \partial T_{kp} / \partial x_p] \} dV \\ &= \int \{ e_{ipk} T_{kp} + e_{ijk} x_j \partial T_{kp} / \partial x_p \} dV, \end{aligned}$$

$e_{ipk} T_{kp} = -e_{ikp} T_{kp}$ are components of twice the dual or axial vector, t^A , of the antisymmetric part of $\mathbf{T}$, i.e.

$$\begin{aligned} 2t^A &= -e_{ijk} T_{jk} e_i \\ &= (T_{32} - T_{23}) e_1 + (T_{13} - T_{31}) e_2 + (T_{21} - T_{12}) e_3 \\ &= \mathbf{T}_a^T - \mathbf{T}_a. \end{aligned}$$

Also, notice that $e_{ijk} x_j \partial T_{kp} / \partial x_p$ are the components of $\mathbf{x} \times \text{div } \mathbf{T}$, so

$$\oint (\mathbf{x}_a \times \mathbf{T}_a \mathbf{n}) dS = \int [\mathbf{x}_a \times \text{div } \mathbf{T}_a + (\mathbf{T}_a^T - \mathbf{T}_a)] dV. \quad (2.37)$$

Then, collecting terms,

$$\begin{aligned} \int \{ \mathbf{x}_a \times \partial(\rho_a \mathbf{v}_a) / \partial t + \mathbf{x}_a \times \mathbf{v}_a \cdot \text{grad}(\rho_a \mathbf{v}_a) + \mathbf{x}_a \times \rho_a \mathbf{v}_a \text{div } \mathbf{v}_a \\ - [\mathbf{x}_a \times \text{div } \mathbf{T}_a + (\mathbf{T}_a^T - \mathbf{T}_a)] - (\mathbf{x} \times \rho_a \mathbf{b}_a) - \dot{\mathbf{M}}_a^+ - \mathbf{x}_a \times \dot{\mathbf{m}}_a^+ \} dV = 0, \end{aligned}$$

and since this must hold for an arbitrary body

$$\begin{aligned} & \mathbf{x}_a \times \partial(\rho_a \mathbf{v}_a)/\partial t + [\mathbf{x}_a \times \mathbf{v}_a \cdot \text{grad}(\rho_a \mathbf{v}_a) + \mathbf{x}_a \times \rho_a \mathbf{v}_a \text{div} \mathbf{v}_a] \\ & - [\mathbf{x}_a \times \text{div} \mathbf{T}_a + (\mathbf{T}_a^T - \mathbf{T}_a)] - (\mathbf{x}_a \times \rho_a \mathbf{b}_a) - \mathbf{M}_a^+ - \mathbf{x}_a \times \mathbf{m}_a^+ = \mathbf{0} \end{aligned}$$

Noting that the first two expressions are just $\mathbf{x}_a \times (\rho_a \mathbf{v}_a)$, the above becomes,

$$\begin{aligned} & \mathbf{x}_a \times (\rho_a \mathbf{v}_a) + \mathbf{x}_a \times \rho_a \mathbf{v}_a \text{div} \mathbf{v}_a - [\mathbf{x}_a \times \text{div} \mathbf{T}_a + (\mathbf{T}_a^T - \mathbf{T}_a)] \\ & - (\mathbf{x}_a \times \rho_a \mathbf{b}_a) - \mathbf{M}_a^+ - \mathbf{x}_a \times [\rho_a \mathbf{v}_a - \text{div} \mathbf{T}_a - \rho_a \mathbf{b}_a + \mathbf{c}_a^+ \mathbf{v}_a] = \mathbf{0}. \end{aligned}$$

Using local form for the balance of linear momentum (Equation 2.32), this reduces to

$$\mathbf{x}_a \times (\rho_a \mathbf{v}_a) + [\mathbf{x}_a \times \rho_a \mathbf{v}_a \text{div} \mathbf{v}_a] - (\mathbf{T}_a^T - \mathbf{T}_a) - \mathbf{M}_a^+ - \mathbf{x}_a \times \mathbf{c}_a^+ \mathbf{v}_a = \mathbf{0},$$

into which the local mass balance for constituent a (Equation 2.26) is substituted,

$$\begin{aligned} & \mathbf{x}_a \times (\rho_a \mathbf{v}_a) + [\mathbf{x}_a \times \rho_a \mathbf{v}_a \text{div} \mathbf{v}_a] - (\mathbf{T}_a^T - \mathbf{T}_a) - \mathbf{M}_a^+ \\ & - \mathbf{x}_a \times (\rho_a + \rho_a \text{div} \mathbf{v}_a) \mathbf{v}_a = \mathbf{0}. \end{aligned}$$

The local form for the angular momentum balance equation for the constituent is

$$\mathbf{M}_a^+ = \mathbf{T}_a - \mathbf{T}_a^T. \quad (2.38)$$

This implies that the partial stress for the constituent is not necessarily symmetric, unless $\mathbf{M}_a^+ = \mathbf{0}$.

Balance of Equilibrated Force for the Constituents

As mentioned earlier, when the volume fraction is adopted as an additional kinematic variable, an additional balance equation is included in

the theory to account for changes in the volume fraction of the constituents. This equation is called the balance of equilibrated force. The global form assumed by Passman, Nunziato and Walsh [1984] and which is adapted from the theory proposed by Goodman and Cowan [1972] for granular materials is

$$\int v_a^+ dV = (\int \rho_a k_a v_a dV) - \oint h_a \cdot n dS - \int \rho_a (g_a + l_a) dV. \quad (2.39)$$

It is readily apparent that this conservation principle is similar in form to the global linear momentum balance equations (Equation 2.34). The terminology used for these equilibrated terms reflects this similarity. Here, v_a^+ represents the equilibrated force interaction, k_a is the equilibrated inertia, v_a is the volume fraction, h_a is the equilibrated stress, g_a is the equilibrated force supply, and l_a is the external equilibrated body force; all of the constituent.

Applying the Reynolds transport theorem (Equation 2.19) to the first term on the right hand side of Equation 2.60 gives

$$(\int \rho_a k_a v_a) = \int \partial[\rho_a k_a v_a] / \partial t dV + \oint \rho_a k_a v_a v_a \cdot n dS, \quad (2.40)$$

then, use of the divergence theorem (Equation 2.25) on the surface integrals in Equations 2.39 and 2.40 yields,

$$\begin{aligned} \oint \rho_a k_a v_a v_a \cdot n dS &= \int \text{div} (\rho_a k_a v_a v_a) dV \\ &= \int \text{grad} (\rho_a k_a v_a) \cdot v_a + \rho_a k_a v_a (\text{div} v_a) dV, \end{aligned} \quad (2.41)$$

and

$$\oint h_a \cdot n dS = \int \text{div} h_a dV. \quad (2.42)$$

Appropriate substitution of Equations 2.41 and 2.42 into 2.39 yields the volume integral,

$$\int [\partial(\rho_a k_a' v_a) / \partial t + \text{grad}(\rho_a k_a' v_a) \cdot v_a + \rho_a k_a' v_a (\text{div } v_a) - \text{div } h_a - (\rho_a(g_a + l_a) - v_a^+)] dV = 0,$$

which, since the body is arbitrary, gives a differential form for the balance of equilibrated force equation for the constituent,

$$\partial(\rho_a k_a' v_a) / \partial t + \text{grad}(\rho_a k_a' v_a) \cdot v_a + \rho_a k_a' v_a (\text{div } v_a) - \text{div } h_a - (\rho_a(g_a + l_a) - v_a^+) = 0. \quad (2.43)$$

Noting that the first two terms in Equation 2.43 are the material derivative of $\rho_a k_a' v_a$, the equation gives

$$\begin{aligned} & (\rho_a k_a' v_a)' + \rho_a k_a' v_a (\text{div } v_a) - \text{div } h_a - \rho_a(g_a + l_a) - v_a^+ = 0 \\ & \rho_a'(k_a' v_a) + \rho_a k_a' v_a + \rho_a k_a' v_a (\text{div } v_a) - \text{div } h_a - \rho_a(g_a + l_a) - v_a^+ = 0 \\ & \rho_a'(k_a' v_a) + k_a' v_a(\rho_a + \rho_a \text{div } v_a) - \text{div } h_a - \rho_a(g_a + l_a) - v_a^+ = 0. \end{aligned}$$

Substituting from the local form for the mass balance of the constituents (Equation 2.26), the local balance of equilibrated force is achieved,

$$v_a^+ = \rho_a'(k_a' v_a) - \text{div } h_a - \rho_a(g_a + l_a) + c_a^+ k_a' v_a. \quad (2.44)$$

Balance of Energy for the Constituents

The energy equation is also frequently referred to as the first law of thermodynamics. The integral form for the conservation of energy of the constituent is given as

$$\begin{aligned}
\int e_a^+ dV = & \left(\int \rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a \nu_a^2 / 2) dV \right. \\
& - \oint (T_a^T \mathbf{v}_a + \mathbf{h}_a \nu_a - \mathbf{q}_a) \cdot \mathbf{n} dS \\
& \left. - \int \rho_a (\mathbf{b}_a \cdot \mathbf{v}_a + l_a \nu_a + r_a) dV, \quad (2.45)
\right.
\end{aligned}$$

where e_a^+ is the energy interaction of the a^{th} constituent with the others, $\mathbf{q}_a$ is the constituent heat flux, r_a is the external heat supply for the constituent, and e_a is the internal energy which represents all of the energy of the constituent exclusive of the kinetic energy.

The Reynolds transport theorem (Equation 2.19) applied to the first integral on the right in Equation 2.45 gives

$$\begin{aligned}
& \left(\int \rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a \nu_a^2 / 2) dV \right) \\
& = \int \{ \partial [\rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a \nu_a^2 / 2)] / \partial t \} dV \\
& \quad + \oint \{ \rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a \nu_a^2 / 2) \mathbf{v}_a \cdot \mathbf{n} \} dS
\end{aligned}$$

and substituting this into the energy balance equation gives

$$\begin{aligned}
\int e_a^+ dV = & \int \partial [\rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a \nu_a^2 / 2)] / \partial t dV + \oint \rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 \\
& + k_a \nu_a^2 / 2) \mathbf{v}_a \cdot \mathbf{n} dS - \oint (T_a^T \mathbf{v}_a + \mathbf{h}_a \nu_a - \mathbf{q}_a) \cdot \mathbf{n} dS \\
& - \int \rho_a (\mathbf{b}_a \cdot \mathbf{v}_a + l_a \nu_a + r_a) dV. \quad (2.46)
\end{aligned}$$

In this, the first integral on the right hand side of the equation indicates the time rate of change of the total instantaneous energy of a , the second indicates the flux of energy across the boundary, the third gives the work rate of the surface tractions, work rate of the tractions due to equilibrated stress and the flux of heat across the surface of the body. The

last term simply adds work or energy due to the body forces and external heat supply.

The surface integrals in Equation 2.46 converted to volume integrals by Equation 2.20 are

$$\begin{aligned}
 & \oint \rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a \nu_a^2 / 2) \mathbf{v}_a \cdot \mathbf{n} \, dS \\
 &= \int \operatorname{div} [\rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a \nu_a^2 / 2) \mathbf{v}_a] \, dV \\
 &= \int [\operatorname{grad} (\rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a \nu_a^2 / 2)) \cdot \mathbf{v}_a \\
 &\quad + \rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a \nu_a^2 / 2) (\operatorname{div} \mathbf{v}_a)] \, dV \\
 &\hspace{15em} (2.47)
 \end{aligned}$$

and

$$\begin{aligned}
 & \oint (\mathbf{T}_a^T \mathbf{v}_a + \mathbf{h}_a \nu_a - \mathbf{q}_a) \cdot \mathbf{n} \, dS = \oint (\mathbf{v}_a \mathbf{T}_a + \mathbf{h}_a \nu_a - \mathbf{q}_a) \cdot \mathbf{n} \, dS \\
 &= \int \operatorname{div} (\mathbf{v}_a \mathbf{T}_a + \mathbf{h}_a \nu_a - \mathbf{q}_a) \, dV \\
 &= \int [\mathbf{v}_a \cdot (\operatorname{div} \mathbf{T}_a) + (\operatorname{grad} \mathbf{v}_a) \cdot \mathbf{T}_a + (\operatorname{div} \mathbf{h}_a) \nu_a \\
 &\quad + \mathbf{h}_a \cdot (\operatorname{grad} \nu_a) - \operatorname{div} \mathbf{q}_a] \, dV \\
 &= \int [(\operatorname{div} \mathbf{T}_a) \cdot \mathbf{v}_a + \mathbf{T}_a \cdot \mathbf{L}_a + (\operatorname{div} \mathbf{h}_a) \nu_a + \mathbf{h}_a \cdot (\operatorname{grad} \nu_a) - \operatorname{div} \mathbf{q}_a] \, dV. \\
 &\hspace{15em} (2.48)
 \end{aligned}$$

Where, in general, the scalar product of two tensors is defined as

$$\mathbf{A} \cdot \mathbf{B} = \operatorname{tr}(\mathbf{AB}) = \operatorname{tr}(\mathbf{BA}) = \mathbf{B} \cdot \mathbf{A}$$

Collecting terms from Equations 2.47 and 2.48 into 2.46 under the volume integral yields

$$\begin{aligned}
& \int \{ \partial [\rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2)] / \partial t \\
& + \operatorname{div} [\rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) \mathbf{v}_a] \\
& - \operatorname{div} (\mathbf{v}_a \mathbf{T}_a + \mathbf{h}_a v_a - \mathbf{q}_a) \\
& - \rho_a (\mathbf{b}_a \cdot \mathbf{v}_a + l_a v_a + r_a) - e_a^+ \} dV = 0,
\end{aligned}$$

and since the region is arbitrary,

$$\begin{aligned}
& \partial [\rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2)] / \partial t + \operatorname{div} [\rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) \mathbf{v}_a] \\
& - \operatorname{div} (\mathbf{v}_a \mathbf{T}_a + \mathbf{h}_a v_a - \mathbf{q}_a) - \rho_a (\mathbf{b}_a \cdot \mathbf{v}_a + l_a v_a + r_a) - e_a^+ = 0.
\end{aligned} \tag{2.49}$$

Applying the material time derivative (Equation 2.11) gives

$$\begin{aligned}
& [\rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2)] - \mathbf{v}_a \operatorname{grad} [\rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2)] + \\
& \operatorname{grad} (\rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2)) \mathbf{v}_a + \rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) (\operatorname{div} \mathbf{v}) \\
& - \operatorname{div} (\mathbf{v}_a \mathbf{T}_a + \mathbf{h}_a v_a - \mathbf{q}_a) - \rho_a (\mathbf{b}_a \cdot \mathbf{v}_a + l_a v_a + r_a) - e_a^+ = 0,
\end{aligned}$$

which leads to

$$\begin{aligned}
& \rho_a' (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) + \rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) \\
& + \rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) (\operatorname{div} \mathbf{v}) - \operatorname{div} (\mathbf{v}_a \mathbf{T}_a + \mathbf{h}_a v_a - \mathbf{q}_a) \\
& - \rho_a (\mathbf{b}_a \cdot \mathbf{v}_a + l_a v_a + r_a) - e_a^+ = 0.
\end{aligned}$$

Substituting from the equation for mass balance of the constituent (Equation 2.33), the energy balance reduces to

$$\begin{aligned}
e_a^+ = & \rho_a (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) + c_a^+ (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) \\
& - \mathbf{v}_a \cdot (\text{div } \mathbf{T}_a) - (\text{grad } v_a) \cdot \mathbf{T}_a - (\text{div } \mathbf{h}_a) v_a - \mathbf{h}_a \cdot (\text{grad } v_a) \\
& + \text{div } \mathbf{q}_a - \rho_a (\mathbf{b}_a \cdot \mathbf{v}_a + l_a v_a + r_a). \quad (2.50)
\end{aligned}$$

Differentiating the first derivative on the right, and using the chain rule gives

$$'(e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) = 'e_a + \mathbf{v}_a \cdot ' \mathbf{v}_a + 'k_a v_a^2 / 2 + k_a v_a'' v_a. \quad (2.51)$$

It will be useful to notice for the upcoming manipulations that,

$$'(k_a v_a) = 'k_a v_a + k_a'' v_a,$$

so that the material time derivative of Equation 2.51 may be written as

$$'(e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) = 'e_a + \mathbf{v}_a \cdot ' \mathbf{v}_a + '(k_a v_a)' v - 'k_a v_a^2 / 2. \quad (2.52)$$

Substituting Equation 2.51 into Equation 2.50 gives

$$\begin{aligned}
e_a^+ = & \rho_a ('e_a + \mathbf{v}_a \cdot ' \mathbf{v}_a + 'k_a v_a^2 / 2 + k_a v_a'' v_a) \\
& + c_a^+ (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) - \mathbf{v}_a \cdot (\text{div } \mathbf{T}_a) - (\text{grad } v_a) \cdot \mathbf{T}_a \\
& - (\text{div } \mathbf{h}_a) v_a - \mathbf{h}_a \cdot (\text{grad } v_a) + \text{div } \mathbf{q}_a - \rho_a \mathbf{b}_a \cdot \mathbf{v}_a - \rho_a l_a v_a - \rho_a r_a.
\end{aligned}$$

This equation is next manipulated in order to get the energy interaction in terms of the other interactions and using Equation 2.52

$$\begin{aligned}
e_a^+ = & c_a^+ (e_a + \mathbf{v}_a \cdot \mathbf{v}_a / 2 + k_a v_a^2 / 2) + c_a^+ (\mathbf{v}_a \cdot \mathbf{v}_a - \mathbf{v}_a \cdot \mathbf{v}_a + k_a v_a^2 \\
& - k_a v_a^2) + \rho_a (\mathbf{v}_a \cdot ' \mathbf{v}_a + '(k_a v_a)' v - 'k_a v_a^2 / 2) + \rho_a 'e_a \\
& - (\text{div } \mathbf{T}_a) \cdot \mathbf{v}_a - \mathbf{T}_a \cdot \mathbf{L}_a - (\text{div } \mathbf{h}_a) v_a - \mathbf{h}_a \cdot (\text{grad } v_a) \\
& + \text{div } \mathbf{q}_a - \rho_a \mathbf{b}_a \cdot \mathbf{v}_a - \rho_a l_a v_a - \rho_a r_a + (\rho_a g_a v_a - \rho_a g_a v_a)
\end{aligned}$$

$$\begin{aligned}
&= c_a^+ (e_a - \mathbf{v}_a \cdot \mathbf{v}_a / 2 - k_a' v_a^2 / 2) + (c_a^+ \mathbf{v}_a + \rho_a' \mathbf{v}_a - \text{div } \mathbf{T}_a - \rho_a' \mathbf{b}_a) \cdot \mathbf{v}_a \\
&\quad + (c_a^+ k_a' v_a + \rho_a' (k_a' v_a) - \text{div } \mathbf{h}_a - \rho_a' (l_a + g_a)) v + \rho_a' e_a - \mathbf{T}_a : \mathbf{L}_a \\
&\quad - \mathbf{h}_a \cdot (\text{grad } v_a) - \rho_a' k_a' v_a^2 / 2 + \rho_a' g_a v_a + \text{div } \mathbf{q}_a - \rho_a' r_a.
\end{aligned}$$

Then, substituting the appropriate interaction terms from Equations 2.32 and 2.44 into this the local form of the energy equation for the constituent is

$$\begin{aligned}
e_a^+ &= c_a^+ (e_a - \mathbf{v}_a \cdot \mathbf{v}_a / 2 - k_a' v_a^2 / 2) + m_a^+ \cdot \mathbf{v}_a + v_a^+ v + \rho_a' e_a - \mathbf{T}_a : \mathbf{L}_a \\
&\quad - \mathbf{h}_a \cdot (\text{grad } v_a) - \rho_a' k_a' v_a^2 / 2 + \rho_a' g_a v_a + \text{div } \mathbf{q}_a - \rho_a' r_a. \quad (2.53)
\end{aligned}$$

Rules for Summing and Mixture Balance Equations

The interaction terms postulated in the theory are considered to be representative of exchanges only among constituents, and as such should all be in balance with each other. In accordance with this, the interaction of all constituents sum to zero.

Summation of the constituent interactions:

$$\sum c_a^+ = 0, \quad (2.54)$$

$$\sum m_a^+ = 0, \quad (2.55)$$

$$\sum H_a^+ = 0, \quad (2.56)$$

$$\sum v_a^+ = 0, \quad (2.57)$$

$$\sum e_a^+ = 0. \quad (2.58)$$

Properties of the mixture should be defined in terms of the properties of the constituents in such a way that the conservation principles for the

mixture are the same as those defined for a single continuum. Summing over all of the constituent balance equations should lead to the standard forms for the balance equations of the mixture. In order to satisfy these requirements, certain restrictions must be imposed. Suitable forms for these restrictions are developed here.

Summing over all of the constituents in the balance of mass equation (Equation 2.26), where, as mentioned previously, the summation $\sum$ symbol implies summation over all of the constituents,

$$\sum c_a^+ = \sum [\rho_a + \rho_a \operatorname{div} \mathbf{v}_a]. \quad (2.59)$$

Imposition of the summation requirement for the mass interaction (Equation 2.54) and using the material time derivative (Equation 2.11) on Equation 2.59 leads to

$$\sum [\partial \rho_a / \partial t + \mathbf{v}_a \cdot \operatorname{grad} \rho_a + \rho_a \operatorname{div} \mathbf{v}_a] = 0$$

$$\sum [\partial \rho_a / \partial t + \operatorname{div} (\rho_a \mathbf{v}_a)] = 0$$

$$\partial (\sum [\rho_a]) / \partial t + \operatorname{div} \sum (\rho_a \mathbf{v}_a) = 0$$

$$\partial \rho / \partial t + \operatorname{div} (\rho \mathbf{v}) = 0$$

$$\partial \rho / \partial t + \mathbf{v} \operatorname{div} \rho + \rho \operatorname{div} \mathbf{v} = 0$$

$$\dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0, \quad (2.60)$$

which is the usual mass balance equation for a single continuum, and therefore for the mixture.

A useful identity which will be used subsequently is the material time derivative for a mixture quantity, Γ , of the form,

$$\Gamma = \sum [\rho_a \Gamma_a] / \rho.$$

Now,

$$\rho\Gamma = \sum [\rho_a \Gamma_a],$$

so that

$$\partial(\rho\Gamma)/\partial t = \sum \partial[\rho_a \Gamma_a]/\partial t,$$

or, using the material time derivative in spatial coordinates for the mixture (Equation 2.18) and for the constituents (Equation 2.11) yields

$$\dot{(\rho\Gamma)} - \mathbf{v} \cdot \text{grad}(\rho\Gamma) = \sum [\dot{(\rho_a \Gamma_a)} - \mathbf{v}_a \cdot \text{grad}(\rho_a \Gamma_a)],$$

$$\rho \dot{\Gamma} - \dot{\rho}\Gamma - \mathbf{v} \cdot \text{grad}(\rho\Gamma) = \sum [\rho_a \dot{\Gamma}_a + \dot{\rho}_a \Gamma_a - \mathbf{v}_a \cdot \text{grad}(\rho_a \Gamma_a)].$$

Substituting from the mass balance equation (Equation 2.33)

$$\begin{aligned} \rho \dot{\Gamma} - \rho\Gamma \text{div } \mathbf{v} - \mathbf{v} \cdot \text{grad}(\rho\Gamma) &= \sum [\rho_a \dot{\Gamma}_a + \Gamma_a (c_a^+ - \rho_a \text{div } \mathbf{v}_a) \\ &\quad - \mathbf{v}_a \cdot \text{grad}(\rho_a \Gamma_a)], \end{aligned}$$

so,

$$\rho \dot{\Gamma} - \text{div}(\rho\Gamma\mathbf{v}) = \sum [\rho_a \dot{\Gamma}_a + \Gamma_a c_a^+ - \text{div}(\rho_a \Gamma_a \mathbf{v}_a)].$$

The material time derivative for Γ may then be written as,

$$\dot{\Gamma} = \{\sum [\rho_a \dot{\Gamma}_a + \Gamma_a c_a^+ - \text{div}(\rho_a \Gamma_a \mathbf{v}_a)] + \text{div}(\rho\Gamma\mathbf{v})\}/\rho. \quad (2.61)$$

Incidentally, this may also be written in terms of the diffusion velocity, $\mathbf{u}_a$, as

$$\dot{\Gamma} = \{\sum [\rho_a \dot{\Gamma}_a + \Gamma_a c_a^+ - \text{div}(\rho_a \Gamma_a \mathbf{u}_a)]\}/\rho.$$

Now, sum over all of the balance of linear momentum equations (Equation 2.32) for the constituents

$$\sum \mathbf{m}_a^+ = \sum [\rho_a \dot{\mathbf{v}}_a - \text{div } \mathbf{T}_a - \rho_a \mathbf{b}_a + c_a^+ \mathbf{v}_a],$$

and define for the mixture,

$$\rho \mathbf{b} = \sum \rho_a \mathbf{b}_a, \quad (2.62)$$

which, in conjunction with Equation 2.55, use of the material time derivative on the mixture (Equation 2.61) gives

$$\rho \dot{\mathbf{v}} - \sum [\mathbf{v}_a c_a^+ - \text{div} (\rho_a \mathbf{v}_a \mathbf{v}_a) + \text{div} (\rho \mathbf{v} \mathbf{v}) + \text{div} \mathbf{T}_a - c_a^+ \mathbf{v}_a] - \rho \mathbf{b} = \mathbf{0}$$

$$\rho \dot{\mathbf{v}} + \sum [\text{div} \{(\rho_a \mathbf{v}_a \mathbf{v}_a) - (\rho \mathbf{v} \mathbf{v}) - \mathbf{T}_a\}] - \rho \mathbf{b} = \mathbf{0}.$$

Define the mixture stress to be related to the partial stresses as

$$\mathbf{T} = \sum [\mathbf{T}_a - (\rho_a \mathbf{v}_a \mathbf{v}_a)] + (\rho \mathbf{v} \mathbf{v}), \quad (2.63)$$

then the standard form for the linear momentum of the mixture is achieved,

$$\rho \dot{\mathbf{v}} = \text{div} \mathbf{T} + \rho \mathbf{b}. \quad (2.64)$$

Summing over the constituents for the local balance of angular momentum equation (Equation 2.38),

$$\sum \mathbf{M}_a^+ = \sum [\mathbf{T}_a - \mathbf{T}_a^T],$$

and applying the angular momentum interaction summation restriction (Equation 2.56) and the stress restriction just stated (Equation 2.63)

$$\mathbf{T} + \sum (\rho_a \mathbf{v}_a \mathbf{v}_a) - (\rho \mathbf{v} \mathbf{v}) = \mathbf{T}^T + \sum (\rho_a \mathbf{v}_a \mathbf{v}_a) - (\rho \mathbf{v} \mathbf{v}).$$

Thus the balance of angular momentum for the mixture is in the usual form for a single material,

$$\mathbf{T} = \mathbf{T}^T. \quad (2.65)$$

The constituent balance of equilibrated force (Equation 2.44), summed over all of the constituents, is

$$\sum \mathbf{v}_a^+ = \sum [\rho_a (k_a \mathbf{v}_a) - \text{div} \mathbf{h}_a - \rho_a (g_a + l_a) + c_a^+ k_a \mathbf{v}_a].$$

Define for the mixture,

$$\rho g = \sum \rho_a g_a, \quad (2.66)$$

and

$$\rho l = \sum \rho_a l_a, \quad (2.67)$$

then substitute for mass interaction from the constituent mass balance equation (Equation 2.26) and impose the summing restriction for the equilibrated force interaction terms (Equation 2.57) to obtain

$$\sum [\rho_a (k_a \cdot v_a) - \text{div } h_a + (\rho_a + \rho_a \text{div } v_a) k_a \cdot v_a] - \rho (g + l) = 0.$$

Using the material time derivative (Equation 2.11)

$$\begin{aligned} \sum [\rho_a \{ \partial(k_a \cdot v_a) / \partial t + v_a \text{grad}(k_a \cdot v_a) \} - \text{div } h_a \\ + (\partial \rho_a / \partial t + v_a \text{grad} \rho_a + \rho_a \text{div } v_a) k_a \cdot v_a] - \rho (g + l) = 0 \end{aligned}$$

$$\begin{aligned} \sum [\rho_a \partial(k_a \cdot v_a) / \partial t + \text{div}(\rho_a k_a \cdot v_a v_a) - \text{div } h_a + k_a \cdot v_a (\partial \rho_a / \partial t)] \\ - \rho (g + l) = 0 \end{aligned}$$

$$\sum [\partial(\rho_a k_a \cdot v_a) / \partial t + \text{div}\{(\rho_a k_a \cdot v_a v_a) - h_a\}] - \rho (g + l) = 0.$$

Define

$$\rho k \cdot v = \sum \rho_a k_a \cdot v_a, \quad (2.68)$$

and,

$$(\rho k \cdot v v) - h = \sum \{(\rho_a k_a \cdot v_a v_a) - h_a\}, \quad (2.69)$$

then,

$$\partial(\rho k \cdot v) / \partial t + \text{div}\{(\rho k \cdot v v) - h\} - \rho (g + l) = 0$$

$$\partial(\rho k \cdot v) / \partial t + v \text{grad}(\rho k \cdot v) + \rho k \cdot v \text{div}(v) - \text{div } h - \rho (g + l) = 0$$

$$\dot{(\rho k \cdot v)} + \rho k \cdot v \operatorname{div}(v) - \operatorname{div} h - \rho(g + l) = 0$$

$$\dot{\rho}(k \cdot v) + \rho \dot{(k \cdot v)} + \rho k \cdot v \operatorname{div}(v) - \operatorname{div} h - \rho(g + l) = 0.$$

Substitution from the balance of mass of the mixture (Equation 2.60) for $\dot{\rho}$, recovers the desired form for the balance of equilibrated force for the mixture,

$$\rho \dot{(k \cdot v)} = \operatorname{div} h + \rho(g + l). \quad (2.70)$$

This is of the correct local form required by the general equation of balance, i.e. the rate of change of the mixture equilibrated inertia is determined by source terms and a flux term.

Finally summing over the constituents for the energy balance (Equation 2.53) yields

$$\begin{aligned} \sum e_a^+ = \sum [c_a^+(e_a - v_a \cdot v_a/2 - k_a \cdot v_a^2/2) + m_a^+ \cdot v_a + v_a^+ \cdot v + \rho_a e_a \\ - T_a \cdot L_a - h_a \cdot (\operatorname{grad} v_a) - \rho_a k_a \cdot v_a^2/2 + \rho_a g_a \cdot v_a + \operatorname{div} q_a - \rho_a r_a], \end{aligned}$$

which may be written in the following form, as is readily seen by referring to the development of the local form from the global for the constituent energy equation, given by Equation 2.49,

$$\begin{aligned} \sum e_a^+ = \sum \{ \partial [\rho_a (e_a + v_a \cdot v_a/2 + k_a \cdot v_a^2/2)] / \partial t + \operatorname{div} [\rho_a (e_a + v_a \cdot v_a/2 \\ + k_a \cdot v_a^2/2) v] - \operatorname{div} (T_a^T v_a + h_a \cdot v_a - q_a) - \rho_a (b_a \cdot v_a + l_a \cdot v_a + r_a) \}, \end{aligned}$$

or

$$\begin{aligned} \{ \partial \sum [\rho_a (e_a + v_a \cdot v_a/2 + k_a \cdot v_a^2/2)] / \partial t + \operatorname{div} \sum [\rho_a (e_a + v_a \cdot v_a/2 \\ + k_a \cdot v_a^2/2) v - T_a^T v_a - h_a \cdot v_a + q_a] - \sum \rho_a (b_a \cdot v_a + l_a \cdot v_a + r_a) \} = 0. \end{aligned}$$

If the following definitions are made,

$$\rho(e + \mathbf{v} \cdot \mathbf{v}/2 + k'v^2/2) = \sum [\rho_a(e_a + \mathbf{v}_a \cdot \mathbf{v}_a/2 + k_a'v_a^2/2)], \quad (2.71)$$

$$\begin{aligned} \mathbf{q} - \mathbf{T}^T \mathbf{v} - \mathbf{h}'v + \rho(e + \mathbf{v} \cdot \mathbf{v}/2 + k'v^2/2)\mathbf{v} \\ = \sum \{ \mathbf{q}_a - \mathbf{T}_a^T \mathbf{v}_a - \mathbf{h}_a'v_a + \rho_a(e_a + \mathbf{v}_a \cdot \mathbf{v}_a/2 + k_a'v_a^2/2)\mathbf{v}_a \}, \end{aligned} \quad (2.72)$$

$$\rho(\mathbf{b} \cdot \mathbf{v} + l'v + r) = \rho_a(\mathbf{b}_a \cdot \mathbf{v}_a + l_a'v_a + r_a), \quad (2.73)$$

then, using Equations 2.71, 2.72 and 2.73 and summation constraint for the energy interaction (Equation 2.58), the energy balance equation for the mixture becomes

$$\begin{aligned} \partial[\rho(e + \mathbf{v} \cdot \mathbf{v}/2 + k'v^2/2)]/\partial t \\ + \text{div} [\mathbf{q} - \mathbf{T}^T \mathbf{v} - \mathbf{h}'v + \rho(e + \mathbf{v} \cdot \mathbf{v}/2 + k'v^2/2)\mathbf{v}] - \rho(\mathbf{b} \cdot \mathbf{v} + l'v + r) = 0. \end{aligned}$$

Applying the material time derivative and expanding the divergence terms as in the development going from the global to local form for the constituents yields,

$$\begin{aligned} \dot{\rho}(e + \mathbf{v} \cdot \mathbf{v}/2 + k'v^2/2) + \rho \dot{(e + \mathbf{v} \cdot \mathbf{v}/2 + k'v^2/2)} \\ - \mathbf{v} \cdot \text{grad}[\rho(e + \mathbf{v} \cdot \mathbf{v}/2 + k'v^2/2)] + \text{div} \mathbf{q} - \text{div} \mathbf{T} \cdot \mathbf{v} - \mathbf{T} \cdot \mathbf{L} - \text{div} \mathbf{h}'v \\ - \mathbf{h} \cdot \text{grad} v + \mathbf{v} \cdot \text{grad}[\rho(e + \mathbf{v} \cdot \mathbf{v}/2 + k'v^2/2)] \\ + \rho(e + \mathbf{v} \cdot \mathbf{v}/2 + k'v^2/2) \text{div} \mathbf{v} - \rho(\mathbf{b} \cdot \mathbf{v} + l'v + r) = 0, \end{aligned}$$

and substituting from the other local balance equations for the mixture Equations 2.60, 2.64 and 2.70,

$$\begin{aligned} (-\rho \text{div} \mathbf{v})(e + \mathbf{v} \cdot \mathbf{v}/2 + k'v^2/2) + \rho(\dot{e} + \dot{\mathbf{v}} \cdot \mathbf{v} + k'\dot{v}^2/2 + k'v''v) + \text{div} \mathbf{q} \\ - (\dot{\rho} \mathbf{v} - \rho \mathbf{b}) \cdot \mathbf{v} - \mathbf{T} \cdot \mathbf{L} - [\dot{\rho}(k'v) - \rho(g + l)]v - \mathbf{h} \cdot \text{grad} v \\ + \rho(e + \mathbf{v} \cdot \mathbf{v}/2 + k'v^2/2) \text{div} \mathbf{v} - \rho(\mathbf{b} \cdot \mathbf{v} + l'v + r) = 0 \end{aligned}$$

$$\rho(\dot{e} + \dot{k} \cdot v^2/2 + \dot{k} \cdot v'' \cdot v) + \text{div } \mathbf{q} - \mathbf{T} \cdot \mathbf{L} - [\rho(\dot{k} \cdot v) - \rho g] \cdot v - \mathbf{h} \cdot \text{grad } v - \rho r = 0$$

$$\rho(\dot{e} + \dot{k} \cdot v^2/2 + \dot{k} \cdot v'' \cdot v) + \text{div } \mathbf{q} - \mathbf{T} \cdot \mathbf{L} - \rho(\dot{k} \cdot v + \dot{k} \cdot v'' \cdot v - g) \cdot v - \mathbf{h} \cdot \text{grad } v - \rho r = 0.$$

This leaves the usual local energy balance equation for the mixture,

$$\rho \dot{e} = \mathbf{T} \cdot \mathbf{L} + \mathbf{h} \cdot \text{grad } v - \rho g \cdot v + \rho \dot{k} \cdot v^2/2 + \text{div } \mathbf{q} + \rho r. \quad (2.74)$$

The summation relationships are collected here in a symmetric form which shows a pleasing and intuitively comprehensible balance between the mixture and the constituents.

Collected rules for summing:

$$\rho \mathbf{b} = \sum \rho_a \mathbf{b}_a, \quad (2.62)$$

$$\mathbf{T} - \rho \mathbf{v} \mathbf{v} = \sum (\mathbf{T}_a - \rho_a \mathbf{v}_a \mathbf{v}_a), \quad (2.63)$$

$$\rho g = \sum \rho_a g_a, \quad (2.66)$$

$$\rho \mathbf{l} = \sum \rho_a \mathbf{l}_a, \quad (2.67)$$

$$\rho \dot{k} \cdot v = \sum \rho_a \dot{k}_a \cdot v_a, \quad (2.68)$$

$$\mathbf{h} - \rho \dot{k} \cdot v \mathbf{v} = \sum (\mathbf{h}_a - \rho_a \dot{k}_a \cdot v_a \mathbf{v}_a), \quad (2.69)$$

$$\rho(e + [1/2] \mathbf{v} \cdot \mathbf{v} + [1/2] \dot{k} \cdot v^2) = \sum \rho_a (e_a + [1/2] \mathbf{v}_a \cdot \mathbf{v}_a + [1/2] \dot{k}_a \cdot v_a^2), \quad (2.71)$$

$$\begin{aligned} \mathbf{q} - \mathbf{T}^T \mathbf{v} - \mathbf{h} \cdot v - \rho(e + [1/2] \mathbf{v} \cdot \mathbf{v} + \dot{k} \cdot v^2) v \\ = \sum \mathbf{q}_a - \mathbf{T}_a^T \mathbf{v}_a - \mathbf{h}_a \cdot v_a - \rho_a (e_a + [1/2] \mathbf{v}_a \cdot \mathbf{v}_a + \dot{k}_a \cdot v_a^2) \mathbf{v}_a, \end{aligned} \quad (2.72)$$

$$\rho(r + \mathbf{b} \cdot \mathbf{v} + \mathbf{l} \cdot v) = \rho_a (r_a + \mathbf{b}_a \cdot \mathbf{v}_a + \mathbf{l}_a \cdot v_a). \quad (2.73)$$

Saturated Mixtures

In the case when there are no voids present, the mixture is said to be saturated. The saturation constraint implies that

$$\sum v_a = v = 1, \quad (2.75)$$

so

$$\dot{v} = 0.$$

This leads to a simplification of the equilibrated force and energy balance equations for the mixture (Equations 2.70 and 2.74). The balance of equilibrated force for a saturated mixture is

$$\text{div } h + p(g + l) = 0, \quad (2.76)$$

and the mixture energy balance reduces to

$$\rho \dot{e} = (T \cdot L) - \text{div } q + pr. \quad (2.77)$$

Following the assertion of Truesdell and Noll [1965] that constraints are maintained by reaction forces, Passman, Nunziato and Walsh [1984] use the assertion that the simplest such reaction forces are those which do no work. They represent the reaction force for the saturation constraint by π and let w_a^+ be the work (actually the working power) done on constituent a by the other constituents as a result of the saturation. They state that the work done on constituent a , is a result of the reaction force π and the rate of change of v . Since

$$\dot{v}_a = \dot{v} + v_a \cdot \text{grad } v_a,$$

then

$$w_a^+ = \pi(\nu_a - \mathbf{v}_a \cdot \text{grad } \nu_a).$$

The extra growth of energy is defined as

$$\begin{aligned} e_a^{+e} &= e_a^+ + w_a^+ \\ &= e_a^+ + \pi(\nu_a - \mathbf{v}_a \cdot \text{grad } \nu_a), \end{aligned} \quad (2.78)$$

and since $\sum \nu_a = 1$, and $\sum e_a^+ = 0$,

$$\sum e_a^{+e} = 0. \quad (2.79)$$

π is interpreted to be the interface pressure which is required to maintain contact between phases. See also Ishii [1975] and Bedford and Drumheller [1978]. Equations 2.53 and 2.78 lead to a constituent energy balance equation of the form

$$\begin{aligned} e_a^{+e} &= c_a^+(e_a - \mathbf{v}_a \cdot \mathbf{v}_a / 2 - k_a \nu_a^2 / 2) + m_a^{+e} \cdot \mathbf{v}_a + v_a^{+e} \nu_a + \rho_a e_a \\ &\quad - \mathbf{T}_a \cdot \mathbf{L}_a - h_a (\nabla \nu_a) - \rho_a k_a \nu_a^2 / 2 + \nabla \cdot \mathbf{q}_a - \rho_a r_a, \end{aligned} \quad (2.80)$$

with the extra momentum interaction given by

$$m_a^{+e} = m_a^+ - \pi \text{grad } \nu_a. \quad (2.81)$$

This additional term in the momentum interaction is often referred to as a buoyancy force, here it represents the microstructural forces near the constituent boundaries. The extra equilibrated force is given by,

$$v_a^{+e} = v_a^+ + \pi + \rho_a g_a. \quad (2.82)$$

These balance equations, with the constraint of saturation, may now be included in the balance of linear momentum equation through Equations 2.32 and 2.81

$$m_a^{+e} = \rho_a \mathbf{v}_a - \text{div } \mathbf{T}_a - \rho_a \mathbf{b}_a + c_a^+ \mathbf{v}_a - \pi \text{grad } \nu_a, \quad (2.83)$$

and the balance of equilibrated force through Equations 2.44 and 2.82

$$v_a^{+e} = \rho_a'(k_a'v_a) - \text{div } h_a - \rho_a l_a + c_a^+ k_a'v_a + \pi. \quad (2.84)$$

Making use of the summation restrictions gives the restrictions,

$$\sum m_a^{+e} = 0 \quad (2.85)$$

and

$$\sum v_a^{+e} = N\pi + \rho g. \quad (2.86)$$

At this point it is useful, in the interest of clarity, to collect the local balance equations for a general saturated multiphase mixture, such as the type under consideration in this dissertation.

Balance equations for the constituents of a saturated mixture:

Balance of Mass for the Constituent

$$c_a^+ = \rho_a + \rho_a \text{div } v_a, \quad (2.26)$$

Balance of Linear Momentum for the Constituent

$$m_a^{+e} = \rho_a'v_a - \text{div } T_a - \rho_a b_a + c_a^+ v_a - \pi \text{grad } v_a, \quad (2.83)$$

Balance of Angular Momentum for the Constituent

$$M_a^+ = T_a - T_a^T, \quad (2.38)$$

Balance of Equilibrated Force for the Constituent

$$v_a^{+e} = \rho_a'(k_a'v_a) - \text{div } h_a - \rho_a l_a + c_a^+ k_a'v_a + \pi, \quad (2.84)$$

Balance of Energy for the Constituent

$$\begin{aligned} e_a^{+e} = & c_a^+(e_a - v_a \cdot v_a / 2 - k_a'v_a^2 / 2) + m_a^{+e} \cdot v_a + v_a^{+e} \cdot v + \rho_a' e_a - T_a : L_a \\ & - h_a \cdot (\nabla' v_a) - \rho_a' k_a'v_a^2 / 2 + \nabla \cdot q_a - \rho_a' r_a. \end{aligned} \quad (2.80)$$

Balance Equations for a Saturated Mixture:

Balance of Mass for the Mixture

$$\dot{\rho} = -\rho \operatorname{div} \mathbf{v}, \quad (2.60)$$

Balance of Linear Momentum for the Mixture

$$\rho \dot{\mathbf{v}} = \operatorname{div} \mathbf{T} + \rho \mathbf{b}, \quad (2.64)$$

Balance of Angular Momentum for the Mixture

$$\mathbf{T} = \mathbf{T}^T, \quad (2.65)$$

Balance of Equilibrated Force for the Mixture

$$0 = \operatorname{div} \mathbf{h} + \rho (\mathbf{g} + \mathbf{l}), \quad (2.76)$$

Balance of Energy for the Mixture

$$\rho \dot{e} = (\mathbf{T} \cdot \mathbf{L}) - \operatorname{div} \mathbf{q} + \rho r. \quad (2.77)$$

The Entropy Inequality

Following an approach analogous to the general balance equation the constituent entropy balance equation is given as,

$$\int \eta_a^+ dV = \left(\int \rho_a \eta_a dV \right) + \oint (\mathbf{q}_a \cdot \mathbf{n} / \theta_a) dS - \int (\rho_a r_a / \theta_a) dV, \quad (2.87)$$

where η_a^+ is the entropy interaction, η_a is the entropy of constituent a , and θ_a is the temperature of the a^{th} constituent.

Applying the Reynolds transport theorem (Equation 2.19) to the first term on the right of Equation 2.87 yields

$$\left(\int \rho_a \eta_a dV \right) = \int \partial(\rho_a \eta_a) / \partial t dV + \oint (\rho_a \eta_a) \mathbf{v}_a \cdot \mathbf{n} dS \quad (2.88)$$

and then utilizing the divergence theorem (Equation 2.20) to convert the surface integrals in Equation 2.88 to volume integrals gives

$$\oint (\rho_a \eta_a) \mathbf{v}_a \cdot \mathbf{n} \, dS = \int [\text{grad}(\rho_a \eta_a) \cdot \mathbf{v}_a + (\rho_a \eta_a) \text{div } \mathbf{v}] \, dV,$$

so that

$$\begin{aligned} \frac{d}{dt} \left(\int \rho_a \eta_a \, dV \right) &= \int \left[\frac{\partial (\rho_a \eta_a)}{\partial t} + \text{grad}(\rho_a \eta_a) \cdot \mathbf{v}_a + (\rho_a \eta_a) \text{div } \mathbf{v} \right] \, dV \\ &= \int \left[\dot{(\rho_a \eta_a)} + (\rho_a \eta_a) \text{div } \mathbf{v} \right] \, dV. \end{aligned} \quad (2.89)$$

Once again applying the divergence theorem (Equation 2.25), to the surface integral in Equation 2.87, yields

$$\oint (\mathbf{q}_a \cdot \mathbf{n} / \theta_a) \, dS = \int \text{div} (\mathbf{q}_a / \theta_a) \, dV.$$

The growth of entropy equation in the global form becomes,

$$\int \left[\dot{\rho}_a \eta_a + \rho_a \dot{\eta}_a + (\rho_a \eta_a) \text{div } \mathbf{v}_a + \text{div} (\mathbf{q}_a / \theta_a) - (\rho_a r_a / \theta_a) - \eta_a^+ \right] dV = 0,$$

but, since this is an arbitrary boundary the local form may be written as

$$\dot{\rho}_a \eta_a + \rho_a \dot{\eta}_a + (\rho_a \eta_a) \text{div } \mathbf{v}_a + \text{div} (\mathbf{q}_a / \theta_a) - (\rho_a r_a / \theta_a) - \eta_a^+ = 0.$$

Substituting the equation for the mass balance of the constituents (Equation 2.33), this becomes

$$\begin{aligned} (c_a^+ - \rho_a \text{div } \mathbf{v}_a) \eta_a + \rho_a \dot{\eta}_a + (\rho_a \eta_a) \text{div } \mathbf{v}_a \\ + \text{div} (\mathbf{q}_a / \theta_a) - (\rho_a r_a / \theta_a) - \eta_a^+ = 0 \end{aligned}$$

or,

$$\eta_a^+ = c_a^+ \eta_a + \rho_a \dot{\eta}_a + \text{div} (\mathbf{q}_a / \theta_a) - (\rho_a r_a / \theta_a).$$

The total entropy is defined as,

$$\rho \eta = \sum \rho_a \eta_a.$$

Following the usual assumption of the second law of thermodynamics, the total entropy growth is non-negative,

$$\sum \eta_a^+ \geq 0,$$

The Entropy Inequality for the mixture may be written as

$$\sum [c_a^+ \eta_a + \rho_a' \eta_a + \text{div} (\mathbf{q}_a / \theta_a) - (\rho_a r_a / \theta_a)] \geq 0. \quad (2.90)$$

Using the balance of energy equation for the constituents (Equation 2.80) to eliminate the term $\rho_a r_a$ from the inequality,

$$\begin{aligned} \sum [c_a^+ \eta_a + \rho_a' \eta_a + \text{div} (\mathbf{q}_a / \theta_a) - \{c_a^+ (e_a - \mathbf{v}_a \cdot \mathbf{v}_a / 2 - k_a' v_a^2 / 2) \\ + m_a^{+e} \cdot \mathbf{v}_a + v_a^{+e} \cdot \mathbf{v} + \rho_a' e_a - T_a' L_a - h_a' (\text{grad } v_a) \\ - \rho_a' k_a' v_a^2 / 2 + \text{div } \mathbf{q}_a - e_a^{+e}\} / \theta_a] \geq 0. \end{aligned} \quad (2.91)$$

Let ψ_a represent the Helmholtz free energy of the constituent, which is defined as,

$$\psi_a \equiv e_a - \theta_a \eta_a, \quad (2.92)$$

so

$$e_a = \psi_a + \theta_a \eta_a.$$

The term "free energy" is used since the Helmholtz free energy sets a maximum on the work energy that can be liberated in a process.

Using the chain rule,

$$\begin{aligned} \text{div} (\mathbf{q}_a / \theta_a) &= \text{div } \mathbf{q}_a / \theta_a + \mathbf{q}_a \cdot \text{grad } (1 / \theta_a) \\ &= \text{div } \mathbf{q}_a / \theta_a - (\mathbf{q}_a / \theta_a^2) \cdot \text{grad } \theta_a, \end{aligned}$$

and substituting this into the dissipation inequality (Equation 2.91)

$$\begin{aligned} \sum [c_a^+ \eta_a + \rho_a \eta_a + \text{div } \mathbf{q}_a / \theta_a - (\mathbf{q}_a / \theta_a^2) \cdot \text{grad } \theta_a \\ - \{c_a^+ (\psi_a + \theta_a \eta_a - \mathbf{v}_a \cdot \mathbf{v}_a / 2 - k_a \nu_a^2 / 2) + m_a^{+e} \cdot \mathbf{v}_a + v_a^{+e} \nu \\ + \rho_a (\psi_a + \theta_a \eta_a + \theta_a' \eta_a) - T_a \cdot \mathbf{L}_a - h_a \cdot (\text{grad } \nu_a) - \rho_a k_a \nu_a^2 / 2 \\ + \text{div } \mathbf{q}_a - e_a^{+e} \} / \theta_a] \geq 0. \end{aligned}$$

$$\begin{aligned} \sum [- (\mathbf{q}_a / \theta_a^2) \cdot \text{grad } \theta_a + \mathbf{q}_a \cdot \text{grad } (1 / \theta_a) - \{c_a^+ (\psi_a - \mathbf{v}_a \cdot \mathbf{v}_a / 2 \\ - k_a \nu_a^2 / 2) + m_a^{+e} \cdot \mathbf{v}_a + v_a^{+e} \nu + \rho_a (\psi_a + \theta_a \eta_a) - T_a \cdot \mathbf{L}_a \\ - h_a \cdot (\text{grad } \nu_a) - \rho_a k_a \nu_a^2 / 2 - e_a^{+e} \} / \theta_a] \geq 0 \end{aligned}$$

$$\begin{aligned} \sum [- (\mathbf{q}_a / \theta_a) \cdot \text{grad } \theta_a - c_a^+ (\psi_a - \mathbf{v}_a \cdot \mathbf{v}_a / 2 - k_a \nu_a^2 / 2) - m_a^{+e} \cdot \mathbf{v}_a \\ - v_a^{+e} \nu - \rho_a (\psi_a + \theta_a \eta_a) + T_a \cdot \mathbf{L}_a + h_a \cdot (\text{grad } \nu_a) \\ + \rho_a k_a \nu_a^2 / 2 + e_a^{+e} \} / \theta_a] \geq 0. \end{aligned}$$

Finally the form used for the entropy inequality for saturated multiphase mixtures is

$$\begin{aligned} \sum [- \rho_a (\psi_a + \eta_a \theta_a) + T_a \cdot \mathbf{L}_a + h_a \cdot \text{grad } \nu_a - \mathbf{q}_a \cdot (\text{grad } \theta_a) / \theta_a \\ - (v_a^{+e} - \rho_a k_a \nu_a^2 / 2) \nu_a + e_a^{+e} - m_a^{+e} \cdot \mathbf{v}_a \\ - c_a^+ (\psi_a - \mathbf{v}_a \cdot \mathbf{v}_a / 2 - k_a \nu_a^2 / 2)] / \theta_a \geq 0. \end{aligned} \quad (2.93)$$

A suitable form for the entropy inequality for each constituent has yet to be developed. The second law of thermodynamics restricts the direction in which a particular process may proceed. This inequality should not be violated by any equations which are developed to describe processes for a particular material. In particular the second law may be used to impose

restrictions on thermomechanical processes and to impose restrictions on allowable forms for the constitutive equations.

CHAPTER III

CONSTITUTIVE PRINCIPLES

Constitutive Assumptions and Restrictions

The constitutive variables for the multiphase mixture do not adhere to the Principle of Equipresence [Truesdell, 1951], which indicates that an independent variable in one constitutive equation should be present in all equations of the same material. Instead, the Principle of Phase Separation [Passman, Nunziato and Walsh, 1984], deemed to be more appropriate for describing the the isolated physical nature of the individual constituents is used. Passman, Nunziato and Walsh state the Principle of Phase Separation as,

"The dependent variables of the a^{th} constituent that are material-specific depend only on the independent variables of the a^{th} constituent. The growth dependent variables depend on all of the independent variables."

The constitutive assumptions chosen are those suggested by Nunziato and Walsh [1980] for multiphase mixtures with chemical reactions and diffusion:

$$(\psi_a, \eta_a, T_a, h_a, q_a) = \mathcal{F}_a(v_a, w_a, v_a, u_a, \theta_a, F_a, g_a, c_a), \quad (3.1)$$

$$(c_a^+, v_a^+, m_a^+, H_a^+, e_a^+) = \mathcal{G}_a(v^\dagger, w^\dagger, v^\dagger, u^\dagger, \theta^\dagger, F^\dagger, g^\dagger, c^\dagger), \quad (3.2)$$

$$k_a = k_a(v_a), \quad (3.3)$$

where the subscript a , as usual, implies a dependence on that particular

constituent, and $\uparrow$ indicates a dependence on all of the constituents. The gradients of the volume fraction and temperature are given as, $\mathbf{w}_a = \text{grad } v_a$, and $\mathbf{g}_a = \text{grad } \theta_a$, and the quantities c_a and c are the mass concentrations for the constituent and mixture respectively. Mass concentration is used as a measurement of how far a chemical reaction has progressed. The mass concentration is defined for diffusing mixtures as

$$c_a = (\rho_a / \rho_R) |\det \mathbf{F}_a|, \quad (3.4)$$

where ρ_R is the reference density of the mixture. Since the sum of the partial densities yields the mixture density (Equation 2.13), then

$$\sum c_a / |\det \mathbf{F}_a| = \rho / \rho_R.$$

Now consider the material time derivative of the Helmholtz free energy, ψ_a , in spatial coordinates, so that it can be used in the entropy inequality,

$$\begin{aligned} \dot{\psi}_a &= \partial \psi_a / \partial t + (\text{grad } \psi_a) \cdot \mathbf{x}_a \\ &= (\partial \psi_a / \partial v_a) (\partial v_a / \partial t) + (\partial \psi_a / \partial v_a) (\text{grad } v_a) \cdot \mathbf{x}_a + (\partial \psi_a / \partial \mathbf{w}_a) (\partial \mathbf{w}_a / \partial t) \\ &\quad + (\partial \psi_a / \partial \mathbf{w}_a) (\text{grad } \mathbf{w}_a) \cdot \mathbf{x}_a + (\partial \psi_a / \partial v_a) (\partial v_a / \partial t) \\ &\quad + (\partial \psi_a / \partial v_a) (\text{grad } v_a) \cdot \mathbf{x}_a + (\partial \psi_a / \partial \mathbf{u}_a) (\partial \mathbf{u}_a / \partial t) \\ &\quad + (\partial \psi_a / \partial \mathbf{u}_a) (\text{grad } \mathbf{u}_a) \cdot \mathbf{x}_a + (\partial \psi_a / \partial \theta_a) (\partial \theta_a / \partial t) \\ &\quad + (\partial \psi_a / \partial \theta_a) (\text{grad } \theta_a) \cdot \mathbf{x}_a + \text{tr}[(\partial \psi_a / \partial \mathbf{F}_a) (\partial \mathbf{F}_a / \partial t) \\ &\quad + (\partial \psi_a / \partial \mathbf{F}_a) (\text{grad } \mathbf{F}_a) \cdot \mathbf{x}_a] + (\partial \psi_a / \partial \mathbf{g}_a) (\partial \mathbf{g}_a / \partial t) \end{aligned}$$

$$\begin{aligned}
& + (\partial\psi_a/\partial\mathbf{g}_a)(\text{grad } \mathbf{g}_a) \cdot \mathbf{x}_a + (\partial\psi_a/\partial c_a)(\partial c_a/\partial t) \\
& + (\partial\psi_a/\partial c_a)(\text{grad } c_a) \cdot \mathbf{x}_a.
\end{aligned}$$

Collecting terms and utilizing the definition of the material derivative, the time derivative in spatial coordinates of the Helmholtz free energy for the constituent is

$$\begin{aligned}
\dot{\psi}_a = & (\partial\psi_a/\partial v_a)\dot{v}_a + (\partial\psi_a/\partial \mathbf{w}_a)\dot{\mathbf{w}}_a + (\partial\psi_a/\partial v_a)v_a + (\partial\psi_a/\partial \mathbf{u}_a)\dot{\mathbf{u}}_a \\
& + (\partial\psi_a/\partial \theta_a)\dot{\theta}_a + \text{tr}[(\partial\psi_a/\partial \mathbf{F}_a)\dot{\mathbf{F}}_a] + (\partial\psi_a/\partial \mathbf{g}_a)\dot{\mathbf{g}}_a + (\partial\psi_a/\partial c_a)\dot{c}_a.
\end{aligned} \tag{3.5}$$

The material time derivatives for the volume fraction and its gradient are,

$$\begin{aligned}
\dot{v}_a & = \partial v_a / \partial t + (\text{grad } v_a) \cdot \mathbf{v}_a \\
& = \partial v_a / \partial t + \mathbf{w}_a \cdot \mathbf{v}_a,
\end{aligned}$$

and

$$\dot{\mathbf{w}}_a = \partial \mathbf{w}_a / \partial t + (\text{grad } \mathbf{w}_a) \cdot \mathbf{v}_a. \tag{3.6}$$

It follows then, that

$$\begin{aligned}
\text{grad } \dot{v}_a & = \text{grad}(\partial v_a / \partial t) + \text{grad}(\mathbf{w}_a \cdot \mathbf{v}_a) \\
& = \partial(\text{grad } v_a) / \partial t + (\text{grad } \mathbf{w}_a) \cdot \mathbf{v}_a + \mathbf{w}_a \cdot \mathbf{L}_a \\
& = \partial \mathbf{w}_a / \partial t + (\text{grad } \mathbf{w}_a) \cdot \mathbf{v}_a + \mathbf{L}_a^T \cdot \mathbf{w}_a,
\end{aligned}$$

and substituting $\partial \mathbf{w}_a / \partial t$ from this into Equation 3.6, gives

$$\dot{\mathbf{w}}_a = \text{grad } \dot{v}_a - \mathbf{L}_a^T \cdot \mathbf{w}_a.$$

Now taking the time derivative of c_a (Equation 3.4) yields

$$\dot{c}_a = (\rho_a/\rho_R) |\det F_a| + (\rho_a/\rho_R) d(|\det F_a|)/dt,$$

and substituting from the mass balance equation for the constituent (Equation 2.26), yields

$$\begin{aligned} \dot{c}_a &= ([c_a^+ - \rho_a \operatorname{div} \mathbf{v}_a] / \rho_R) |\det F_a| + (\rho_a/\rho_R) d(|\det F_a|)/dt \\ &= [c_a^+ |\det F_a|] / \rho_R + (\rho_a/\rho_R) [\operatorname{div} \mathbf{v}_a |\det F_a| - d(|\det F_a|)/dt]. \end{aligned} \quad (3.7)$$

But, expanding in indicial notation, on the time derivative for the determinant of the deformation gradient, yields

$$\begin{aligned} d(|\det F_a|)/dt &= d|F_{iJ}|/dt \\ &= \det \begin{bmatrix} F_{1J} \\ F_{2J} \\ F_{3J} \end{bmatrix} + \det \begin{bmatrix} F_{1J} \\ F_{2J} \\ F_{3J} \end{bmatrix} + \det \begin{bmatrix} F_{1J} \\ F_{2J} \\ F_{3J} \end{bmatrix} \\ &= \det \begin{bmatrix} (\partial v_1/\partial x_1) F_{1J} \\ F_{2J} \\ F_{3J} \end{bmatrix} + \det \begin{bmatrix} F_{1J} \\ (\partial v_2/\partial x_2) F_{2J} \\ F_{3J} \end{bmatrix} + \det \begin{bmatrix} F_{1J} \\ F_{2J} \\ (\partial v_3/\partial x_3) F_{3J} \end{bmatrix} \\ &= (\partial v_1/\partial x_1 + \partial v_2/\partial x_2 + \partial v_3/\partial x_3) \det |F_{iJ}| \\ &= (\operatorname{div} \mathbf{v}_a) \det |F_a|, \end{aligned}$$

so that Equation 3.7 reduces to

$$\dot{c}_a = (|\det F_a|/\rho_R) c_a^+. \quad (3.8)$$

Equation 3.8 is then appropriately substituted into the material time derivative of the Helmholtz free energy (Equation 3.5) which is entered into the entropy inequality (Equation 2.93). Making these substitutions the

inequality becomes

$$\begin{aligned}
 & \sum \{ -\rho_a [(\partial \psi_a / \partial \theta_a) + \eta_a] \theta_a - \rho_a (\partial \psi_a / \partial v_a) v_a - \rho_a (\partial \psi_a / \partial u_a) u_a \\
 & - \rho_a (\partial \psi_a / \partial g_a) g_a + \text{tr} \{ [T_a - \rho_a F_a (\partial \psi_a / \partial F_a) + \rho_a (\partial \psi_a / \partial w_a) w_a] L_a \\
 & + [h - \rho_a (\partial \psi_a / \partial w_a)] \cdot \text{grad } v_a - q_a \cdot g_a / \theta_a - (v_a^{+e} - \rho_a k_a v_a / 2 \\
 & + \rho_a \partial \psi_a / \partial v_a) v_a + e_a^{+e} - m_a^{+e} \cdot v_a - c_a^+ (\rho_a (\partial \psi_a / \partial c_a) (|\det F_a| / \rho_R) \\
 & + \psi_a - v_a \cdot v_a / 2 - k_a v_a^2 / 2) \} / \theta_a \geq 0.
 \end{aligned}
 \tag{3.9}$$

An examination of the term associated with the mass interaction shows that,

$$\begin{aligned}
 \rho_a (\partial \psi_a / \partial c_a) (|\det F_a| / \rho_R) + \psi_a &= c_a (\partial \psi_a / \partial c_a) + \psi_a \\
 &= \partial (\psi_a c_a) / \partial c_a,
 \end{aligned}$$

or

$$\mu_a = \partial (\psi_a c_a) / \partial c_a, \tag{3.10}$$

which is the definition of the chemical potential.

Using the argument established by Coleman and Noll [1963] some restrictions are implied by the second law since, for specified values of v_a , w_a , v_a , u_a , θ_a , F_a , g_a , c_a , the variables θ_a , v_a , u_a , g_a , $\text{grad } v_a$, and L_a are arbitrarily independent. This implies that the coefficients for these variables in the entropy inequality must go to zero, to insure that the inequality is not violated. This necessitates the following restrictions:

$$\eta_a = -\partial\psi_a / \partial\theta_a, \quad (3.11)$$

$$\partial\psi_a / \partial v_a = 0, \quad (3.12)$$

$$\partial\psi_a / \partial u_a = 0, \quad (3.13)$$

$$\partial\psi_a / \partial g_a = 0, \quad (3.14)$$

$$T_a = \rho_a F_a (\partial\psi_a / \partial F_a) - \rho_a (\partial\psi_a / \partial w_a) w_a, \quad (3.15)$$

$$h_a = \rho_a \partial\psi_a / \partial w_a. \quad (3.16)$$

These restrictions indicate a reduction in the allowed dependence of the constitutive variables and provide specific forms for constitutive relations for T_a , η_a and h_a . The allowed dependence on the variables in Equations 3.1 and 3.2 is reduced to

$$(\psi_a, \eta_a, T_a, h_a) = \mathcal{F}(v_a, w_a, \theta_a, F_a, c_a), \quad (3.17)$$

$$q_a = q_a(v_a, w_a, v_a, u_a, \theta_a, F_a, g_a, c_a),$$

$$(c_a^+, v_a^+, m_a^+, H_a, e_a^{++}) = \mathcal{G}(v^\dagger, w^\dagger, v^\dagger, u^\dagger, \theta^\dagger, F^\dagger, g^\dagger, c^\dagger).$$

The reduced form for the entropy inequality is,

$$\begin{aligned} \sum_a \{ & -q_a \cdot g_a / \theta_a - (v_a^{+e} - \rho_a k_a v_a / 2 + \rho_a \partial\psi_a / \partial v_a) v_a + e_a^{+e} \\ & - m_a^{+e} \cdot v_a - c_a^+ (\mu_a - v_a \cdot v_a / 2 - k_a v_a^2 / 2) \} / \theta_a \geq 0. \end{aligned} \quad (3.18)$$

Thermochemical Equilibrium

The entropy inequality must be satisfied at all states, and the results which led to the reduced form must remain valid, even under nonequilibrium

conditions. At this point an examination of the restrictions imposed at thermochemical equilibrium are examined. An equilibrium state is attained when constituent temperatures are equal, constant and uniform, the velocities and mass interactions are identically zero, and the mass concentrations, deformation gradients and volume fractions are constant. An asterisk, *, will be used to indicate an equilibrium state, so that,

$$(\theta_a)^* \Rightarrow \theta_1 = \theta_2 = \dots = \theta_n = \theta^*, \quad (3.19)$$

$$(\mathbf{g}_a)^* = \mathbf{0}, \quad (3.20)$$

$$(\mathbf{v}_a)^* = \mathbf{0}, \quad (3.21)$$

$$(\mathbf{v}_a)^* = \mathbf{0}, \quad (3.22)$$

$$(c_a^+)^* = 0. \quad (3.23)$$

Define the internal dissipation of the mixture,

$$\delta = \delta(s),$$

as being equal to the entropy inequality for the mixture,

$$\begin{aligned} \delta(s) = \sum \{ & -\mathbf{q}_a \cdot \mathbf{g}_a / \theta_a - (v_a^{+e} - \rho_a k_a v_a / 2 + \rho_a \partial \psi_a / \partial v_a) v_a + e_a^{+e} \\ & - m_a^{+e} \cdot \mathbf{v}_a - c_a^+ (\mu_a - \mathbf{v}_a \cdot \mathbf{v}_a / 2 - k_a v_a^2 / 2) \} / \theta_a \geq 0, \end{aligned} \quad (3.24)$$

where s is the state,

$$s = (v\uparrow, \mathbf{w}\uparrow, v\uparrow, \mathbf{u}\uparrow, \theta\uparrow, F\uparrow, \mathbf{g}\uparrow, c\uparrow).$$

As can be seen from the entropy inequality, the internal dissipation will vanish at thermochemical equilibrium and will be greater than or equal to zero in a neighborhood of equilibrium,

$$\delta(s^*) = 0,$$

$$\delta(s^* + \xi s^P) \geq 0,$$

This can be readily verified by observing that $\sum e_a^{+e} = 0$ (Equation 2.79) and that all other terms in Equation 3.24 vanish at equilibrium. The superscript, P , indicates perturbation and ξs^P represents a slight perturbation from the equilibrium state, s^* , ξ is a scalar of arbitrarily small magnitude. The internal dissipation is therefore a local minimum at equilibrium. For ease and clarity of presentation in this part of the development let

$$\begin{aligned} \delta' &= \delta(s^* + \xi s^P) \\ &= \sum \{ -q_a (g_a^* + \xi g_a^P) / (\theta_a^* + \xi \theta_a^P) - [v_a^{+e} - \rho_a k_a (v_a^* + \xi v_a^P) / 2 \\ &\quad + \rho_a \partial \psi_a / \partial v_a] (v_a^* + \xi v_a^P) + e_a^{+e} - m_a^{+e} (v_a^* + \xi v_a^P) \\ &\quad - c_a [\mu_a - (v_a^* + \xi v_a^P)^2 / 2 - k_a (v_a^* + \xi v_a^P)^2 / 2] \} / (\theta_a^* + \xi \theta_a^P) \geq 0. \end{aligned}$$

Using this notation, a consequence of the local minimum condition is,

$$(d\delta'/d\xi) \big|_{\xi=0} = 0,$$

and,

$$(d^2\delta'/d\xi^2) \big|_{\xi=0} \geq 0.$$

The derivative of the internal dissipation is,

$$d\delta' = (\partial\delta'/\partial[s^* + \xi s^P]) d[s^* + \xi s^P],$$

so in general,

$$\begin{aligned} d\delta'/d\xi \big|_{\xi=0} &= \{ (\partial\delta'/\partial[s^* + \xi s^P]) (d[s^* + \xi s^P]/d\xi) \} \big|_{\xi=0} \\ &= (\partial\delta'/\partial[s^* + \xi s^P]) \big|_{\xi=0} s^P \\ &= (\partial\delta'/\partial s)^* s^P \end{aligned}$$

$$\begin{aligned}
&= \sum_a [(-\theta_a^p/[\theta^*]^2) \{ -q_a \cdot g_a / \theta_a - (v_a^{+e} - \rho_a k_a v_a / 2 \\
&\quad + \rho_a \partial \psi_a / \partial v_a) v_a + e_a^{+e} - m_a^{+e} \cdot v_a - c_a^+ (\mu_a - v_a \cdot v_a / 2 \\
&\quad - k_a v_a^2 / 2) \}^* + \sum_b (1/\theta^*) \{ [\partial(-q_a / \theta_a) / \partial s_b]^* s_b^p \cdot g_a^* \\
&\quad - \{ \partial(g_a) / \partial g_b \}^* g_b^p (q_a / \theta_a)^* - \{ \partial(v_a^{+e} - \rho_a k_a v_a / 2 \\
&\quad + \rho_a \partial \psi_a / \partial v_a) / \partial s_b \}^* s_b^p v_a^* - (v_a^{+e} - \rho_a k_a v_a / 2 \\
&\quad + \rho_a \partial \psi_a / \partial v_a)^* [\partial(v_a) / \partial v_b]^* v_b^p + (\partial e_a^{+e} / \partial s_b)^* s_b^p \\
&\quad - [\partial(m_a^{+e}) / \partial s_b]^* s_b^p \cdot v_a^* - m_a^{+e*} \cdot [\partial v_a / \partial v_b]^* v_b^p \\
&\quad - c_a^{+*} [\partial(\mu_a - v_a \cdot v_a / 2 - k_a v_a^2 / 2) / \partial s_b]^* s_b^p \\
&\quad - (\partial c_a^+ / \partial s_b) s_b^p (\mu_a - v_a \cdot v_a / 2 - k_a v_a^2 / 2) \}^*] \\
&= \sum_a [(-\theta_a^p/[\theta^*]^2) \{ e_a^{+e} \}^* + \sum_b (1/\theta^*) \{ - \{ \partial(g_a) / \partial g_b \}^* g_b^p (q_a / \theta_a)^* \\
&\quad - (v_a^{+e} + \rho_a \partial \psi_a / \partial v_a)^* [\partial(v_a) / \partial v_b]^* v_b^p + (\partial e_a^{+e} / \partial s_b)^* s_b^p \\
&\quad - m_a^{+e*} \cdot [\partial v_a / \partial v_b]^* v_b^p - (\partial c_a^+ / \partial s_b)^* s_b^p \mu_a^* \}].
\end{aligned}$$

Now, imposing the equilibrium restrictions given by Equations 3.19 - 3.23, and using the fact that summation over all of the energy interaction terms is zero by Equation 2.79, then

$$\begin{aligned}
\sum_a \sum_b (\partial e_a^{+e} / \partial s_b)^* s_b^p &= \sum_b (\partial [\sum_a e_a^{+e}] / \partial s_b)^* s_b^p \\
&= 0.
\end{aligned}$$

Writing out the differentiation in more detail and noting that the terms for the volume fraction, equilibrated stress and the deformation do not necessarily go to zero or any particular value at equilibrium,

perturbations away from the equilibrium state for these terms are meaningless, then

$$\begin{aligned}
 0 &= d\delta'/d\xi \big|_{\xi=0} \\
 &= \sum_a [-(\theta_a^P/\theta^*)\{e_a^{+e}\}^* - g_a^P(q_a/\theta)^* - (v_a^{+e} + p_a \partial\psi_a/\partial v_a)^* \cdot v_a^P \\
 &\quad - m_a^{+e*} v_a^P - \mu_a^* \sum_b \{(\partial c_a^+/\partial v_b)^* \cdot v_b^P + (\partial c_a^+/\partial v_b)^* \cdot v_b^P \\
 &\quad + (\partial c_a^+/\partial \theta_b)^* \theta_b^P + (\partial c_a^+/\partial g_b)^* \cdot g_b^P + (\partial c_a^+/\partial c_b)^* c_b^P].
 \end{aligned}$$

In addition, what is termed a strong equilibrium condition requires that the chemical potentials for all of the constituents be equal [Nunziato and Walsh 1980],

$$(\mu_a)^* \Rightarrow (\mu_1)^* = (\mu_2)^* = \dots = (\mu_n)^*.$$

This in conjunction with the fact that the sum of the mass interaction terms will be zero, yields,

$$\begin{aligned}
 0 &= d\delta'/d\xi \big|_{\xi=0} \\
 &= \sum_a [-(\theta_a^P/\theta^*)\{e_a^{+e}\}^* - g_a^P(q_a/\theta)^* - (v_a^{+e} + p_a \partial\psi_a/\partial v_a)^* \cdot v_a^P \\
 &\quad - m_a^{+e*} v_a^P],
 \end{aligned}$$

which places some additional restrictions on the forms for the constitutive equations at thermomechanical equilibrium. In particular at strong equilibrium

$$(v_a^{+e})^* = (-p_a \partial\psi_a/\partial v_a)^*, \quad (3.25)$$

This is the negative of the form for the configuration pressure as presented by Baer, Benner, Gross and Nunziato [1985] and Passman, Nunziato

and Walsh [1984] indicated that it represents the elastic response of the particle assembly to compression. Additional requirements of equilibrium are,

$$\{e_a + e\}^* = 0, \quad (3.26)$$

$$q_a^* = 0, \quad (3.27)$$

$$m_a + e^* = 0. \quad (3.28)$$

As noted earlier, additional restrictions on the sign of some terms will result from the second derivative on the perturbations. Examining this in general,

$$\begin{aligned} (d^2\delta'/d\xi^2) \big|_{\xi=0} &= d[(\partial\delta'/\partial[s^* + \xi s^P])(d[s^* + \xi s^P]/d\xi)]/d\xi \big|_{\xi=0} \\ &= d[(\partial\delta'/\partial[s^* + \xi s^P]) s^P]/d\xi \big|_{\xi=0} \\ &= (\partial^2\delta'/\partial[s^* + \xi s^P]^2) d[s^* + \xi s^P]/d\xi s^P \\ &\quad + \partial\delta'/\partial[s^* + \xi s^P] ds^P/d\xi \big|_{\xi=0} \\ &= s^P \cdot (\partial^2\delta'/\partial[s^* + \xi s^P]^2 s^P) \big|_{\xi=0} \\ &= s^P \cdot \{(\partial^2\delta/\partial s^2)^* s^P\}, \end{aligned}$$

and for the constituents this is written as

$$(d^2\delta'/d\xi^2) \big|_{\xi=0} = \sum_{\alpha} \sum_i \sum_j s_i^P (\partial^2\delta_a/\partial s_i \partial s_j)^* s_j^P,$$

where the summations are all from 1 to n.

Due to the notational complexity of presentation, the second derivative development will not be carried out in as general a form as was shown for the first order case. Instead, several specific cases involving individual variables will be demonstrated here, which show the tedious

procedure followed in order to obtain the proper results. For example consider the a constituent of 'v' from among the constitutive variables. The first derivative is,

$$\begin{aligned} \partial \delta / \partial v_a = \sum_{\alpha} \{ & - \partial[q_{\alpha}]/\partial v_a \cdot g_{\alpha}/\theta_{\alpha} - (\partial[v_{\alpha}^{+e}]/\partial v_a - \rho_{\alpha} k_{\alpha}/2) v_{\alpha} \\ & - (v_a^{+e} - \rho_a k_a v_a/2 + \rho_a \partial \psi_a / \partial v_a) + \partial[e_{\alpha}^{+e}]/\partial v_a \\ & - \partial[m_{\alpha}^{+e}]/\partial v_a \cdot v_{\alpha} - \partial[c_{\alpha}^{+}]/\partial v_a (\mu_{\alpha} - v_{\alpha} \cdot v_{\alpha}/2 - k_{\alpha} v_{\alpha}^2/2) \\ & - c_{\alpha}^{+} (\partial[\mu_{\alpha}]/\partial v_{\alpha} - v_{\alpha} \cdot v_{\alpha}/2 - k_{\alpha} v_{\alpha}) \} / \theta_{\alpha} \end{aligned}$$

The second partial derivative evaluated at equilibrium is,

$$\begin{aligned} (\partial^2 \delta / \partial v_a^2)^* = \sum_{\alpha} \{ & - \partial^2[q_{\alpha}]/\partial v_a^2 \cdot g_{\alpha}/\theta_{\alpha} - (\partial[v_{\alpha}^{+e}]^2/\partial v_a^2) v_{\alpha} \\ & - 2(\partial[v_{\alpha}^{+e}]/\partial v_a - \rho_{\alpha} k_{\alpha}/2) + \partial^2[e_{\alpha}^{+e}]/\partial v_a^2 \\ & - \partial[m_{\alpha}^{+e}]^2/\partial v_a^2 \cdot v_{\alpha} - \partial[c_{\alpha}^{+}]^2/\partial v_a^2 (\mu_{\alpha} - v_{\alpha} \cdot v_{\alpha}/2 \\ & - k_{\alpha} v_{\alpha}^2/2) - 2 \partial[c_{\alpha}^{+}]/\partial v_{\alpha} (\partial[\mu_{\alpha}]/\partial v_{\alpha} - v_{\alpha} \cdot v_{\alpha}/2 \\ & - k_{\alpha} v_{\alpha}) - c_{\alpha}^{+} (\partial[\mu_{\alpha}]^2/\partial v_{\alpha}^2 - k_{\alpha}) \} / \theta_{\alpha} \}^* v_a^2. \end{aligned}$$

Imposing the equilibrium conditions, as indicated by Equations 3.19 - 3.23, reduces this to

$$\begin{aligned} (\partial^2 \delta / \partial v_a^2)^* = \sum_{\alpha} \{ & - 2(\partial[v_{\alpha}^{+e}]/\partial v_a) + \partial^2[e_{\alpha}^{+e}]/\partial v_a^2 \\ & - \partial[c_{\alpha}^{+}]^2/\partial v_a^2 (\mu_{\alpha}) \\ & - 2 \partial[c_{\alpha}^{+}]/\partial v_a (\partial[\mu_{\alpha}]/\partial v_a) \} / \theta_{\alpha} \}^* v_a^2. \end{aligned}$$

But remembering that $\theta_1^* = \theta_2^* = \dots = \theta_n^*$,

$$\begin{aligned}\sum_{\alpha} (\partial^2 [e_{\alpha}^{+e}] / \partial v_a^2)^* &= (\partial^2 [\sum_{\alpha} e_{\alpha}^{+e}] / \partial v_a^2)^* \\ &= 0,\end{aligned}$$

since $\sum_{\alpha} e_{\alpha}^{+e} = 0$ (Equation 2.79).

Also,

$$\begin{aligned}\sum_{\alpha} \llbracket \partial [c_{\alpha}^{+}]^2 / \partial v_a^2 (\mu_{\alpha}) \rrbracket^* &= \mu_a^* \partial [\sum_{\alpha} c_{\alpha}^{+}]^2 / \partial v_a^2 \\ &= 0,\end{aligned}$$

since the chemical potentials for the constituents are all equal at strong equilibrium and Equation 2.54.

Similarly,

$$\begin{aligned}\sum_{\alpha} \llbracket \partial [c_{\alpha}^{+}] / \partial v_a (\partial [\mu_{\alpha}] / \partial v_a) \rrbracket^* &= \llbracket \partial [\sum_{\alpha} c_{\alpha}^{+}] / \partial v_a (\partial [\mu_a] / \partial v_a) \rrbracket^* \\ &= 0.\end{aligned}$$

Then,

$$v^D \cdot \{ (\partial^2 \delta / \partial v_a^2)^* v^D \} = - 2 (\partial [v_a^{+e}] / \partial v_a)^* (v_a)^2,$$

which leaves as an equilibrium constraint,

$$(\partial [v_a^{+e}] / \partial v_a)^* \leq 0. \quad (3.29)$$

Proceeding as above for the velocity term. The first derivative is

$$\begin{aligned}\partial \delta / \partial v_a &= \sum_{\alpha} \{ - \partial [q_{\alpha}] / \partial v_a \cdot g_{\alpha} / \theta_{\alpha} - (\partial [v_{\alpha}^{+e}] / \partial v_a) v_{\alpha} + \partial [e_{\alpha}^{+e}] / \partial v_a \\ &\quad - \partial [m_{\alpha}^{+e}] / \partial v_a \cdot v_{\alpha} - m_{\alpha}^{+e} - \partial [c_{\alpha}^{+}] / \partial v_a (\mu_{\alpha} - v_{\alpha} \cdot v_{\alpha} / 2 \\ &\quad - k_{\alpha} v_{\alpha}^2 / 2) - c_{\alpha}^{+} (\partial [\mu_{\alpha}] / \partial v_a - v_{\alpha}) \} / \theta_{\alpha}\end{aligned}$$

and the second partial derivative evaluated at equilibrium is,

$$\begin{aligned}
(\partial^2 \delta / \partial \mathbf{v}_a^2)^* &= \sum_{\alpha} \left[\left\{ -\partial^2 [q_{\alpha}] / \partial \mathbf{v}_a^2 \cdot \mathbf{g}_{\alpha}' / \theta_{\alpha} - (\partial^2 [v_{\alpha}^{+e}] / \partial \mathbf{v}_a^2) \cdot \mathbf{v}_{\alpha} \right. \right. \\
&\quad + \partial^2 [e_{\alpha}^{+e}] / \partial \mathbf{v}_a^2 - \partial^2 [m_{\alpha}^{+e}] / \partial \mathbf{v}_a^2 \cdot \mathbf{v}_{\alpha} - 2 \partial [m_{\alpha}^{+e}] / \partial \mathbf{v}_a \\
&\quad - \partial^2 [c_{\alpha}^{+}] / \partial \mathbf{v}_a^2 (\mu_{\alpha} - \mathbf{v}_{\alpha} \cdot \mathbf{v}_{\alpha} / 2 - k_{\alpha} v_{\alpha}^2 / 2) \\
&\quad - 2 \partial [c_{\alpha}^{+}] / \partial \mathbf{v}_a (\partial [\mu_{\alpha}] / \partial \mathbf{v}_a - \mathbf{v}_{\alpha}) \\
&\quad \left. \left. - c_{\alpha}^{+} (\partial^2 [\mu_{\alpha}] / \partial \mathbf{v}_a^2 - 1) \right\} / \theta_{\alpha} \right]^* \\
&= \sum_{\alpha} \left[\left\{ \partial^2 [e_{\alpha}^{+e}] / \partial \mathbf{v}_a^2 - 2 \partial [m_{\alpha}^{+e}] / \partial \mathbf{v}_a - \partial^2 [c_{\alpha}^{+}] / \partial \mathbf{v}_a^2 (\mu_{\alpha}) \right. \right. \\
&\quad \left. \left. - 2 \partial [c_{\alpha}^{+}] / \partial \mathbf{v}_a (\partial [\mu_{\alpha}] / \partial \mathbf{v}_a) - c_{\alpha}^{+} (\partial^2 [\mu_{\alpha}] / \partial \mathbf{v}_a^2 - 1) \right\} / \theta_{\alpha} \right]^*.
\end{aligned}$$

Since the temperatures are all equal at equilibrium, the other terms can be evaluated,

$$\begin{aligned}
\sum_{\alpha} (\partial^2 [e_{\alpha}^{+e}] / \partial \mathbf{v}_a^2)^* &= (\partial^2 [\sum_{\alpha} e_{\alpha}^{+e}] / \partial \mathbf{v}_a^2)^* \\
&= 0,
\end{aligned}$$

and

$$\begin{aligned}
\sum_{\alpha} \left[\partial^2 [c_{\alpha}^{+}] / \partial \mathbf{v}_a^2 (\mu_{\alpha}) \right]^* &= (\mu_{\alpha})^* (\partial^2 [\sum_{\alpha} c_{\alpha}^{+}] / \partial \mathbf{v}_a^2)^* \\
&= 0,
\end{aligned}$$

$$\begin{aligned}
\sum_{\alpha} \left[\partial [c_{\alpha}^{+}] / \partial \mathbf{v}_a (\partial [\mu_{\alpha}] / \partial \mathbf{v}_a) \right]^* &= \left[\partial [\sum_{\alpha} c_{\alpha}^{+}] / \partial \mathbf{v}_a (\partial [\mu_a] / \partial \mathbf{v}_a) \right]^* \\
&= 0,
\end{aligned}$$

$$\begin{aligned}
\sum_{\alpha} c_{\alpha}^{+} (\partial^2 [\mu_{\alpha}] / \partial \mathbf{v}_a^2 - 1) &= (\partial^2 [\mu_a] / \partial \mathbf{v}_a^2 - 1) \sum_{\alpha} c_{\alpha}^{+} \\
&= 0.
\end{aligned}$$

So that,

$$\mathbf{v}_a \cdot \{ (\partial^2 \delta / \partial \mathbf{v}_a^2)^* \mathbf{v}_a \} = -2 \mathbf{v}_a \cdot (\partial [m_{\alpha}^{+e}] / \partial \mathbf{v}_a)^* \mathbf{v}_a,$$

and the constraint result is,

$$\mathbf{n}_a \cdot (\partial[\mathbf{m}_\alpha^{+e}]/\partial \mathbf{v}_a)^* \mathbf{n}_a \leq 0. \quad (3.30)$$

Carrying out a similar process for all of the other constitutive variables including the cross product terms will give additional restrictions on the direction of equilibrium processes. These results are collected below,

$$(\partial[v_a^{+e}]/\partial v_a)^* \leq 0, \quad (3.29)$$

$$\mathbf{v}_a \cdot (\partial[\mathbf{m}_\alpha^{+e}]/\partial \mathbf{v}_a)^* \mathbf{v}_a \leq 0, \quad (3.30)$$

$$(\partial[c_a^{+}]/\partial c_a)^* \leq 0, \quad (3.31)$$

$$\mathbf{n}_a \cdot (\partial \mathbf{q}_a / \partial \mathbf{g}_a)^* \mathbf{n}_a \leq 0. \quad (3.32)$$

In these terms, the usual forms for the drag coefficient,

$$-\partial[\mathbf{m}_\alpha^{+e}]/\partial \mathbf{v}_a = \text{drag coefficient} \quad (3.33)$$

and, the thermal conductivity,

$$-\partial \mathbf{q}_a / \partial \mathbf{g}_a = \text{thermal conductivity}, \quad (3.34)$$

are indicated by the second derivative restrictions from the entropy inequality.

CHAPTER IV

SPECIFICATION TO SNOW AS A TWO PHASE MIXTURE

Assumptions for Snow

In the previous chapters the development has been approached in a very general manner. At this point, some assumptions which are appropriate to describing snow as a specific material are discussed. The mixture (snow) is assumed to be a porous material comprised of two constituents, a solid and a vapor. The solid constituent characterizes the ice phase, while the air and water vapor which fill the pores constitute the vapor constituent. The ice constituent is considered to be incompressible for the environment under consideration, but the vapor density may vary. As a consequence of the incompressibility of the ice the material density, ρ_i , is a constant, but ρ_v can vary. The ice and vapor are both considered to be isotropic.

Many of the terms associated with the equilibrated force equations are not well understood yet, but interpretations for some have been postulated. Much of the interpretation for these terms are derived from the granular theory of Goodman and Cowin [1972], upon which the present theory for mixtures is based. The equilibrated stress is related to the variation of the Helmholtz free energy with the volume fraction gradient, as is apparent from the form generated by the second law, equation (3.24). Nunziato and

Cowen [1979], and Nunziato and Walsh [1980] state that $h = 0$ when the matrix material is incompressible. Also, for slightly different application of the same theory, Passman, Nunziato and Walsh [1984] assert that for fluid suspensions, h_a is not significant except for highly concentrated nonhomogeneous suspensions. Based on this foregoing work the equilibrated stress term will be set to zero in this development,

$$h_a = 0. \quad (4.1)$$

Velocities involved in snow metamorphism are very low and the matrix material is incompressible, so the microstructural inertia effects are assumed to be insignificant, that is the equilibrated inertia is negligible,

$$k_a = 0. \quad (4.2)$$

The equilibrated force supply, according to Nunziato and Walsh [1980] is somehow related to the pressure in the void and the material properties of the matrix. However, in the present situation for a porous material where the matrix material is self supporting with little assistance from the vapor and since the curvature effects of the grains will be considered to some degree by the interface pressure, the equilibrated force supply is ignored in the formulation:

$$g_a = 0. \quad (4.3)$$

The external equilibrated body force for the mixture, l , which is related to an externally controlled body force or pore pressure [Jenkins, 1975], is considered in the formulation. The manner in which it enters the

theory is presented in the following section. All of these assumptions however will impose restrictions on the equilibrated force supply. The balance of extra equilibrated force (Equation 2.84), with the imposed restrictions (Equations 4.1 and 4.2), becomes

$$v_a^{+e} = -\rho_a l_a + \pi. \quad (4.4)$$

So that in the present development the extra equilibrated force gives the interface pressure between the constituents which is necessary for the phases to remain in contact, minus the term involving the external equilibrated body force.

Assuming the helmholtz free energy, ψ_a , is isotropic implies that T_a is symmetric, so the angular momentum for the constituent is identically zero,

$$H_a = 0. \quad (4.5)$$

Heat Flux and the Interaction Terms

In order to come up with some allowable forms for the rest of the constitutive equations, the dissipation inequality (Equation 3.26) is again utilized. The second law expanded explicitly for the two constituents is

$$\begin{aligned} & \{-\mathbf{q}_i \cdot \mathbf{g}_i / \theta_i - (v_i^{+e} - \rho_i k_i v_i / 2 + \rho_i \partial \psi_i / \partial v_i) v_i + e_i^{+e} - \mathbf{m}_i^{+e} \cdot \mathbf{v}_i \\ & - c_i^+(\mu_i - \mathbf{v}_i \cdot \mathbf{v}_i / 2 - k_i v_i^2 / 2) / \theta_i + \{-\mathbf{q}_V \cdot \mathbf{g}_V / \theta_V \\ & - (v_V^{+e} - \rho_V k_V v_V / 2 + \rho_V \partial \psi_V / \partial v_V) v_V + e_V^{+e} - \mathbf{m}_V^{+e} \cdot \mathbf{v}_V \\ & - c_V^+(\mu_V - \mathbf{v}_V \cdot \mathbf{v}_V / 2 - k_V v_V^2 / 2) / \theta_V \geq 0, \end{aligned}$$

where the subscript, i , indicates the ice, and v , indicates the vapor constituent.

A sufficient, although not a necessary, condition that the entropy inequality is not violated is that each of the individual terms is positive semi-definite. Using the fact that the two constituent interaction terms, for the mass (Equation 2.54) and for the linear momentum (Equation 2.55), are negative values of each other and that the time rate of change of the volume fractions are also negatives of each other, the inequality may be written in the form,

$$\begin{aligned}
 & -\mathbf{q}_i \cdot \mathbf{g}_i / \theta_i^2 - \mathbf{q}_v \cdot \mathbf{g}_v / \theta_v^2 - \{(v_i^{+e} - \rho_i k_i v_i / 2 + \rho_i \partial \psi_i / \partial v_i) / \theta_i \\
 & - (v_v^{+e} - \rho_v k_v v_v / 2 + \rho_v \partial \psi_v / \partial v_v) / \theta_v\} v_i + [(1/\theta_i) - (1/\theta_v)] e_i^{+e} \\
 & - \{(\mathbf{v}_i / \theta_i) - (\mathbf{v}_v / \theta_v)\} m_i^{+e} - \{(\mu_i - \mathbf{v}_i \cdot \mathbf{v}_i / 2 - k_i v_i^2 / 2) / \theta_i \\
 & - (\mu_v - \mathbf{v}_v \cdot \mathbf{v}_v / 2 - k_v v_v^2 / 2) / \theta_v\} c_i^{+e} \geq 0.
 \end{aligned}
 \tag{4.6}$$

Requiring positive coefficients, the terms are now chosen to insure that the inequality is satisfied. To arrive at a suitable form for the constituent heat flux, set,

$$\mathbf{q}_i = -q_{i0} \mathbf{g}_i, \tag{4.7}$$

and

$$\mathbf{q}_v = -q_{v0} \mathbf{g}_v, \tag{4.8}$$

so that the heat flux is proportional to the temperature gradient, and the proportionality constant, q_{a_i} , is the thermal conductivity which, as stated

earlier (Equation 3.34), is $q_{a_1} = -\partial q_a / \partial g_a$.

Next, examine the terms associated with the energy exchange term in Equation 4.6. If $(1/\theta_i) - (1/\theta_v) < 0$, then obviously, $\theta_i > \theta_v$, on the other hand if, $(1/\theta_i) - (1/\theta_v) > 0$, then, $\theta_i < \theta_v$, so that an appropriate equation describing the extra energy interaction would be,

$$e_i^{+e} = -e_v^{+e} = e_{i_0}^{+e}(\theta_v - \theta_i). \quad (4.9)$$

This form is analogous to Newton's law of cooling. Newton's law of cooling is generally used for calculating the heat flux from a surface when convection of the fluid is involved. This will govern the rate and direction in which the energy interaction will go, determined by the constituent temperatures.

The the extra interaction of linear momentum has as a suitable form to satisfy the requirement of Equation 4.6

$$m_i^{+e} = -m_v^{+e} = m_{i_0}^{+e} \{ (v_v/\theta_v) - (v_i/\theta_i) \}. \quad (4.10)$$

Where $m_i^{+e} = -\partial m_a / \partial u_a$ is the previously mentioned drag coefficient, which is consistent with Darcy's law if $m_{i_0}^{+e}$ is assumed to be of the form,

$$m_i^{+e} = v_i^2 \zeta \theta_v / \kappa, \quad (4.11)$$

where ζ is the fluid viscosity and κ is the permeability.

The form for the mass interaction as implied by the inequality (Equation 4.7) is

$$c_i^+ = -c_v^+ \\ = c_{i_0}^+ \{ (\mu_v - \mathbf{v}_v \cdot \mathbf{v}_v / 2 - k_v' v_v^2 / 2) / \theta_v - (\mu_i - \mathbf{v}_i \cdot \mathbf{v}_i / 2 - k_i' v_i^2 / 2) / \theta_i \}.$$

In the case under consideration here, where the equilibrated inertia is assumed negligible,

$$c_i^+ = -c_v^+ = c_{i_0}^+ \{ (\mu_v / \theta_v - \mu_i / \theta_i) + (1/2)(\mathbf{v}_i \cdot \mathbf{v}_i / \theta_i - \mathbf{v}_v \cdot \mathbf{v}_v / \theta_v) \}. \quad (4.12)$$

The mass interaction then is governed by the differences in the chemical potentials for the two constituents, differences in kinetic energy terms, and temperature difference effects.

It is important to note that the forms arrived at for the heat fluxm (Equations 4.7 and 4.8), extra energy interaction (Equation 4.9), extra momentum interaction (Equation 4.10) and mass interaction (Equation 4.12) all go to zero at equilibrium as required, when it is assured that the chemical potentials are equal at equilibrium.

Finally the term associated with the equilibrated inertia should satisfy,

$$K'v_i = -\{ (v_i^{+e} - \rho_i' k_i' v_i / 2 + \rho_i \partial \psi_i / \partial v_i) / \theta_i - (v_v^{+e} - \rho_v' k_v' v_v / 2 + \rho_v \partial \psi_v / \partial v_v) / \theta_v \},$$

where K is some positive value.

Rearranging terms to get things in relation to the extra equilibrated force of the ice,

$$v_i^{+e} = \{ (v_v^{+e} - \rho_v' k_v' v_v / 2 + \rho_v \partial \psi_v / \partial v_v) / \theta_v - K'v_i \} \theta_i \\ - (- \rho_i' k_i' v_i / 2 + \rho_i \partial \psi_i / \partial v_i),$$

Now using the relationships from Equation 2.82 gives:

$$v_i^+ + p_i g_i + \pi = \{ (v_v^+ + p_v g_v + \pi - p_v' k_v' v_v / 2 + p_v \partial \psi_v / \partial v_v) / \theta_v \\ - K' v_i \} \theta_i - (- p_i' k_i' v_i / 2 + p_i \partial \psi_i / \partial v_i).$$

Manipulating this, and using the constraint, $v_i^+ = -v_v^+$ (Equation 2.57),

$$v_i^+ \{ 1 + (\theta_i / \theta_v) \} = (p_v g_v + \pi - p_v' k_v' v_v / 2 + p_v \partial \psi_v / \partial v_v) (\theta_i / \theta_v) - K' v_i \theta_i \\ - (- p_i' k_i' v_i / 2 + p_i \partial \psi_i / \partial v_i) - p_i g_i - \pi,$$

so the equilibrated force is,

$$v_i^+ = \{ (p_v g_v + \pi - p_v' k_v' v_v / 2 + p_v \partial \psi_v / \partial v_v) \theta_i - K' v_i \theta_i \theta_v - (- p_i' k_i' v_i / 2 \\ + p_i \partial \psi_i / \partial v_i + p_i g_i + \pi) \theta_v \} / \{ \theta_v + \theta_i \}.$$

As a check a similar manipulation gives a form for the equilibrated force of the vapor which is properly the negative of this. However, the development for the saturated mixture being used here is in terms of the extra equilibrated force v_i^{+e} so,

$$v_i^{+e} = \{ (p_v g_v + \pi - p_v' k_v' v_v / 2 + p_v \partial \psi_v / \partial v_v) \theta_i - K' v_i \theta_i \theta_v \\ - (- p_i' k_i' v_i / 2 + p_i \partial \psi_i / \partial v_i + p_i g_i + \pi) \theta_v \} / \{ \theta_v + \theta_i \} + p_i g_i + \pi,$$

and

$$v_v^{+e} = \{ - (p_v g_v + \pi - p_v' k_v' v_v / 2 + p_v \partial \psi_v / \partial v_v) \theta_i + K' v_i \theta_i \theta_v \\ + (- p_i' k_i' v_i / 2 + p_i \partial \psi_i / \partial v_i + p_i g_i + \pi) \theta_v \} / \{ \theta_v + \theta_i \} + p_v g_v + \pi.$$

This satisfies the summation restriction proposed for the mixture earlier in the dissertation by Equation 2.86.

Similarly neglecting the appropriate terms in the extra equilibrated force equation just developed,

$$- \rho_i l_i = \{(\pi + \rho_v \partial \psi_v / \partial v_v) \theta_i - K' v_i \theta_i \theta_v - (\rho_i \partial \psi_i / \partial v_i + \pi) \theta_v\} / \{\theta_v + \theta_i\}.$$

Notice that,

$$v_a^+ = - \rho_a l_a, \quad (4.13)$$

in this somewhat simplified development. For the two constituents under consideration here,

$$v_i^+ + v_v^+ = - \rho_i l_i - \rho_v l_v,$$

and since the sum of the interaction terms is zero,

$$\rho_i l_i = - \rho_v l_v. \quad (4.14)$$

so that

$$\begin{aligned} v_i^+ &= \{(\pi + \rho_v \partial \psi_v / \partial v_v) \theta_i - K' v_i \theta_i \theta_v - (\rho_i \partial \psi_i / \partial v_i + \pi) \theta_v\} / \{\theta_v + \theta_i\} \\ &= - v_v^+. \end{aligned}$$

The balance of equilibrated force for the ice is

$$v_i^{+e} = v_i^+ + \pi,$$

and for the vapor,

$$v_v^{+e} = v_v^+ + \pi = - v_i^+ + \pi.$$

A satisfactory form for the extra equilibrated force for the ice, using the assumptions in this dissertation is

$$\begin{aligned} v_i^{+e} &= \{(\pi + \rho_v \partial \psi_v / \partial v_v) \theta_i - K' v_i \theta_i \theta_v \\ &\quad - (\rho_i \partial \psi_i / \partial v_i + \pi) \theta_v\} / \{\theta_v + \theta_i\} + \pi, \end{aligned} \quad (4.15)$$

and the extra equilibrated force for the vapor is,

$$\begin{aligned} v_v^{+e} = & - \{ (\pi + p_v \partial \psi_v / \partial v_v) \theta_i - K' v_i \theta_i \theta_v \\ & - (\rho_i \partial \psi_i / \partial v_i + \pi) \theta_v \} / \{ \theta_v + \theta_i \} + \pi. \end{aligned} \quad (4.16)$$

Helmholtz Free Energies and Associated Terms

If the Helmholtz free energy is known, then forms for the entropy, partial stress and the equilibrated stress are immediately determined through the equations dictated by the second law (Equations 3.11, 3.15 and 3.16). Consequently, a correct form for the Helmholtz function is crucial to the theory.

Snow is considered as a fully symmetric material. This isotropy indicates that a static density preserving alteration of the reference configuration will not alter the material response. The manner in which the assumed constitutive variables enter the formulation should satisfy the material symmetry group. Based on the work of Cross [1973] dealing with mixtures of fluids and isotropic solids, a suitable choice of functions for the constitutive variables may be chosen to be,

$$(\psi_a, \eta_a, T_a) = f(v_a, w_a, \theta_a, E_a, \rho_a), \quad (4.17)$$

where,

$$E_i = (1/2)(F_i^T F_i - 1). \quad (4.18)$$

E_i is the finite strain tensor sometimes called the Lagrangian strain tensor.

Constitutive equations may depend on these variables without

violating any principles, however it does not imply that they must all be included. Dependence on variables which affect one of the constituents is not necessarily appropriate to describing all constituents. This is apparent through consideration of the principle of phase separation for multiphase mixtures, which takes into account the discrete nature of the individual constituents.

The vapor constituent is not considered to be affected by the deformation gradient and therefore the elastic strain E (Equation 4.18) of the ice constituent, so this term is not included in the constitutive assumptions for the vapor. The ice constituent is taken as incompressible, therefore including both the volume fraction and the dispersed density as variables for the ice is redundant. The constitutive variable which will be used here is the dispersed density, ρ_i , of the ice constituent.

The form for the Helmholtz free energy for both the ice and the vapor are approximated here as second order Taylor series expansions. The Helmholtz free energy expansion for the ice is,

$$\begin{aligned}
 \psi_i = & [\psi_{i1}(\text{tr } E) + \psi_{i2}(\theta_i - \theta_R) + \psi_{i3}(\rho_i - \rho_{iR}) + \psi_{i4}|\mathbf{w}_i|] \\
 & + (1/2)[\psi_{i5}[\text{tr}(E_i)]^2 + 2\psi_{i6}\text{tr}(E_i)^2 + 2\psi_{i7}(\theta_i - \theta_R)\text{tr}(E_i) \\
 & + \psi_{i8}(\theta_i - \theta_R)^2 + 2\psi_{i9}(\theta_i - \theta_R)(\rho_i - \rho_{iR}) + 2\psi_{i10}(\rho_i - \rho_{iR})\text{tr}(E_i) \\
 & + \psi_{i11}(\rho_i - \rho_{iR})^2 + \psi_{i12}(\mathbf{w}_i \cdot \mathbf{w}_i) + \psi_{i13}(|\mathbf{w}_i|(\text{tr } E)) \\
 & + \psi_{i14}|\mathbf{w}_i|(\theta_i - \theta_R) + \psi_{i15}|\mathbf{w}_i|(\rho_i - \rho_{iR})] + \psi_{iR},
 \end{aligned} \tag{4.19}$$

and for the vapor,

$$\begin{aligned}
\psi_V = & \psi_{V1}(\nu_V - \nu_{VR}) + \psi_{V2}(\theta_V - \theta_R) + \psi_{V3}(\rho_V - \rho_{VR}) + \psi_{V4}|\mathbf{w}_i| \\
& + (1/2)[\psi_{V5}(\nu_V - \nu_{VR})^2 + 2\psi_{V6}(\theta_V - \theta_R)(\nu_V - \nu_{VR}) + \psi_{V7}(\theta_V - \theta_R)^2 \\
& + 2\psi_{V8}(\theta_V - \theta_R)(\rho_V - \rho_{VR}) + 2\psi_{V9}(\rho_V - \rho_{VR})(\nu_V - \nu_{VR}) \\
& + \psi_{V10}(\rho_V - \rho_{VR})^2 + \psi_{V11}(\mathbf{w}_V \cdot \mathbf{w}_V) + \psi_{V12}(|\mathbf{w}_V|(\nu_V - \nu_{VR})) \\
& + \psi_{V13}|\mathbf{w}_V|(\theta_V - \theta_R) + \psi_{V14}|\mathbf{w}_i|(\rho_V - \rho_{VR})] + \psi_{VR}. \quad (4.20)
\end{aligned}$$

Without loss of generality the reference temperature θ_R will be taken as the same for both constituents.

Using the previously stated assumption (Equation 4.1) that the equilibrated stress is insignificant, $\mathbf{h}_i = \mathbf{0}$, but by Equation 3.16

$$\mathbf{h}_i = \rho_i \partial \psi_i / \partial \mathbf{w}_i,$$

so through Equation 4.19

$$\begin{aligned}
\mathbf{0} = & \{\rho_i \{\psi_{i4} + (1/2)[2\psi_{i13}(\text{tr } \mathbf{E}) + \psi_{i14}(\theta_i - \theta_R) \\
& + \psi_{i15}(\rho_i - \rho_{iR})]\} \mathbf{1} + \psi_{i12} \mathbf{w}_i.
\end{aligned}$$

This will hold true is if all of the coefficients are assumed zero. Similarly for the equilibrated stress for the vapor,

$$\mathbf{h}_V = \mathbf{0},$$

but

$$\mathbf{h}_V = \rho_V \partial \psi_V / \partial \mathbf{w}_V,$$

so through Equation 4.20

$$\mathbf{0} = \{\psi_{V4} + (1/2)[\psi_{V12}(\nu_V - \nu_{VR}) + \psi_{V13}(\theta_V - \theta_R) + \psi_{V14}(\rho_V - \rho_{VR})]\} \mathbf{1}$$

$$+ \psi_{v_{11}} w_v$$

which is equal to zero, as above, if all of the coefficients go to zero.

This then effectively eliminates the gradient of the volume fraction from the Helmholtz free energy (Equations 4.19 and 4.20) and therefore from the partial stress and entropy, Equations 3.15 and 3.11 respectively.

The form for the partial stress of the ice (Equation 3.15) which has been developed is,

$$T_i = \rho_i F_i (\partial \psi_i / \partial F_i) - \rho_i (\partial \psi_i / \partial w_i) w_i.$$

An application of the chain rule and the fact that the equilibrated stress is not considered significant, gives a form for the stress under the imposed restrictions,

$$\begin{aligned} T_i &= \rho_i F_i (\partial \psi_i / \partial F_i) \\ &= \rho_i F_i \{ (\partial \psi_i / \partial E_i) (\partial E_i / \partial F_i) \} \\ &= \rho_i F_i \{ (\partial \psi_i / \partial E_i) F_i \}^T. \end{aligned}$$

Now, if only small strains are imposed, the deformation gradient is approximated by $F \approx 1$. This small strain assumption implies that the Cauchy and the first and second Piola-Kirchoff stress are equivalent, so there is no difficulty posed in dealing with the Lagrangian strain tensor. The stress is then given by,

$$\begin{aligned} T_i &= \rho_i (\partial \psi_i / \partial E_i) \\ &= \rho_i \{ \psi_{i_1} \mathbf{1} + \psi_{i_5} \text{tr}(\mathbf{E}_i) \mathbf{1} + 2 \psi_{i_6} \mathbf{E}_i + \psi_{i_7} (\theta_i - \theta_R) \mathbf{1} + \psi_{i_{10}} (\rho_i - \rho_{iR}) \mathbf{1} \}. \end{aligned} \quad (4.21)$$

Taking the strain to be zero in the reference state leaves,

$$\rho_i \psi_{i_1} \mathbf{1} = \mathbf{T}_{iR},$$

as the reference stress of the ice.

This form for the stress is similar to the Duhamel-Neumann law [Sokolnikoff, 1956] for a thermoelastic material, but is further complicated by the reference stress and the term involving the partial density. This provides a way to obtain values for several of the coefficients. Using λ and G as the Lamé constants and α as the coefficient of linear expansion, direct comparison with the Duhamel-Neumann law yields

$$\rho_i \psi_{i_5} = \lambda,$$

$$\rho_i \psi_{i_6} = G,$$

and

$$\psi_{i_7} = -\alpha(3\lambda + 2G).$$

G is also known as the modulus of rigidity or shear modulus. These Lamé constants are related to Young's modulus, Y and Poisson's ratio, Φ , as,

$$\lambda = \Phi Y / ((1 + \Phi)(1 - 2\Phi))$$

and

$$G = Y / 2(1 + \Phi).$$

The entropy of the ice, by Equation 3.11, is $\eta_i = -\partial\psi_i / \partial\theta_i$, so for this expansion,

$$\eta_i = -[\psi_{i_2} + \psi_{i_7} \text{tr}(\mathbf{E}_i) + \psi_{i_8}(\theta_i - \theta_R) + \psi_{i_9}(\rho_i - \rho_{iR})]. \quad (4.22)$$

This then gives,

$$-\psi_{i2} = \eta_{iR},$$

as the reference entropy.

At equilibrium the equilibrated force for the ice is given by

$$\begin{aligned} (v_i^{+e})^* &= (-\rho_i \partial \psi_i / \partial v_i)^* \\ &= [-\rho_i \gamma_i \{ \psi_{i3} + \psi_{i9} (\theta_i - \theta_R) + \psi_{i10} \text{tr}(E_i) + \psi_{i11} (\rho_i - \rho_{iR}) \}]^*, \end{aligned}$$

so that

$$-\rho_{iR} \gamma_i \psi_{i3} = v_{iR}^{+e},$$

gives the reference equilibrated force.

This will allow ψ_{i3} to be determined as,

$$\psi_{i3} = -(2\pi - \gamma_{iR} \theta_R) / (\rho_{iR} \gamma_i), \quad (4.23)$$

which will be shown when the reference equilibrated force for the vapor is determined.

Since, $\psi_a = e_a - \theta_a \eta_a$ (Equation 2.92), the internal energy may immediately be written,

$$\begin{aligned} e_i &= [\psi_{i1} (\text{tr } E) + \psi_{i2} (\theta_i - \theta_R) + \psi_{i3} (\rho_i - \rho_{iR})] + (1/2) [\psi_{i5} [\text{tr}(E_i)]^2 \\ &\quad + 2 \psi_{i6} \text{tr}(E_i)^2 + 2 \psi_{i7} (\theta_i - \theta_R) \text{tr}(E_i) + \psi_{i8} (\theta_i - \theta_R)^2 \\ &\quad + 2 \psi_{i9} (\theta_i - \theta_R) (\rho_i - \rho_{iR}) + 2 \psi_{i10} (\rho_i - \rho_{iR}) \text{tr}(E_i) + \psi_{i11} (\rho_i - \rho_{iR})^2] \\ &\quad + \psi_{iR} - \theta_i [\psi_{i2} + \psi_{i7} \text{tr}(E_i) + \psi_{i8} (\theta_i - \theta_R) + \psi_{i9} (\rho_i - \rho_{iR})] \end{aligned}$$

$$\begin{aligned}
&= [\psi_{i_1}(\text{tr } \mathbf{E}) - \psi_{i_2}\theta_R + \psi_{i_3}(\rho_i - \rho_{iR})] + (1/2)[\psi_{i_5}[\text{tr}(\mathbf{E}_i)]^2 + 2\psi_{i_6}\text{tr}(\mathbf{E}_i)^2 \\
&\quad - 2\psi_{i_7}\theta_{i_0}\text{tr}(\mathbf{E}_i) - \psi_{i_8}(\theta_i^2 - \theta_R^2) - 2\psi_{i_9}\theta_{i_0}(\rho_i - \rho_{iR}) \\
&\quad + 2\psi_{i_{10}}(\rho_i - \rho_{iR})\text{tr}(\mathbf{E}_i) + \psi_{i_{11}}(\rho_i - \rho_{iR})^2] + \psi_{iR}.
\end{aligned}$$

Following the example of Passman and Batra [1984] and using an approach similar to that used for the time derivative for the Helmholtz free energy which was developed earlier, $'e_i$ is,

$$\begin{aligned}
'e_i &= \text{tr}[(\partial e_i / \partial \mathbf{E}_i)' \mathbf{E}_i] + (\partial e_i / \partial \theta_i)' \theta_i + (\partial e_i / \partial \rho_i)' \rho_i \\
&= \text{tr}('e_{i_1}' \mathbf{E}_i) + 'e_{i_2}' \theta_i + 'e_{i_3}' \rho_i,
\end{aligned} \tag{4.24}$$

where, as an exception to the usual notation, the lower case boldface $\mathbf{e}$ will represent a tensor in this case.

The coefficient associated with the time derivative of the temperature, $'e_{i_2}$, is related to the specific heat of ice at constant volume. The other coefficients in Equation 4.24 represent the latent heats as a result of strain and partial density. This will allow some additional insight into the coefficients in the Helmholtz equation. Latent heat of the ice with respect to the strain is given by,

$$\begin{aligned}
'e_{i_1} &= \partial e_i / \partial \mathbf{E}_i \\
&= [\psi_{i_1} + \psi_{i_5}[\text{tr}(\mathbf{E}_i)] + 2\psi_{i_6}\mathbf{E}_i - \psi_{i_7}\theta_{i_0} + \psi_{i_{10}}(\rho_i - \rho_{iR})].
\end{aligned}$$

Specific heat of the ice is,

$$\begin{aligned}
'e_{i_2} &= (\partial e_i / \partial \theta_i) \\
&= -\psi_{i_8}\theta_i.
\end{aligned}$$

Latent heat due to a change in dispersed density is,

$$\begin{aligned} e_{i3} &= (\partial e_i / \partial \rho_i) \\ &= [\psi_{i3} - \psi_{i9} \theta_{i0} + \psi_{i10} \text{tr}(\mathbf{E}_i) + \psi_{i11} (\rho_i - \rho_{iR})]. \end{aligned}$$

The chemical potential of the ice may be written in terms of the derivative of the expansion for the Helmholtz free energy as,

$$\begin{aligned} \mu_i &= \partial(\rho_i \psi_i) / \partial \rho_i \\ &= \psi_i + \rho_i \partial \psi_i / \partial \rho_i \\ &= \psi_{i1} (\text{tr } \mathbf{E}) + \psi_{i2} (\theta_i - \theta_R) + \psi_{i3} (\rho_i - \rho_{iR}) + (1/2) [\psi_{i5} [\text{tr}(\mathbf{E}_i)]^2 \\ &\quad + 2 \psi_{i6} \text{tr}(\mathbf{E}_i)^2 + 2 \psi_{i7} (\theta_i - \theta_R) \text{tr}(\mathbf{E}_i) + \psi_{i8} (\theta_i - \theta_R)^2 \\ &\quad + 2 \psi_{i9} (\theta_i - \theta_R) (\rho_i - \rho_{iR}) + 2 \psi_{i10} (\rho_i - \rho_{iR}) \text{tr}(\mathbf{E}_i) + \psi_{i11} (\rho_i - \rho_{iR})^2] \\ &\quad + \psi_{iR} + \rho_i [\psi_{i3} + \psi_{i9} (\theta_i - \theta_R) + \psi_{i10} \text{tr}(\mathbf{E}_i) + \psi_{i11} (\rho_i - \rho_{iR})] \\ &= \psi_{i1} (\text{tr } \mathbf{E}) + \psi_{i2} (\theta_i - \theta_R) + \psi_{i3} (2\rho_i - \rho_{iR}) + (1/2) [\psi_{i5} [\text{tr}(\mathbf{E}_i)]^2 \\ &\quad + 2 \psi_{i6} \text{tr}(\mathbf{E}_i)^2 + 2 \psi_{i7} (\theta_i - \theta_R) \text{tr}(\mathbf{E}_i) + \psi_{i8} (\theta_i - \theta_R)^2 \\ &\quad + 2 \psi_{i9} (\theta_i - \theta_R) (2\rho_i - \rho_{iR}) + 2 \psi_{i10} (2\rho_i - \rho_{iR}) \text{tr}(\mathbf{E}_i) \\ &\quad + \psi_{i11} (3\rho_i^2 - 4\rho_i \rho_{iR} + \rho_{iR}^2)] + \psi_{iR}. \end{aligned} \tag{4.25}$$

The reference Helmholtz free energy is determined in this development by assuming it is valued such that it will yield a zero chemical potential at reference. This gives the reference Helmholtz free energy as,

$$\psi_{i3} \rho_{iR} = -\psi_{iR}.$$

The manner in which $\psi_{i1} (\text{tr } \mathbf{E})$ and $\psi_{i10} (2\rho_i - \rho_{iR}) \text{tr}(\mathbf{E}_i)$ should effect

the chemical potential is not known, so in the interest of simplification it is assumed that when the partial density is equal to the reference value, these terms will cancel each other in the chemical potential equation, thus,

$$\psi_{i10} = -\psi_{i1}/\rho_{iR}$$

The Taylor series representation which is to be used for the Helmholtz free energy is assumed to be an approximation of the form for the free energy given for an ideal gas as represented by the form given in Sears and Salinger [1975]. A similar appropriate representation for the ice is not available, so in order to maintain a compatibility between the equations for the ice and vapor, the approximating expansion is used for both. The form given in Sears and Salinger for an ideal gas is,

$$\begin{aligned}\psi_V &= C(\theta_V - \theta_R) - C\theta_V \ln[\theta_V/\theta_R] - R\theta_V(\ln[\alpha_{VR}/\alpha_V]) - \eta_{VR}(\theta_V - \theta_R) + \psi_{V0} \\ &= C(\theta_V - \theta_R) - C\theta_V [\ln\theta_V - \ln\theta_R] - R\theta_V(\ln\alpha_{VR} + \ln[v_V/\rho_V]) \\ &\quad - \eta_{VR}(\theta_V - \theta_R) + \psi_{VR}\end{aligned}$$

where C is the specific heat capacity at constant volume, R is the gas constant, and η is the entropy.

Evaluating the coefficients in the usual way for the Taylor series expansion results with:

$$\psi_{V1} = \partial\psi_V/\partial v_V|_R$$

$$= -R\theta_R/v_{VR}$$

$$\psi_{V2} = \partial\psi_V/\partial\theta_V|_R$$

$$= -\eta_{VR}$$

$$\psi_{v_3} = \partial \psi_V / \partial p_V |_R$$

$$= R \theta_R / p_{VR}$$

$$\psi_{v_5} = \partial^2 \psi_V / \partial v_V^2 |_R$$

$$= R \theta_R / v_{VR}^2$$

$$\psi_{v_6} = \partial^2 \psi_V / \partial \theta_V \partial v_V |_R$$

$$= -R / v_{VR}$$

$$\psi_{v_7} = \partial^2 \psi_V / \partial \theta_V^2 |_R$$

$$= -C / \theta_R$$

$$\psi_{v_8} = \partial^2 \psi_V / \partial \theta_V \partial p_V |_R$$

$$= R / p_{VR}$$

$$\psi_{v_9} = \partial^2 \psi_V / \partial p_V \partial v_V |_R$$

$$= 0$$

$$\psi_{v_{10}} = \partial^2 \psi_V / \partial p_V^2 |_R$$

$$= -R \theta_R / p_{VR}^2$$

Substitution of these coefficients into Equation 4.20 gives

$$\begin{aligned} \psi_V = & - (R \theta_R / v_{VR}) (v_V - v_{VR}) - \pi_{VR} (\theta_V - \theta_R) + (R \theta_R / p_{VR}) (p_V - p_{VR}) \\ & + (1/2) [(R \theta_{VR} / v_{VR}^2) (v_V - v_{VR})^2 - (2R / v_{VR}) (\theta_V - \theta_R) (v_V - v_{VR}) \\ & - (C / \theta_{VR}) (\theta_V - \theta_R)^2 + (2R / p_{VR}) (\theta_V - \theta_R) (p_V - p_{VR}) \\ & - (R \theta_R / p_{VR}^2) (p_V - p_{VR})^2] + \psi_{VR} \end{aligned}$$

The objective form for the partial stress in the vapor as shown in Nunziato and Walsh [1980] is

$$\mathbf{T}_V = -\rho_V^2(\partial\psi_V/\partial\rho_V)\mathbf{I} - \rho_V(\partial\psi_V/\partial\mathbf{w}_V)\mathbf{w}_V,$$

since $\mathbf{h}_V = \mathbf{0}$ the partial stress for the vapor is,

$$\begin{aligned}\mathbf{T}_V &= -\rho_V^2(\partial\psi_V/\partial\rho_V)\mathbf{I} \\ &= -\rho_V^2[\psi_{V3} + \psi_{V8}(\theta_V - \theta_R) + \psi_{V10}(\rho_V - \rho_{VR})]\mathbf{I} \\ &= -\rho_V^2[(R\theta_R/\rho_{VR}) + (R/\rho_{VR})(\theta_V - \theta_R) - (R\theta_{VR}/\rho_{VR}^2)(\rho_V - \rho_{VR})]\mathbf{I} \\ &= -R\theta_R \rho_V^2/\rho_{VR}[2 - (\rho_V/\rho_{VR}) + (\theta_V - \theta_R)/\theta_{VR}]\mathbf{I}. \quad (4.26)\end{aligned}$$

In the reference state this yields a stress which is simply the negative partial pressure for an ideal gas,

$$\mathbf{T}_{VR} = -R\theta_R \rho_{VR} \mathbf{I}.$$

At equilibrium the equilibrated force for the vapor is given by

$$\begin{aligned}(v_V^{+e})^* &= (-\rho_V \partial\psi_V/\partial v_V)^* \\ &= -\rho_V[\psi_{V1} + \psi_{V5}(v_V - v_{VR}) + \psi_{V6}(\theta_V - \theta_R)] \\ &= -\rho_V[-(R\theta_R/v_{VR}) + (R\theta_{VR}/v_{VR}^2)(v_V - v_{VR}) - (R/v_{VR})(\theta_V - \theta_R)].\end{aligned}$$

Examination of this at the reference state, gives the reference extra equilibrated force,

$$\begin{aligned}(v_{VR}^{+e})^* &= \rho_V(R\theta_R/v_{VR}) \\ &= \gamma_V R\theta_R,\end{aligned}$$

which is the pressure for an ideal gas.

A slight retrogression at this point is helpful in ascertaining an appropriate value for the reference equilibrated force of the ice. Since with the assumptions which have been made,

$$\sum v_a^{+e} = N\pi,$$

then,

$$(v_{iR}^{+e})^* = 2\pi_R^* - \gamma_V R \theta_R,$$

and

$$\psi_{i3} = -(2\pi_R^* - \gamma_V R \theta_R) / (\rho_{iR} \gamma_i),$$

as stated previously in Equation 4.23.

The vapor entropy is by Equation 3.11 is

$$\begin{aligned} \eta_V &= -\partial\psi_V / \partial\theta_V \\ &= -[\psi_{V2} + \psi_{V6}(v_V - v_{VR}) + \psi_{V7}(\theta_V - \theta_R) + \psi_{V8}(\rho_V - \rho_{VR})] \\ &= \eta_{VR} + (R/v_{VR})(v_V - v_{VR}) + (C/\theta_R)(\theta_V - \theta_R) - (R/\rho_{VR})(\rho_V - \rho_{VR}), \end{aligned} \quad (4.27)$$

and since, $\psi_a = e_a - \theta_a \eta_a$ (Equation 2.92), the internal energy may be written as

$$\begin{aligned} e_V &= \psi_{V1}(v_V - v_{VR}) + \psi_{V2}(\theta_V - \theta_R) + \psi_{V3}(\rho_V - \rho_{VR}) + (1/2)[\psi_{V5}(v_V - v_{VR})^2 \\ &\quad + 2\psi_{V6}(\theta_V - \theta_R)(v_V - v_{VR}) + \psi_{V7}(\theta_V - \theta_R)^2 + 2\psi_{V8}(\theta_V - \theta_R)(\rho_V - \rho_{VR}) \\ &\quad + \psi_{V10}(\rho_V - \rho_{VR})^2] + \psi_{VR} - \theta_V[\psi_{V2} + \psi_{V6}(v_V - v_{VR}) + \psi_{V7}(\theta_V - \theta_R) \\ &\quad + \psi_{V8}(\rho_V - \rho_{VR})] \end{aligned}$$

$$\begin{aligned}
&= \psi_{v1}(\nu_v - \nu_{vR}) - \psi_{v2}\theta_R + \psi_{v3}(\rho_v - \rho_{vR}) + (1/2)[\psi_{v5}(\nu_v - \nu_{vR})^2 \\
&\quad - 2\psi_{v6}\theta_R(\nu_v - \nu_{vR}) - \psi_{v7}(\theta_v^2 - \theta_R^2) - 2\psi_{v8}\theta_R(\rho_v - \rho_{vR}) \\
&\quad + \psi_{v10}(\rho_v - \rho_{vR})^2] + \psi_{vR} \\
&= - (R\theta_R/\nu_{vR})(\nu_v - \nu_{vR}) + \eta_{vR}\theta_R + (R\theta_{vR}/\rho_{vR})(\rho_v - \rho_{vR}) \\
&\quad + (1/2)[(R\theta_R/\nu_{vR}^2)(\nu_v - \nu_{vR})^2 + (2R/\nu_{vR})(\nu_v - \nu_{vR}) \\
&\quad + (C/\theta_{vR})(\theta_v^2 - \theta_R^2) - (2R/\rho_{vR})\theta_R(\rho_v - \rho_{vR}) \\
&\quad - (R\theta_R/\rho_{vR}^2)(\rho_v - \rho_{vR})^2] + \psi_{vR}. \tag{4.28}
\end{aligned}$$

Using a development similar to that for the ice (Equation 4.52), the time rate of change for the internal energy of the vapor is,

$$e_v = e_{v1}\nu_v + e_{v2}\theta_v + e_{v3}\rho_v. \tag{4.29}$$

Latent heat due to a change in the volume fraction is,

$$\begin{aligned}
e_{v1} &= \partial e_v / \partial \nu_v \\
&= \psi_{v1} + \psi_{v5}(\nu_v - \nu_{vR}) - \psi_{v6}\theta_R \\
&= - (R\theta_R/\nu_{vR}) + (R\theta_R/\nu_{vR}^2)(\nu_v - \nu_{vR}) + (R/\nu_{vR})\theta_R \\
&= (R\theta_R/\nu_{vR}^2)(\nu_v - \nu_{vR}).
\end{aligned}$$

The specific heat of the vapor in Equation 4.29 is given by

$$\begin{aligned}
e_{v2} &= \partial e_v / \partial \theta_v \\
&= - \psi_{v7}\theta_v \\
&= (C/\theta_R)\theta_v.
\end{aligned}$$

At the reference state this yields the specific heat, as it must,

$$e_{v2} = C.$$

The latent heat with respect to the partial density of the vapor in Equation 4.29 is

$$\begin{aligned} e_{v3} &= \partial e_v / \partial \rho_v \\ &= \psi_{v3} - \psi_{v8} \theta_R + \psi_{v10} (\rho_v - \rho_{vR}) \\ &= (R\theta_R / \rho_{vR}) - (R / \rho_{vR}) \theta_R - (R\theta_{vR} / \rho_{vR}^2) (\rho_v - \rho_{vR}) \\ &= - (R\theta_{vR} / \rho_{vR}^2) (\rho_v - \rho_{vR}). \end{aligned}$$

The chemical potential of the vapor using the final constitutive variables [Nunziato and Walsh, 1980] is

$$\begin{aligned} \mu_v &= \partial(\rho_v \psi_v) / \partial \rho_v \\ &= \psi_v + \rho_v \partial \psi_v / \partial \rho_v \\ &= \psi_{v1} (\nu_v - \nu_{vR}) + \psi_{v2} (\theta_v - \theta_R) + \psi_{v3} (\rho_v - \rho_{vR}) + (1/2) [\psi_{v5} (\nu_v - \nu_{vR})^2 \\ &\quad + 2\psi_{v6} (\theta_v - \theta_R) (\nu_v - \nu_{vR}) + \psi_{v7} (\theta_v - \theta_R)^2 + 2\psi_{v8} (\theta_v - \theta_R) (\rho_v - \rho_{vR}) \\ &\quad + 2\psi_{v9} (\rho_v - \rho_{v0}) (\nu_v - \nu_{vR}) + \psi_{v10} (\rho_v - \rho_{v0})^2] + \psi_{vR} \\ &\quad + \rho_v [\psi_{v3} + \psi_{v8} (\theta_v - \theta_R) + \psi_{v9} (\nu_v - \nu_{vR}) + \psi_{v10} (\rho_v - \rho_{vR})] \\ &= \psi_{v1} (\nu_v - \nu_{vR}) + \psi_{v2} (\theta_v - \theta_R) + \psi_{v3} (2\rho_v - \rho_{vR}) + (1/2) [\psi_{v5} (\nu_v - \nu_{vR})^2 \\ &\quad + 2\psi_{v6} (\theta_v - \theta_R) (\nu_v - \nu_{vR}) + \psi_{v7} (\theta_v - \theta_R)^2 + 2\psi_{v8} (\theta_v - \theta_R) (2\rho_v - \rho_{vR}) \\ &\quad + 2\psi_{v9} (2\rho_v - \rho_{vR}) (\nu_v - \nu_{vR}) + \psi_{v10} (3\rho_v^2 - 4\rho_v \rho_{vR} + \rho_{vR}^2)] + \psi_{vR}. \end{aligned} \tag{4.30}$$

As for the ice, the reference Helmholtz free energy is determined in this development by assuming it is valued such that it will yield a zero chemical potential at reference. This requires the reference Helmholtz free energy to be,

$$\psi_{VR} = -\psi_{V3}\rho_{VR}$$

At equilibrium the temperatures of the two constituents are the same, $\theta_V = \theta_i = \theta$, and the chemical potentials must at be equal, so

$$\begin{aligned} & [\psi_{i1}(\text{tr } E) + \psi_{i2}(\theta - \theta_R) + \psi_{i3}(2\rho_i - \rho_{iR})] + (1/2)[\psi_{i5}[\text{tr}(E_i)]^2 \\ & + 2\psi_{i6}\text{tr}(E_i)^2 + 2\psi_{i7}(\theta - \theta_R)\text{tr}(E_i) + \psi_{i8}(\theta - \theta_R)^2 \\ & + 2\psi_{i9}(\theta - \theta_R)(2\rho_i - \rho_{iR}) + 2\psi_{i10}(2\rho_i - \rho_{iR})\text{tr}(E_i) \\ & + \psi_{i11}(3\rho_i^2 - 4\rho_i\rho_{iR} + \rho_{iR}^2)] + \psi_{iR} \\ & = \psi_{V1}(\nu_V - \nu_{VR}) + \psi_{V2}(\theta - \theta_R) + \psi_{V3}(2\rho_V - \rho_{VR}) \\ & + (1/2)[\psi_{V5}(\nu_V - \nu_{VR})^2 + 2\psi_{V6}(\theta - \theta_R)(\nu_V - \nu_{VR}) \\ & + \psi_{V7}(\theta - \theta_R)^2 + 2\psi_{V8}(\theta - \theta_R)(2\rho_V - \rho_{VR}) \\ & + 2\psi_{V9}(2\rho_V - \rho_{VR})(\nu_V - \nu_{VR}) \\ & + \psi_{V10}(3\rho_V^2 - 4\rho_V\rho_{VR} + \rho_{VR}^2)] + \psi_{VR} \end{aligned}$$

At this point, ψ_{i9} and ψ_{i11} are still undefined. The necessity of equivalence of the chemical potentials at equilibrium suggests a means to ascertain possible values for these terms. The terms are examined in the reference state for all variables except the temperature, since this should

be the dominant term indicating the difference in chemical potential. This is an artificial means to determine the values, but, the reference conditions in the solution will be chosen as the initial values for the variables, so that, except for the temperature these values will not stray very far from the reference values for the time duration and conditions to be considered. First, ψ_{i11} , is arbitrarily set to zero since an appropriate value for it is not known, and $\psi_{i11}(3\rho_i^2 - 4\rho_i\rho_{iR} + \rho_{iR}^2)$, will not contribute appreciably as long as the partial density of the ice does not vary far from the reference. A value for ψ_{i9} is determined by equating coefficients of similar variables. Although this forces a dependence of the ice coefficient on the vapor constituent, choosing the value at the reference state fixes it as constant, and it is assumed that the resulting value would be the appropriate one for this ice coefficient, independent of the vapor.

Examining everything in the reference state except temperature and collecting the remaining temperature related terms from the chemical potential (Equations 4.25 and 4.30) at equilibrium,

$$\begin{aligned} (\psi_{i2} + \psi_{i9} \rho_{iR})(\theta - \theta_R) + \psi_{i8}(\theta - \theta_R)^2 \\ = (\psi_{v2} + \psi_{v8} \rho_{vR})(\theta - \theta_R) + \psi_{v7}(\theta - \theta_R)^2, \end{aligned}$$

so that by equating coefficients, ψ_{i9} can be determined in terms of known quantities,

$$\psi_{i9} = (\psi_{v2} - \psi_{i2} + \psi_{v8}\rho_{v0})/\rho_{iR},$$

but another implication is that,

$$\psi_{i_8} = \psi_{v_7}.$$

This last result requires that the specific heats for the ice and vapor must be equal, in order to satisfy the requirement that the chemical potentials are equivalent at equilibrium. Although this is probably inappropriate in general, this constraint will be adhered to in the present case, until more precise values for the other coefficients can be developed, which will presumably balance the equilibrium chemical potential, to make this requirement unnecessary.

Material Frame Indifference

Equations describing a material response, the constitutive equations, should not change based on any particular choice of reference frame. This is the basis for the principle of material frame indifference, also called the principle of material objectivity. Material frame indifference does not require that a time dependent change of reference, such as Newton's Second Law of Motion, be invariant, only those equations describing the material response must remain unchanged under a change of reference frame. Two different frames of reference are considered equivalent if they agree about: i) the distance between two points in a body, ii) the order in which events occur, iii) the orientation of a line segment, and iv) the time interval between events.

Consider two reference frames RF and $(RF)^*$, and define $\mathbf{c}(t)$ as the position vector relating the origin of RF, O , from the origin of $(RF)^*$, O^* , and $\mathbf{Q}(t)$ as the orthogonal tensor which rotates the reference frame $(RF)^*$

into the orientation of the other reference frame (RF). Scaler point functions are not affected by a change of frame. Functions and fields are material frame indifferent, if while scaler values remain unchanged, vector, and tensor functions transform according to the following rules for a change of frame [Malvern, 1969]:

$$1. \text{ Events } \{\mathbf{x}, t\} : \mathbf{x}^* = \mathbf{c}(t) + \mathbf{Q}(t) \mathbf{x} \\ t^* = t - a$$

$$2. \text{ Vectors } \mathbf{v} : \mathbf{v}^* = \mathbf{Q}(t) \mathbf{v} \\ (\text{here } \mathbf{v} \text{ implies any general vector})$$

$$3. \text{ Second order tensors } \mathbf{T} \text{ or } \mathbf{S} \text{ regarded as linear vector transformations:}$$

$$\mathbf{u} = \mathbf{T} \mathbf{v} \text{ or } \mathbf{u} = \mathbf{v} \mathbf{S} \\ \mathbf{T}^* = \mathbf{Q}(t) \mathbf{T} \mathbf{Q}(t)^T \\ \mathbf{S}^* = \mathbf{Q}(t) \mathbf{S} \mathbf{Q}(t)^T$$

(here the notation implies general vectors and tensors)

$$4. \text{ Deformation gradient } \mathbf{F}(\mathbf{X}, t) \\ \mathbf{F}^* = \mathbf{Q}(t) \mathbf{F}$$

(This two-point tensor transforms as a vector under a change of frame at time t)

Now the specific constitutive equations which have been developed are examined to see if they are objective. The the constitutive equations are

$$\psi_a, \eta_a, \mathbf{T}_a, \mathbf{q}_a, c_a^+, v_a^+, \mathbf{m}_a^+, e_a^+.$$

Since $\psi_a, \eta_a, c_a^+, v_a^+, e_a^+$ are scaler functions, they will automatically be satisfied. The partial stress for the ice is given by Equation 4.24 as

$$\mathbf{T}_i = p_i \{ \psi_{i1} \mathbf{1} + \psi_{i5} \text{tr}(\mathbf{E}_i) \mathbf{1} + 2 \psi_{i6} \mathbf{E}_i + \psi_{i7} (\theta_i - \theta_R) \mathbf{1} + \psi_{i10} (\rho_i - \rho_{iR}) \mathbf{1} \}.$$

By orthogonality $\mathbf{Q}^T = \mathbf{Q}^{-1}$, so

$$\mathbf{I}^* = \mathbf{Q} \mathbf{I} \mathbf{Q}^T$$

$$= \mathbf{I}.$$

The only other thing to be shown for the partial stress of the ice is E_i (Equation 4.18), where

$$E_i = (1/2)(\mathbf{F}_i^T \mathbf{F}_i - \mathbf{I}),$$

so,

$$\begin{aligned} E_i^* &= (1/2)(\mathbf{F}_i^{T*} \mathbf{F}_i^* - \mathbf{I}^*) \\ &= (1/2)(\mathbf{F}_i^T \mathbf{Q}^T \mathbf{Q} \mathbf{F}_i - \mathbf{I}) \\ &= (1/2)(\mathbf{F}_i^T \mathbf{F}_i - \mathbf{I}) \end{aligned}$$

and

$$E_i^* = E_i.$$

The partial stress for the vapor (Equation 4.26) is material frame indifferent since it contains only the identity tensor.

For the heat flux,

$$\begin{aligned} \mathbf{q}_a^* &= (\theta_a \nabla_{\mathbf{x}^*})(\nabla_{\mathbf{x}^*} \mathbf{x}) \\ &= (\theta_a \nabla_{\mathbf{x}^*}) \mathbf{Q}^{-1} \\ &= \mathbf{g}_a \mathbf{Q}^T \\ &= \mathbf{Q} \mathbf{g}_a. \end{aligned}$$

The constitutive equation for the momentum interaction which was earlier derived from the dissipation inequality is,

$$\mathbf{m}_i^{+e} = -\mathbf{m}_v^{+e} = m_{i_0}^{+e} \{(\mathbf{v}_v/\theta_v) - (\mathbf{v}_i/\theta_i)\}.$$

For either velocity, say simply $\mathbf{v}_i = \mathbf{v}_V = \mathbf{v}$, then for a change of frame,

$$\mathbf{x}^* = \mathbf{c} + \mathbf{Q}\mathbf{x},$$

The material time derivative gives the velocity,

$$\mathbf{v}^* = \dot{\mathbf{c}} + \dot{\mathbf{Q}}\mathbf{x} + \mathbf{Q}\mathbf{v}.$$

So the velocity is not objective.

It is argued here that the non-objectivity of the constitutive form for the extra momentum interaction is not inappropriate, since it enters the theory through a fundamental law of dynamics, the equation of motion (balance of linear momentum equation), which itself is not material frame indifferent. However, as an aside, it is pointed out that if the temperatures are equal, the velocity difference term which results, is frame indifferent,

$$\begin{aligned} \mathbf{v}_V^* - \mathbf{v}_i^* &= \dot{\mathbf{c}} + \dot{\mathbf{Q}}\mathbf{x}_V + \mathbf{Q}\mathbf{v}_V - \dot{\mathbf{c}} - \dot{\mathbf{Q}}\mathbf{x}_i - \mathbf{Q}\mathbf{v}_i \\ &= \dot{\mathbf{Q}}\mathbf{x}_V + \mathbf{Q}\mathbf{v}_V - \dot{\mathbf{Q}}\mathbf{x}_i - \mathbf{Q}\mathbf{v}_i, \end{aligned}$$

but $\mathbf{x}_V = \mathbf{x}_i$, so

$$\mathbf{v}_V^* - \mathbf{v}_i^* = \mathbf{Q}(\mathbf{v}_V - \mathbf{v}_i).$$

CHAPTER V

APPLICATION OF THE THEORY

One Dimensional Solution

Application of the theory which has been developed for snow, is carried out in one dimension. This one dimensional approach is applied in the vertical, slope normal direction, simulating a snowpack on a horizontal field. This one dimensional model is obviously limiting to the scope of problems, as well as being inadequate to properly describe some processes. However, this is the logical first step toward implementing the theory of multiphase mixtures with phase change to physical problems.

In this application the velocity of the ice is assumed negligible, since the settlement velocity due to gravity would be very slow. Also, given the granular nature of the material, settlement involves a closer packing of grains as they move laterally and downward into voids, an effect which is not applicable in a one dimensional model. Vapor velocity is considered in the formulation, but the one dimensional approach cannot account for convection cells. Since the vapor is considered as a single constituent, any diffusion of water vapor through the air is not independently calculated, but is included as a part of the total vapor flux.

In the numerical solution to the problem, derivatives are put in a finite difference form. The derivatives on space are in general central differenced, except at the bottom and top nodes where they are

appropriately forward and backward differenced. The derivatives on time are forward differenced.

The basic approach to the explicit numerical solution used, is quite straight forward. Values for variables which do not involve time derivatives are calculated at the initial or current time for each time interval iteration or program loop. The balance equations are then used to find the rate of change of those variables which explicitly vary with time as indicated by the equations. For each iteration or loop, variables are recalculated to reflect what the value is at the end of the period which is used to step forward in time. These updated values are then assumed as the variables which are used in the balance equations for the next loop. This iterative process is progressively stepped forward in time, until the desired total time is achieved.

Proceeding as above, the manner in which the balance equations are utilized should be noted. The time rate of change for the volume fraction of the ice is directly calculated through the equation of mass balance for the ice, and the time rate of change of the partial density of the vapor is given by the mass balance for the vapor (Equation 3.26):

Since the ice velocity is assumed always zero, the acceleration is zero, and the linear momentum balance equation (2.26) may be used to calculate the partial stress of the ice constituent. Then, since a form for the stress is also given through the derivative of the Helmholtz free energy, as required by the second law (Equation 4.21), the strain of the ice may be calculated. Using this calculated strain in conjunction with the strain from the previous iteration, an approximation to the strain rate is

found, which is needed in the energy balance equation (Equation 2.80). The vapor velocity is approximated from the linear momentum balance for the vapor (Equation 2.83), the manner in which this is accomplished is outlined below.

The equilibrated force interaction for the ice and vapor is given by the balance equations for the equilibrated force (Equations 4.15 and 4.16). It is important to note that the time rate of change of the volume fraction must be calculated prior, since it is necessary in order to solve the balance of equilibrated force equations. Time rate of change of temperature for the ice and vapor is calculated through the constituent energy balance equations (Equation 2.80), prior to which the mass balance equations and the momentum balance for the ice must be solved, since the time rate of change of these variables are needed.

Boundary and initial conditions must be assumed in order to solve the system of equations. At both the upper and lower boundaries the temperatures for the ice and vapor are taken to be constant and equal. Holding the temperatures constant is reasonable for the steady state problem, but the assumption that the boundary constituent temperatures remain equal is quite likely incorrect. No physical data are available to suggest what realistic constituent temperature differences might be, therefore, the constituent temperatures at the boundary are taken to be equal, while the temperatures within the pack are permitted to vary separately. Although this equality at the boundary surely effects how the constituent temperature difference varies throughout the pack, it is perhaps the most reasonable assumption to use until reliable data become

available. The vapor velocity at the ground is assumed to remain zero, simulating an impermeable boundary.

Initially, the vapor velocity is assumed zero everywhere. The initial temperature conditions within the pack, excluding the upper surface boundary, are assumed isothermal with the temperature at the ground-snow interface boundary. The upper and lower surface temperatures are fixed at whatever temperature is desired to simulate the prescribed thermal regime, and the stress on the ice surface is a constant.

Numerical determination of the vapor velocity is the most unsatisfying aspect of the entire development presented in this dissertation. The balance of linear momentum (Equation 2.83) is used to calculate the velocity of the vapor, but due to difficulties encountered in the numerical evaluation, a discussion of this balance equation is required. A standard finite difference equation using the boundary and initial conditions as mentioned above was at first attempted, but instantaneously imposing accelerations due to gravity and the pressure gradient gave values for the velocity which were too large, and caused program instability. An attempt to provide initial density gradients to compensate for the initial assumptions were found to give results which were numerically unstable. This instability is attributed to the rounding errors inherent to numerical analysis which involved a series of calculations involving small differences of very large numbers. This gave numerical values which are very close to zero, with random oscillation of sign.

The initial values for the vapor velocities, as stated, are all assumed zero. When instantaneous accelerations are imposed through the linear

momentum equation, large velocity values are immediately calculated. To smooth these sudden velocity jumps, which result from the imposition of instantaneous accelerations, the vapor velocity was solved for directly, using an analytic solution to the differential equation. Details of the solution to the differential equation is shown in appendix A. However, the transient effects for the velocity calculated from the balance of linear momentum seemingly react much more quickly than do the other balance equations. Due to the coupling of equations, this causes the entire program to become numerically unstable. The dominant terms determining the vapor velocities are the difference in the gradient of the partial vapor stress and gravity effects. In fact if these terms are not allowed to effect the linear momentum equation, a zero vapor velocity will be maintained in the case of a homogeneous snowcover.

In order to slow the vapor velocity response at each incremental time adjustment, the particular part of the solution is artificially scaled down. The "a" coefficient noted in the appendix is chosen as the scaling multiplier. This is used, although somewhat arbitrarily, because it is the value which was divided through the original differential equation to achieve a form for the cubic equation which is used to find the particular solution. This coefficient is always positive and should not effect the direction of the calculated vapor flow, only the magnitude. The necessity of this artificial adjustment of the vapor velocity magnitude is displeasing. But, with this computational problem noted, results from the theory are presented, looking toward a resolution in future work.

The value for the interface pressure, π , the pressure necessary in a saturated mixture for the phases to remain in contact, is assumed to be approximated by the vapor pressure over a surface at equilibrium. The equilibrium vapor pressure over an ice grain will vary with temperature, θ , and the mean radius of curvature, r [Colbeck, 1980]. The well known Clausius-Clapeyron and Kelvin equations may be used in a combined form to give the equilibrium vapor pressure over a grain in terms of the desired variables [Adams and Brown, 1982; 1983; Gubler, 1985]. The Clausius-Clapeyron equation which gives the vapor pressure as a function of temperature is,

$$P(\theta) = P_R \exp[L/R(\theta^{-1} - \theta_R^{-1})],$$

where P is the equilibrium vapor pressure over the surface and L is the latent heat of sublimation. The vapor pressure in terms of the mean radius of curvature, ω , is given by Kelvin's equation,

$$P(\omega) = P_R \exp[2\sigma/\gamma_i R \theta_R \omega],$$

where σ is the interfacial energy. Assuming the fixed reference temperature is the same as the reference temperature to be used in the Clausius-Clapeyron equation, the two equations may be combined,

$$P(\theta, \omega) = P_R \exp[2\sigma/\gamma_i R \theta_R \omega] \exp[L/R(\theta^{-1} - \theta_R^{-1})].$$

The leading coefficient involved in the mass interaction equation, $c_{i_0}^+$, is assumed to be proportional to this interface pressure as well. The magnitude of the proportionality is assumed small since the density change in snow as the result of metamorphism in dry snow is small. Although the coefficient for the energy is not known, it is arbitrarily assumed to be on

an order of magnitude equivalent for Newton's law of cooling for air flowing over a flat plate.

Young's Modulus is approximated by fitting to a curve in Mellor's Review of Basic Snow Mechanics [1974]. The equation used in the calculations presented here to approximate the curve for a density range of approximately, 150 kg/m^3 to 375 kg/m^3 , is

$$Y = 10 \exp(10\nu_i + 4).$$

Material values used for the ice and vapor are shown in the input file listed with the program in appendix B. These values are for ice and vapor which is considered to be water vapor saturated air at 273°C .

Results from the Analysis

Several idealized situations for snow are examined in order to ascertain the success of the theoretical model which has been presented. Two ideal snowpacks of one meter depth are considered: a perfectly homogeneous sample and a sample exhibiting stratigraphic density layering. The homogeneous snow is taken to have an ice volume fraction of 0.3, which is equivalent to snow with a density of approximately 276 kg/m^3 . The other is considered to be of the same overall density as the homogeneous, but with two distinct, isolated layers 15 cm thick. One of these layers is greater and one is of lesser density than the rest of the snowpack. The high density layer is assumed to have an ice volume fraction of 0.4, which corresponds to a snow density of 368 kg/m^3 , while the low density layer is represented by an ice volume fraction of 0.2, or a snow density 184 kg/m^3 . These densities are in a range typical for alpine snow.

The variation of snowcover properties of these snowpack types are examined, using the theory, for initial isothermal conditions of 0°C throughout, and for a snowpack with a temperature of 0°C from the base up to, but not including, the surface, which is at a temperature of -20°C . Boundary temperatures for both the ice and the vapor are held constant and equal. The actual calculations are made using the Kelvin temperature scale. Stress on the ice at the surface is assumed to be equal to the same atmospheric pressure in all situations.

Sign convention for stress is used in the normal engineering manner, which implies a positive sign for tension and a negative for compression. Stress for both the ice and vapor are considered in this manner. This is pointed out, since a frequent usage when considering pressure scalars, as is common in fluid and vapor analysis, is to consider pressure to be positive in compression. This paper considers all values noted, of both constituents, to be in terms of the stress sign convention. Likewise, strain is, correspondingly, negative in compression. Measurement of position in the snowpack is from the ground upward toward the surface.

Examination of the homogeneous snowpack with the equal thermal boundary conditions gives results which are characteristic of a purely mechanical system. The results are illustrated in figures 4 - 7. The partial stress of the ice constituent is shown to increase in magnitude in a linear fashion from top to bottom (Figure 4). This increase is logically the result of the overburden of the snowpack itself. There is a variation in the strain (Figure 5) which corresponds directly to the stress distribution as a result of the mechanical loading. Strain in the ice at the top surface is nonzero,

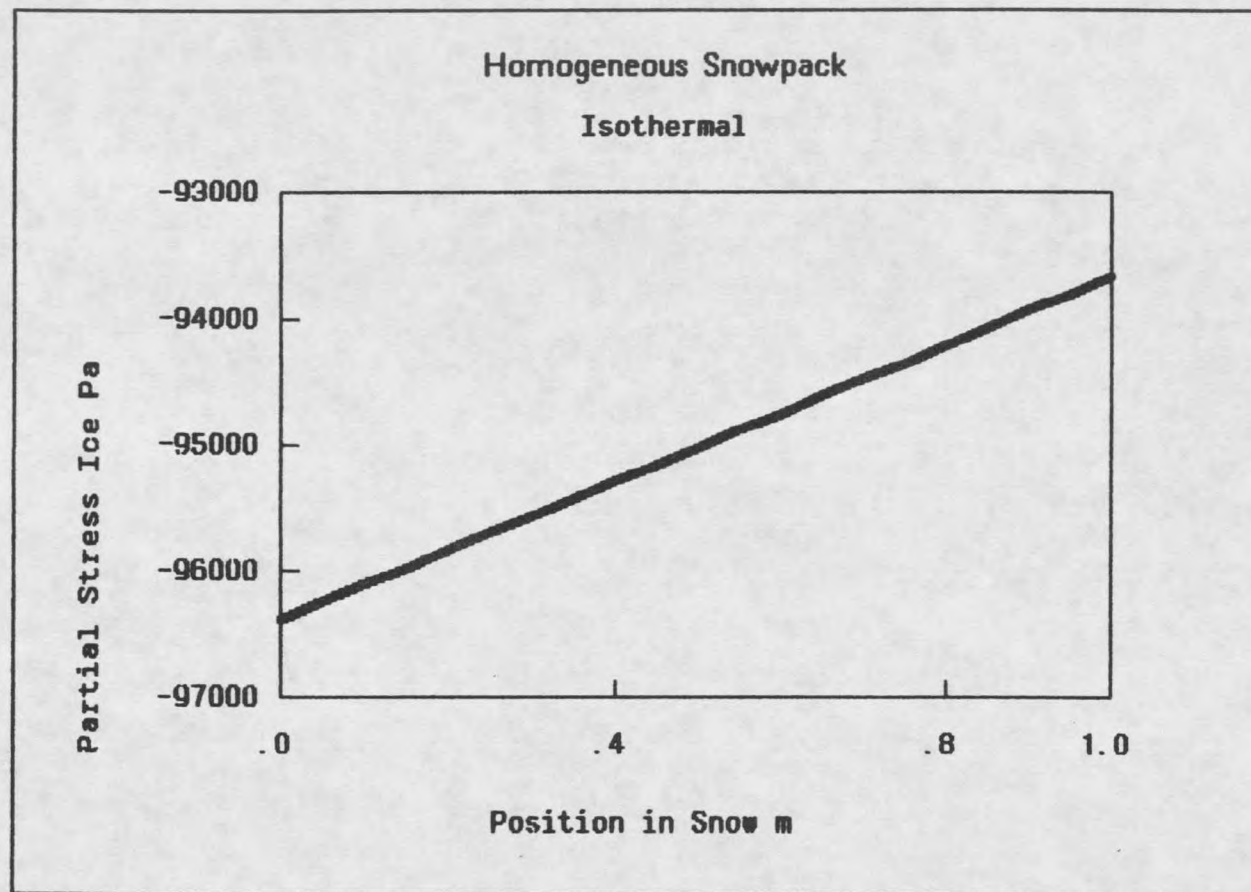


Figure 4. Partial stress of the ice relative to position in an isothermal homogeneous snowpack. Stress is negative in compression.

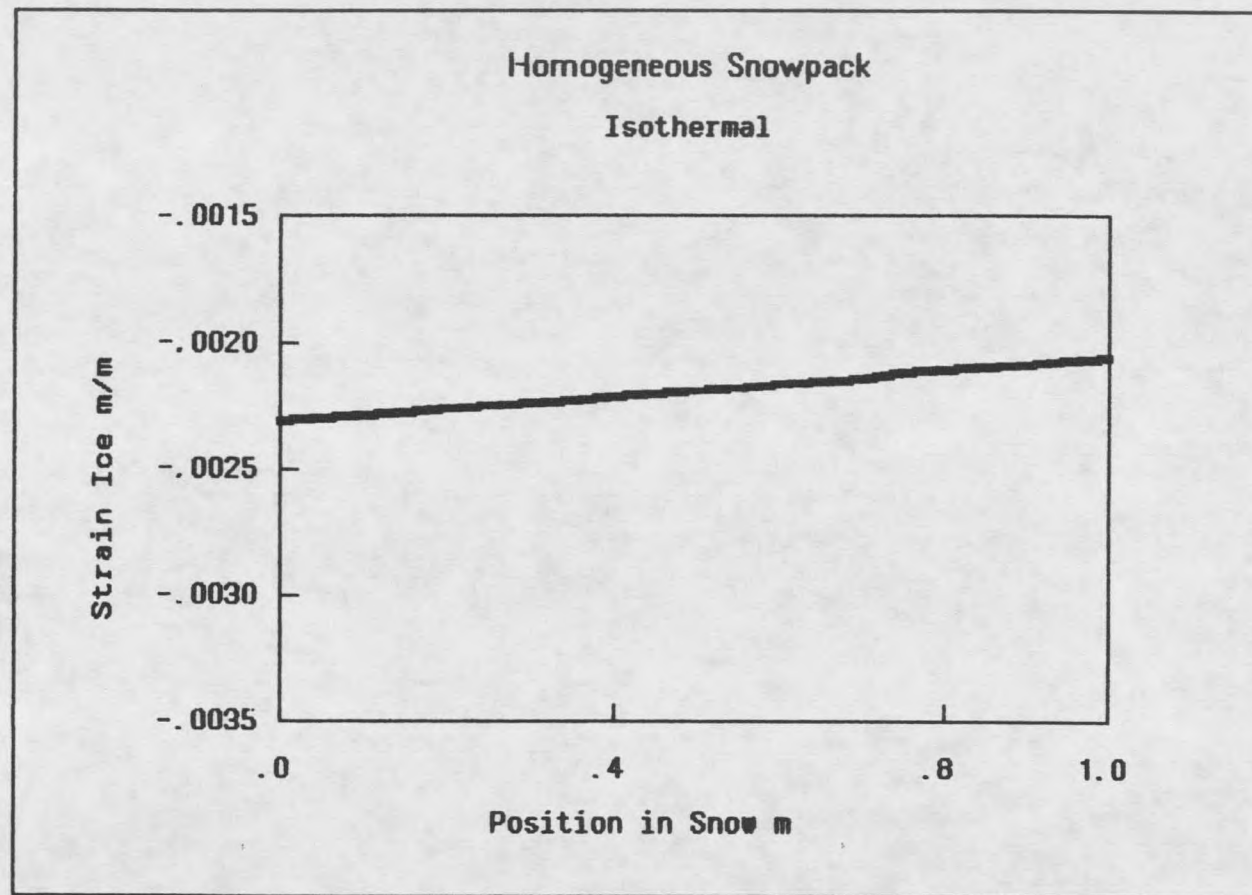


Figure 5. Strain in the ice relative to position in an isothermal homogeneous snowpack. Strain is negative in compression.

since a partial stress is applied to the ice constituent by atmospheric pressure.

The partial stress considered for the vapor constituent is constant throughout, since the description for the vapor stress did not include the gradient due to gravity. The stress considered is absolute stress measured relative to a zero stress environment (i.e. it is not a gauge pressure type of value). No vapor velocity is established in the homogeneous isothermal snowpack.

The time rate of change of the volume fraction for the homogeneous isothermal consideration, on inspection of figure 6, reveals that there will be an overall decrease in the portion of the total volume occupied by the ice, and that this decrease is amplified with depth. This phenomena is the result of the the difference of the chemical potentials of the constituents, caused by the variation in the strain of the ice on the chemical potential of that constituent. The effect is relatively slight, and as will be seen in the non-isothermal situation, is so small as to not have any meaningful effect on the results in that case.

The equilibrated force is included in this theory to account for those dynamical effects which occur in conjunction with volume fraction changes of the constituents. The development presented here for the equilibrated force interaction of a constituent is derived to be equal to the negative of the external equilibrated body force times the partial density, for that same constituent, it is also the negative of the equilibrated force interaction for the other constituent.

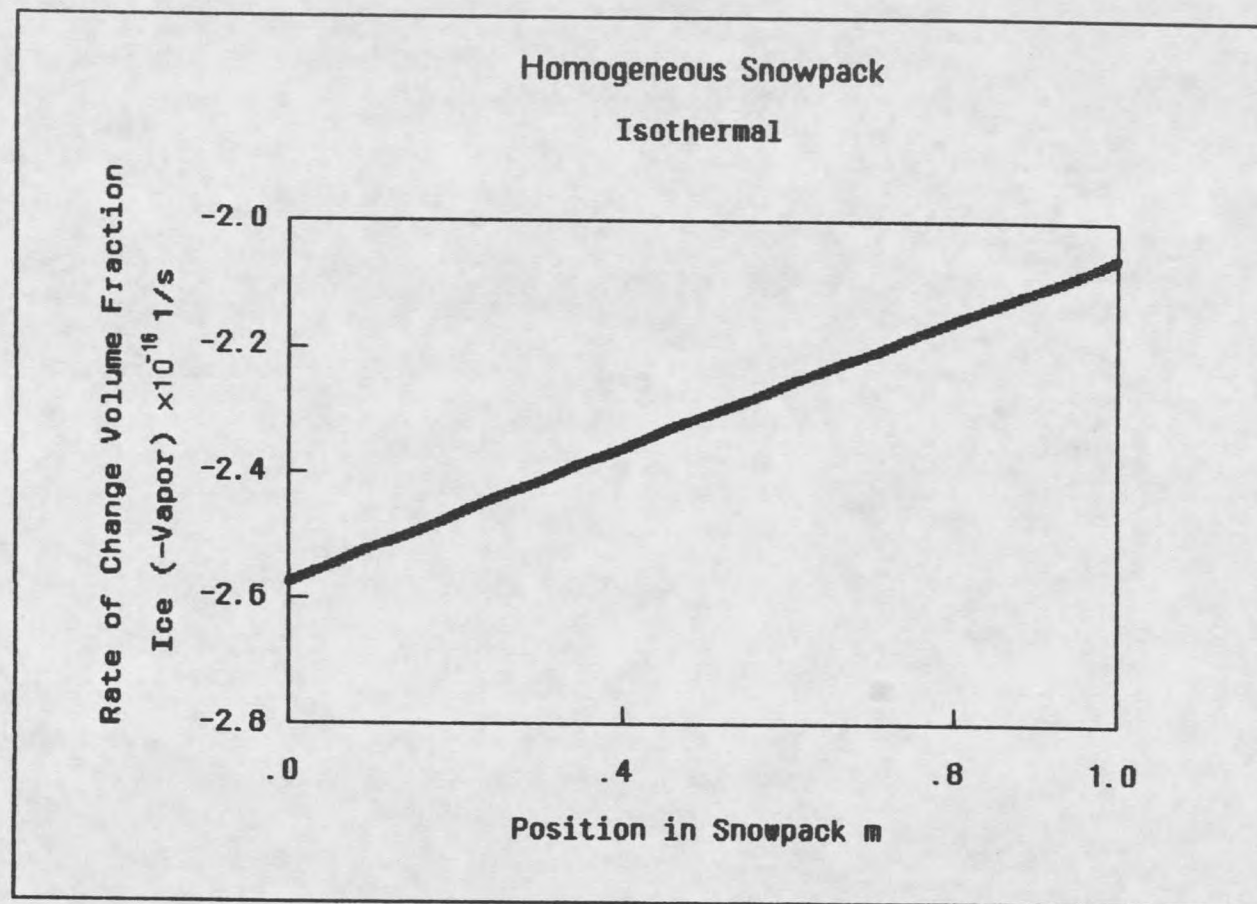


Figure 6. Time rate of change of the volume fraction of the ice relative to position in an isothermal homogeneous snowpack.

As stated earlier the, the external equilibrated body force for the mixture has been related in some manner to an externally controlled pore pressure, but a clear understanding particularly in regard to the constituents has not yet been established. Values calculated for the equilibrated force interaction terms are presented here (Figure 7), but an indication of whether or not these values are reasonable cannot be determined based on any physical or intuitive knowledge, at this time. Current research on granular materials is attempting to define these variables more precisely.

Now consider this same homogeneous snowpack subjected to the initial and boundary conditions. For both constituents the lower boundary temperature is set and held at 0°C , the upper boundary is held at -20°C and initially the rest of the snow is set to 0°C . Partial stress of the ice at the surface is assumed constant. Initial vapor velocities are all assumed zero and the lower boundary velocity is held at this value. Values of calculated results are shown for several time increments after the initial, so that the transient variation may be observed. These are illustrated in figures 8 - 19.

Variation of temperature for the vapor (Figure 8) and ice (Figure 9) are seen to react quite reasonably. At the end of a very short time period, 1 hour, most of the snow remains at the initial temperature with a very large temperature variation in the uppermost region. Passing of time shows the temperature profile with respect to position to be migrating toward a linear function.

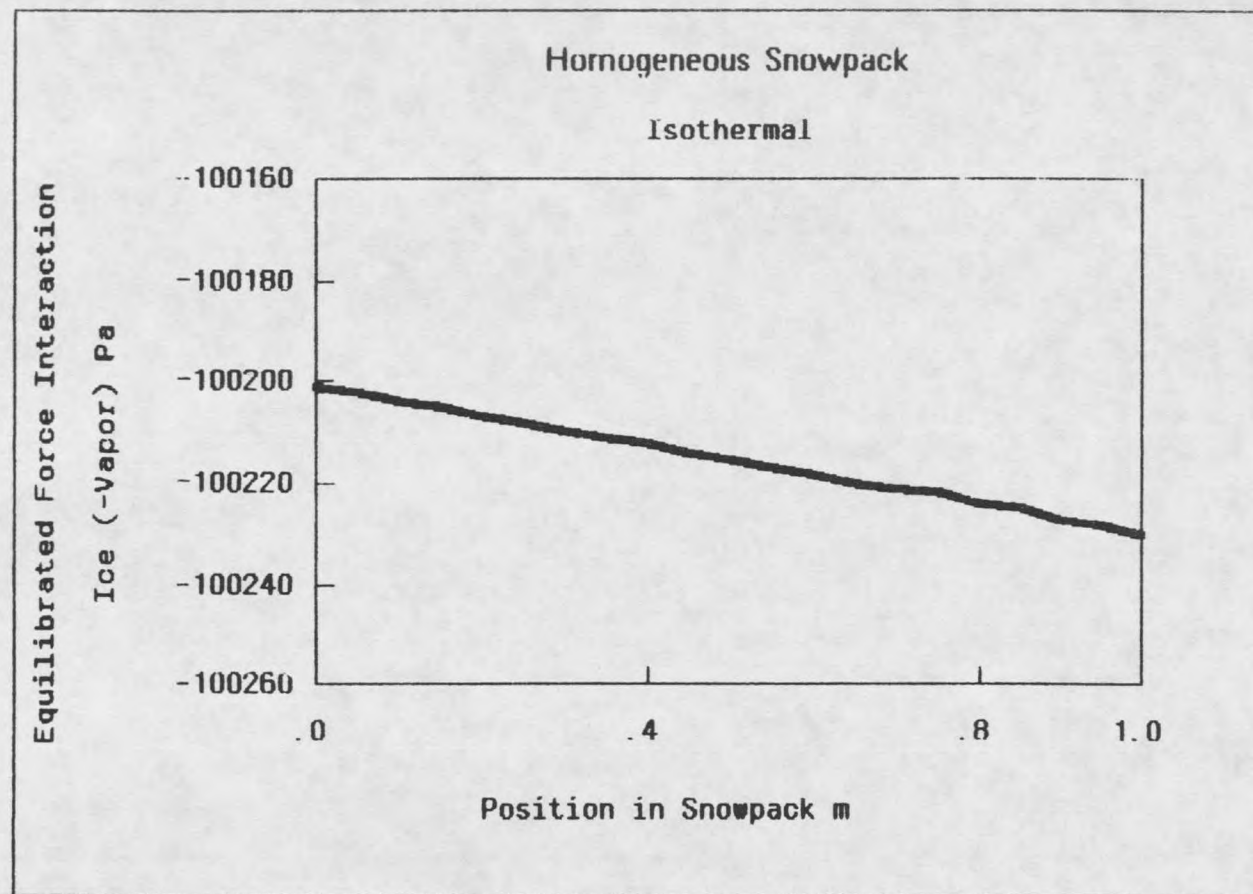


Figure 7. Equilibrated force interaction of the ice relative to position in an isothermal homogeneous snowpack.

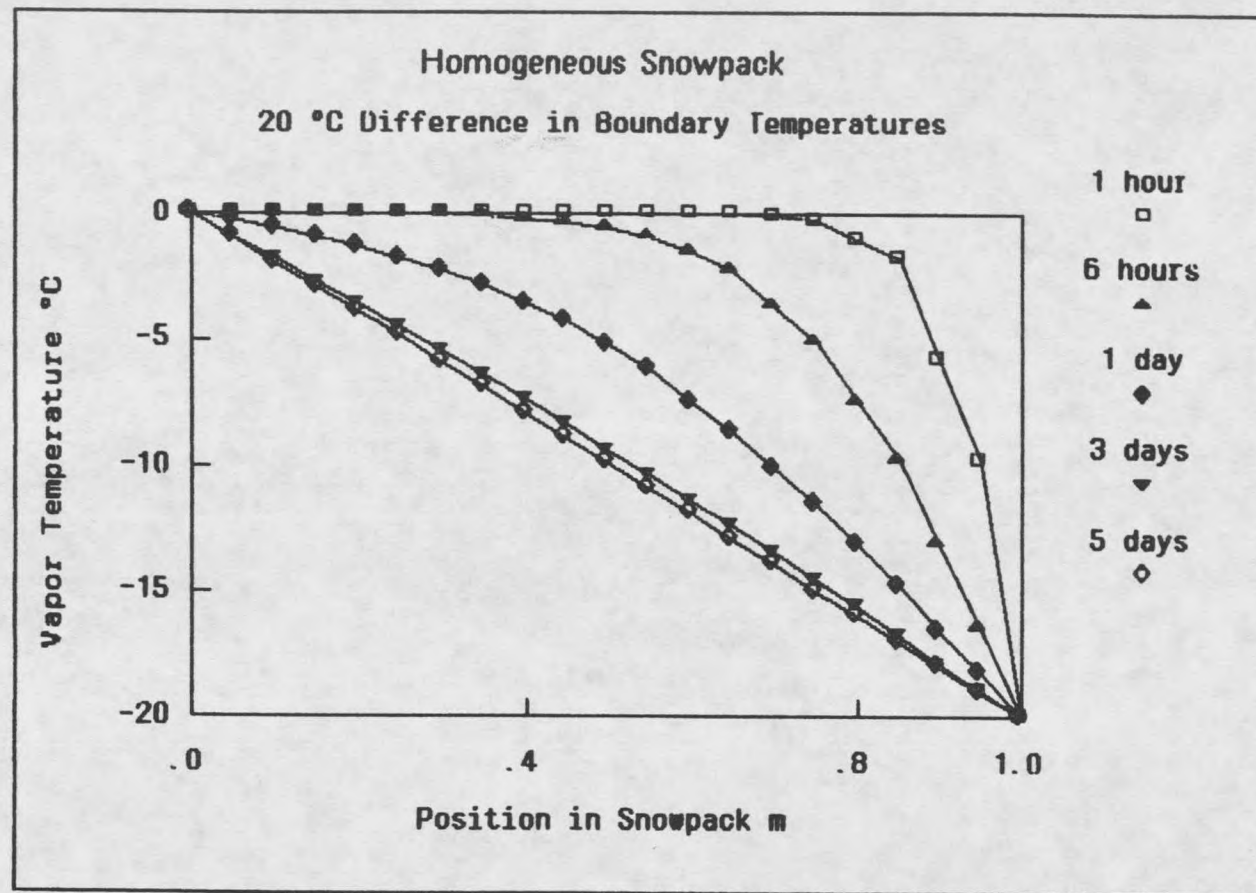


Figure 8. Temperature of the vapor relative to position in a homogeneous snowpack.

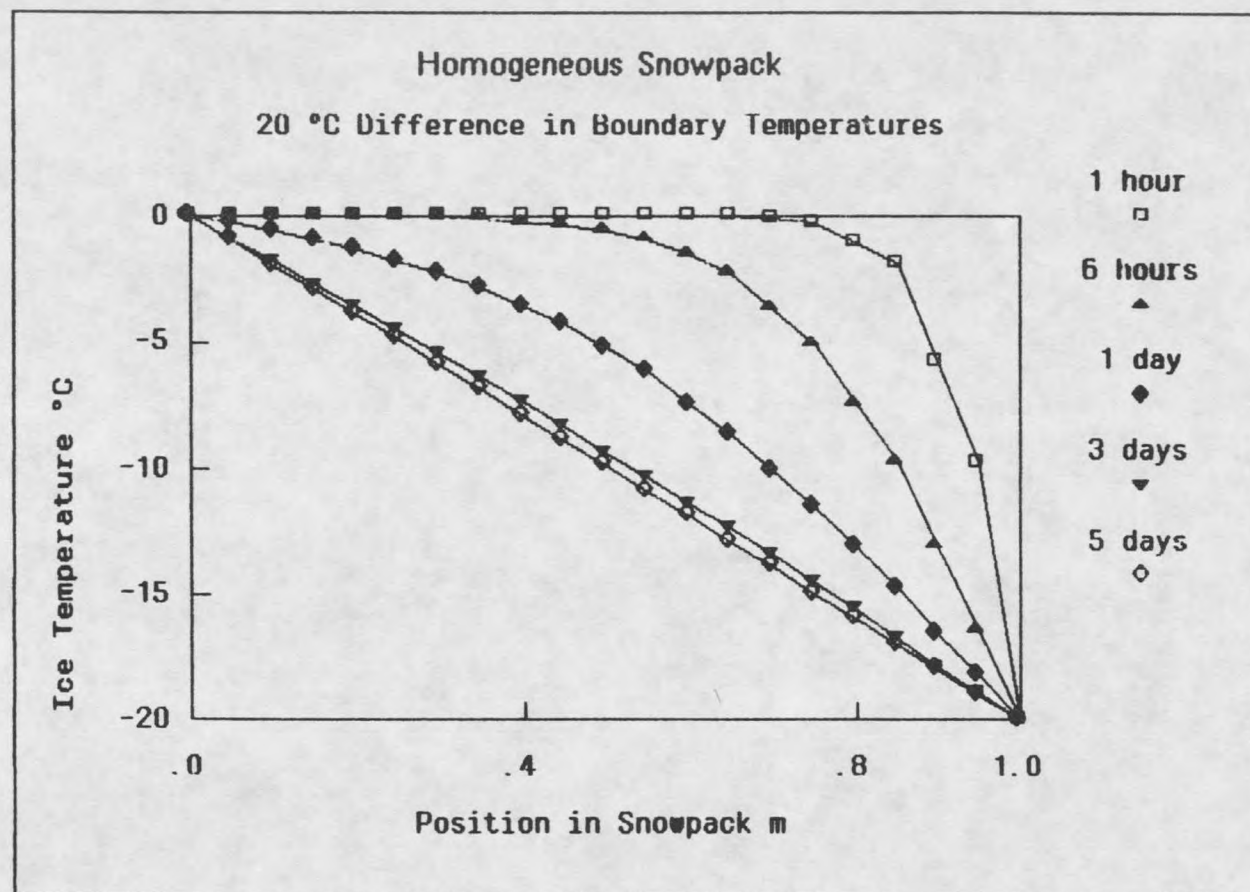


Figure 9. Temperature of the ice relative to position in a homogeneous snowpack.

Corresponding to this temperature curve is the temperature gradient variation with position (Figures 10, 11, and 12). A very large negative temperature gradient is established in the upper region of the snowpack for a short time. This temperature gradient in the uppermost section begins to lower with the passage of time, as the temperature permeates deeper into the snow, inducing a gradient throughout the snowpack. This thermal gradient which is larger near the surface and lower near the bottom gradually moves toward a constant value which is the same as the gross initial value measured across the full meter, $-20^{\circ}\text{C}/\text{m}$ (Figure 13).

When the surface of the snowpack is suddenly cooled as in the situation presented here, where the surface is initially 20°C colder than the rest of the snow, the underlying snowpack temperature will begin to be lowered also, as has just been demonstrated in the model. But, the mixture is composed of two distinct materials with differing thermal conductivities. These constituents should not be expected to change temperature at the same rate. Here too the model seems to be predicting some very plausible results (Figure 13), although no known physical data exist for snow in regard to differences in temperature between the ice and vapor phases. Notice in the figure that it is early in the developing situation and in the upper, more active region where the most substantial difference in constituent temperatures is occurring.

Ice has a much higher thermal conductivity than does the vapor and consequently will react to the imposed boundary temperature more quickly. This is the reason the vapor is at a warmer temperature than the ice, and the temperature difference between the phases is most pronounced when

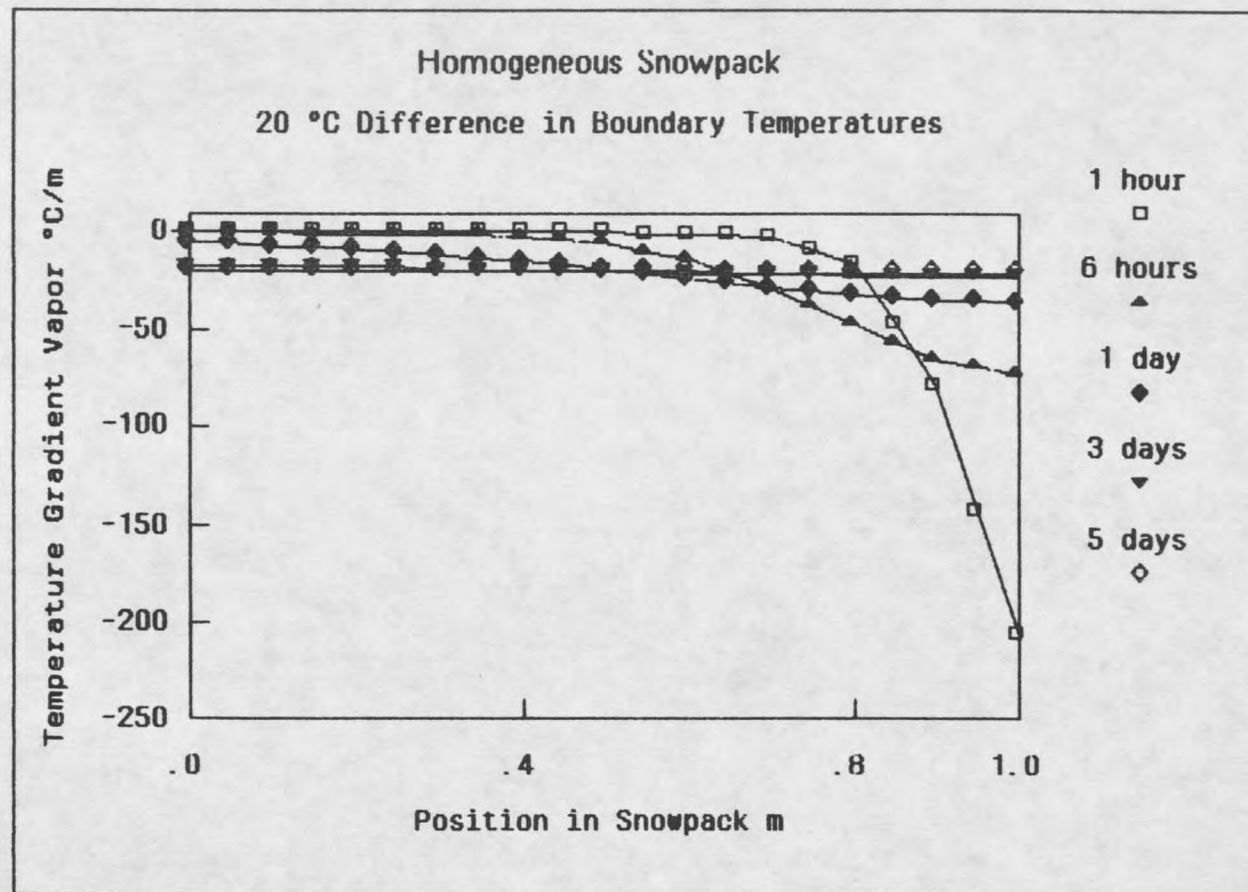


Figure 10. Temperature gradient of the vapor relative to position in a homogeneous snowpack, with base temperature 0 °C and surface temperature -20 °C.

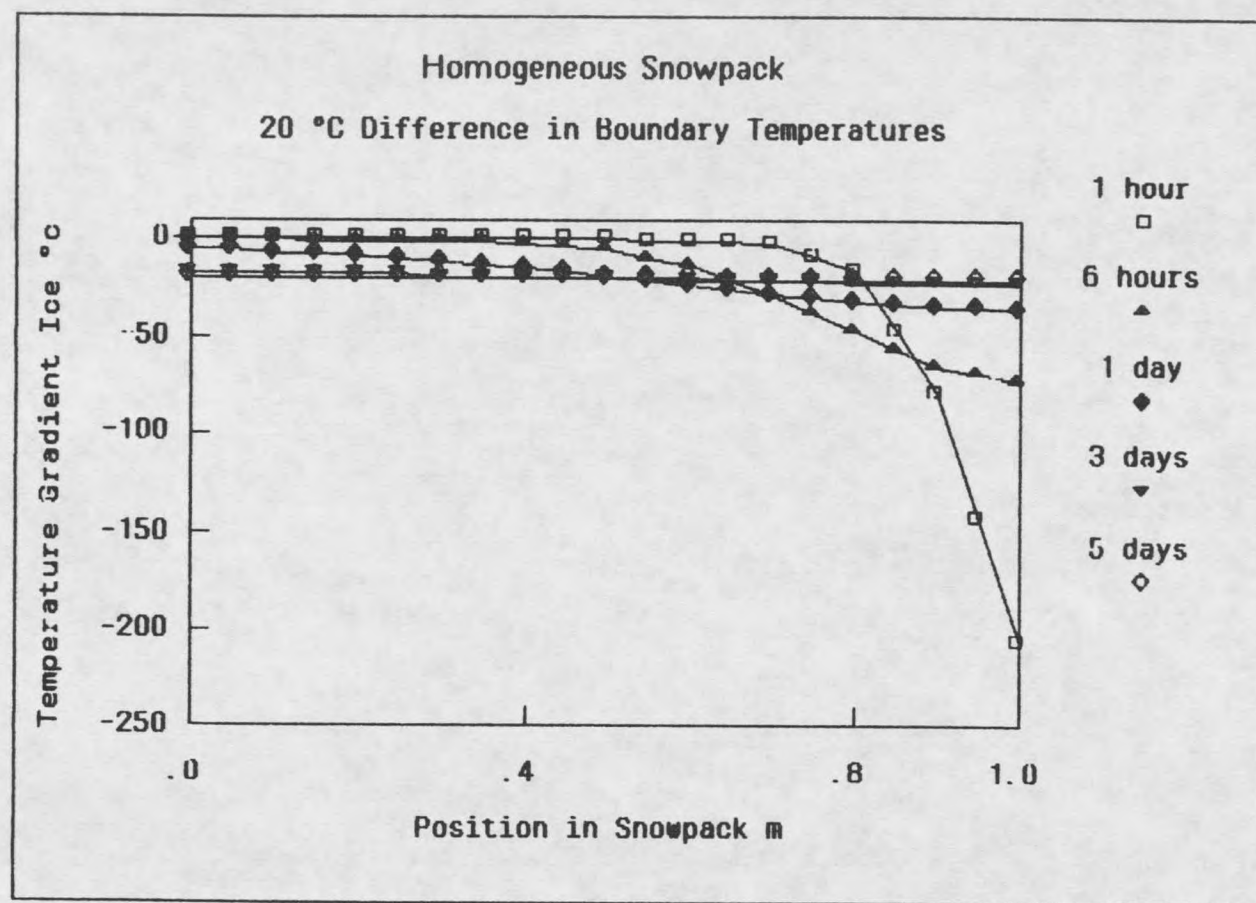


Figure 11. Temperature gradient of the ice relative to position in a homogeneous snowpack, with base temperature 0 °C and surface temperature -20 °C.

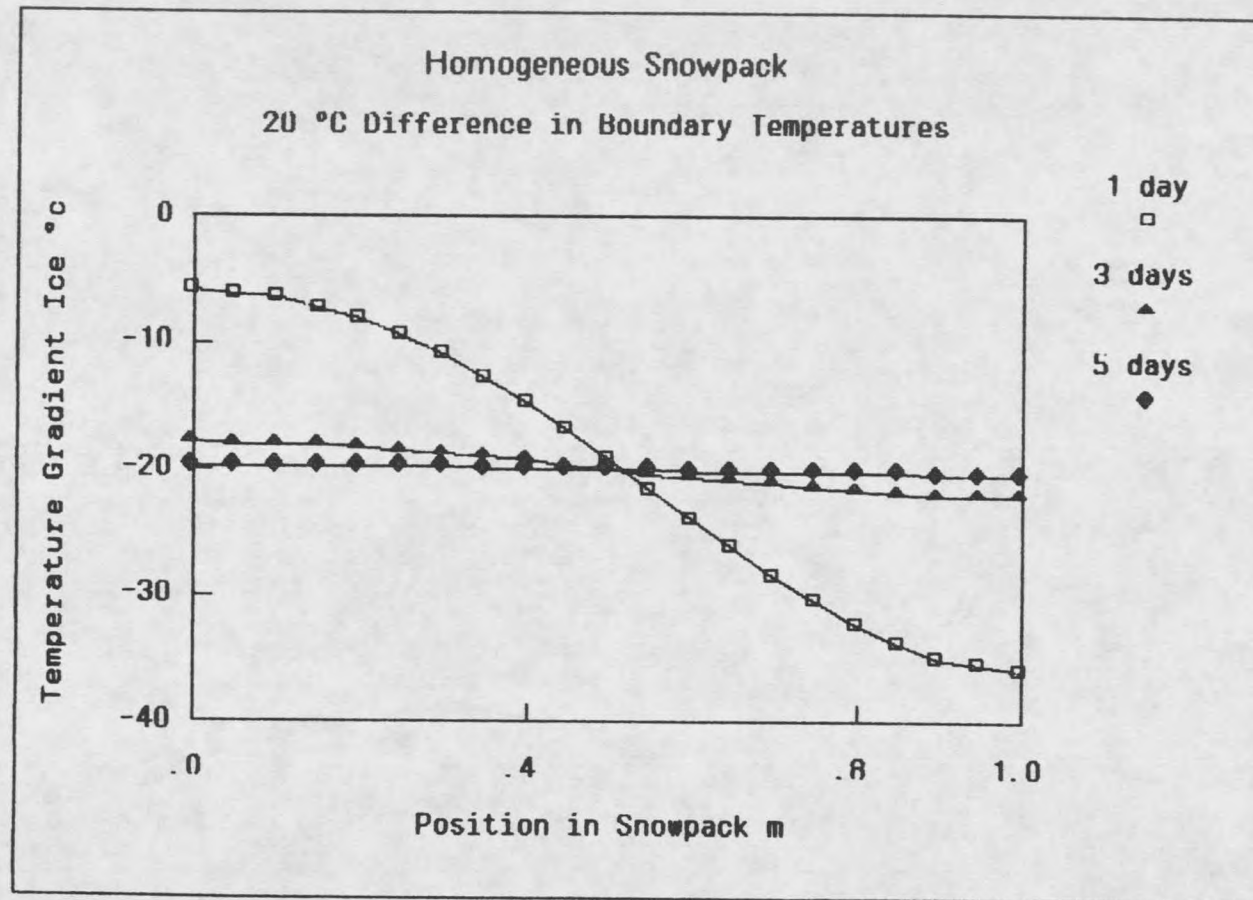


Figure 12. Temperature gradient of the ice relative to position in a homogeneous snowpack, with base temperature 0 °C and surface temperature -20 °C. Same as figure 11, but with the first two transient profiles removed to increase resolution.

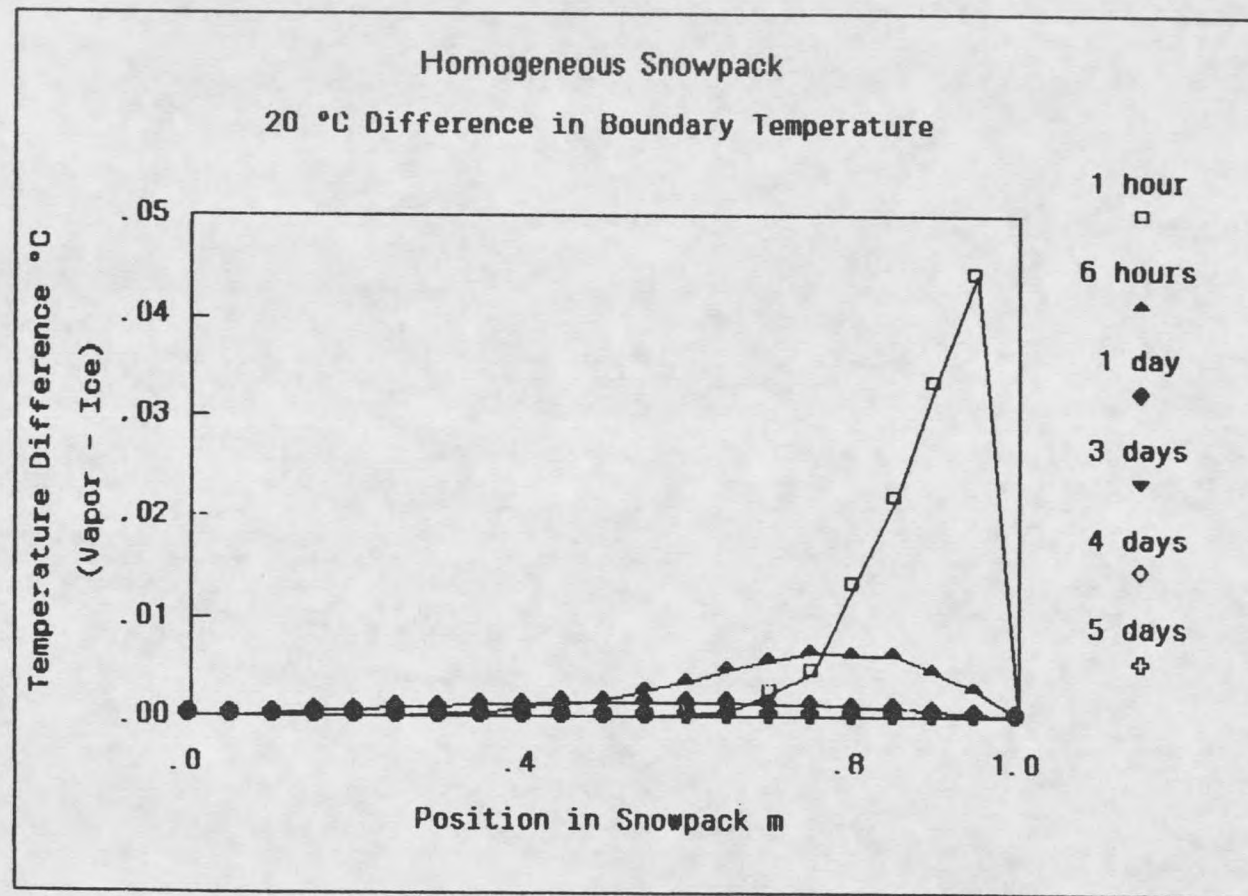


Figure 13. Difference in constituent temperature, $(\theta_v - \theta_i)$, relative to position in a homogeneous snowpack, with base temperature 0 °C and surface temperature -20 °C.

the temperature gradient is the largest. As a result of the boundary temperatures being held constant and equal for both constituents, it may be readily seen that, as the processes move toward a steady state situation the constituent temperatures tend to equilibrate (Figure 14).

Partial stress in the ice, calculated through the linear momentum balance equation does not yield values, for this case, which constitute a perceptible change from the isothermal values, so the figure will not be represented again. Strain, computed through the derived form analogous to the Duhamel-Neumann law for a thermoelastic material is dependent on the calculated stress and temperature. Recall that the strain in the ice for the isothermal problem was found to increase slightly in magnitude with depth (Figure 5), as expected for a purely mechanical situation. Strain resulting from simply the overburden of the snow itself however is not as large as that imposed through thermal contraction, for the depth and snow density considered here. Strain then, in accordance with the variation in temperature for the present situation, will be a maximum in the coldest region at the surface (Figure 15).

Partial stress in the vapor (i.e. the negative of the partial vapor pressure) is highly temperature dependent and follows a transient pattern which varies in a manner similar to that described for the thermal regime (Figure 16). At the end of the first time period examined, the partial vapor stress in the lower portion of the snowpack is unaffected, and as the colder region near the surface is approached, the magnitude of the stress decreases abruptly over a short span. Examination of the variation with time shows that this large gradient near the surface decreases, with the

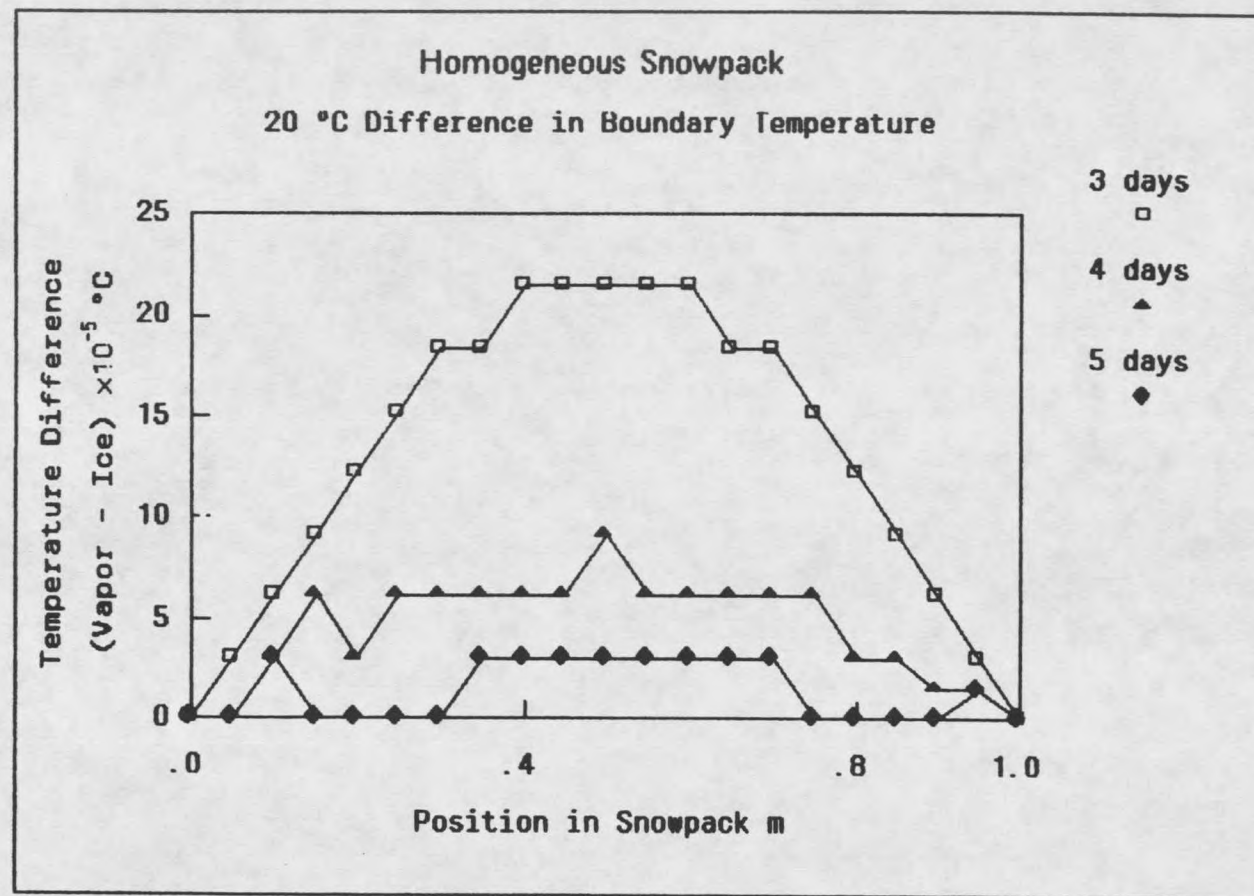


Figure 14. Difference in constituent temperature, $(\theta_v - \theta_i)$, relative to position in a homogeneous snowpack, with base temperature $0 \text{ } ^\circ\text{C}$ and surface temperature $-20 \text{ } ^\circ\text{C}$. Same as figure 13, but with the first two transient profiles removed to increase resolution.

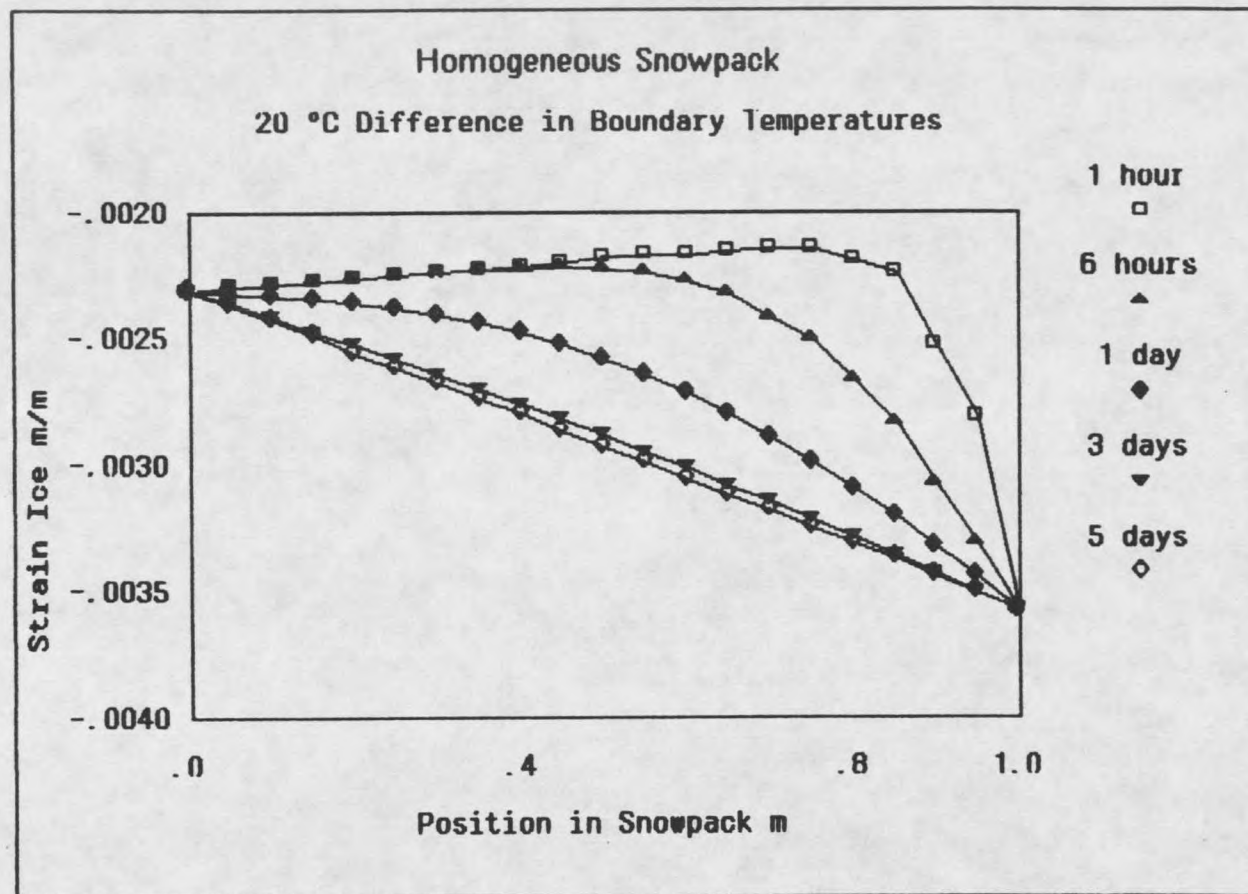


Figure 15. Strain in the ice relative to position in a homogeneous snowpack, with base temperature 0 °C and surface temperature -20 °C.

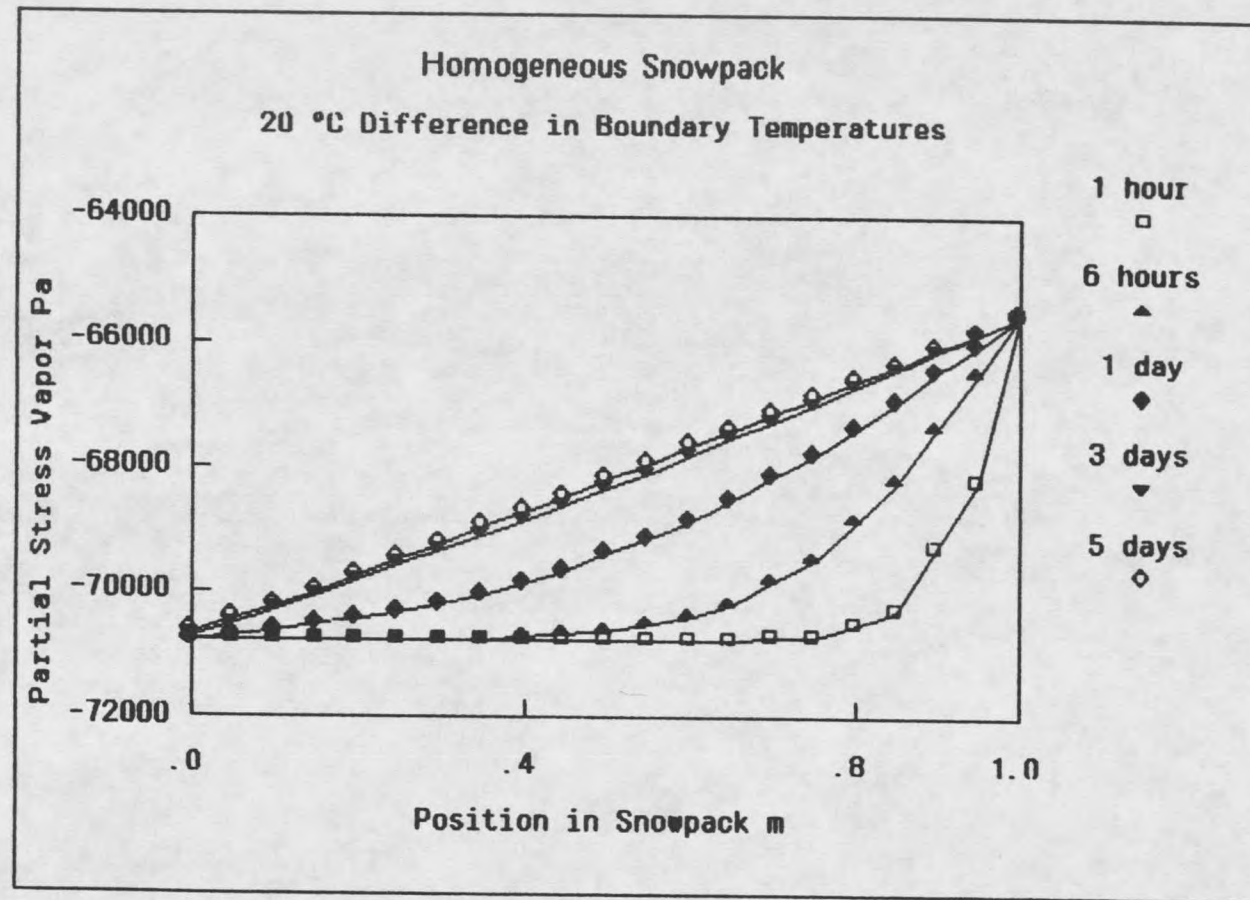


Figure 16. Partial stress of the vapor constituent relative to position in a homogeneous snowpack, with base temperature 0 °C and surface temperature -20 °C.

partial stress in the vapor finally settling toward a linear profile across this homogeneous snowpack. The greatest stress is at the warmer base.

Inspection of the time rate of change of the volume fraction of the ice (Figure 17) indicates that for a short time after the initial conditions have been imposed, there is a relatively rapid loss of ice volume in the very thermodynamically active region located in the upper transitional zone of the snowpack. This relatively rapid volume loss is then substantially lowered with the advance of time, as the gradient terms and temperature difference between constituents are reduced. An active zone for ice volume loss, indicated by a bulge in the curve, migrates down through the snowpack with time, but at a greatly reduced magnitude. Finally, as the steady state is approached the region of maximum ice volume loss is located at the bottom of the snowpack, where the temperature is the warmest, and it is the most thermodynamically active.

At this point, the assumption is made that this calculated loss in volume fraction of the ice is indicative of the development of depth hoar. This kinetic growth form as indicated in the introduction is known to be most apparent in conjunction with large temperature gradients and warm temperatures. Recrystallization is generally seen to develop at or near the ground, but it is also seen in conjunction with abrupt stratigraphic layering. Although a change in density has not been measured in conjunction with temperature gradient metamorphism, this loss of density might be too small to be measured with the instrumentation used, or could well be slight enough to be offset by gravity settlement on this weakened structure. In any case, it is certainly plausible and intuitively probable

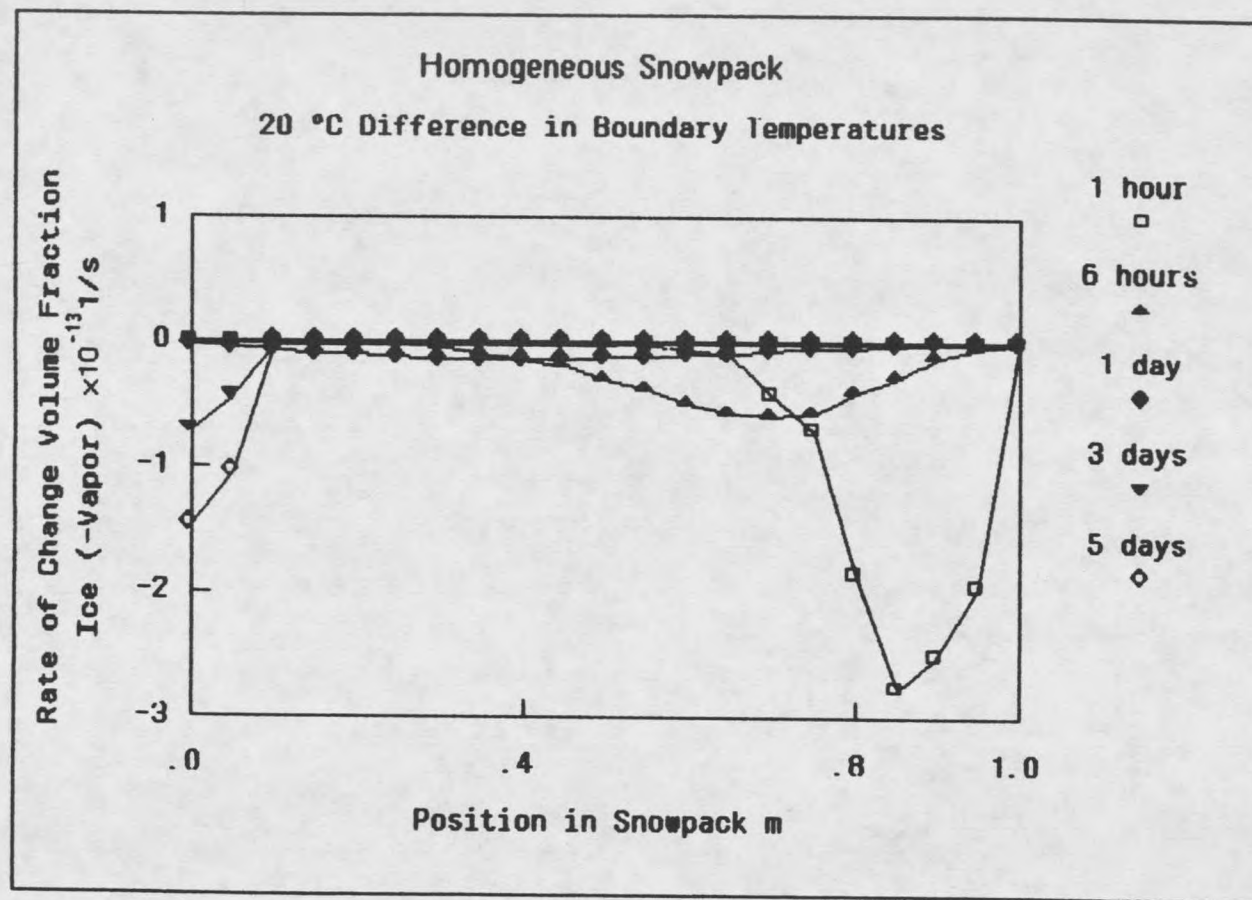


Figure 17. Time rate of change of the volume fraction of the ice relative to position in a homogeneous snowpack, with base temperature 0 °C and surface temperature -20 °C.

that there is some loss of the ice mass in conjunction with this metamorphic recrystallization process.

Consider the isothermal situation again, in regard to the error implied in the time rate of change of the volume fraction (Figure 6). It can be seen now that the magnitude of the error introduced is negligible when examining situations where the temperature gradient effect is significant.

The influence of the transient pattern which has been established among all of the interconnected processes, is apparent also in the values calculated here for the vapor velocity. It is during the early transitional period when the largest vapor velocities are attained, as expected, in the very active upper region of the snowpack, with no effect being felt in the lower regions at this stage (Figure 18). Subsequent transient vapor velocity profiles show the velocity becoming established, progressively deeper in the pack. Eventually, as the steady state is approached, the velocity profile becomes more linear, and is the greatest near the warmer base. Recall that the velocity at the lower boundary was chosen to be zero. This boundary condition may not be realistic for a snowcover resting on top of a porous moist soil base.

Examination of the equilibrated force interaction, reveals that this derived term has a transient variation similar in pattern to the temperature (Figure 19). Boundary values remain essentially unchanged from the initial ones as the profile varies in the now familiar transition from a steep gradient near the top, with no change in the lower regions, to a linear additional overburden loading which, accumulating, is then maintained until the high density layer is encountered. The effect of this layer on the

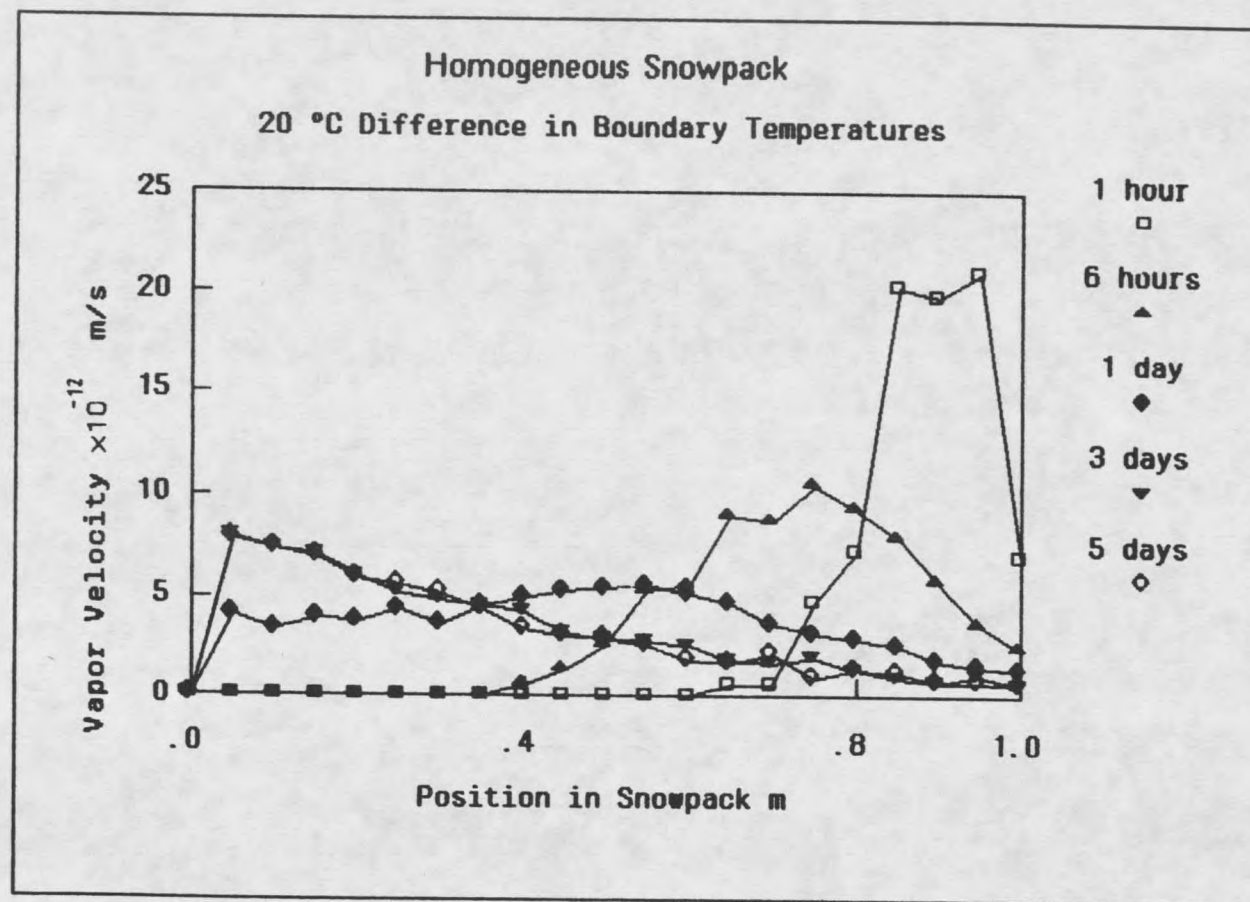


Figure 18. Vapor velocity relative to position in a homogeneous snowpack, with base temperature 0 °C and surface temperature -20 °C.

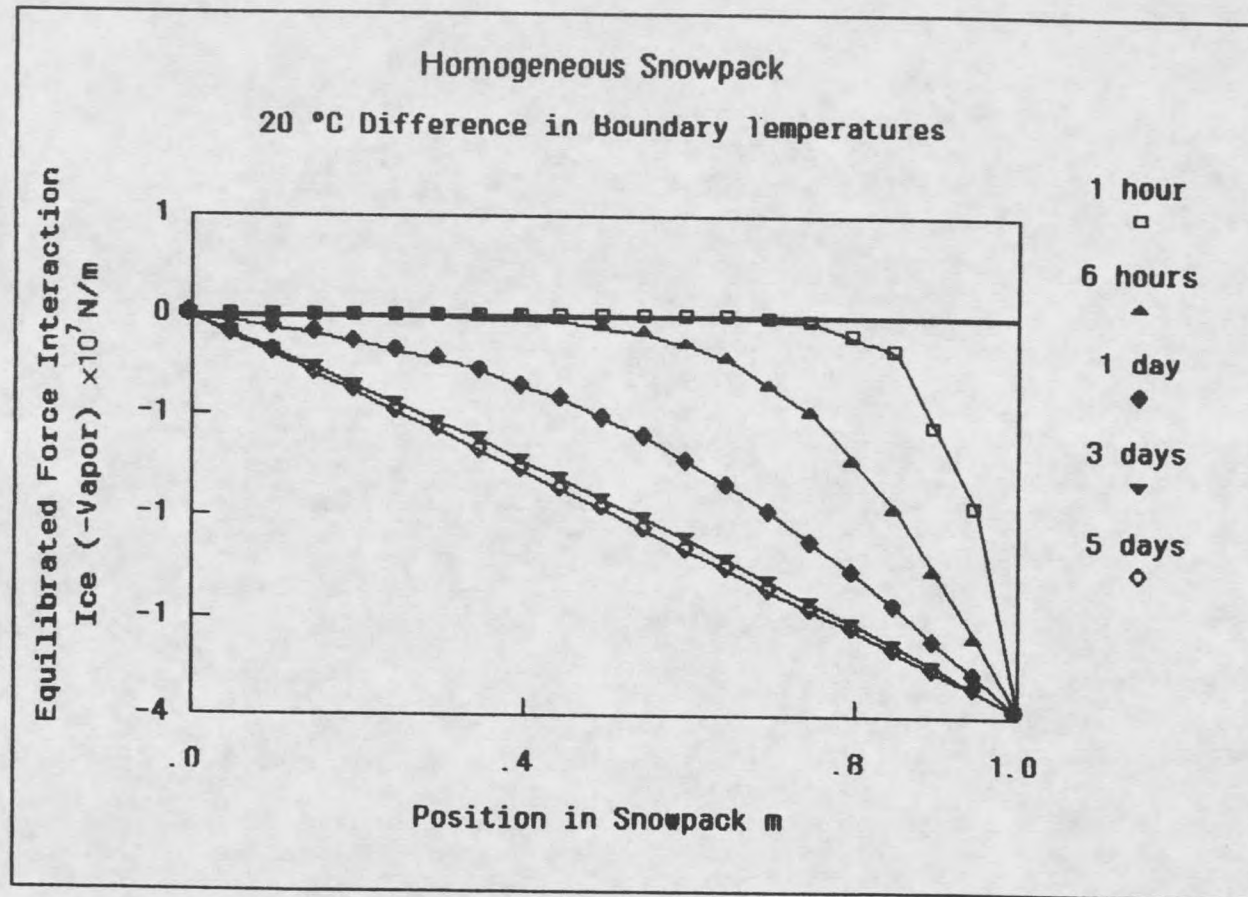


Figure 19. Equilibrated force interaction of the ice relative to position in a homogeneous snowpack, with base temperature 0°C and surface temperature -20°C .

profile between the upper and lower values. The final base value and the calculated early transient values removed from the surface effects are the same as for the isothermal condition.

Next the more complicated idealized stratigraphically layered snowpack (Figure 20) is considered under isothermal conditions. This environment, as expected, reveals no change for the direct thermal values calculated, but mechanical effects due to the layering produce some very reasonable results. Partial vapor stress values for this nonhomogeneous snowpack vary directly with the layering (Figure 21). Since this term is reckoned with respect to constituent fraction of the mixture, the largest magnitude is in the low mixture density layer which corresponds to the region with the largest vapor fraction.

Partial stress of the ice is also shown to vary with the imposed layering (Figure 22). The top section varies in precisely the same manner as the corresponding section of the homogeneous sample (Figure 23), then the gradient of partial stress at the transition to the low density layer abruptly decreases. This is caused by the sudden change in the volume fraction at the interface and the interface pressure term at that point. A linear profile exists through the low density layer, but with a gradient which is slightly less than that in the upper section. This lower gradient is simply the result of the fact that the accumulating additional weight of the lower density overburden snow through this section is less. The change in volume fraction at the lower interface between the layers is the result of the same term in the linear momentum balance equation which caused the transition at the upper surface. A constant gradient in keeping with the

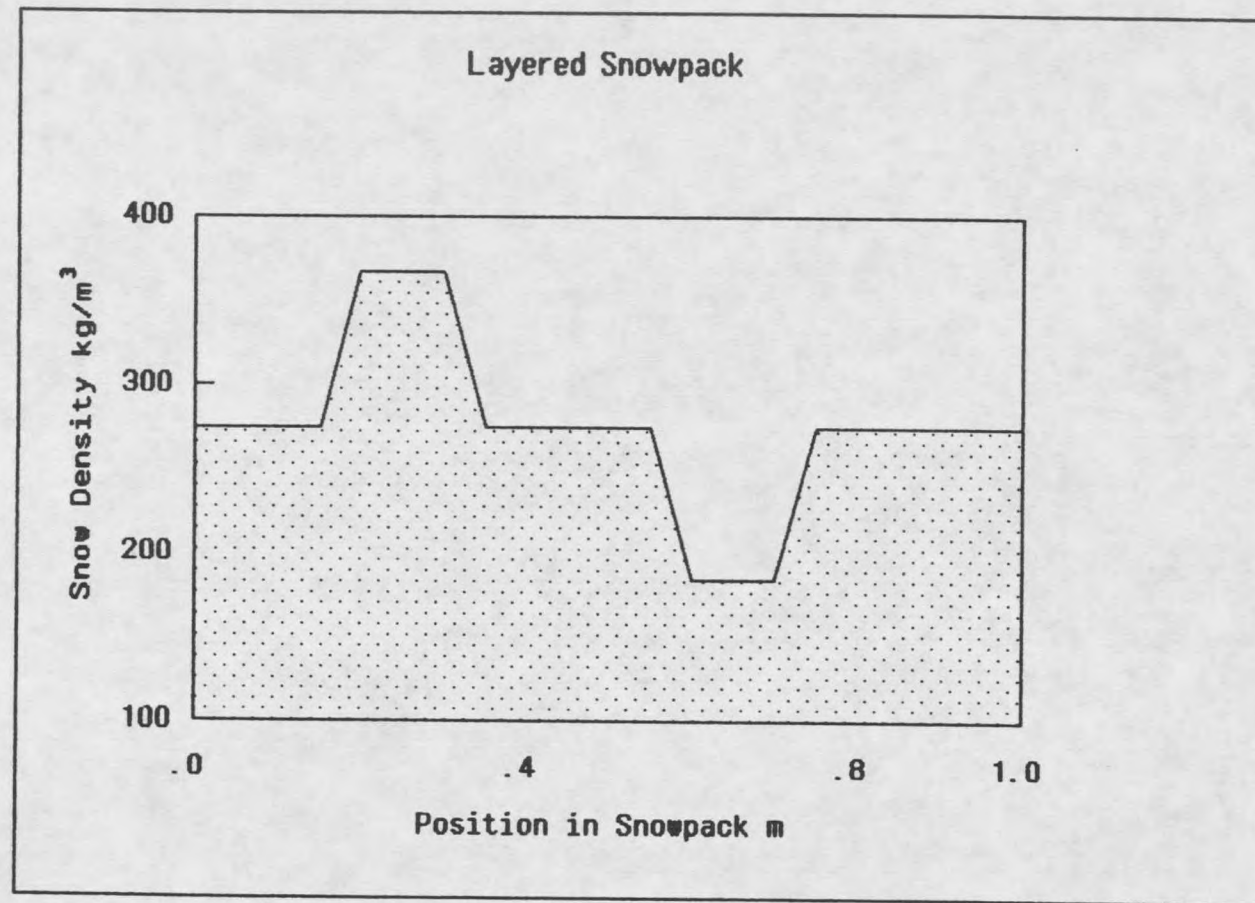


Figure 20. Idealized density profile which is examined.

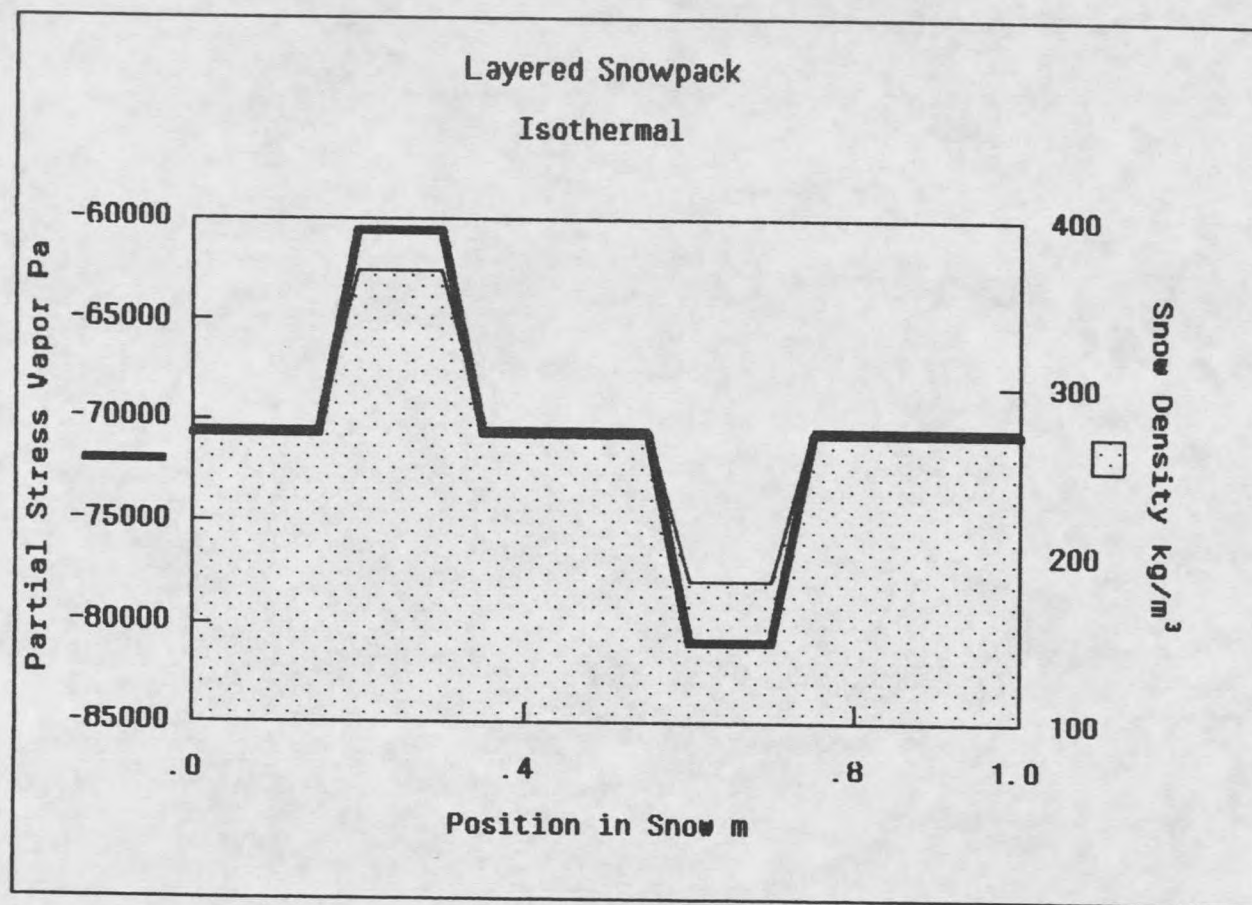


Figure 21. Partial stress of the vapor relative to position in a layered isothermal snowpack.

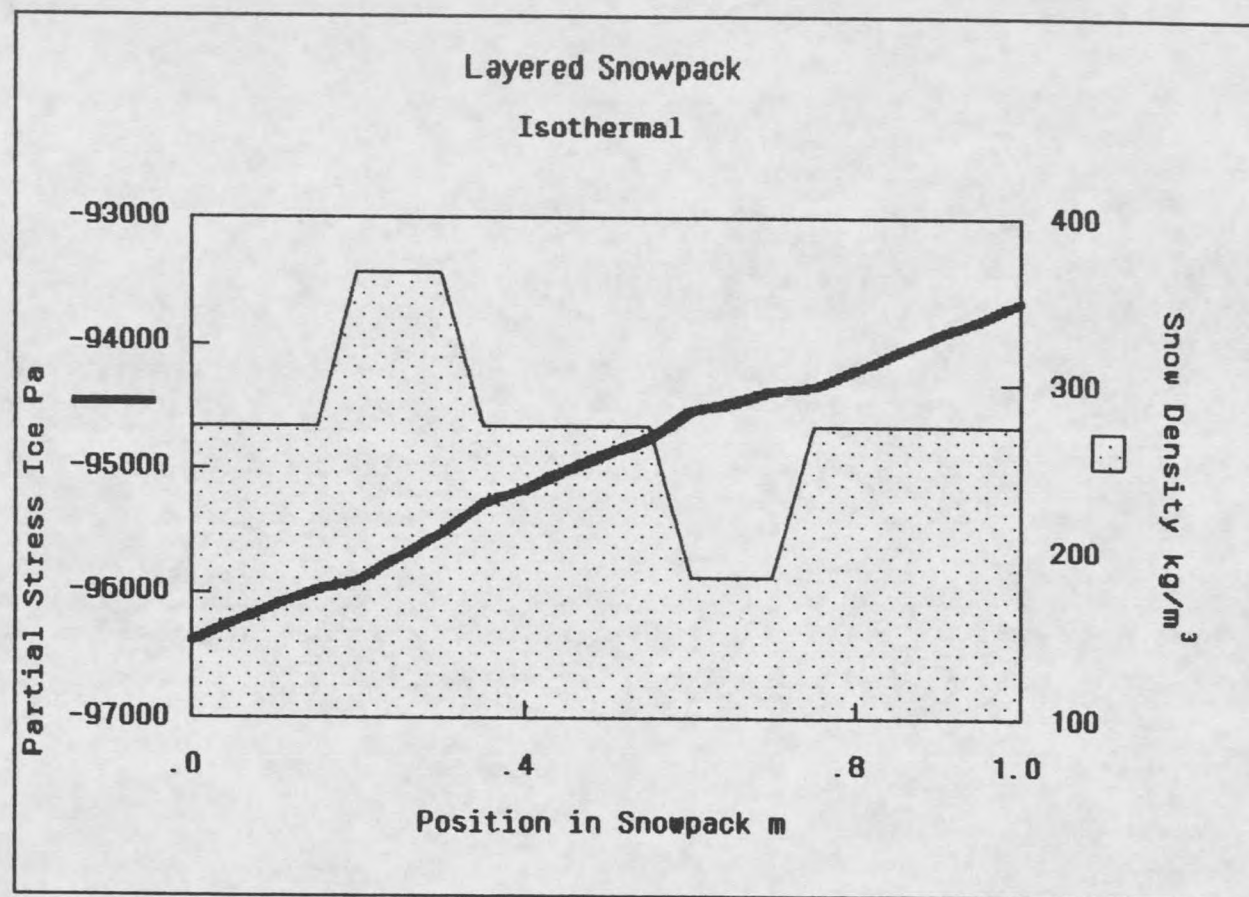


Figure 22. Partial stress of the ice relative to position in a layered isothermal snowpack.

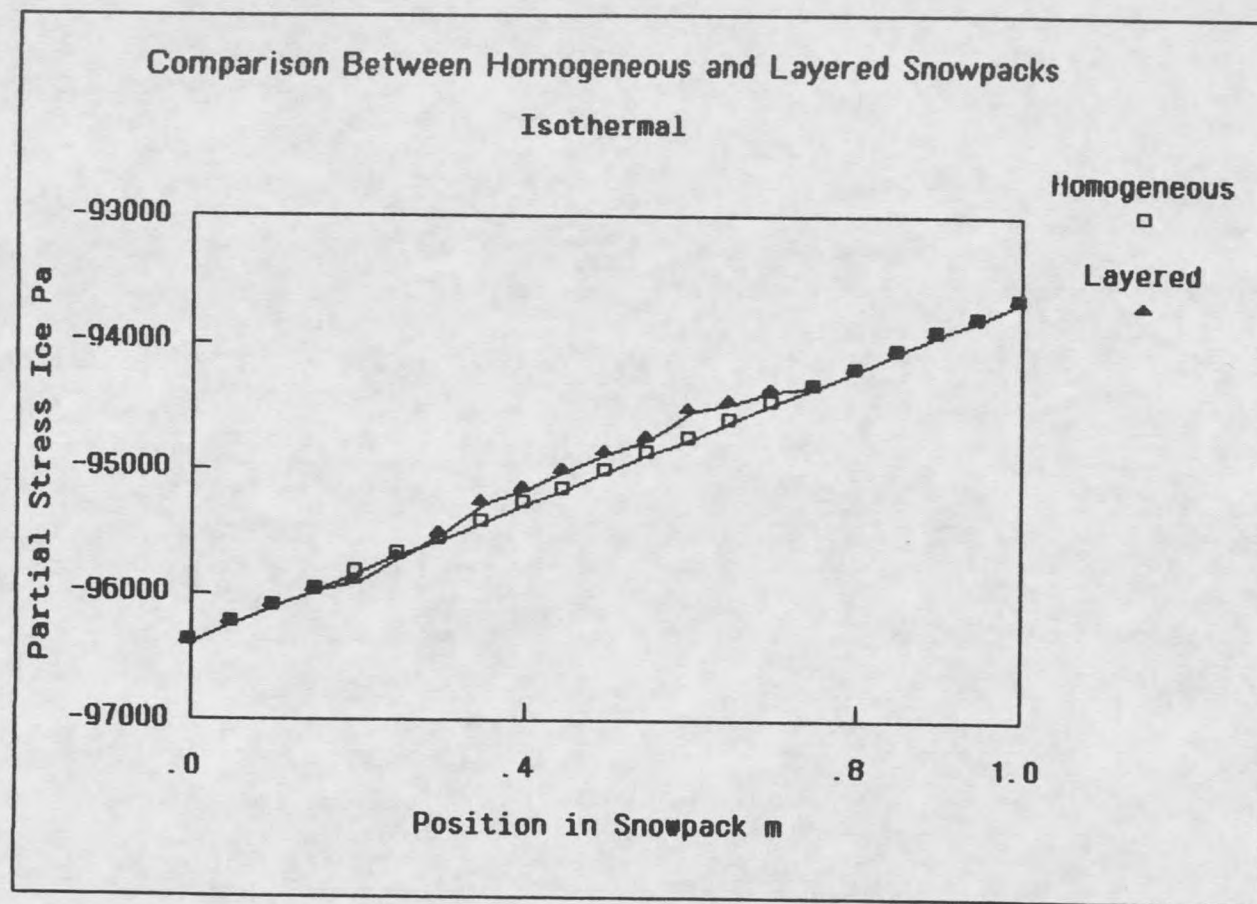


Figure 23. Comparison of the partial stresses in the ice relative to position in isothermal homogeneous and layered snowpacks.

ice partial stress profile may be described by direct comparison with that explained for the low density, but with the obvious transposition. Total snow overburden is the same for corresponding position in the two snowpacks at the lowest zone, so the partial stress for the homogeneous and layered samples are equal.

The ice must account for the structural integrity of the snow. It seems intuitive then, that for the same loading, a lower density layer would be expected to support a higher stress in the ice and conversely for a high density zone. Although not readily apparent at first examination of the partial stress profile, this is implicitly accounted for in the volume fraction theory.

It is instructive, as an aside to the theory being considered, to examine the stress referenced to a complete unit of ice, instead of as the partial fraction of the mixture. This is accomplished by simply dividing the partial stress with that fraction of the whole mixture which it represents. This gives an indication of what the stress would be for a unit composed totally of the ice constituent, i.e. the type of stress which the ice alone would be expected to experience in a more traditional analysis (Figure 24). The stress variation when examined in this manner indeed satisfies the intuitive sense.

A similar examination of the partial stress for the vapor, yields a constant value for the total stress of the vapor when considered in the same sense as for the total stress in the ice. The inference is that, as expected intuitively, the total stress attributed to only the vapor in any individual pore space, for isothermal conditions is the same.

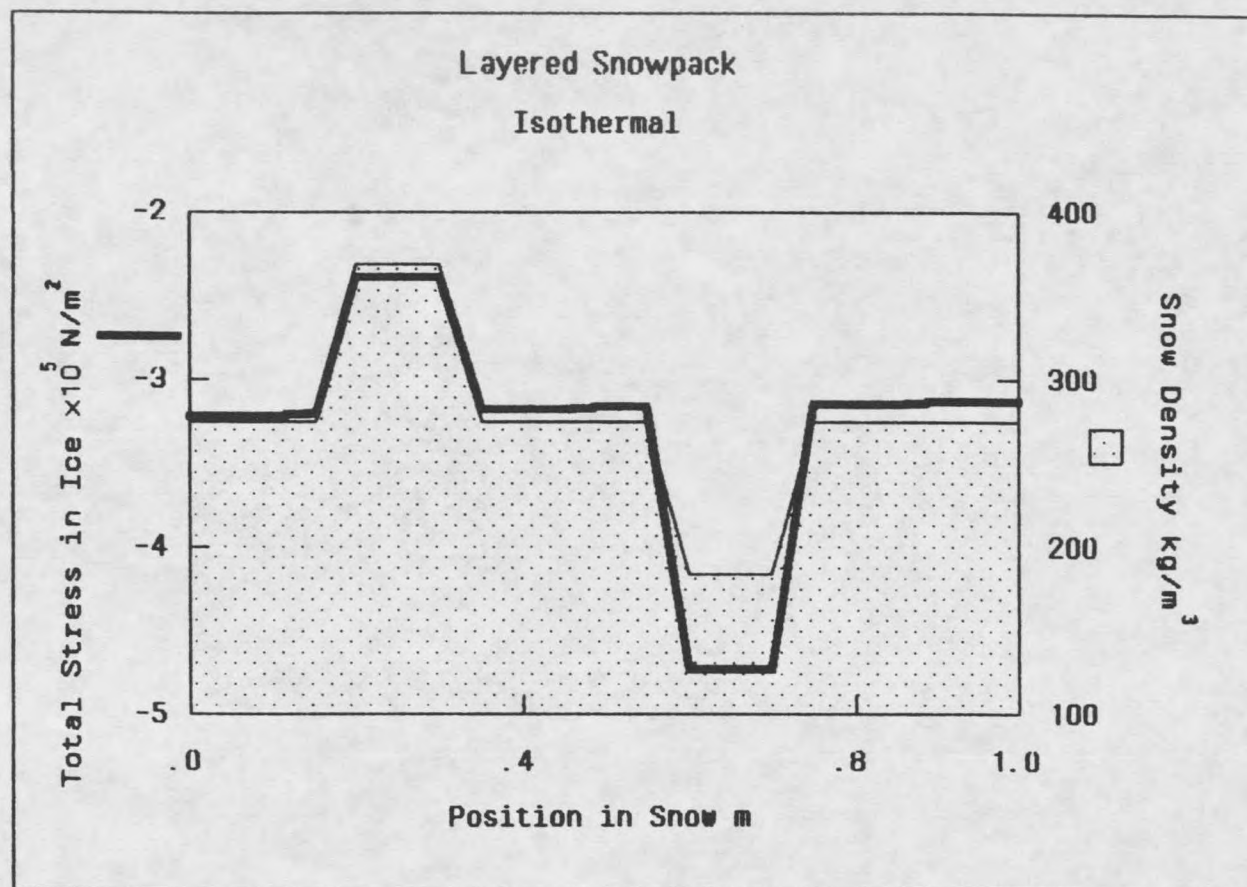


Figure 24. Total stress of the ice alone, relative to position in a layered isothermal snowpack.

Strain in the ice is greatest in the low density layer and minimum in the high density layer (Figure 25). The Young's modulus which was used, as stated previously, is based on values determined for snow. This is appropriate in the present context, since these values are essentially determined by the ice constituent alone, and based on the snow density or volume fraction of the ice.

The time rate of change of the volume fraction for the isothermal situation in a layered snowpack (Figure 26), is seen to vary with the strain in the ice (Figure 25). This is caused, as discussed for the homogeneous isothermal snowpack, by the effect of the strain on the chemical potential of the ice. As the strain becomes more negative, the chemical potential for the ice responds accordingly. The strain, in this isothermal case, sufficiently effects the difference in chemical potentials between constituents to produce the noted results. This effect is negligible when compared to snow with a significant temperature gradient. This will be seen when the layered snowpack with an imposed temperature is examined.

Vapor velocities are indicated, at the interfaces of abrupt changes in the snow density (Figure 27). These velocities are generated by the large gradient in the volume fraction at these inter-layer zones. Vapor flow is from lower density toward higher density regions.

The equilibrated force interaction (Equation 28) is seen to be affected by the layering, with a demonstrated increase in the lower density region and is conversely influenced in the high density zone. Corresponding positions in the homogeneous and layered snowpack which are of equal density give equivalent values for the equilibrated force interaction.

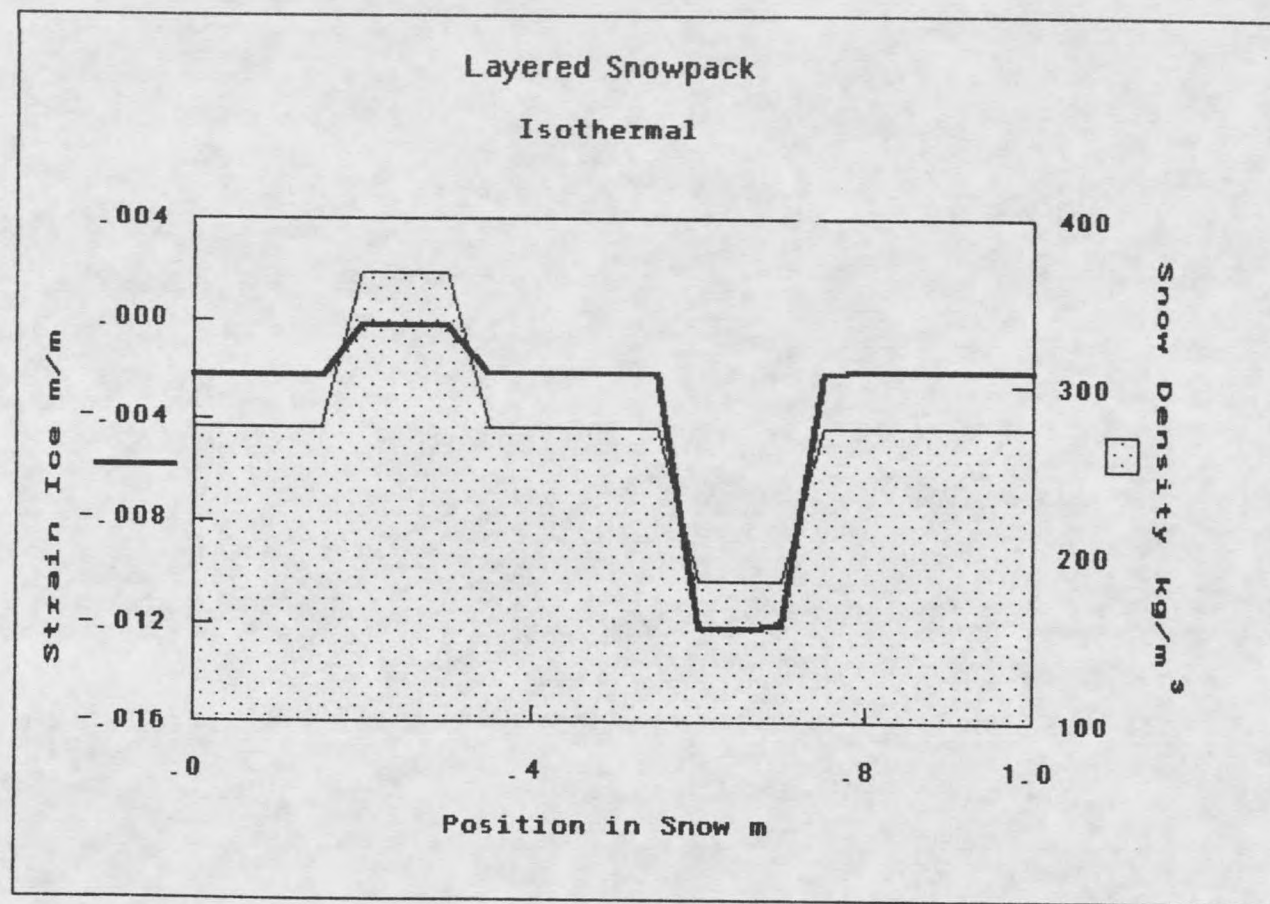


Figure 25. Strain in the ice relative to position in a layered isothermal snowpack.

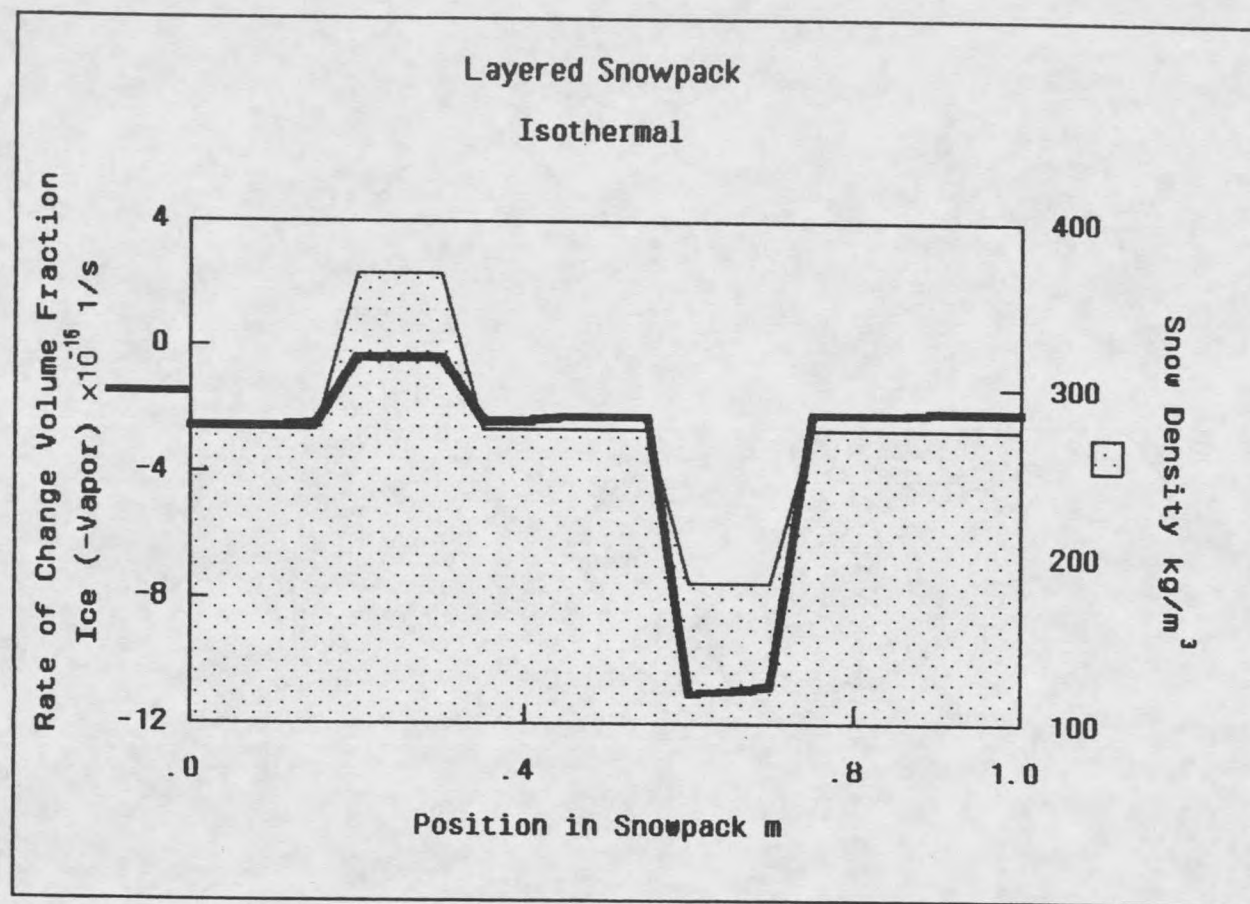


Figure 26. Time rate of change of the volume fraction of ice relative to position in a layered isothermal snowpack.

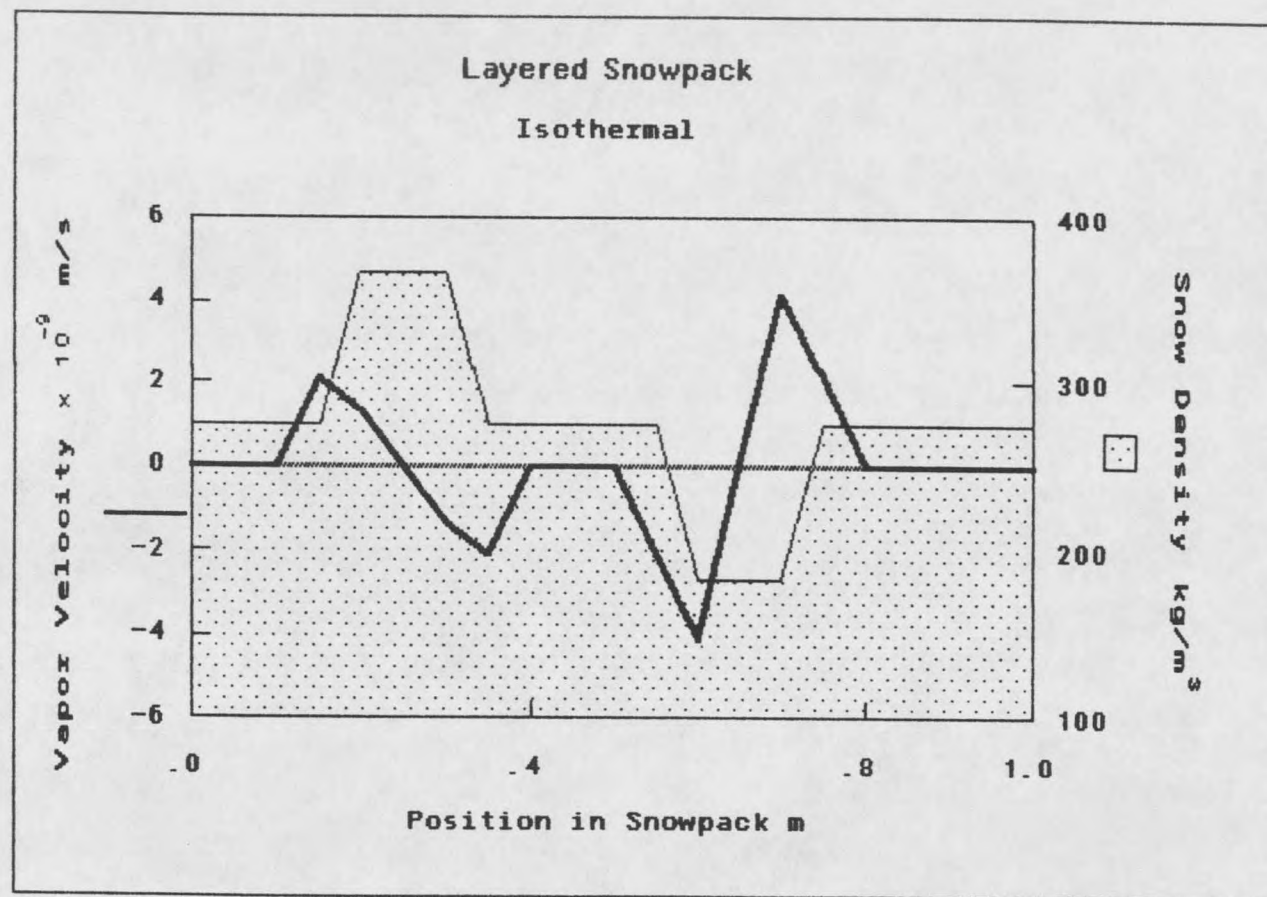


Figure 27. Vapor velocity relative to position in a layered isothermal snowpack.

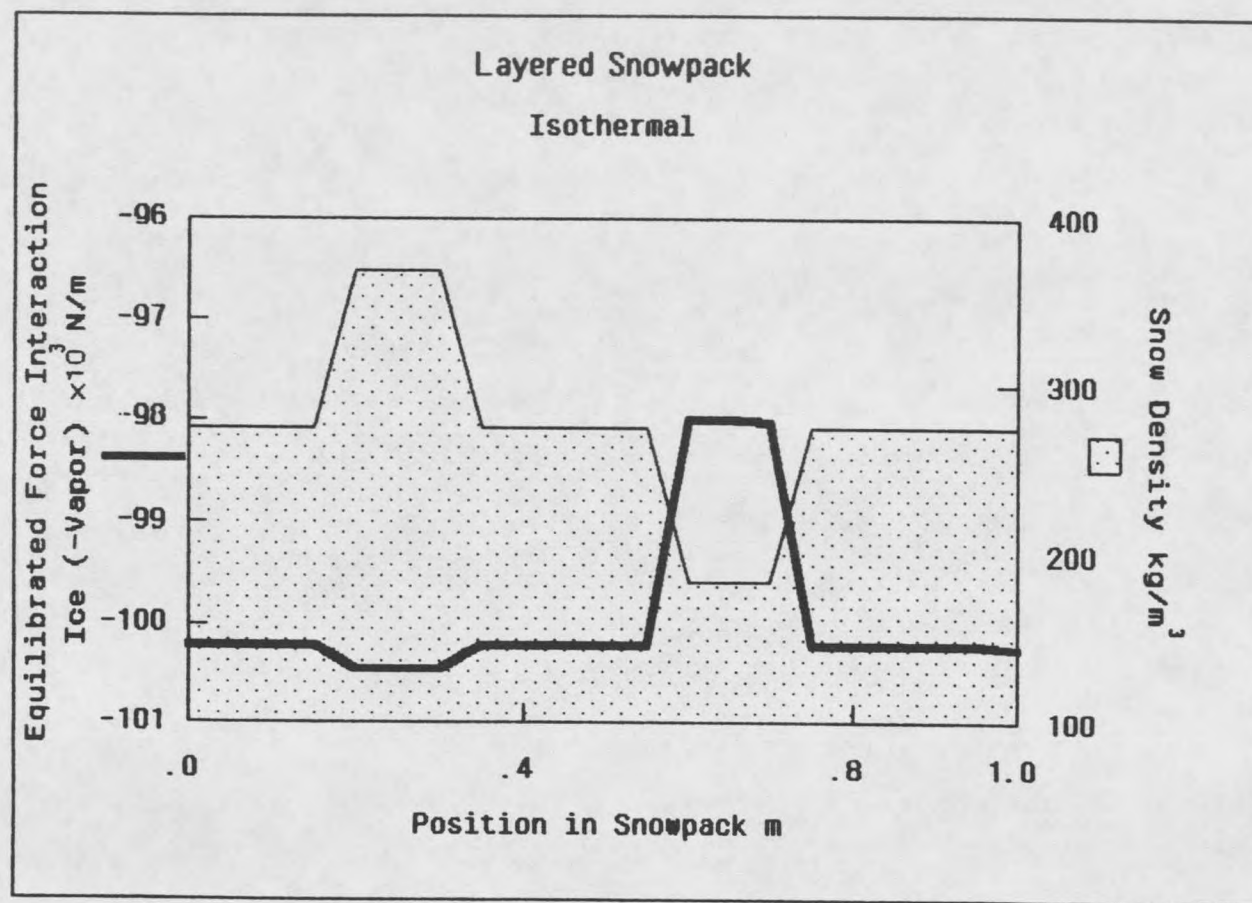


Figure 28. Equilibrated force interaction of the ice relative to position in a layered isothermal snowpack.

As for the case of the homogeneous sample with the imposed thermal boundary conditions, the transient solutions for the layered snowpack are considered. Temperature variations for the vapor and the ice (Figures 29 and 30) reveal trends which are similar to that demonstrated in the homogeneous example. In the early calculations no change in the temperature from the initial conditions have taken place in the lower section, but the upper region shows large temperature changes between nodes. However, as the temperature advances downward settling into the steady state, instead of developing a perfectly linear profile as for the homogeneous snowpack, perturbations from the linear are seen in conjunction with the disrupting layers.

The gradient of these transient temperature profiles (Figures 31 and 32) show that after a relatively short time period the very large gradient in the upper region drops as the temperature effects permeate more deeply into the snow. The gradient through the lower density layer which is located higher in the pack is greater than in the surrounding snow, and as the temperature becomes established in the lower region, the temperature gradient in the higher density layer is less than in the adjoining snow (Figure 33).

This result is what should be expected, since the thermal conductivity of snow is known to be governed to a large extent by the snow density [Mellor, 1964]. Calculations in this model however, did not rely on this information but naturally handled it through consideration of only the volume fraction and the individual conductivities of the constituents. Refinements could be made for variations in snow type, by considering how

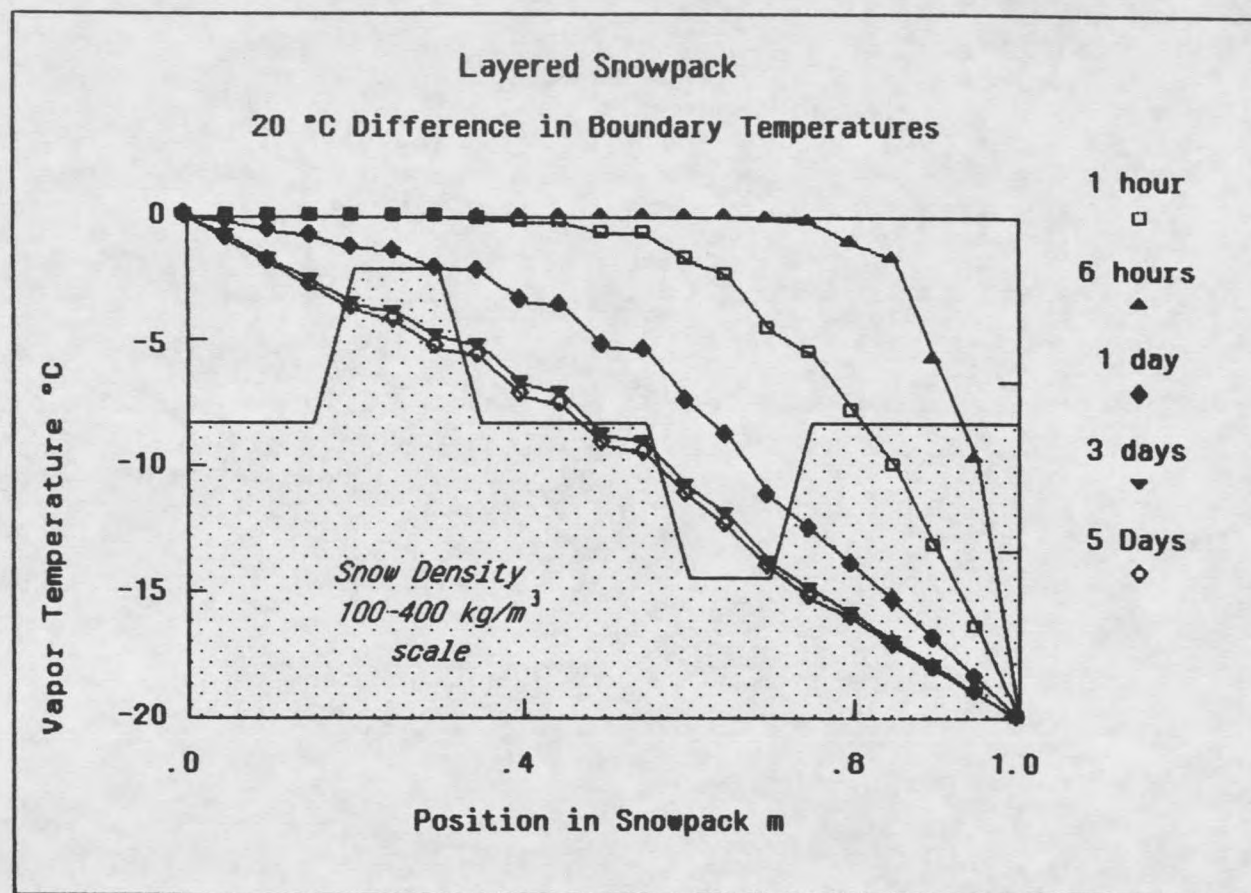


Figure 29. Temperature of the vapor relative to position in a layered snowpack.

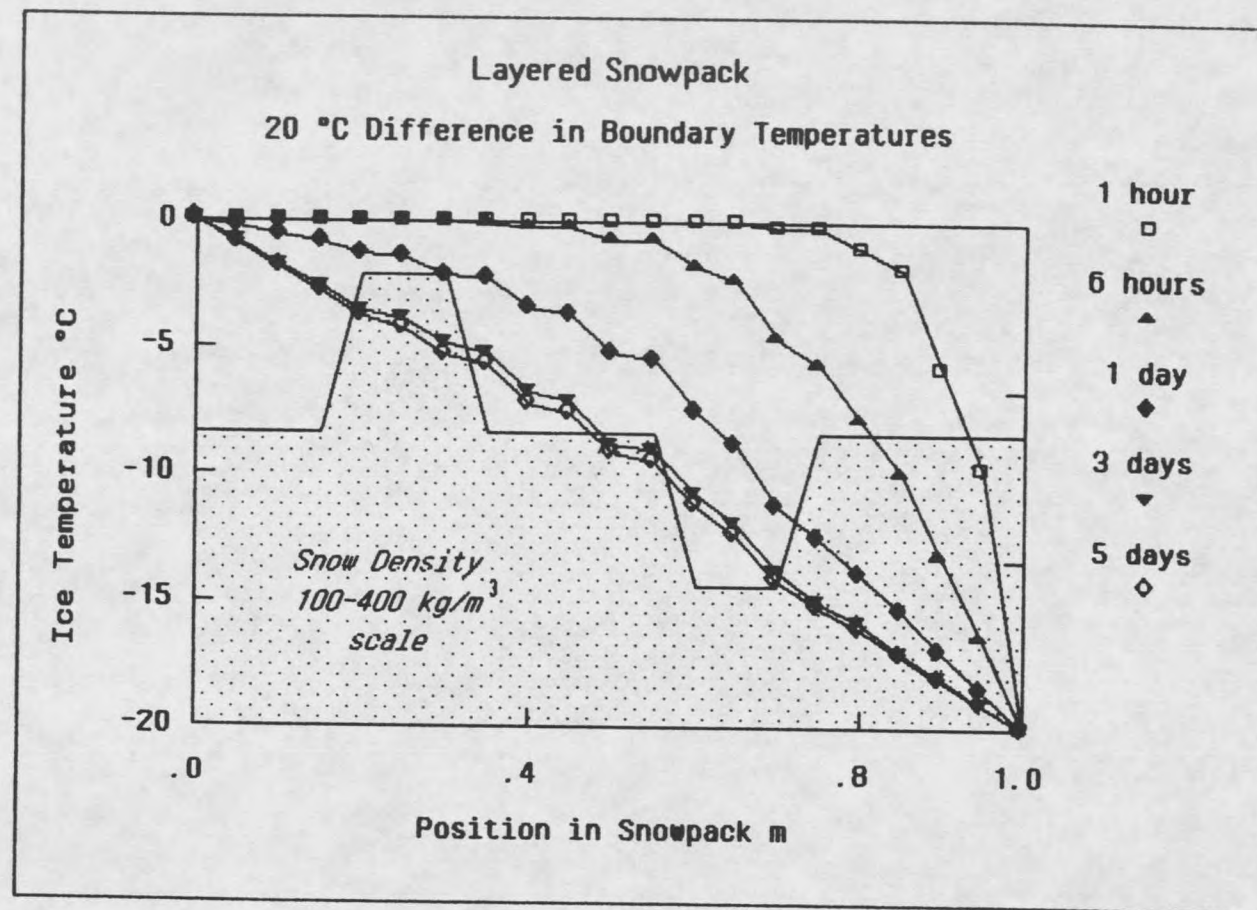


Figure 30. Temperature of the ice relative to position in a layered snowpack.

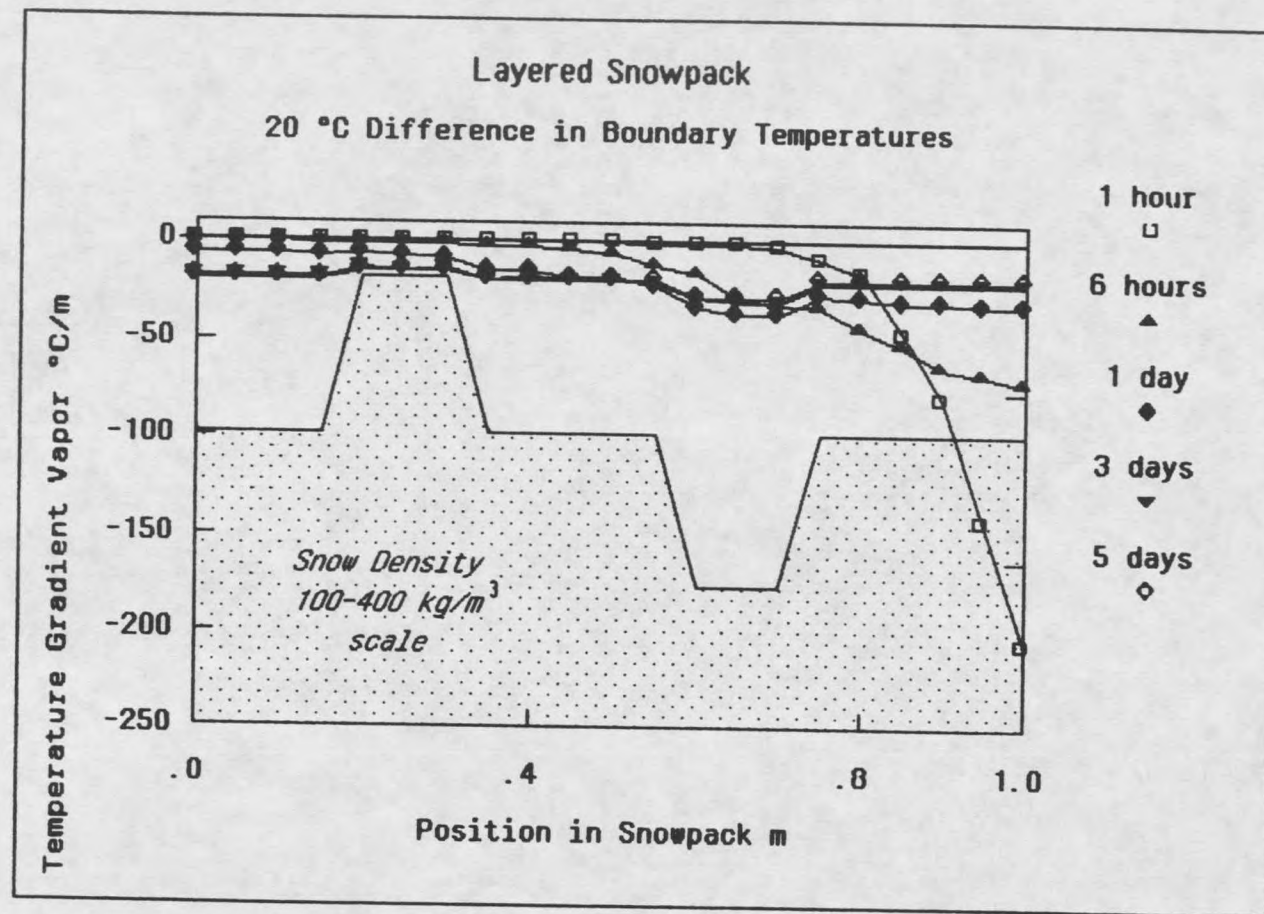


Figure 31. Temperature gradient of the vapor relative to position in a layered snowpack, with base temperature 0 °C and surface temperature -20 °C.

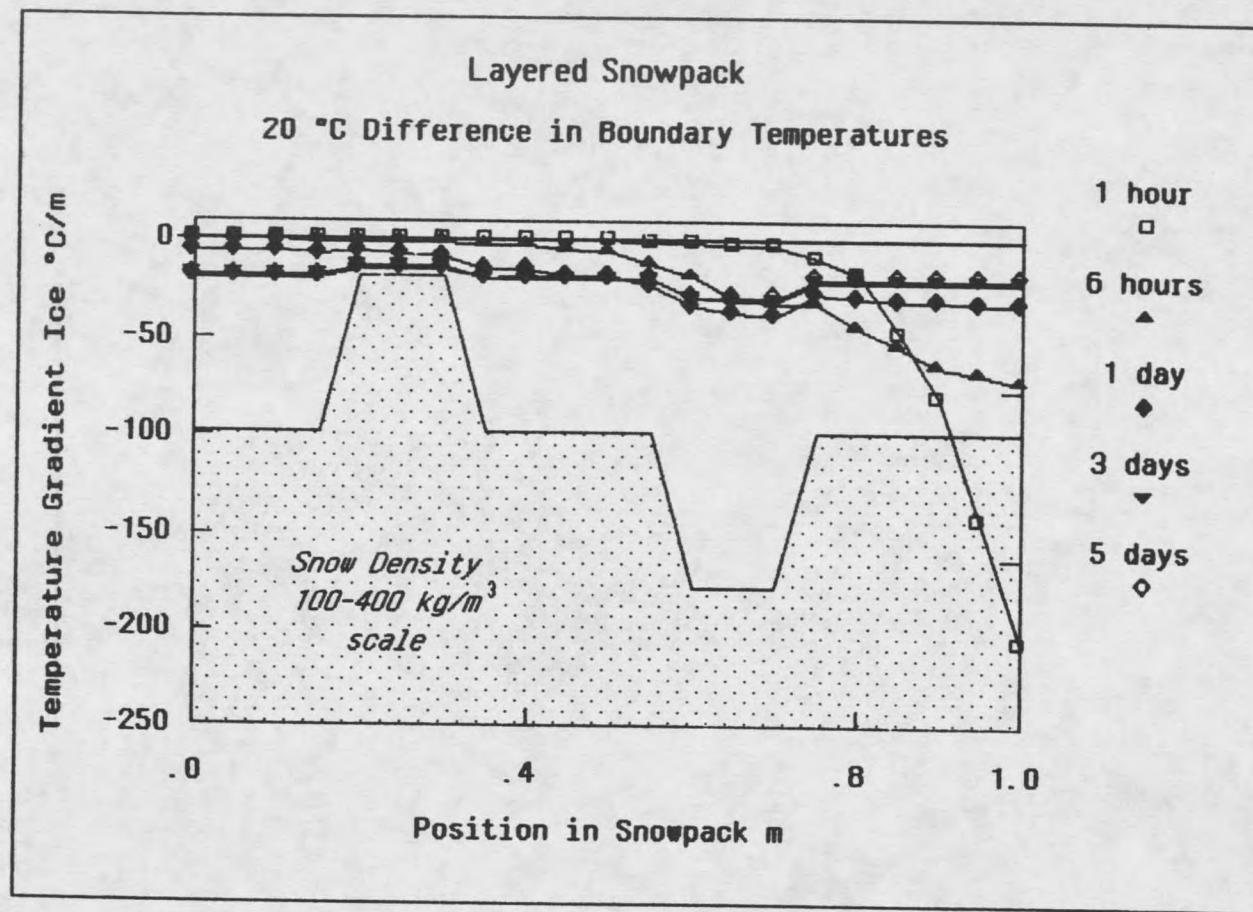


Figure 32. Temperature gradient of the ice relative to position in a layered snowpack, with base temperature 0 °C and surface temperature -20 °C.

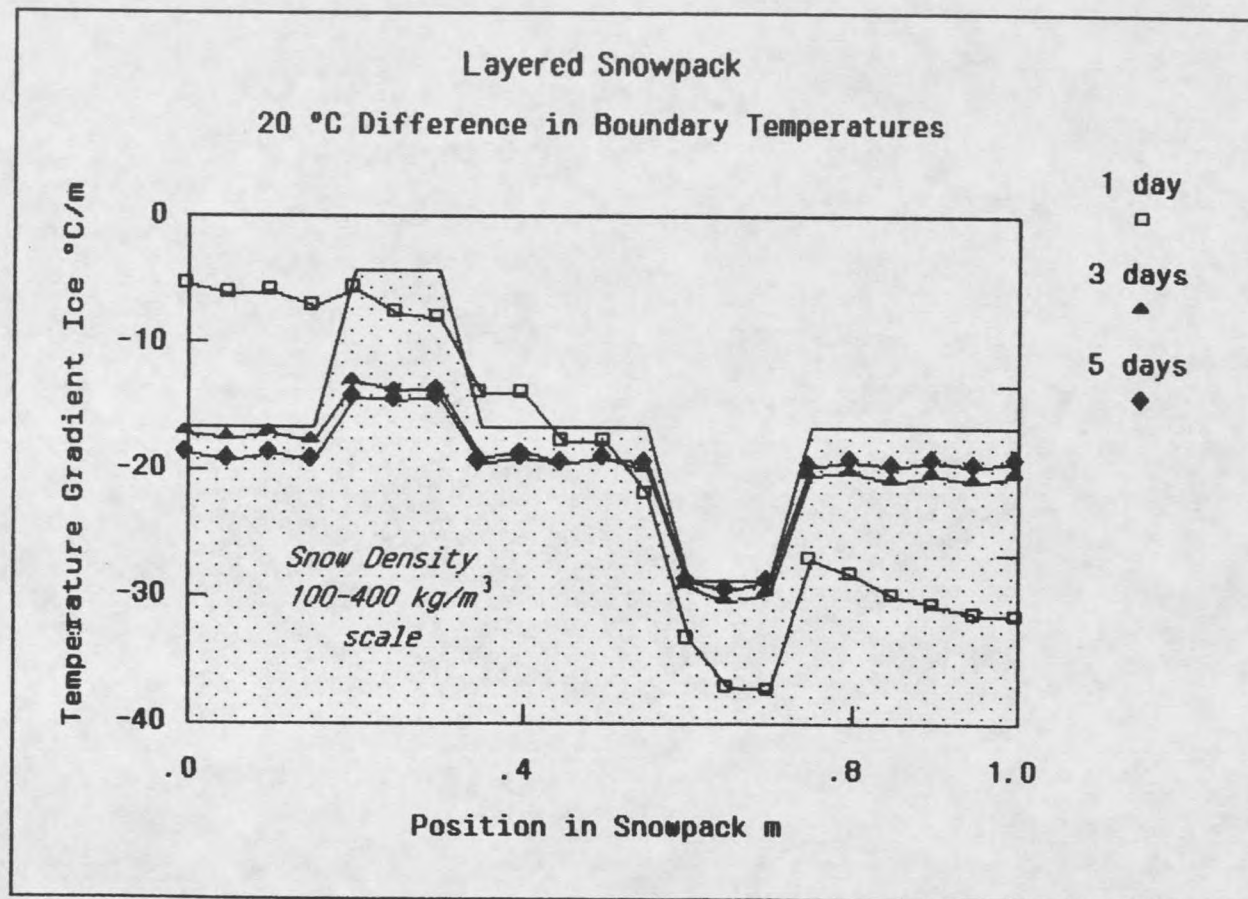


Figure 33. Temperature gradient of the ice relative to position in a layered snowpack. Same as in figure 32, but with first two transient profiles removed to increase resolution.

bonding and grain configuration might affect the thermal conductivities of the constituents.

The manner in which layering affects how the calculated individual constituent temperatures vary with respect to each other (Figure 34) is quite interesting. Temperature differences computed after the first hour display the expected large temperature difference expected in the upper region, with the higher thermal conductivity of the ice causing it to cool more quickly than the vapor. At the upper interface of the lower density layer for this same time frame however, there is another smaller jump in the difference, with the ice at a lower temperature than the vapor. Six hours after the start, this temperature difference jump is accentuated and another jump just below this layer has developed, but here the vapor is cooler than the ice.

Migration of the temperature down into the snowpack with the passage of additional time reveals that a similar but opposite trend, involving the magnitude of the temperature difference jumps, has developed in conjunction with the high density layer. Above the high density layer the vapor is cooler, and below it the ice is. While this situation is developing in the lower region, where the reaction to the transient temperature penetration is being felt most strongly, temperature differences nearer to the surface are becoming smaller as the temperatures in this upper region begin to equilibrate. This anomaly is felt to be induced by the vapor velocity which is associated with the layering, as described earlier for the isothermal layering situation. Recall that the direction of this vapor flux is from the lower toward the higher density snow. The effect of this on

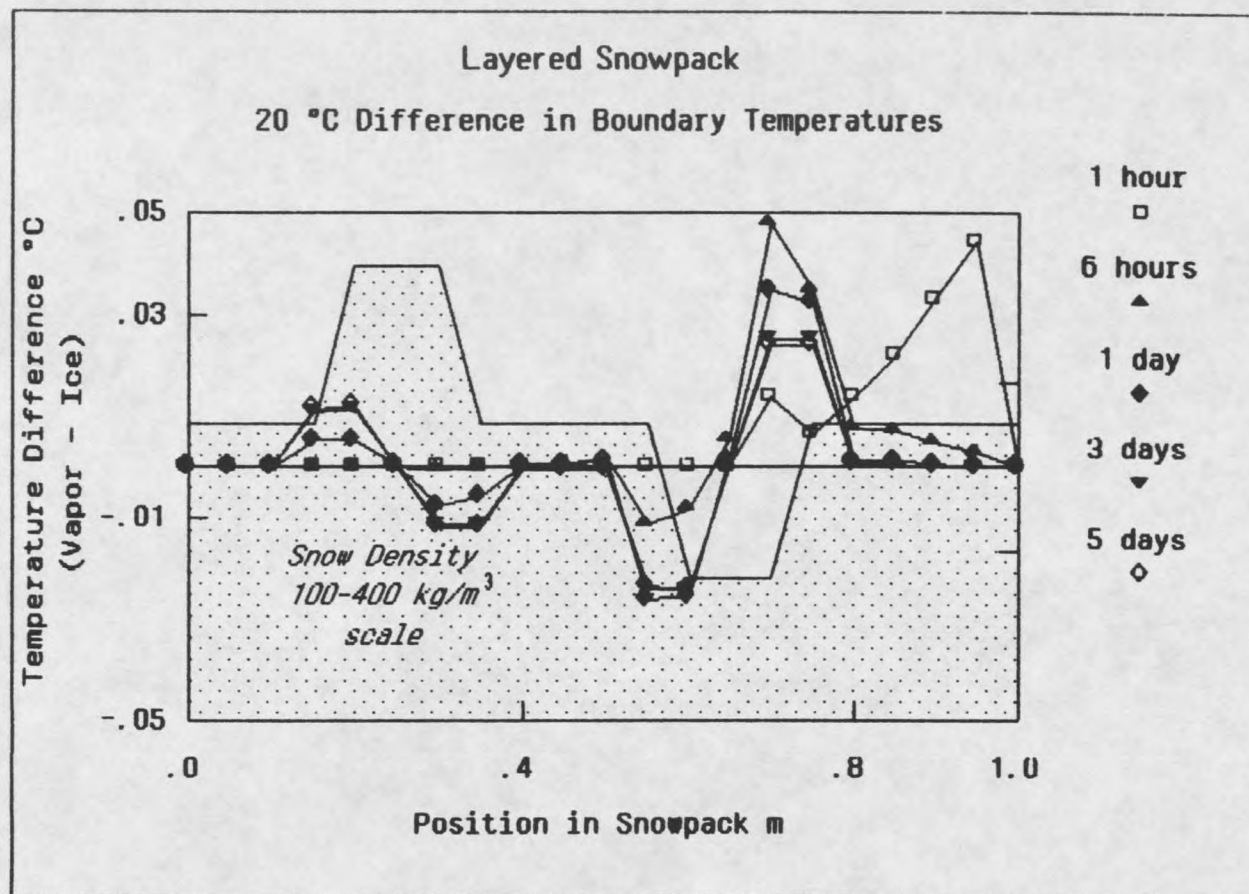


Figure 34. Difference in constituent temperatures, $(\theta_v - \theta_i)$, relative to position in a layered snowpack, base temperature 0 °C and surface temperature -20 °C.

the temperature differences is postulated as follows. As the imposed upper surface boundary temperature penetrates the snowpack, thermal conduction will cause the more highly conductive ice to change temperature more readily than the vapor. However, when there is even slight vapor motion, such as that which exists for the vapor at the layer interfaces, the heat flux will be effected.

In the instance where the lower density snow overlain with the higher density snow is initially being impacted by the thermal changes, the upward heat flux due to the vapor velocity will impede the rate at which the vapor will cool, since the warmer vapor is being transported upward from below. In the reverse situation where the low density snow is on top, the combination of the downward vapor velocity in conjunction with the conductive heat flux causes the vapor to cool more rapidly than the ice.

The partial stress profiles of the ice does not differ perceptibly from the stress profiles for the isothermal case. The strain (Figure 35) and the partial stress of the vapor (Figure 36) are influenced by the thermal variation in a similar manner to that previously discussed for the homogeneous snow, with the obvious variation due to the effect of layering as noted for the isothermal instance. The maximum strain in the layered snowpack, initially in the low density layer, remains there and becomes more pronounced when the temperature is lowered. The partial stress of the vapor as noted earlier is temperature sensitive and decreases in magnitude as it cools.

Indication of some interesting phenomena are demonstrated in the results calculated for the time rate of change of the volume fraction

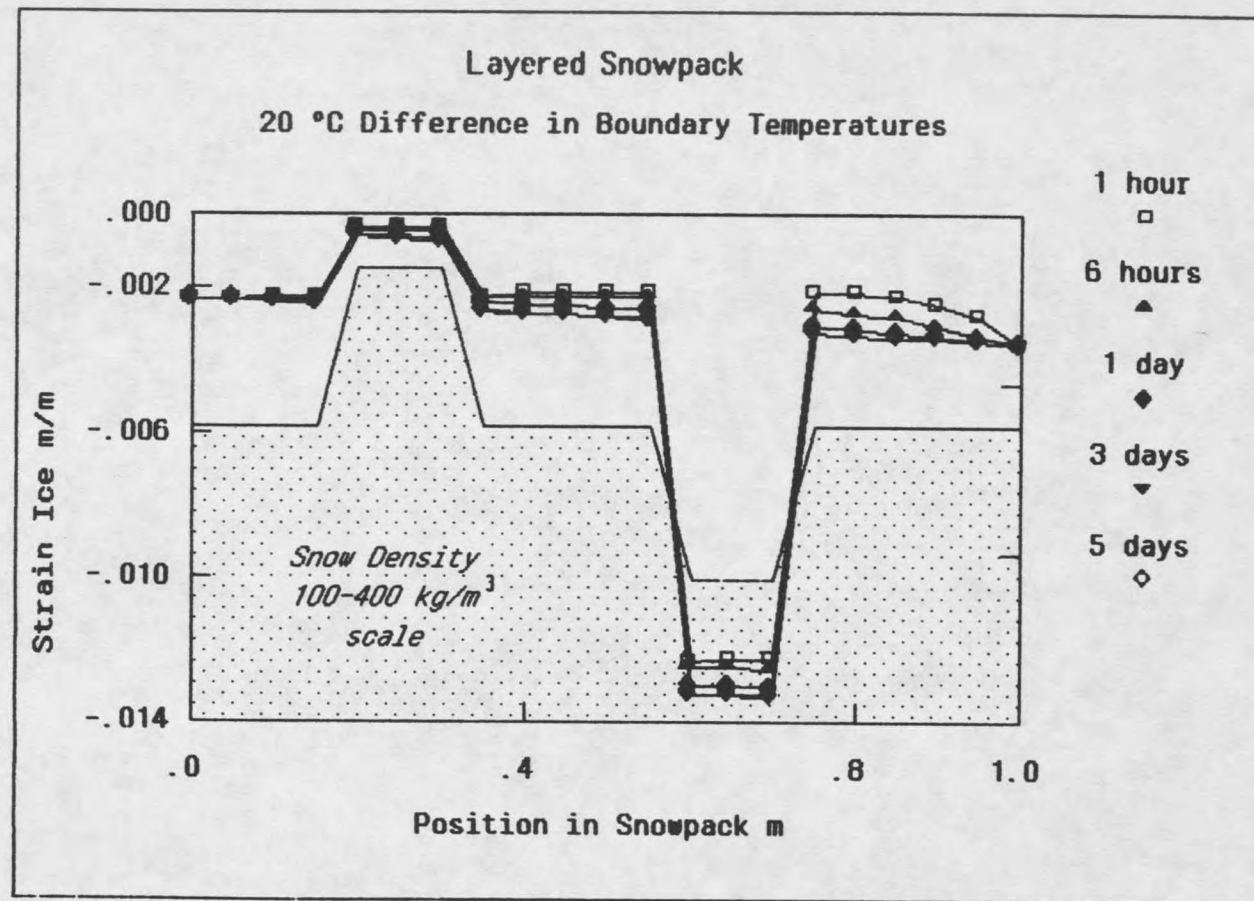


Figure 35. Strain in the ice relative to position in a layered snowpack, with base temperature 0 °C and surface temperature -20 °C.

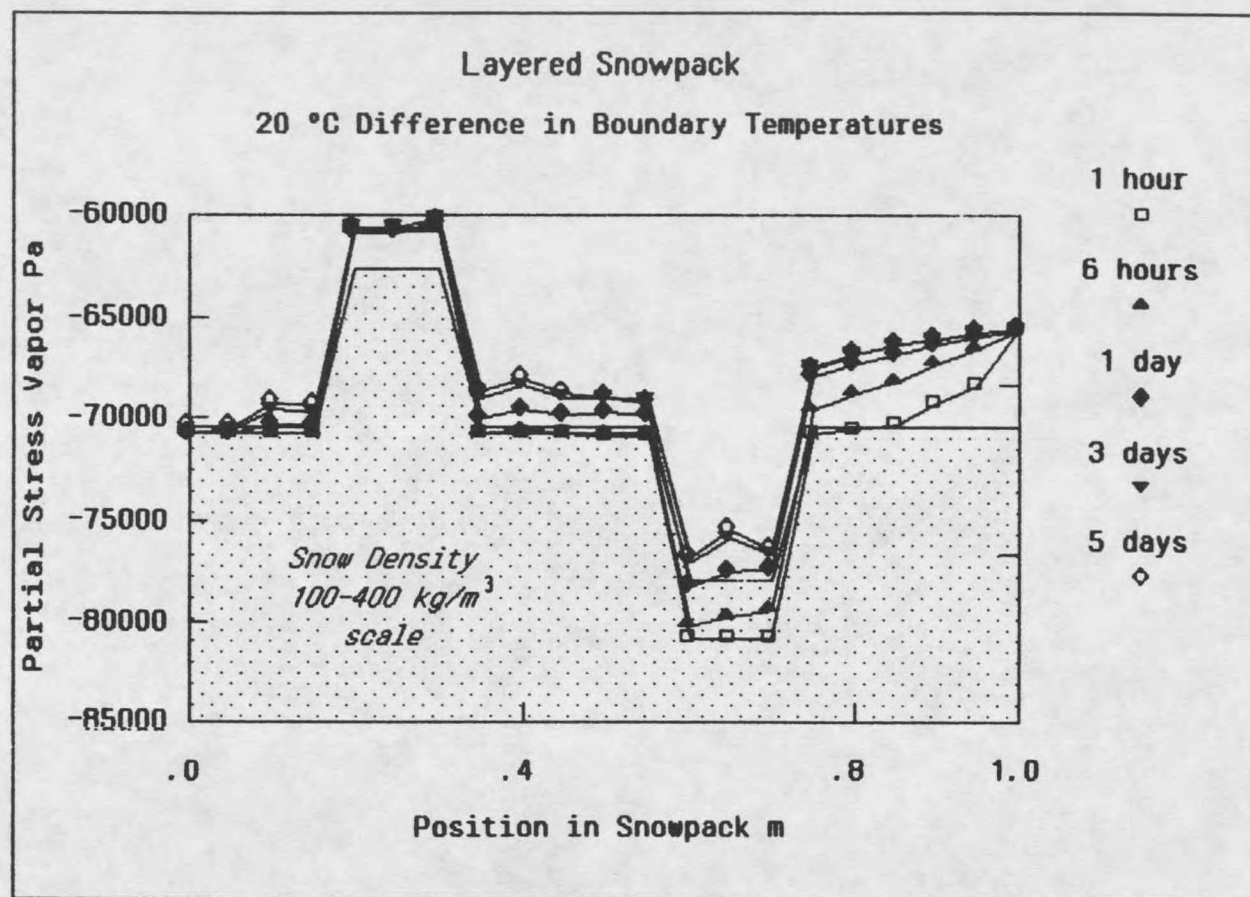


Figure 36. Partial stress of the vapor relative to position in a layered snowpack, with base temperature 0 °C and surface temperature -20 °C.

(Figure 37). The upper surface is once again indicated to be the most active zone as the initial changes are taking place. However, of particular interest is the way in which layering affects the change in volume fraction, since it is in apparent agreement with observed physical phenomena. Depth hoar crystals have been observed in the natural environment to grow above and below dense layers and crusts [Perla, 1978], and have been observed by the author as well. Regions of high density such as compacted snow from a ski track have been observed to increase in density at the obvious expense of the lower density snow surrounding it [Reid, 1984; Oakberg, personal communication].

Using the assumption asserted earlier, that a rapid decrease in ice volume fraction implies development of depth hoar, the indicated effect of the layering is to enhance depth hoar growth above and below the high density layer as well as in the low density snow and at the base. Also indicated by the model is the increase in density of the higher density snow, at the expense of the lower. It should be noted that these phenomena are particularly pronounced during the period when the thermal effects are being established. The indication of these trends are encouraging since the phenomena indicated by the model are indeed real. However, it is felt that the rates of change indicated may be too large relative to the magnitude of the results given for the temperature gradient effects alone. Until precise physical measurements of the density change for the various situations are taken, no conclusive judgement as to the what the relative rates for the different conditions should be, can be made.

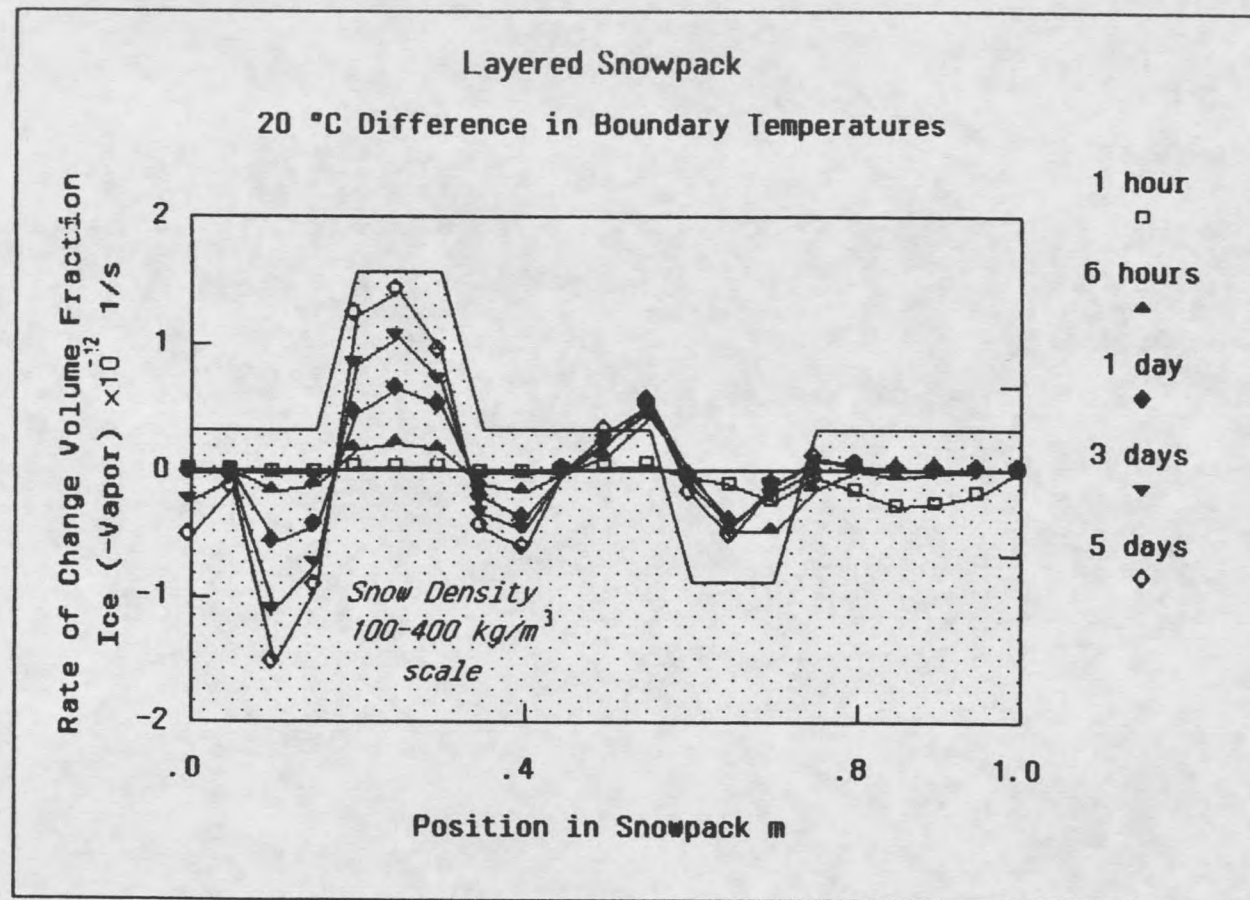


Figure 37. Time rate of change of the volume fraction relative to position in a layered snowpack, with base temperature 0 °C and surface temperature -20 °C.

The vapor velocity for the layered snowpack (Figure 38) has its maximum values initially at the transition interface between the density layers. Then, as the thermal effects of the imposed surface temperature infiltrate the snow the magnitude of the velocity decreases markedly. Finally, the effects of layering on the equilibrated force interaction (Figure 39) are seen to deviate from the trends noted for the homogeneous snow in much the same manner that noted for the temperature profile as the result of layering.

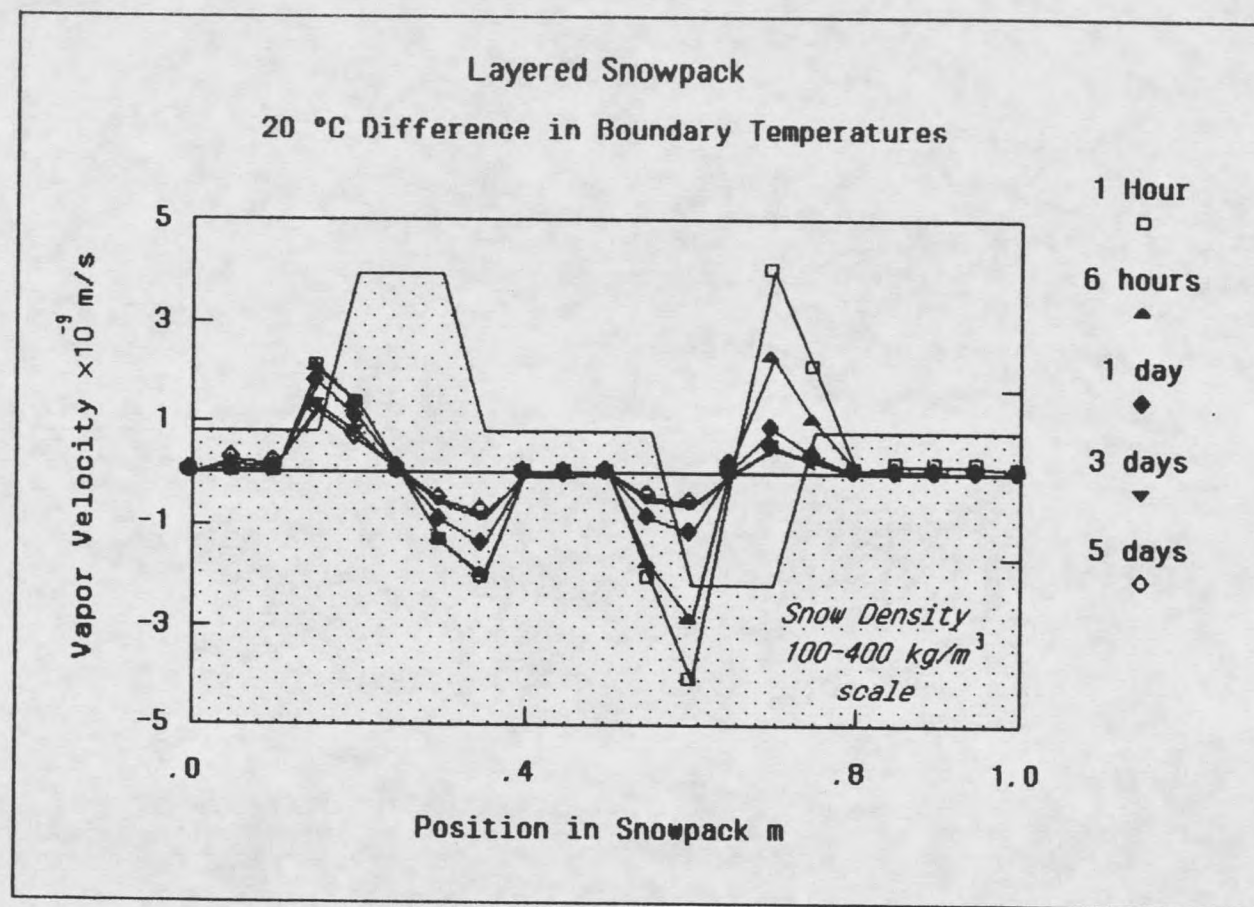


Figure 38. Vapor velocity relative to position in a layered snowpack, with base temperature 0 °C and surface temperature -20 °C.

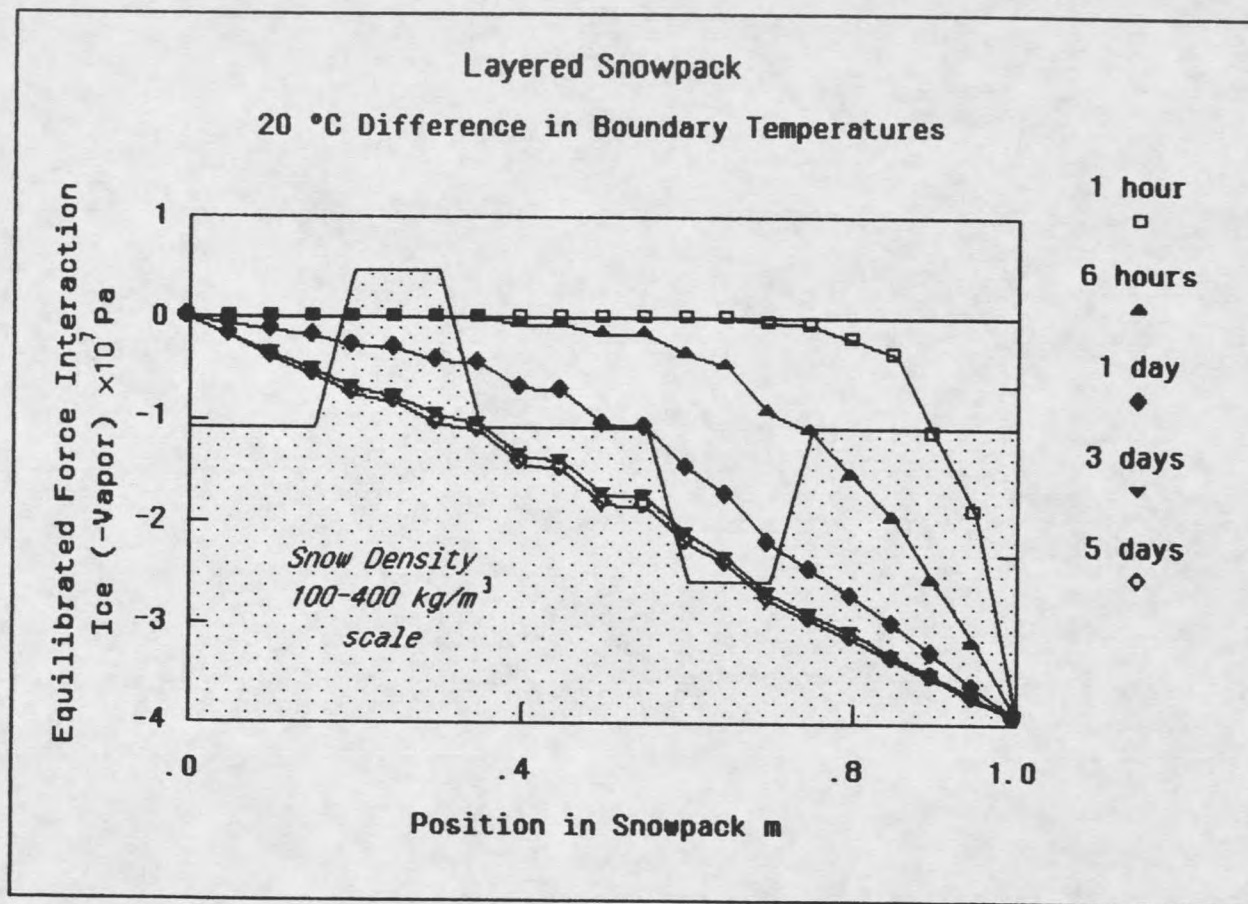


Figure 39. Equilibrated force interaction of the ice relative to position in a layered snowpack, with base temperature 0 °C and surface temperature -20 °C.

Chapter VI

SUMMARY

Recommendations

Since the equations used in the application have been developed entirely within the guidelines governing the modern theory of multiphase mixtures, a number of the coefficients involved in these newly established equations are not yet well understood. In light of this, continuing research which would yield more accurate values for the coefficients are warranted.

In the formulation presented here, the interaction terms as generated from the second law produce equations which intuitively seem appropriate. The fact that these equations are generated through the dissipation inequality within the framework of the theory is appealing, since it serves to sustain the coherent nature of the approach.

Although the forms derived for the interaction terms are reasonable, the positive coefficients involved in the equations are not in general well known. Even the most straight forward coefficients, when applied to a mixture, may be less transparent than for a single constituent. For example, the coefficient relating to the heat flux, the thermal conductivity, requires a closer examination. The usual thermal conductivity coefficients for the ice and vapor are used in the application. As a result of the volume fraction concept, the thermal conductivity of the snow mixture varies with

the snow density. This is in keeping with the usual concept associated with thermal conductivity in snow. Density is most commonly considered to be the predominant variable affecting thermal conduction in a snowpack [Mellor, 1964]. Future work however, should consider the manner in which temperature, grain bonding and configuration affect the constituent thermal conductivity coefficients.

The coefficient used for the energy interaction is based on Newton's law for cooling, and might be refined in future applications. The K coefficient involved in the extra equilibrated force term is not known or understood, and consequently it was arbitrarily chosen to be fairly small. The positive mass interaction coefficient which is used in this paper is assumed to be proportional to the interface pressure, since this term varies with temperature and grain configuration. The proportionality used is assumed to be very small, in order to maintain a mass exchange between constituents which is plausible. Snow density change due to metamorphic processes alone are so small that they have not yet been physically measured. Future investigation would appropriately work toward a more complete understanding of this coefficient.

Part of the appeal of the theory presented is the coherent, self contained nature of the approach. Central to this is the manner in which the Helmholtz free energy directly and naturally defines the stresses, entropy and equilibrated stress, based on the general theoretical requirements. The Helmholtz energies are approximated by a Taylor series expansion, as explained in the development presented previously in the text.

The ideal gas law is assumed to apply to the vapor free energy and is used to ascertain values for the coefficients of the series. A number of coefficients for the ice are arrived at by similarity to established forms. For example, similarity of the form arrived at for the stress with a thermoelastic material was utilized. Other coefficients for the free energy of the ice were calculated by equating suitable values to arrive at a balance with the chemical potential for the vapor at equilibrium. This method of determining coefficients, i.e. by comparison with processes involved for a separate constituent, offers a method to calculate values at certain conditions. The results, seem to indicate that these values are also appropriate at states other than those for which the coefficients were chosen to satisfy. These might be chosen by more independent methods in future work.

A significant stumbling block which must be addressed in future work, is the numerical calculation of the vapor velocity. The predominant emphasis of the present work is theoretical in nature with a fairly straight forward numerical approach. Continuation of the research should perhaps involve a more sophisticated numerical analysis, which would better address the instability associated with the balance of linear momentum equation for the vapor. Examination of the assumption of zero equilibrated stress might be addressed in future work, since it effects the calculation of vapor stress through Equations 3.15 and 3.16 and therefore may effect the vapor velocity which is calculated through the balance of linear momentum.

Solutions to the homogeneous snow problem appear to be extremely good. As stated in the discussion of results, the effects of layering appear to be correctly described by the theory developed here. The predicted results correspond quite nicely with physical evidence showing that dense layers adjacent to layers of lower density snow become more dense at the expense of the lower density layer. Although the model predicts this process correctly, the rate at which it is calculated is felt to be too high, relative to the calculated rate governed by temperature gradient effects. Further physical and analytic investigation is required for a resolution of this possible discrepancy. Until additional research is accomplished, whether or not these calculated values are indeed too large cannot with any certainty be determined.

The theoretical development presented in the dissertation is for a fully dimensional model. However, the numerical scheme which is used to test the formulation, simplified the application to one dimension. There are obvious limitations imposed when this is done. An expansion of the quantitative analysis to two and three dimensions would be a logical extension of the application presented here.

The ice constituent in the present development is considered as a thermoelastic material. When considering an extended time frame, modeling the ice as a thermo-viscoelastic material would be a desirable approach in a more sophisticated analysis.

Finally, the vapor, which is considered as a single constituent might be successfully subdivided, considering the air and water vapor as two

distinct constituents. This obviously implies a three constituent mixture, which is necessarily more complicated. The three constituent model would have the advantage of distinguishing between the more thermodynamically active water vapor which is changing phase, and the essentially inert air constituent. The relative diffusion between the two vapor constituents could then be distinguished as well. It is quite possible that treating the air and water vapor as independent constituents would lead to more suitable values when determining the velocities as calculated through the linear momentum equations. As a word of caution on this approach; since the vapors are not physically separated it may not be suitable to apply the immiscible assumption to these two constituents.

Conclusions

Perhaps the most appealing aspect of the theory presented is the fact that it is essentially self contained. Following the basic tenants of standard continuum mechanics, including the very important restrictions imposed by the entropy inequality, a set of intricately interconnected relationships are developed.

Development of the multiphase mixture theory to snow is the product of a straightforward approach following guidelines set down in previous theoretical work. Strict adherence to the basic principles of continuum mechanics with assurance that requisite requirements or restrictions are not violated, led to a model which is specialized to snow. Although considerable manipulation and specialized formulation are considered, it is

all carried out within the established framework of the theory of multiphase mixtures.

The strength of the theory is in its completeness. It does not isolate individual processes for examination, but instead requires that interrelationships be accounted for. Consideration of the snow as a continuum does not explicitly indicate the type of crystal development which is occurring, except by inference to the physical growth which is associated with the conditions predicted by the model.

The description of snow, or any material, as a mixture consisting of two constituents allows for considerable simplification over a mixture requiring additional constituents. This is particularly evident in reference to the constituent interaction terms. These interaction terms are the negative values of each other, when only two constituents are considered. Consequently, when a form for one term is established, values for both are immediately known. The time rate of change of the volume fraction for each constituent will also be negatives of each other.

Consideration of physically separated phases as autonomous materials except in reference to the constituent interaction terms, is important when making the transition from theory to application. This independent consideration of the individual constituents does not produce equations which are so unwieldy as to be impractical. The demonstration that this immiscible mixture concept may yield plausible results for physical situations such as the one examined in this paper, adds credence to the approach.

The theory is applied to several idealized snow conditions. Homogeneous and layered snowpacks one meter in depth are considered for isothermal conditions and with the boundary temperatures held constant, 20 °C apart. Initially the snowpack is assumed to be at the same temperature throughout, except at the upper surface. The processes such as temperature change, mass interaction, vapor flux, etc. and their transition from the initial conditions are evaluated. Results from the theory presented are quite good.

The idealized homogeneous sample gives very plausible results. An ice volume fraction of 0.3 is assumed, which corresponds to a snow density of approximately 275 kg/m³. The isothermal condition gives results which show little variation throughout the snowpack for predominantly thermodynamic processes, as would be expected for this simple situation. With only mechanical effects driving them, processes such as the partial stress and strain of the ice are seen to increase in magnitude with depth from simply the overburden of the snow above. The partial stress of the vapor is constant throughout and the vapor velocity is zero.

The homogeneous snowpack is examined to see the transitory variation of processes with time, after the initial thermal boundary conditions are imposed. Inspection of the homogeneous model one hour after the start, shows the processes near the surface to be very active. Large gradients of the temperature, vapor pressure, thermal strain and equilibrated force interaction near the surface are apparent as well as relatively large vapor velocities and a rapid decrease in the volume

fraction of the ice. Because it has a higher thermal conductivity, the ice cools more rapidly than the vapor, and near the surface the temperature of the ice drops substantially below that of the vapor constituent at the same location. At the end of the first hour, there is very little change from the initial conditions further down into the snowpack.

Inspection of the processes as time progresses reveals a particularly active zone, similar to those in the upper region noted after one hour, which moves downward with time in a wavelike fashion. However, the abrupt radical jumps in the terms described are less pronounced as this active zone moves downward through the snowpack. After five days the steady state is being approached, indicated by the approach of constant gradients for the terms mentioned above, and the equilibrating of constituent temperatures at corresponding layers.

Interestingly, the strain profile, in accordance with the changing temperature regime, has been altered as the result of thermal expansion, to the point where the magnitude of the strain becomes greater as the cooler surface is approached.

The time rate of change of the ice volume fraction is most pronounced for the homogeneous situation in the lower warmer, more thermodynamically active region. The decreasing volume fraction of the ice is assumed in this application to indicate the development of the kinetic growth form.

The idealized snowpack used to test the effect of stratigraphy is considered to be a snowpack of predominantly 0.3 ice volume fraction with

a 15 cm layer of 0.4 ice volume fraction and a lower density layer of the same thickness with an ice volume fraction of 0.2. These correspond to approximately 367 kg/m^3 and 183 kg/m^3 snow densities respectively.

When the stratigraphically layered snow is considered as initially isothermal, temperatures remain constant and equal. The greatest strain for the ice constituent is calculated in the low density layer, and the least is in the high density layer. The partial vapor stress varies with the layering, but as discussed in the previous chapter, when considered with respect to a unit of pure vapor it remains constant throughout. That is if only the vapor were to be considered the vapor stress in all of the individual pores would be equal. Partial stress for the ice increases in magnitude with depth and exhibits perturbations through the layering. Scrutinizing this ice stress, it is seen that larger stresses per unit of the ice alone are sustained in lower density snow.

Vapor velocity is everywhere zero, except at the interfaces between layers. The direction of the velocities at the interfaces shows a flow from lower density regions toward zones of higher density.

When the differing boundary temperatures are imposed on the layered snowpack, a transient pattern similar to that seen in the homogeneous snow takes place. This similarity exists in the sense that there are initially large gradient and rate functions near the surface, which become less pronounced as this initial wave of transition physically progresses downward through the snow with time. There are, as expected, notable differences due to the varied stratigraphy. Curve profiles of processes

varying with position are not smooth functions progressing toward a linear form, as in the homogeneous example. There are perturbations which coincide with the layering.

Temperature gradients develop which are strongest through the low density layer and weakest in the high. The change in volume fraction indicates that a dense layer sandwiched between lower density snow will become more dense as the adjacent lower density snow decreases in density. Similarly, the lower density snow will lose ice as the adjacent higher density snow gains. This result is encouraging, since it has been observed in natural snowcover [Reid, 1984; Oakberg, personal communication, 1984]. Although the anomaly is quite likely real, it is felt that the effect of layering indicated by the model is too large relative to the calculated temperature gradient effects. Although, as stated earlier, without further research this question cannot be answered.

Ice stresses are essentially the same as those calculated for the isothermal, and the partial vapor stress maintains the same basic response as for the isothermal situation, but decreases somewhat along with temperature. The vapor velocity response to layering remains after the thermal processes have permeated the snowpack, but is shown to slow with time.

The theory of multiphase mixtures offers a unified, coherent, comprehensive approach to analyzing the myriad of intricately interrelated processes involved in thermodynamically active granular or porous materials. Results from the initial attempt presented in this dissertation

to model snow on the ground by application of the theory are quite promising. Of course, considerable future work remains in development of the application, but the thesis demonstrates that this relatively new theoretical approach may be successfully used for modeling processes as complex as the one presented. The thrust of this paper is concerned with an ongoing development of an enhanced understanding of snow as a material. But, the most significant accomplishment is quite probably the demonstration of the usefulness of the potentially powerful theory, which has had relatively few applications, to a broad range of problems.

NOTATION AND NOMENCLATURE

Notation

In general, except where explicitly noted in the text, bold upper case symbols indicate second order tensors, bold lower case symbols indicate vectors and scalars are represented by standard print symbols. A backward prime preceding a symbol, $\cdot T_a$, indicates a material time derivative on the constituent property, and a preceding superscript dot preceding a symbol, $\dot{T}$, indicates a material time derivative for the mixture.

Subscripts associated with symbols imply a property associated with the constituent, and symbols without a subscript imply a property associated with the mixture. Subscripts for specific constituents i and v (T_i and T_v) represent the ice and vapor respectively. A subscript R implies a reference state.

Nomenclature

B_a	configuration of constituent a .
B_{aR}	reference configuration of constituent a
$\mathbf{b}_a, \mathbf{b}$	body force
c_a, c	mass concentrations
c_a^+	mass interaction
E_a	strain tensor for constituent a
e_a, e	internal energy
e_a^+	energy interaction
e_a^{+e}	extra energy interaction
F_a, F	deformation gradients
G	Lame' constant, modulus of rigidity
g_a, g	equilibrated force supply

g_a	temperature gradient
h_a, h	equilibrated stress
k_a, k	equilibrated inertia
L_a, L	velocity gradients
L	heat of sublimation
l_a, l	external equilibrated body force
M_a^+	angular momentum interaction
m_a^+	momentum interaction
m_a^{+e}	extra momentum interaction
n_a, n	unit normal vector directed outward
q_a, q	heat flux
R	gas constant
r_a, r	external heat supply
s	the state of a variable
s^*	equilibrium state
s^D	perturbation away from the equilibrium state
T_a, T	stress tensors
t	time
u_a	diffusion velocity for constituent a
v_a, x_a, v, x	velocity vectors
w_a, w	volume fraction gradient
X_a, X	position vectors in the reference configuration
x_a, x	position vectors in spacial coordinates
Y	Young's modulus
α	coefficient of linear expansion
β_a, β	body of constituent a, mixture body
Γ_a, Γ	any general scalar, vector or tensor valued property
ϱ_a	material density of constituent a
δ	internal dissipation of the mixture
δ'	slight perturbation from equilibrium state of δ

ζ	fluid viscosity
η_a, η	entropy
η_a^+	entropy interaction
θ_a	constituent temperature
θ_R	reference temperature
κ	permeability
λ	Lame's constant
μ_a	chemical potential
v_a, v	volume fraction
ξ	scalar of arbitrarily small magnitude
π	interphase pressure between phases
ρ	bulk density of the mixture
ρ_a	partial density of constituent a
$\S$	a general source term
σ	interfacial energy
Υ	a general flux term
v_a^+	equilibrated force interaction
v_a^{+e}	extra equilibrated force interaction
Φ	Poisson's ratio
Ψ	a general property
ψ_a	Helmholtz free energy
ω	mean radius of curvature

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APPENDICES

APPENDIX A

Vapor Velocity from the Balance of Linear Momentum Equation

The one dimensional balance of linear momentum equation for the vapor is

$$m_v^+ = \rho_v v_v - \partial T_v / \partial x_v - \rho_v b_v + c_v^+ v_v - \pi \partial v_v / \partial x_v,$$

or, rearranging terms

$$v_v = (\partial T_v / \partial x_v + \rho_v b_v - c_v^+ v_v + \pi \partial v_v / \partial x_v + m_v^+) / \rho_v.$$

Substituting for the interaction terms gives

$$\begin{aligned} v_v = & (\partial T_v / \partial x_v + \rho_v b_v + [c_{i_0}^+ \{(\mu_v - v_v v_v / 2 - k_v v_v^2 / 2) / \theta_v \\ & - (\mu_i - v_i v_i / 2 - k_i v_i^2 / 2) / \theta_i\}] v_v + \pi \partial v_v / \partial x_v \\ & - [m_{i_0}^{+e} \{ (v_v / \theta_v) - (v_i / \theta_i) \}]) / \rho_v. \end{aligned}$$

Rearranging and collecting terms

$$\begin{aligned} v_v + [c_{i_0}^+ / (2\theta_v \rho_v)] v_v^3 + \{- [c_{i_0}^+ \{(\mu_v - k_v v_v^2 / 2) / \theta_v \\ - (\mu_i - v_i v_i / 2 - k_i v_i^2 / 2) / \theta_i\} + m_{i_0}^{+e} / \theta_v] / \rho_v\} v_v \\ = [\partial T_v / \partial x_v + \rho_v b_v + \pi \partial v_v / \partial x_v + m_{i_0}^{+e} (v_i / \theta_i)] / \rho_v, \end{aligned}$$

or with the obvious substitutions

$$v_v + a v_v^3 + b v_v = c.$$

This is a first order but nonlinear differential equation. However, the homogeneous part is readily solved since it is in the class of Bernoulli Equations.

Multiplying the homogeneous part by v_v^{-3} gives

$$v_v^{-3} v_v + b v_v^{-2} = -a.$$

Now set $y = v_v^{-2}$ so that

$$v_V^{-3} 'v_V = - 'y/2,$$

and the equation to be solved is simply

$$'y - 2b y = 2a,$$

which has the solution

$$y = k \exp(2bt) - a/b,$$

so that the homogeneous solution to the original differential equation is

$$v = [k \exp(2bt) - a/b]^{-1/2}.$$

The particular solution is arrived at by finding the cube root of the equation

$$v^3 + d v + e = 0,$$

where

$$d = b/a \quad \& \quad e = -c/a.$$

For the solution to the cubic equation, let

$$A = \left[-e/2 + [(e^2/4) + (d^3/27)]^{1/2} \right]^{1/3}$$

and

$$B = \left[-e/2 - [(e^2/4) + (d^3/27)]^{1/2} \right]^{1/3}$$

and since

$$e^2/4 + d^3/27 > 0,$$

(this is continuously checked in the computer program) there is only one real root, which is used as the particular solution p ,

$$p = A + B.$$

The complete solution to the differential equation is then

$$v = [k \exp(2bt) - a/b]^{-1/2} + p.$$

Using as an initial condition

$$@ t = 0; \quad v = v_{\text{initial}}.$$

yields

$$v_{\text{initial}} = [k - a/b]^{-1/2} + p,$$

so

$$k = (v_{\text{initial}} - p)^{-2} + a/b,$$

and finally

$$v = \{[(v_{\text{initial}} - p)^{-2} + a/b] \exp(2bt) - a/b\}^{-1/2} + p.$$

APPENDIX B

Computer Program

Figure 40. Computer program, EASNOMIX, which is used to calculate results.

```

PROGRAM EASNOMIX(INPUT,OUTPUT,EACOE,EAOUT);

CONST N=21;
      M=7;

TYPE VECTOR=ARRAY[1..N] OF REAL;

VAR GAMMAI,R,TEMPR,SPHTV,SPHTI,THERMEXP,KIR,KVR,MASINSCALE,
    ENTROPVR,ENTROPIR,ENERINTR,DT,DTH,DZ,
    BF,TIME,TOTLTIME,VISC,PERMEAB,PIR,SIGMA,L,PSIV2,PSI12,
    HEIGHT,POISSON,K:REAL;

    I,J,IK,CK,OUTINTV:INTEGER;

    NUU,NUI,ROI,ROV,UU,TEMPV,TEMPI,E,GAMMAV,MUV,MUI,MASINTI,MOMINTI,
    ENERINTI,PI,DPDNI,DPDNV,EQFR1,EQFRINI,EQFRINV,EQFSV,STRESSI,STRESSS,
    STRESSV,ENTROPI,ENTROPV,ENGYI,ENGYV,QI,QV,LV,MOMINTR,TRCNUI,TRCROV,
    TRCTEMPI,TRCTEMPV,LATHTROI,LATHTNUV,LATHTROV,LATHTSTR,
    TRCE,EPRE,KI,KV,NUVR,NUIR,GAMMAVR,ROVR,ROIR,
    PSIVR,PSIV1,PSIV3,PSIV5,PSIV6,PSI110,PSI18,MASINTR,
    PSIV8,PSIV10,PSI1R,PSI1I,PSI13,PSI15,PSI16,PSI17,PSI19,RADIUS,BND,KON,
    TGI,TGV,YOUNGMOD,LAMBDA,SHRMOD,PSIV7,PRESS,VS,DVV,DVI,ROS,ROOTEST,
    ACOEF,BCOEF,CCOEF,DCOEF,ECOEF,VVPARTA,VVPARTB,VVPARTIC,CUBEA,CUBEB:VECTOR;

    INCOEF,OUTFILE,OutfileI,OutfileV,OutfileS,OutfileX:TEXT;

PROCEDURE INITIAL;
VAR I:INTEGER;
BEGIN

```

DEGIN

PSIV2:=-ENTROPVR;
PSII2:=-ENTROPIR;
Writeln(OutfileI,N,M);
Writeln(OutfileV,N,M);
Writeln(OutfileS,N,M);
Writeln(OutfileX,N,M);

FOR I:=1 TO N DO

BEGIN

ROI[I]:=NUI[I]*GAMMAI;
NUV[I]:=1-NUI[I];
NUIR[I]:=NUI[I];
NUVR[I]:=NUV[I];
GAMMAV[I]:=1.29;
GAMMAVR[I]:=GAMMAV[I];
ROV[I]:=NUV[I]*GAMMAV[I];
ROS[I]:=ROI[I]+ROV[I];
ROIR[I]:=ROI[I];
ROVR[I]:=ROV[I];
PI[I]:=PIR*(EXP((2*SIGMA)/(GAMMAI*R*TEMPR*RADIUS[I]))
EXP((L/R)((1/TEMPR)-(1/TEMPI[I]))));

PSIV1[I]:=-R*TEMPR/NUVR[I];
PSIV3[I]:=R*TEMPR/ROVR[I];
PSIV5[I]:=R*TEMPR/SQR(NUVR[I]);
PSIV6[I]:=-R/NUVR[I];

PSIV8[I]:=R/ROVR[I];
PSIV10[I]:=R*TEMPR/SQR(ROVR[I]);
PSII1[I]:=-R*TEMPR*ROVR[I]/ROIR[I];
PSII10[I]:=-PSII1[I]/ROIR[I];
PSIV7[I]:=-SPHTV/TEMPR;
PSII8[I]:=-SPHTI/TEMPR;

```

PSI13[I]:=-(2*PI[I]-GAMMAVR[I]*R*TEMPR)/(ROIR[I]*GAMMAI);
YOUNGMOD[I]:=EXP((10*NUI[I]+4)*LN(10));
LAMBDA[I]:=(YOUNGMOD[I]*POISSON)/((1+POISSON)*(1-2*POISSON));
SHRMOD[I]:=YOUNGMOD[I]/(2*(1+POISSON));
PSI15[I]:=LAMBDA[I]/ROIR[I];
PSI16[I]:=SHRMOD[I]/ROIR[I];
PSI17[I]:=-THERMEXP*(3*PSI15[I]+2*PSI16[I]);
PSI19[I]:=((PSIV2-PSI12)+PSIV8[I]*ROVR[I])/ROIR[I];
PSIVR[I]:=-PSIV3[I]*ROVR[I];
PSIIR[I]:=(PSIVR[I]+PSIV3[I]*ROVR[I])-ROIR[I]*PSI13[I];

VV[I]:=0;
VS[I]:=0;
DVI[I]:=0;
DVV[I]:=0;
TRCE[I]:=0;
LV[I]:=0;
STRESSS[I]:=0;
END;

STRESSI[N]:=-GAMMAVR[N]*253*R;
FOR I:=N-1 DOWNT0 1 DO
BEGIN
  STRESSI[I]:=(STRESSI[I+1]+(BF*ROI[I])*DZ+PI[I]*(NUI[I+1]-NUI[I]));
END;
FOR I:=1 TO N DO
BEGIN
  EI[I]:=(STRESSI[I]/ROI[I]-PSI11[I]-PSI17[I]*(TEMPI[I]-TEMPR)-PSI110[I]
    *(ROI[I]-ROIR[I]))/(PSI15[I]+2*PSI16[I]);
END;
END;

```

```

PROCEDURE INTERACT; (CALCULATE VALUES FOR INTERACTION TERMS)
VAR I:INTEGER;
BEGIN
  FOR I:=1 TO N DO
    BEGIN
      YOUNGMOD[I]:=EXP((10*NUI[I]+4)*LN(10));
      LAMBDA[I]:=(YOUNGMOD[I]*POISSON)/((1+POISSON)*(1-2*POISSON));
      SHRMOD[I]:=YOUNGMOD[I]/(2*(1+POISSON));
      PSII5[I]:=LAMBDA[I]/ROIR[I];
      PSII6[I]:=SHRMOD[I]/ROIR[I];
      PSII7[I]:=-THERMEXP*(3*PSII5[I]+2*PSII6[I]);
      LATHTNUV[I]:=PSIV5[I]*(NUV[I]-NUVR[I]);
      LATHTROV[I]:=PSIV10[I]*(ROV[I]-ROVR[I]);
      LATHTROI[I]:=PSII3[I]-PSII9[I]*TEMPR+PSII10[I]*E[I];
      LATHTSTR[I]:=(PSII1[I]+(PSII5[I]+2*PSII6[I])*E[I]-PSII7[I]*TEMPR+PSII10[I]*
        (ROI[I]-ROIR[I]));
      KI[I]:=BND[I]*KIR*NUI[I];
      KV[I]:=KVR*NUV[I];

      MUV[I]:=PSIV1[I]*(NUV[I]-NUVR[I])+PSIV2*(TEMPV[I]-TEMPR)+PSIV3[I]
        *(2*ROV[I]-ROVR[I])+
        (1/2)*(PSIV5[I]*SQR(NUV[I]-NUVR[I])+2*PSIV6[I]*(TEMPV[I]-TEMPR)*
        (NUV[I]-NUVR[I])+PSIV7[I]*SQR(TEMPV[I]-TEMPR)+2*PSIV8[I]*(TEMPV[I]-TEMPR)*
        (2*ROV[I]-ROVR[I])+PSIV10[I]*(3*SQR(ROV[I])-4*ROV[I]*ROVR[I]+
        SQR(ROVR[I])))+PSIVR[I];
      MUI[I]:=PSII1[I]*E[I]+PSII2*(TEMPI[I]-TEMPR)+PSII3[I]*(2*ROI[I]-ROIR[I])+
        (1/2)*((PSII5[I]+2*PSII6[I])*SQR(E[I])+2*PSII7[I]*(TEMPI[I]-
        TEMPR)*E[I]+PSII8[I]*SQR(TEMPI[I]-TEMPR)+2*PSII9[I]*(TEMPI[I]-TEMPR)*
        (2*ROI[I]-ROIR[I])+2*PSII10[I]*(2*ROI[I]-ROIR[I])*E[I]+PSIIR[I];
      MASINTR[I]:=MASINSCALE*PI[I];
      MASINTI[I]:=MASINTR[I]*(MUV[I]/TEMPV[I]-MUI[I]/TEMPI[I]
        -(SQR(VV[I])/TEMPV[I])/2);
      MOMINTR[I]:=(SQR(NUI[I])*TEMPV[I]*VISC)/(PERMEAB);
      MOMINTI[I]:=MOMINTR[I]*(VV[I]/TEMPV[I]);
    END
  END

```

```

ENERINTI[I]:=ENERINTR*(TEMPV[I]-TEMPI[I]);
DPDNI[I]:=GAMMAI*(PSII3[I]+PSII9[I]*(TEMPI[I]-TEMPR)+PSII10[I]*E[I]);
DPDNV[I]:=PSIV1[I]+PSIV5[I]*(NUV[I]-NUVR[I])+PSIV6[I]*(TEMPV[I]-TEMPR);
STRESSV[I]:=(-SQR(RQV[I])*(PSIV3[I]+PSIV8[I]*(TEMPV[I]-TEMPR)+
    PSIV10[I]*(ROV[I]-ROVR[I])));
ENTROPI[I]:=-(PSII2+PSII7[I]*E[I]+PSII8[I]*(TEMPI[I]-TEMPR)+PSII9[I]
    *(ROI[I]-ROIR[I]));
ENTROPV[I]:=-(PSIV2+PSIV6[I]*(NUIR[I]-NUI[I])+PSIV7[I]*(TEMPV[I]-TEMPR)
    +PSIV8[I]*(ROV[I]-ROVR[I]));
ENGYV[I]:=PSIV1[I]*(NUV[I]-NUVR[I])-PSIV2*TEMPR+PSIV3[I]*(ROV[I]-ROVR[I])+
    (1/2)*(PSIV5[I]*SQR(NUV[I]-NUVR[I])-2*PSIV6[I]*TEMPR*(NUV[I]-NUVR[I])
    -PSIV7[I]*(SQR(TEMPV[I])-SQR(TEMPR))-2*PSIV8[I]*TEMPR*(ROV[I]-ROVR[I])+
    PSIV10[I]*SQR(ROV[I]-ROVR[I]))+PSIVR[I];
ENGYI[I]:=PSII1[I]*E[I]-PSII2*TEMPR+PSII3[I]*(ROI[I]-ROIR[I])+
    (1/2)*((PSII5[I]+2*PSII6[I])*SQR(E[I])-2*PSII7[I]*TEMPR*E[I]
    -PSII8[I]*(SQR(TEMPI[I])-SQR(TEMPR))-2*PSII9[I]*TEMPR*(ROI[I]-ROIR[I])+
    2*PSII10[I]*(ROI[I]-ROIR[I])*E[I])+PSIIR[I];

```

END;

END;

PROCEDURE BALANCE;

VAR I:INTEGER;

BEGIN

I:=1;(NODE AT THE GROUND USE FORWARD DIFFERENCE)

TGI[I]:=(TEMPI[I+1]-TEMPI[I])/(DZ);

TGV[I]:=(TEMPV[I+1]-TEMPV[I])/(DZ);

QI[I]:=-KI[I]*(TEMPI[I+1]-TEMPI[I])/(DZ);

QV[I]:=-KV[I]*(TEMPV[I+1]-TEMPV[I])/(DZ);

LV[I]:=(VV[I+1]-VV[I])/(DZ);

TRCNUI[I]:=MASINTI[I]/GAMMAI;

TRCROV[I]:=-MASINTI[I]-ROV[I]*(VV[I+1]-VV[I])/DZ;

EQFR1[I]:=((PI[I]+ROV[I]*DPDNV[I])*TEMPI[I]-(PI[I]+ROI[I]*DPDNI[I])
 *TEMPV[I]-K*TEMPI[I]*TEMPV[I]*TRCNUI[I])/(TEMPV[I]+TEMPI[I]);

EQFRINI[I]:=EQFR1[I]+PI[I];

EQFRINV[I]:=-EQFR1[I]+PI[I];

VV[I]:=0;

```

TRCTEMP[I]:=0;
TRCTEMPV[I]:=0;

I:=N;(NODE AT THE SURFACE USE BACK DIFFERENCE)
TGI[I]:=(TEMP[I]-TEMP[I-1])/DZ;
TGV[I]:=(TEMPV[I]-TEMPV[I-1])/DZ;
QI[I]:=-KI[I]*(TEMP[I]-TEMP[I-1])/DZ;
QV[I]:=-KV[I]*(TEMPV[I]-TEMPV[I-1])/DZ;
LV[I]:=(VV[I]-VV[I-1])/DZ;
TRCNUI[I]:=MASINTI[I]/GAMMAI;
TRCROV[I]:=-MASINTI[I]-ROV[I]*(VV[I]-VV[I-1])/DZ;
ACOEFI[I]:=MASINTR[I]/(2*ROV[I]*TEMPV[I]);
BCOEFI[I]:=((MOMINTR[I]/TEMPV[I]-MASINTR[I]*(MUV[I]/TEMPV[I])
-(MUI[I]/TEMP[I])))/ROV[I];
CCOEFI[I]:=((STRESSV[I]-STRESSV[I-1])/DZ+ROV[I]*BF+
PI[I]*(NUV[I]-NUV[I-1])/DZ)/ROV[I];
DCOEFI[I]:=BCOEFI[I]/ACOEFI[I];
ECCOEFI[I]:=(-CCOEFI[I]/ACOEFI[I]);
ROOTEST[I]:=(SQRT(-CCOEFI[I])/4)+(SQRT(BCOEFI[I]*DCOEFI[I])/27);
IF ROOTEST[I]<0 THEN
  WRITELN(OUTFILE,'THREE REAL ROOTS',ROOTEST[I]);
CUBEAI[I]:=-ECCOEFI[I]+(1/ACOEFI[I])*SQRT(ROOTEST[I]);
CUBEBI[I]:=-ECCOEFI[I]-(1/ACOEFI[I])*SQRT(ROOTEST[I]);
VVPARTAI[I]:=EXP((1/3)*LN(ABS(CUBEAI[I])));
IF CUBEAI[I]<0 THEN
  VVPARTAI[I]:=-VVPARTAI[I];
VVPARTBI[I]:=EXP((1/3)*LN(ABS(CUBEBI[I])));
IF CUBEBI[I]<0 THEN
  VVPARTBI[I]:=-VVPARTBI[I];
VVPARTICI[I]:=ACOEFI[I]*(VVPARTAI[I]+VVPARTBI[I]);

EQFR1[I]:=((PI[I]+ROV[I]*DPDNV[I])*TEMP[I]-(PI[I]+ROI[I]*DPDNI[I])
*TEMPV[I]-K*TEMP[I]*TEMPV[I]*TRCNUI[I])/TEMPV[I]+TEMP[I];
EQFRINI[I]:=EQFR1[I]+PI[I];
EQFRINV[I]:=-EQFR1[I]+PI[I];

```

```

TRCTEMP1[I]:=0;
TRCTEMPV[I]:=0;

FOR I:=2 TO N-1 DO
BEGIN
  TGI[I]:=(TEMP1[I+1]-TEMP1[I-1])/(2*DZ);
  TGV[I]:=(TEMPV[I+1]-TEMPV[I-1])/(2*DZ);
  QI[I]:=-KI[I]*(TEMP1[I+1]-TEMP1[I-1])/(2*DZ);
  QV[I]:=-KV[I]*(TEMPV[I+1]-TEMPV[I-1])/(2*DZ);
END;

FOR I:=2 TO N-1 DO
BEGIN
  TRCNUI[I]:=MASINTI[I]/GAMMAI;
  TRCROV[I]:=-MASINTI[I]-ROV[I]*(VV[I+1]-VV[I-1])/(2*DZ);

  ACOEF[I]:=MASINTR[I]/(2*ROV[I]*TEMPV[I]);
  BCOEF[I]:=((MOMINTR[I]/TEMPV[I]-MASINTR[I]*(MUV[I]/TEMPV[I])
    -(MUI[I]/TEMP1[I])))/ROV[I];
  CCOEF[I]:=((STRESSV[I+1]-STRESSV[I-1])/(2*DZ)+ROV[I]*BF
    +PI[I]*(NUV[I+1]-NUV[I-1])/(2*DZ))/ROV[I];
  DCOEF[I]:=BCOEF[I]/ACOEF[I];
  ECOEF[I]:=(-CCOEF[I]/ACOEF[I]);
  ROOTEST[I]:=(SQR(-CCOEF[I])/4)+(SQR(BCOEF[I]*DCOEF[I])/27);
  IF ROOTEST[I]<0 THEN

    WRITELN(OUTFILE,'THREE REAL ROOTS',ROOTEST[I]);
    CUBEAI[I]:=-ECOEF[I]+(1/ACOEF[I])*SQR(ROOTEST[I]);
    CUBEBI[I]:=-ECOEF[I]-(1/ACOEF[I])*SQR(ROOTEST[I]);
    VVPARTAI[I]:=EXP((1/3)*LN(ABS(CUBEAI[I])));
    IF CUBEAI[I]<0 THEN
      VVPARTAI[I]:=-VVPARTAI[I];
    VVPARTBI[I]:=EXP((1/3)*LN(ABS(CUBEBI[I])));
    IF CUBEBI[I]<0 THEN
      VVPARTBI[I]:=-VVPARTBI[I];

```

```

VVPARTIC[I]:=ACOEFI[I]*(VVPARTA[I]+VVPARTB[I]);
EQFR[I]:=(PI[I]+ROV[I]*DPDNV[I])*TEMPI[I]-(PI[I]+ROI[I]*DPDNI[I])
          *TEMPV[I]-K*TEMPI[I]*TEMPV[I]*TRCNUI[I]/(TEMPV[I]+TEMPI[I]);
EQFRINI[I]:=EQFR[I]+PI[I];
EQFRINV[I]:=-EQFR[I]+PI[I];
TRCTEMP[I]:=(-LATHTSTR[I]*TRCE[I]-LATHTROI[I]*GAMMAI*TRCNUI[I]
             -(QI[I+1]-QI[I-1])/(2*DZ)-MASINTI[I]*
             (ENGY[I])+ENERINTI[I]-
             EQFRINI[I]*TRCNUI[I])/(ROI[I]*SPHTI);
TRCTEMPV[I]:=(LATHTNUV[I]*TRCNUI[I]-LATHTROV[I]*TRCROV[I]+STRESSV[I]
              *LV[I]-(QV[I+1]-QV[I-1])/(2*DZ)+MASINTI[I]*(ENGYV[I]-SQR(VV[I])/2)
              +MOMINTI[I]*VV[I]-ENERINTI[I]+EQFRINV[I]*TRCNUI[I])/(ROV[I]*SPHTV);

```

```

END;
END;

```

PROCEDURE UPDATE;

VAR I:INTEGER;

BEGIN

FOR I:= 1 TO N DO

BEGIN

EPRE[I]:=E[I];

NUI[I]:=TRCNUI[I]*DT+NUI[I];

NUV[I]:=(1-NUI[I]);

ROI[I]:=GAMMAI*NUI[I];

ROV[I]:=TRCROV[I]*DT+ROV[I];

ROS[I]:=ROI[I]+ROV[I];

GAMMAV[I]:=ROV[I]/(1-NUI[I]);

TEMPI[I]:=TRCTEMP[I]*DT+TEMPI[I];

TEMPV[I]:=TRCTEMPV[I]*DT+TEMPV[I];

VV[I]:=1/(SQR(((1/(SQR(VV[I]-VVPARTIC[I])))+ACOEFI[I]/BCOEFI[I])
 *EXP(2*BCOEFI[I]*DT)-ACOEFI[I]/BCOEFI[I]))+VVPARTIC[I];

VS[I]:=ROV[I]*VV[I]/ROS[I];

DVV[I]:=VV[I]-VS[I];

```

    DV[I]:= -VS[I];
    PI[I]:= PIR*(EXP((2*SIGMA)/(GAMMA1*R*TEMPR*RADIUS[I]))
        *EXP((L/R)*((1/TEMPR)-(1/TEMPI[I]))));
END;

VV[I]:= 0;

STRESSI[N]:= -GAMMAVR[N]*253*R+MOMINTI[N]*DZ+PI[N]*(NUI[N]-NUI[N-1]);
FOR I:=N-1 DOWNT0 1 DO
BEGIN
    STRESSI[I]:= (STRESSI[I+1]+(BF*ROI[I]+MOMINTI[I])*DZ+PI[I]*(NUI[I+1]-NUI[I]));
END;

FOR I:=1 TO N DO
BEGIN
    E[I]:= (STRESSI[I]/ROI[I]-PSII1[I]-PSII7[I]*(TEMPI[I]-TEMPR)-PSII10[I]
        *(ROI[I]-ROIR[I]))/(PSII5[I]+2*PSII6[I]);
    TRCE[I]:= (E[I]-EPRE[I])/DT;
    STRESSS[I]:= STRESSI[I]+STRESSV[I]+(ROV[I]*SQR(VV[I]))*
        (1-(ROV[I]/(ROV[I]+ROI[I])));
END;

FOR I:=2 TO N-1 DO
BEGIN
    LV[I]:= (VV[I+1]-VV[I-1])/(2*DZ);
END;
LV[1]:= (VV[2]-VV[1])/DZ;
LV[N]:= (VV[N]-VV[N-1])/DZ;
END;

BEGIN (MAIN PROGRAM)

    RESET(INCOEF, '-#12-EACDEF.TEXT');
    REWRITE(OUTFILE, '-#12-EAOUT.TEXT');
    Rewrite(OutfileI, '-#12-(T19871)Ice.TEXT');

```

```

Rewrite(OutfileV,'-#12-(T19881)Vapor.TEXT');
Rewrite(OutfileS,'-#12-(T19891)Snow.TEXT');
Rewrite(OutfileX,'-#12-(T19901)XTRA.TEXT');
READLN(INCOEF,OUTINTV);
READLN(INCOEF,DTH);READLN(INCOEF,DZ);READLN(INCOEF,TOTLTIME);READLN(INCOEF,GAMMAI);
READLN(INCOEF,ENTROPVR);READLN(INCOEF,ENTROPIR);
READLN(INCOEF,R);READLN(INCOEF,TEMPR);READLN(INCOEF,POISSON);
READLN(INCOEF,THERMEXP);READLN(INCOEF,SPHTV);READLN(INCOEF,SPHTI);
READLN(INCOEF,KIR);READLN(INCOEF,KVR);
READLN(INCOEF,MASINSCALE);READLN(INCOEF,ENERINTR);
READLN(INCOEF,BF);READLN(INCOEF,K);READLN(INCOEF,VISC);READLN(INCOEF,PERMEAB);
READLN(INCOEF,SIGMA);READLN(INCOEF,PIR);READLN(INCOEF,L);

FOR I:=1 TO N DO
  READLN(INCOEF,NUI[I],RADIUS[I],BND[I],TEMPI[I],TEMPV[I]);

INITIAL;(CALL PROCEDURE)

DT:=DTH*60;
TIME:=0;(TIMESTEP)
IK:= 0;
CK:= OUTINTV;
WHILE TIME < TOTLTIME DO
  BEGIN
    INTERACT;(CALL PROCEDURE)
    BALANCE;(CALL PROCEDURE)
    UPDATE;(CALL PROCEDURE)
    TIME:=TIME+DTH;

    IK:= IK + 1;
    IF IK = CK THEN
      BEGIN
        CK:= CK + OUTINTV;

```

```

WRITELN(OUTFILE,'-----TIME = ',TIME,' MIN');

HEIGHT:=0;
FOR I:=1 TO N DO
BEGIN
  WriteLn(OutfileI,Height,ROI[I],Temp[I],TGI[I],TRCNUI[I],
    STRESSI[I],EI[I]);
  WriteLn(OutfileV,Height,ROV[I],TEMPV[I],TGV[I],TRCROV[I],STRESSV[I],
    VVI[I]);
  WriteLn(OutfileS,Height,ROSI[I],STRESSSI[I],MASINTI[I],MOMINTI[I],
    ENERINTI[I],EQFR1[I]);
  WriteLn(OutfileX,Height,PI[I],EQFRINI[I],EQFRINV[I],MUI[I],
    MUV[I],GAMMAV[I]);

  HEIGHT:=HEIGHT+DZ;
END;
END;
CLOSE(INCOEF,LOCK);
CLOSE(OUTFILE,LOCK);
Close(outfileI,lock);
Close(outfileV,lock);
Close(outfileS,lock);
Close(outfileX,lock);

END.

```

Figure 41. Sample input file used in conjunction with EASNOMIX.

7200	OUTINTV [TO INCREMENT OUTPUT]
1	DTH (MINUTES)
0.05	DZ (METER)
7200	TOTLTIME (MINUTES)
917	GAMMAI (ICE DENSITY)
6.867E3	ENTROPVR (REFERENCE ENTROPY VAPOR)
2.306E3	ENTROPIR (REFERENCE ENTROPY VAPOR)
287	R (GAS CONSTANT)
273	TEMPR (REFERENCE TEMPERATURE)
2E-1	POISSON (POISSON'S RATIO)
50E-6	THERMEXP (THERMAL EXPANSION OF ICE)
2065	SPHTV (SPECIFIC HEAT OF VAPOR)
2065	SPHTI (SPECIFIC HEAT IF ICE "CHOSEN AS FOR VAPOR SEE TEXT")
2.2	KIR (THERMAL CONDUCTIVITY ICE)
0.0026	KVR (THERMAL CONDUCTIVITY ICE)
1E-12	MASINSCL (COEFFICIENT FOR MASS INTERACTION)
10	ENERINTR (COEFFICIENT FOR ENERGY INTERACTION)
-9.81	BF (BODY FORCE, GRACITY)
1E-6	K (COEFFICIENT FOR EQUILIBRATED FORCE INTERACTION)
1.3E-5	VISC KINOMATIC (KINEMATIC VISCOSITY)
1E-8	PERMEA (PERMEABILITY)
109E-3	SIGMA (INTERFACE ENERGY)
600	PIR (REFERENCE PRESSURE)
2.831E6	L (LATENT HEAT OF SUBLIMATION)

0.3 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.4 0.005 1.0 273.0 273.0
0.4 0.005 1.0 273.0 273.0
0.4 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.2 0.005 1.0 273.0 273.0
0.2 0.005 1.0 273.0 273.0
0.2 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.3 0.005 1.0 273.0 273.0
0.3 0.005 1.0 253.0 253.0

(INITIAL INPUT VALUES FOR ICE VOLUME FRACTION,
GRAIN RADIUS, BOND VALUE, ICE TEMPERATURE,
VAPOR TEMPERATURE)

(ALL VALUES IN SI UNITS - MKS)

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