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PROBLEMS

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Das Standardwerk der Wetterkunde

Gösta H. Liljequist und Konrad Cehak

Allgemeine Meteorologie


Die internationalen Forschungen der letzten Jahre, vor allem mittels Satelliten, haben unsere Kenntnis über Abläufe in der höheren Atmosphäre sprunghartig erweitert. Die Auswertung der Ergebnisse lassen nun exaktere Prognosen oder doch wenigstens fundiertere Theorien über das großräumige Wetterscheinen zu.

Gösta L. Liljequist vom Meteorologischen Institut der Universität Uppsala und Konrad Cehak vom Meteorologischen Institut der Universität Wien, beide in der Forschung wie in der Lehre engagierte Wissenschaftler, tragen dieser Wissensverweiterung Rechnung.
Transport Equations for Heat and Moisture in the Soil and their Application to Boundary Layer Problems

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Abstract:
The methods of irreversible thermodynamics are used to obtain a consistent set of transport equations for heat and moisture in the soil. Microscopic arguments verify the results. It is found that the empirical diffusion laws for moisture are in harmony with the requirements of the linear Onsager theory. On the other hand, the heat flux parameterization of previous papers seems to be somewhat incomplete.
The new set of prognostic equations is subjected to thermodynamic filtering and is then coupled to a model of the atmospheric boundary layer. Extensive calculations are carried out to determine the influence of soil type and moisture on the atmospheric variables of state.

Zusammenfassung: Die Transportgleichungen für Wärme und Feuchte im Erdboden und deren Anwendung auf atmosphärische Grenzschichtprobleme

Résumé: Equations de transfert de chaleur et d’humidité dans le sol et leur application à des problèmes relatifs à la couche limite atmosphérique.
On utilise les méthodes de la thermodynamique irréversible pour obtenir un système cohérent d’équations de transfert de chaleur et d’humidité dans le sol. Des arguments microscopiques appuient les résultats. On trouve que les lois empiriques de diffusion pour l’humidité sont en harmonie avec les exigences de la théorie linéaire d’Onsager. Par ailleurs, la paramétrisation du flux de chaleur adoptée dans des travaux précédents ne semble pas complète.
Le nouveau système d’équations pronostiques est soumis à un filtrage thermodynamique et est alors couplé à un modèle de la couche limite atmosphérique. Des calculs numériques détaillés sont effectués pour déterminer l’influence du type de sol et de l’humidité du sol sur les variables d’état atmosphériques.

1 Introduction

Numerical models of the atmospheric boundary layer require realistic boundary statements for heat- and mass fluxes at the interface earth-atmosphere. Most of the former models restrict their analysis to empirical formulas to state the soil moisture boundary condition. Often this is accomplished by
prescribing the soil moisture at the interface or by specifying the BOWEN ratio. Still other models prefer empirical evaporation formulas of the PENMAN type.

For various meteorological problems this empirical approach is not satisfactory. Particularly, the modeling of such phenomena as radiation fog and moist convection requires a more detailed treatment of evaporation at the interface which critically determines the temperature at the soil surface and the air layer near the ground.

To determine the influence of soil type and moisture upon atmospheric variables of state, a detailed knowledge of soil temperature and moisture distribution is necessary. For this reason, it is mandatory to formulate prognostic equations for soil state variables. The main purpose of this paper is to present a thermodynamic treatment of the soil based on the arguments of the linear ONSAGER theory (LOT) of irreversible processes.

A fundamental model of transport processes in the soil was developed by PHILIP and De VRIES (1957) which formed the basis of various investigations due to PHILIP (1957), SASAMORI (1970), ZDUNKOWSKI et al. (1975) and others. However, the original model of PHILIP and De VRIES (1957) was incomplete in various ways, particularly the heat equation was insufficient. In a more advanced version De VRIES (1958) included the heat transport associated with the diffusion of water vapor.

In Chapter 2 of the present paper the pertinent prognostic equations and flux parameterizations are re-derived from the view point of irreversible thermodynamics and on the basis of a more complete energy budget. A comparison with the investigations carried out by De VRIES reveals a discrepancy in the formulation of the heat flux. For this reason, results obtained from irreversible thermodynamics are confirmed using independent microscopic arguments. For application purposes the prognostic equations for soil temperature and moisture are subjected to thermodynamical filtering.

In Chapter 3 the boundary layer equations of the atmosphere are briefly introduced and coupled to the soil system using proper continuity conditions. Model results for temperature, moisture and wind are presented for two bare soils and two geostrophic wind speeds to demonstrate the applicability of the method. Finally, the results are compared with data derived from a simplified soil model.

2 Theory of the soil system

2.1 Basic notation, the moisture potential

Before proceeding with the discussion, some notation will be introduced. The soil system treated here consists of four components: dry air, water vapor, liquid water and the soil matrix. Various quantities appearing in connection with these components will be designated with the subscript or superscript $k$ as listed next.

$k = 0$ dry air 
$k = 1$ water vapor 
$k = 2$ liquid water 
$k = 3$ soil matrix

$R_k$, gas constant; $k = 0,1$

$M_k$, $M$ partial mass, total mass with $M = \sum_{k=0}^{3} M_k$

$V_{k}, V_{air}$ volume occupied by component $k$ resp. by moist air with $V_0 = V_1 = V_{air}$

$V_{1c}$ volume taken up by water vapor if it condenses completely

$V$ total volume with $V = V_{air} + V_2 + V_3$

$w_k$ velocity of component $k$ averaged over the occupied volume

$\pi$ porosity of the soil with $\pi = (V - V_3)/V$

$p_0^0, p_1^1$ partial pressure of dry air and of water vapor, total pressure with $p = p_0^0 + p_1^1$

$p_2^{21}, p_3^{21}$ saturation pressure with respect to a flat surface, saturation vapor pressure within the soil.
Among other things, the soil is characterized by the following measures and fluxes

\[ \rho^k = \frac{M^k}{V} \quad \text{partial density of component } k \text{ with respect to total volume} \]  
\[ \rho_k = \frac{M^k}{V_k} \quad \text{partial density with respect to occupied volume} \]  
\[ m^k = \frac{M^k}{M} \quad \text{mass concentration} \]  
\[ p^k = \rho_k R_k T \quad \text{gas equation; } k = 0, 1 \]  
\[ \eta^2 = \frac{V_2}{V} \quad \text{volumetric liquid water content} \]  
\[ \eta^1 = \frac{V_1 c}{V} = \frac{\rho^1}{\rho_2} = \frac{\pi - \eta^2}{\rho_2} \cdot \frac{p^1}{R_1 T} \]  
\[ I^k \quad \text{phase transition flux per unit volume and time; } \]  
\[ I^0 = I^3 = 0, \quad I^1 + I^2 = 0 \]  
\[ \mathcal{J}^k = \rho^k (\omega_k - w_3) = \rho^k v_k \quad \text{diffusion flux referred to the velocity } \omega_3 = 0; \quad k = 0, 1, 2, 3. \]  

In order to give a thermodynamical treatment of soil water EDLEFSEN and ANDERSON (1943) used the concept of the soil moisture potential \( \psi \) which is an essential quantity in the following analysis. Due to the existence of a large surface/volume ratio within the soil, Van der WAALS forces (adsorption, surface tension) are not negligible so that the chemical potential \( \mu_2 \) of the soil water differs significantly from that of free water \( \tilde{\mu}_2 \). The soil moisture potential \( \psi \) is related to \( \mu_2, \tilde{\mu}_2 \) by

\[ \mu_2 = \tilde{\mu}_2 + \psi. \]  

In a microscopic picture \( \psi \) originates from the potential of forces holding the liquid water within the soil and causing a depression of the saturation vapor pressure as compared to bulk water with a flat surface. Since the soil water is in a lower energy state than the free water, \( \psi \) is always a negative quantity. The behavior of \( \psi \) versus the volumetric water content \( \eta^2 \) will be described lateron.

### 2.2 Prognostic equations

The transport processes in the soil are governed by continuity equations of its four mass components and by the heat equation. Solution effects are not taken into account.

In the reference system in which the soil matrix is at rest, the continuity equations are given by

\[ \frac{\partial \rho^0}{\partial t} + \nabla \cdot \mathcal{J}^0 = 0 \]  
\[ \frac{\partial \rho^1}{\partial t} + \nabla \cdot \mathcal{J}^1 = \rho_2 \frac{\partial \eta^1}{\partial t} + \nabla \cdot \mathcal{J}^1 = I^1 \]  
\[ \frac{\partial \rho^2}{\partial t} + \nabla \cdot \mathcal{J}^2 = \rho_2 \frac{\partial \eta^2}{\partial t} + \nabla \cdot \mathcal{J}^2 = I^2 \]  
\[ \frac{\partial \rho^3}{\partial t} = 0 \]  

with

\[ \rho^1 = \eta^1 \rho_2 \quad \text{and} \quad \rho^2 = \eta^2 \rho_2. \]
Here and in the following derivations the liquid water is considered incompressible. The quantities \( I^1 \), \( I^2 \), (\( I^1 = -I^2 \)) are the phase transition rates of water per unit volume and time. The diffusion fluxes refer to the velocity \( w_3 = 0 \), i.e. \( \mathbf{J}^k = \rho^k w_k \). All quantities are considered macroscopic averages over a large number of pores.

An appropriate and sufficient starting point for the derivation of the heat equation is the budget equation for the total energy per unit mass \( E \), given by

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot \mathbf{J}^E = 0
\]  

(8)

where \( \mathbf{J}^E \) is the flux density of the total energy again referred to the velocity \( w_3 = 0 \). The quantity \( E \) is the macroscopic average of the internal energies of the soil components plus the free surface energy of the water film, the energy due to the Van der Waals forces acting between the liquid and the soil matrix and the potential energy \( \Phi \) of gravitation. The kinetic energy of diffusion is neglected.

Introducing a macroscopic internal energy \( e \) and enthalpy \( h \) by the definitions

\[
e = E - \Phi
\]

(9)

\[
h = e + p/\rho
\]

(10)

equation (8) transforms to

\[
\frac{\partial}{\partial t} (\rho h) + \nabla \cdot \mathbf{J}^q = \frac{\partial p}{\partial t} - \sum_{k=0}^{2} \mathbf{J}^k \cdot \nabla \Phi
\]

(11)

where use has been made of \( \partial \Phi/\partial t = 0 \) and of the continuity equation

\[
\frac{\partial \rho}{\partial t} + \sum_{k=0}^{2} \nabla \cdot \mathbf{J}^k = 0
\]

(12)

(sum of Equations 3 to 6). The flux \( \mathbf{J}^q \) defined by

\[
\mathbf{J}^q = \mathbf{J}^E - \Phi \sum_{k=0}^{2} \mathbf{J}^k
\]

(13)

is interpreted as macroscopic heat flux. Note that the sum of diffusion fluxes does not vanish since these are not referred to the center of mass velocity.

To carry on the analysis, the enthalpy \( h \) will be partitioned as

\[
\rho h = \sum_{k=0,1,3} \rho^k h_k + \rho^2 \bar{h}_2 - \rho_2 \int_0^{\eta_2} W(T,\bar{\eta}^2) d\eta^2
\]

(14)

with \( \bar{h}_2 \) referring to free bulk water and \( W \) the differential of wetting. The integral appears since each sublayer of the water film surrounding soil particles is characterized by a different \( W \). The differential of wetting and the moisture potential \( \psi \) are related by

\[
W = -\psi + T \frac{\partial \psi}{\partial T}
\]

(15)
as follows from the definition
\[ h_2 = h_2 - W \]  
and the thermodynamic identity
\[ h_2 = \mu_2 - T \frac{\partial \mu_2}{\partial T} \]  
if use is made also of Equation (2).

Formula (14) is differentiated with respect to time. The result is
\[ \frac{\partial}{\partial t} \rho \phi = \sum_{k=0,1,3} \rho^k \frac{\partial h_k}{\partial t} + \rho^2 \frac{\partial h_2}{\partial t} - h_0 \nabla \cdot \mathbf{J}^0 - h_1 \left( \nabla \cdot \mathbf{J}^1 + I^2 \right) \]
\[ -h_2 \left( \nabla \cdot \mathbf{J}^2 - I^2 \right) - \rho_2 W(T, \mathbf{\eta}^2) \frac{\partial \eta^2}{\partial t} - \rho_2 \frac{\partial}{\partial T} \left( \int_0^{\eta^2} W(T, \mathbf{\eta}^2) d\mathbf{\eta}^2 \right) \frac{\partial T}{\partial t} \]  
where use was made of Equations (3) to (6). Substituting (18) into (11) and expanding \( h_k (p, T) \) results in the following prognostic equation,
\[ c \frac{\partial T}{\partial t} - \rho_2 W(T, \mathbf{\eta}^2) \frac{\partial \eta^2}{\partial t} + \nabla \cdot (\mathbf{J}^q - \sum_{k=0,1} h_k \mathbf{J}^k - h_2 \mathbf{J}^2) = \]
\[ \frac{\partial p}{\partial t} \left( 1 - \sum_{k=0,1,3} \rho^k \frac{\partial h_k}{\partial p} - \rho^2 \frac{\partial h_2}{\partial p} \right) - I^2 (h_2 - h_1) - \sum_{k=0,1} \mathbf{J}^k \cdot \nabla (h_k + \Phi) - \mathbf{J}^2 \cdot \nabla (h_2 + \Phi) \]  
where
\[ c = \sum_{k=0,1,3} \rho^k \frac{\partial h_k}{\partial T} + \rho^2 \frac{\partial h_2}{\partial T} - \rho_2 \frac{\partial}{\partial T} \left( \int_0^{\eta^2} W(T, \mathbf{\eta}^2) d\mathbf{\eta}^2 \right) \]  
is the heat capacity of the soil system.

Equation (19) reduces to the heat equation given by De Vries (1958, Equation 15) if the terms containing \( \mathbf{J}^0, \partial p/\partial t, \nabla \Phi \) are neglected. In the next sections a parameterization for the heat flux \( \mathbf{J}^q \) will be derived using arguments of the linear ONSAGER theory (LOT) of irreversible transport processes. Compared with the heat flux equation introduced by De Vries there appears an additional term. For this reason, the result of LOT is validated by microscopic arguments. Finally, Equation (19), using Formulas (5) and (14), can be transformed into the more suitable form of the prognostic temperature equation,
\[ c \frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{J}^q - \sum_{k=0} h_k \mathbf{J}^k) = \frac{\partial p}{\partial t} \left( 1 - \sum_{k=0} \rho^k \frac{\partial h_k}{\partial p} \right) \]
\[ - I^2 (h_2 - h_1) - \sum_{k=0} \mathbf{J}^k \cdot \nabla (h_k + \Phi). \]
2.3 Entropy production, heat flux

2.3.1 The effective system

The aim of the following sections is the derivation of the heat flux parameterization from basic principles of the linear ONSAGER theory of irreversible transport processes. However, a direct use of the pertinent LOT equations is not possible since these are derived for multi-component systems without velocity constraints. The soil system, however, is governed by $ω = 0$ instead of an equation of motion. Furthermore, within the framework of LOT, diffusion and heat fluxes refer to the center of mass velocity $\mathbf{w} = \Sigma \rho^k \mathbf{w}_k / \rho$ while $\mathbf{j}^k$, $\mathbf{j}^q$ of Equations (3) to (5) and (11) pertain to $ω = 0$.

Nevertheless, the formulas of LOT are applicable to the soil system by introducing a certain artifice. As will be shown, the soil system is physically equivalent to a fictitious multi-component system without a velocity constraint. This system will be referred to as the effective system, and its variables will be designated by a superscript tilde. They must be introduced in such a way that $ω = 0$ is satisfied automatically.

The governing equations of the effective system are assumed to be given by

$$\frac{\partial}{\partial t} \tilde{\rho}^k + \nabla \cdot \tilde{\rho} \tilde{\mathbf{v}}^k + \nabla \cdot \tilde{\mathbf{j}}^k = \tilde{\Gamma}^k, k = 0, 1, 2, 3$$

(22)

$$\frac{\partial}{\partial t} \tilde{\rho} + \nabla \cdot \tilde{\rho} \tilde{\mathbf{v}} + \nabla \cdot \tilde{\mathbf{j}}^q = \frac{\partial \tilde{\rho}}{\partial t} + \tilde{\rho} \cdot \frac{\partial \tilde{\mathbf{v}}}{\partial t} + \tilde{\mathbf{v}} \cdot \tilde{\mathbf{j}}^q - \sum_{k=0}^{3} \tilde{\mathbf{j}}^k \cdot \tilde{\mathbf{F}}^k.$$  

(23)

They must be compatible with the governing Equations (3) to (6) and (11) of the original system. $\tilde{\mathbf{v}}$ is the effective center of mass velocity, $\tilde{\mathbf{F}}$ the viscous stress tensor, and $\tilde{\mathbf{F}}^k$ external forces. The diffusion and heat fluxes $\tilde{\mathbf{j}}^k$, $\tilde{\mathbf{j}}^q$ refer to $\tilde{\mathbf{v}}$. The validity of basic thermodynamic relations such as $\tilde{h} = \hat{h} + \tilde{\rho} \tilde{\mathbf{v}}$, $\tilde{\mu} = \hat{\mu} - \tilde{\rho} \tilde{\mathbf{v}}$, $\tilde{\rho} \tilde{\mathbf{h}} = \Sigma \tilde{\rho}^k \tilde{\mathbf{h}}_k$ etc., of course, must be retained.

How to proceed is indicated by the requirement that the force equation $F^k_x = \rho^3 \tilde{\mathbf{a}}_3$ should be valid where $F^k_x$ is the force per unit volume and $\mathbf{a}_3$ the acceleration. Since $F^k_x$ does not produce any acceleration, the soil matrix behaves effectively as if its density were infinitely large. By the definition

$$\tilde{\rho}^3 = \lim_{\rho \to \infty} \rho^3$$

(24)

it is achieved that $\omega$ vanishes always if it vanishes initially, i.e. the constraint $\omega = 0$ is satisfied automatically. The additional definitions

$$\tilde{\rho}^k = \rho^k; k = 0, 1, 2$$

(25)

$$\tilde{\rho} = \sum_{k=0}^{3} \tilde{\rho}^k$$

(26)

assure that together with vanishing $\omega$ also the center of mass velocity $\tilde{\mathbf{w}}$ vanishes, i.e.

$$\tilde{\omega} = \sum_{k=0}^{3} \tilde{\rho}^k \mathbf{w}_k / \tilde{\rho} = \omega = 0.$$  

(27)

The definition of variables is completed by

$$\tilde{\mathbf{p}} = \mathbf{p}; \quad \tilde{T} = T$$

$$\tilde{\rho} \tilde{\mathbf{X}} = \rho \mathbf{X}; \quad \tilde{\rho}^k \tilde{\mathbf{X}}_k = \rho^k \mathbf{X}_k$$

(28)

(29)

where $X$, $X_k$ are quantities per unit mass, e.g. total and partial internal energies $e$, $e_k$ enthalpies $h$, $h_k$, and others. It is easily seen that (24) to (29) retain the validity of basic thermodynamic relations. Finally, one has to show that the governing Equations (22) and (23) are compatible with (3) to (6) and (11). Using $\dot{w} = 0$ one finds that the following identifications are required

$$
\begin{align*}
\tilde{T}^k &= J^k \text{ for } k = 0, 1, 2; \quad \tilde{T}^3 &= -\sum_{k=0}^{2} J^k \\
\tilde{T}^0 &= \tilde{T}^3 = 0; \quad \tilde{T}^1 = 1^1; \quad \tilde{T}^2 = 1^2 = -1^1 \\
\tilde{F}^q &= J^q \\
\tilde{F}_k &= -\nabla \Phi = \psi \text{ for } k = 0, 1, 2; \quad \tilde{F}^3 = 0.
\end{align*}
$$

The stress tensor $\tilde{\mathbf{D}}$ remains underdetermined; this quantity, however, is not needed in the subsequent analysis. With this remark the equivalence proof is complete.

### 2.3.2 Entropy production rate

The entropy production rate $\sigma$ in a multi-component system with external forces as formulated, for example, by De Groot and Mazur (1962) is given by

$$
\sigma = -\frac{T}{\mu_k J^k} - \frac{T}{\mathbf{q}} \cdot \nabla \nabla T - \sum_{k=0}^{2} J^k \cdot (\nabla \mu_k - \mathbf{F}_k) - \mathbf{F} : \nabla \omega \geq 0
$$

with

$$
\begin{align*}
\mathbf{q}^q &= J^q - \sum_{k} h_k J^k; \quad \nabla \mu_k &= \frac{\partial \mu_k}{\partial T} \rho, m_k \nabla T.
\end{align*}
$$

Using the definitions and identifications associated with the effective system, the entropy production rate in this system assumes the simpler form

$$
\tilde{T}\tilde{\sigma} = 1^1(\mu_2 - \mu_1) - \frac{T}{\mathbf{q}} \cdot \nabla \nabla T - \sum_{k=0}^{2} J^k \cdot (\nabla \mu_k + \nabla \Phi) \geq 0.
$$

This equation provides the basis for the formulation of the phenomenological laws. In general, each thermodynamic “flux” $(1^1, J^k, \mathbf{q}^q)$ is a linear function of each thermodynamic “force” $(\mu_2 - \mu_1, \nabla T/T, \nabla \mu_k + \nabla \Phi)$.

If the soil matrix is assumed to be isotropic, the following two inequalities must hold independently

$$
\begin{align*}
1^1(\mu_2 - \mu_1) &\geq 0 \\
- \{J^q \cdot \nabla \frac{T}{T} + \sum_{k=0}^{2} \tilde{J}^k \cdot (\nabla \mu_k + \nabla \Phi)} &\geq 0.
\end{align*}
$$

(according to the CURIE theorem).

Thus the phenomenological laws simplify to

$$
1^1 = L_1(\mu_2 - \mu_1)
$$

with $L_1 \geq 0$

$$J^q_k = - L_{qq} \frac{\nabla T}{T} - \sum_{k=0}^{2} L_{kk}(\nabla T \mu_k + \nabla \Phi)$$  \hspace{1cm} (36)$$

$$J^k = - L_{kk} \frac{\nabla T}{T} - \sum_{l=0}^{2} L_{kl}(\nabla T \mu_l + \nabla \Phi); \hspace{0.5cm} k = 0, 1, 2$$  \hspace{1cm} (37).$$

where the $L_1, L_{qq}, L_{kk}, L_{kl}, L_{kl}$ are the so-called phenomenological coefficients. These coefficients with exception of $L_1$ will be determined from comparison with the flux equations that may be formulated on the basis of observational evidence (NAKANO and MIYASAKI, 1979; HILLEL and Van BAVEL, 1976). The coefficient $L_1$ is not needed since the phase flux $I^1$ lateron will be eliminated by chemical filtering.

### 2.4 Empirical laws

The diffusion of the gaseous components may be viewed as the superposition of two different processes, flow of the moist air as a whole relative to the soil and diffusion of water vapor with respect to the dry air.

I. Flow of the moist air with respect to the soil

This flow may be viewed as a diffusion flux, parameterized as

$$J^0 + J^1 = - \frac{D^{\text{air}}}{R_0 T} \{ \nabla p - (\rho_0 + \rho_1) g \} \hspace{1cm} (38)$$

were $D^{\text{air}}$ is a diffusion coefficient pertaining to the flow of moist air relative to the soil matrix. The denominator $R_0 T$ is introduced for dimensional reasoning. The quantity $D^{\text{air}}$, usually not available, depends mainly on the structure of the soil matrix and on $\eta^2$. It should be measured by applying a horizontal pressure gradient to a test volume of the soil. Using the identity

$$\nabla p = \rho_0 \nabla T \mu_0 + \rho_1 \nabla T \mu_1$$  \hspace{1cm} (39)$$
valid for a mixture of ideal gases (proof of (39) is given in the Appendix), Equation (38) may be written in the alternative form

$$J^0 + J^1 = - \frac{D^{\text{air}}}{R_0 T} \{ \rho_0 (\nabla T \mu_0 - g) + \rho_1 (\nabla T \mu_1 - g) \} \hspace{1cm} (40)$$

which is more suitable for comparison with Equation (37).

II. Diffusion of water vapor with respect to dry air

This process is usually parameterized as

$$\dot{J}^1 = - \frac{D^{\text{vap}}}{R_1 T} \nabla p^1 \hspace{1cm} (41)$$

where $\dot{J}^1$ is defined with respect to the center of mass velocity $w_{\text{air}}$ of the moist air, i.e.

$$\dot{J}^1 = \rho^1 (w^1 - w_{\text{air}}) \hspace{1cm} (42)$$

with

$$w_{\text{air}} = \frac{J^0 + J^1}{\rho^0 + \rho^1}.$$  \hspace{1cm} (43)
$D^{\text{vap}}$ is the diffusion coefficient of water vapor with respect to dry air within the soil pores. It is related to the coefficient $D^{\text{vap}}_{\text{bulk}}$ for the bulk diffusion of water vapor in air by means of $D^{\text{vap}} = \alpha (\pi - \eta^2) D^{\text{vap}}_{\text{bulk}}$. Thereby $\alpha$ is a correction factor due to the tortosity of the diffusion path and $\pi - \eta^2 = \frac{w_{\text{sff}}}{\bar{w}}$ is a volume correction. Equation (41) may be considered as a limiting case valid for $\rho_1 / \rho_0 \to 0$ of the more general diffusion law

$$\mathbf{j}^1 = -\frac{D^{\text{vap}}}{R_1 T} \cdot \frac{\rho_0 \rho_1}{\rho_0 + \rho_1} \nabla_I (\mu_1 - \mu_0)$$

(44)

as is obvious from consideration of the thermodynamic identity

$$\frac{\rho_0 \rho_1}{\rho_0 + \rho_1} \nabla_I (\mu_1 - \mu_0) = \nabla_P \cdot \frac{\rho_1}{\rho_0 + \rho_1} \nabla_P$$

(45)

valid for a mixture of ideal gases. Returning to the soil matrix system by means of the definition (43) one obtains from Equation (42)

$$\mathbf{j}^1 = \mathbf{j}^1 + \frac{\rho_1}{\rho_0 + \rho_1} \left( \mathbf{j}^0 + \mathbf{j}^1 \right) = \mathbf{j}^1 + \frac{\rho_1}{\rho_0 + \rho_1} \left( \mathbf{j}^0 + \mathbf{j}^1 \right).$$

(46)

Solving (40), (44) and (46) for $\mathbf{j}^0$ and $\mathbf{j}^1$ yields the results

$$\mathbf{j}^0 = -\frac{D^{\text{air}}}{R_0 T} \cdot \frac{\rho_0}{\rho_0 + \rho_1} \left[ \rho_0 \left( \nabla_I \mu_0 - \mathbf{g} \right) + \rho_1 \left( \nabla_I \mu_1 - \mathbf{g} \right) \right]$$

$$+ \frac{D^{\text{vap}}}{R_1 T} \cdot \frac{\rho_0 \rho_1}{\rho_0 + \rho_1} \left( \left( \nabla_I \mu_1 - \mathbf{g} \right) - \left( \nabla_I \mu_0 - \mathbf{g} \right) \right)$$

(47)

$$\mathbf{j}^1 = -\frac{D^{\text{air}}}{R_0 T} \cdot \frac{\rho_1}{\rho_0 + \rho_1} \left[ \rho_0 \left( \nabla_I \mu_0 - \mathbf{g} \right) + \rho_1 \left( \nabla_I \mu_1 - \mathbf{g} \right) \right]$$

$$- \frac{D^{\text{vap}}}{R_1 T} \cdot \frac{\rho_0 \rho_1}{\rho_0 + \rho_1} \left( \left( \nabla_I \mu_1 - \mathbf{g} \right) - \left( \nabla_I \mu_0 - \mathbf{g} \right) \right).$$

(48)

With respect to the diffusion of liquid water observational evidence indicates that the flux $\mathbf{j}^2$ obeys Darcy's law,

$$\mathbf{j}^2 = -\frac{K \rho_2}{g} \nabla (\psi + \phi + p / \rho_2)$$

(49)

where the empirical coefficient $K$, having the dimension of a velocity, is known as the (unsaturated) hydraulic conductivity and $g = |\mathbf{g}|$. For comparison with Equation (37), Formula (49) may be written in the equivalent forms

$$\mathbf{j}^2 = -\frac{K \rho_2}{g} \left( \nabla_I \mu_2 + \nabla \psi - \mathbf{g} \right) = -\frac{K \rho_2}{g} \left( \nabla_I \mu_2 + T \frac{\partial \psi}{\partial T} \frac{\nabla T}{T} - \mathbf{g} \right).$$

(50)

Comparison of (47), (48) and (50) with the general Equation (37) yields the following relations, listed in Table 1, between the phenomenological coefficients $L_{\alpha \beta}$ and the empirical coefficients $D^{\text{air}}, D^{\text{vap}}$ and $K$. An inspection shows that the Onsager symmetry requirements $L_{ik} = L_{ki}$ are satisfied for $i, k = 0, 1, 2$. Furthermore, the inequalities $L_{ii} > 0$ and $L_{ii} L_{kk} - L_{ik}^2 \geqslant 0$ hold if $D^{\text{air}}, D^{\text{vap}}$ and $K$ are positive quantities.
The as yet undetermined coefficients \( L_{q0}, L_{q1} \) and \( L_{q2} \) of the heat flux Equation (36) are specified in such a way that the reciprocity relations \( L_{qk} = L_{kq} \) are satisfied. The resulting form of the heat flux equation is

\[
\mathbf{q}^q = -\frac{L_{qq}}{T} \nabla T - \frac{K\rho_2}{g} T \frac{\partial \psi}{\partial T} (\nabla T \mu_2 - \mathbf{g}) \text{ with } L_{qq} > 0
\]  

(51)
i.e. there should exist a cross effect of the LUDWIG-SORET type. For the total heat flux one obtains from (51) (compare with (15), (16) and (31))

\[
\mathbf{q} = \mathbf{q}^q + \sum_{k=0}^{2} h_k \mathbf{q}^k = -\frac{L^*_q}{T} \nabla T + h_0 \mathbf{q}^0 + h_1 \mathbf{q}^1 + (h_2 + \psi) \mathbf{q}^2
\]

(52)

where

\[
L^*_q = L_{qq} - \frac{K\rho_2}{g} (T \frac{\partial \psi}{\partial T})^2 > 0.
\]  

(53)

A comparison with the heat flux parameterization of De VRIES (1958) shows that in (52) there appears the flux \((h_2 + \psi) \mathbf{q}^2\) instead of \((h_2 - W) \mathbf{q}^2\). i.e. according to (15) an additional term \(-T \partial \psi / \partial T \mathbf{q}^2\).

### 2.5 Microscopic interpretation of the moisture potential

From a microscopic point of view the wetting energy \( W \) is a consequence of attractive Van der WAALS forces \( \mathbf{F}_{vdW} \) acting between the soil matrix and the liquid water film. In a microscopic picture of the soil system these forces may be taken into account as external forces acting on the liquid film. Thereby it is assumed that the direct influence of \( \mathbf{F}_{vdW} \) is restricted to the film so that the microscopic pressure differs from the macroscopic value \( p \) only within the film. Furthermore, the assumption is made that \( \mathbf{F}_{vdW} \) can be derived from a potential \( \Phi_{vdW} \), i.e.

\[
\mathbf{F}_{vdW} = - \nabla \Phi_{vdW}.
\]

(54)

Assuming local chemical equilibrium between the water phases one may write

\[
\mu_2 (p_2^m, T) + \Phi_{vdW} = \mu_1 (p, T)
\]

(55)
where \( p^m_2 \) is the strongly position dependent microscopic pressure within the film, and \( \tilde{\mu}_2 \) is the chemical potential of bulk water. In the following derivation the identity

\[
\tilde{\mu}_2(p^*, T) = \tilde{\mu}_2(T) + p^*/\rho_2
\]

is used which is valid under the assumption of incompressibility. \( \tilde{\mu}_2 \) is the temperature dependent part of \( \mu_2 \). The quantity \( p^* \) is an arbitrary pressure. Specifying \( p^* = p \) and \( p^* = p^m_2 \) successively and subtracting results one obtains from (55) and (56)

\[
\tilde{\mu}_2(p, T) + \frac{p^m_2 - p}{\rho_2} + \Phi_{vdW} = \mu_1(p, T).
\]

A comparison of Equations (57) and (2) identifies \( \psi \), i.e.

\[
\psi = \frac{p^m_2 - p}{\rho_2} + \Phi_{vdW}
\]

which is a macroscopic function of the soil even though microscopic properties appear.

Next a microscopic derivation of Darcy's law will be given. The sum of forces \( F_2 \) per unit mass acting on a microscopic element of the liquid film is given by

\[
F_2 = F_{vdW} + \psi \frac{1}{\rho_2} \nabla p^m_2.
\]

The following interpretation seems reasonable. The liquid element remains at rest if \( F_2 \) vanishes. If \( F_2 \neq 0 \) the liquid will be accelerated until equilibrium between \( F_2 \) and viscous forces is reached. Averaging over a sufficient number of pores and assuming that the average viscous forces are proportional to \( -\omega_2 \) one obtains for the final steady state

\[
\mathbf{J}^2 = \nabla(\psi + \Phi + p/\rho_2)
\]

i.e. Darcy's law in its generalized form (49). Use has been made of \( \mathbf{J}^2 = \rho^2 \omega_2 \) and of Equation (58).

So far the entire analysis refers to the normal case that the soil contains air and liquid water. In the special situation that all pores in the soil are completely filled with water, \( \nabla \psi \) is approximately zero so that (48) transforms to the conventional form of Darcy's law. In the latter case other simplifications occur such as \( \eta^1 = 0 \) and \( \mathbf{J}^0, \mathbf{J}^1 = 0 \).

### 2.6 Microscopic interpretation of the heat flux \( \mathbf{J}^q \)

To obtain an expression for the macroscopic heat flux \( \mathbf{J}^q \), one considers a soil volume element \( \Delta V \) whose total energy can be changed by one or more of the following microscopic flux densities \( \Pi_n \) acting on the surface \( \partial \Delta V \) of \( \Delta V \), i.e.

\[
\frac{\partial}{\partial t} \int_{\Delta V} \text{Ed}V = - \int_{\partial \Delta V} \Pi_n \cdot d\mathbf{F}
\]

The microscopic flux densities are

I. Fluxes due to heat conduction in the soil matrix \( \Pi_s^q \), the liquid \( \Pi_l^q \) and the gas \( \Pi_g^q \).

II. Advective fluxes of internal energy, i.e.

\[
\Pi_0^m = \rho_0^m e_0 w_0^m; \quad \Pi_1^m = \rho_1^m e_1 w_1^m; \quad \Pi_2^m = \rho_2^m \hat{e}_2 w_2^m
\]

where the \( w_k^m \) are the actual microscopic velocities within the pores. The quantities \( \rho_k^m \) which vanish for points outside of \( V_k \) are the microscopic densities. \( \hat{e}_2 = \hat{e}_2(T) \) refers to bulk water.
III. Adveective fluxes of the potential energies $\Phi$ and $\Phi_{vdw}$

\[
\Pi_0^\Phi = \rho_0^m \Phi w_0^m; \quad \Pi_1^\Phi = \rho_1^m \Phi w_1^m; \quad \Pi_2^\Phi = \rho_2^m (\Phi - \Phi_{vdw}) w_2^m
\]  

(62)

IV. Energy fluxes due to compression work, i.e.

\[
\Pi^E = \rho^0 w_0^m; \quad \Pi_1^E = \rho^1 w_1^m; \quad \Pi_2^E = \rho^2 w_2^m
\]  

(63)

The kinetic energy of the diffusion fluxes is small and neglected. The average value of the sum of all of these fluxes over a sufficiently large cross-section is the total energy flux $\mathcal{J}^E$. After some arrangement one obtains

\[
\mathcal{J}^E = \mathcal{J}^q + \Phi \sum_{k=0}^2 \mathcal{J}^k + h_0 \mathcal{J}^0 + h_1 \mathcal{J}^1 + h_2 \mathcal{J}^2 + \psi \mathcal{J}^2
\]  

(64)

where

\[
\mathcal{J}^q = \Pi_s^q + \Pi_i^q + \Pi_b^q, \quad \mathcal{J}^k = \rho_k^m \Phi w_k^m \quad \text{and} \quad h_2 = \frac{\dot{e}_2(T)}{r} + \frac{p}{\rho_2}.
\]

Use has been made of Equation (58)

Using the definition (13) one obtains the following expression

\[
\mathcal{J}^q = \mathcal{J}_1^q + h_0 \mathcal{J}^0 + h_1 \mathcal{J}^1 + (h_2 + \psi) \mathcal{J}^2.
\]  

(65)

With the natural assumption that the heat conduction flux $\mathcal{J}^q$ is proportional to $-\nabla T$, (65) is in total agreement with the result (52) derived from LOT.

2.7 The prognostic system under chemical equilibrium

According to the moisture potential concept it is required that the air within the soil is always saturated. From the equilibrium condition $\mu_1 = \mu_2$ one obtains

\[
p^1 = p_2^{21}(T, \eta^2) = p^{21}(T) e^{\psi(T, \eta^2)} / R_1 T
\]  

(66)

e.g. EDLEFSEN and ANDERSON (1943).

As a consequence it follows

\[
\eta^4 = \eta^1(T, \eta^2) = \frac{\pi - \eta^2}{\rho_3 R_1 T} p^{21} \cdot h^* \quad \text{with} \quad h^* = e^{\psi(T, \eta^2)} / R_1 T
\]  

(67)

The phase flux $\mathcal{J}^2$ is eliminated from Equations (5) and (21) with the aid of (4) and (67). This results in the coupled equations

\[
\rho_2(1 + a) \frac{\partial \eta^2}{\partial t} + b \frac{T}{\partial t} = -\nabla \cdot (\mathcal{J}^1 + \mathcal{J}^2)
\]  

(68)

and

\[
(c + l_1 b) \frac{\partial T}{\partial t} + l_1 a \rho_2 \frac{\partial \eta^2}{\partial t} + \nabla \cdot (\mathcal{J}^q + T \frac{\partial \psi}{\partial T} \mathcal{J}^2) + l_21 \nabla \cdot \mathcal{J}^1
\]

\[
= (\pi - \eta^2) \frac{\partial p}{\partial t} - \sum_{k=0}^2 \mathcal{J}^k \cdot \nabla (h_k + \Phi)
\]  

(69)


69
with
\[ l_{21} = h_1 - h_2 = h_1 - \rho_2 + W = \hat{\eta}_{21} + W \]
\[ a = \left( \frac{\partial \eta^1}{\partial T} \right)_T = \frac{p_{21} h^*}{\rho_2 R_1 T} \left( \frac{1}{R_1 T} \right) \left( \frac{\partial \psi}{\partial \eta^2} \right)_T - 1 \]
\[ b = \rho_2 \left( \frac{\partial \eta^1}{\partial T} \right)_T = \frac{h^* (\pi - \eta^2)}{R_1 T} \left( \frac{dp_{21}}{dT} \right)_T + \frac{p_{21}}{R_1 T} \left( \frac{\partial \psi}{\partial T} \right)_T \cdot \eta^2 - \frac{\psi}{T} - R_1 \].

Equations (68) and (69) show that \( \partial \eta^2 / \partial t, \partial T / \partial t \) can be decoupled, but the resulting expressions are lengthy and therefore not given here.

Equations (47), (48) and (49) are rather general but not easily evaluated. For numerical purposes some simplifications are mandatory. Assuming \( \mathbf{q}^0 \approx \mathbf{0} \) and \( \mathbf{V}^1 \gg \rho_1 / (\rho_0 + \rho_1) \mathbf{V}^1 \mathbf{p}^1 \) one obtains from (44), (45) and (46)
\[ \mathbf{J}^1 \approx - \frac{\rho_0}{\rho_0 + \rho_1} \left( \frac{D^\text{np}}{R_1 T} \mathbf{V}^1 \right). \]

Using the equilibrium condition (66) one gets
\[ \mathbf{J}^1 = - \frac{\rho_0}{\rho_0 + \rho_1} \left( \frac{h^* p_{21}(T) D^\text{np}}{(R_1 T)^2} \right) \left( \frac{l_{21}}{T} \mathbf{V} + \left( \frac{\partial \psi}{\partial \eta^2} \right)_T \mathbf{V}^2 \right). \]

The diffusion flux \( \mathbf{J}^2 \) is best evaluated from (49) assuming \( \mathbf{V}^1 \ll \rho_2 \mathbf{V}^1 + \mathbf{V} \psi + \mathbf{V} \Phi \)
\[ \mathbf{J}^2 = - \frac{K \rho_2}{\bar{g}} \left( \left( \frac{\partial \psi}{\partial T} \right)_T \mathbf{V} + \left( \frac{\partial \psi}{\partial \eta^2} \right)_T \mathbf{V}^2 - \bar{g} \right). \]

The diagnostic-prognostic set (68), (69), (73) and (74) is completed with the heat flux equation
\[ \mathbf{J}^q = - \frac{L_q}{T} \mathbf{V}^q = - \lambda \mathbf{V} T \]
where \( \lambda \) is the thermal conductivity, DeVries (1963) and Baver, Gardner and Gardner (1972).

3 The atmospheric model

3.1 The prognostic model

The prognostic model consists of the usual set of Eulerian conservation equations for horizontal momentum per unit mass \( w_H \), the potential temperature \( \theta \) and the specific humidity \( q \),
\[ \frac{\partial w_H}{\partial t} + \nabla \cdot (w_H \mathbf{V} - w_g) = \frac{\partial}{\partial z} \left( K_m \frac{\partial w_H}{\partial z} \right) \]
\[ \frac{\partial \theta}{\partial t} = - \frac{(p_0/p)^k}{\rho c_p} \frac{\partial F_N}{\partial z} + \frac{\partial}{\partial z} \left( K_h \frac{\partial \theta}{\partial z} \right) - \frac{\hat{\eta}_{21}}{\rho c_p (p_0/p)^k} \mathbf{I}^1 \]
\[ \frac{\partial q}{\partial t} = \frac{\partial}{\partial z} \left( K_q \frac{\partial q}{\partial z} \right) + \frac{\mathbf{I}^1}{\rho}. \]

An Equation analogous to (78), but without source term is valid for aerosol. The notation of the variables is standard; \( K_m \) and \( K_h = K_q \) are exchange coefficients for momentum and heat, \( \mathbf{I}^1 \) is the transition rate of water per unit volume and time. The net flux \( F_N \) of radiation comprises the entire solar and infrared emission spectrum and includes the contribution of water vapor, carbon...
dioxide, ozone, molecules and aerosols. Overlap of gases and multiple scattering are accounted for. The
radiation model is described by ZDUNKOWSKI et al. (1976, 1980). As can be seen in (76) – (78) the
fluxes appearing in the conservation equations are parameterized as gradient laws. The exchange co-
efficient for neutral conditions is modelled according to SHIR (1973). Stratification is accounted for with
the aid of the MONIN-OBUKHOV profile functions, see ZDUNKOWSKI et al. (1976). The phase transition
flux 1\textsuperscript{1} is eliminated using MCDONALD’s (1963) adjustment procedure.

Boundary conditions are modelled as follows.

\[
\begin{align*}
\omega_H &= \begin{cases} 
0 & z = 0 \\
\omega_g & z = 3 \text{ km}
\end{cases} \\
\frac{\partial \theta}{\partial t} &= 0.35 \text{ K/100 m} \quad \text{at} \quad z = 3 \text{ km} \\
\frac{\partial q}{\partial z} &= \alpha q_{N-1} \quad \text{at} \quad z = 3 \text{ km}
\end{align*}
\]

where \( q_{N-1} \) refers to the specific humidity one grid point below the upper boundary. The constant
\( \alpha \) is evaluated from MÖLLER (1973).

### 3.2 The interface conditions

Two interface conditions are used, one for heat and the other one for mass flow. The heat flux
interface condition at \( z = 0 \) is modelled according to

\[
F_N + J_A^3 - J_1^3 + (J_A^1 - J_1^1)(\psi_{21} - \psi) = 0
\]

where \( J_A^3, J_A^1, J_1^3, J_1^1 \) are the vertical components of the sensible atmospheric heat and water vapor
fluxes, the heat conduction and the water vapor flux in the soil, respectively. The mass flux budget for
water at \( z = 0 \) is taken as

\[
J_A^1 - J_1 = J_2 = 0
\]

where \( J_2 \) is the vertical component of the liquid water flux in the soil. Upward fluxes are taken positive,
downward fluxes negative. The interface conditions contain the temperature, the liquid water content
and the specific humidity at the soil surface. Assuming continuity of temperature and specific humidity
at the surface, these quantities may be determined from (79) and (80) and the additional relation (66)
between \( q \) resp. \( p_1 \) and \( \eta^2 \). Since (66) is a transcendental equation, an iterative procedure is used to
obtain \( T(z = 0), q(z = 0) \) and \( \eta^2 (z = 0) \).

The numerical treatment of the atmospheric and the soil equations was previously described by ZDUN-
KOWSKI et al. (1976) except that the present investigation uses a fully implicit scheme. Height variables
were subjected to logarithmic and square root transforms in the atmosphere and in the soil, respectively,
to obtain sufficient resolution near the interface.

### 4 Discussion of results

#### 4.1 Soil moisture data

Fundamental to all calculations is the knowledge of the moisture potential \( \psi \) and the coefficient
of hydraulic conductivity \( K \). For two soil types these quantities are displayed in Figure 1. The
shaded area refers to the region of \( \psi \) which defines a range of \( \eta^2 \)-values known as the field capacity. For
sand and loam the field capacity ranges from 0.07—0.21 and 0.17—0.43, respectively. In the region of
the field capacity, the forces of the potential $\psi$ are of such magnitude as to compensate gravitational effects so that the liquid water in the soil is not removed by seepage. This definition holds true only in the absence of appreciable evaporation. Both quantities $\psi$ and $K$ vary very rapidly with $\eta^2$.

### 4.2 Model results

For both soil types and two geostrophic winds of 7 and 12 m/s, atmospheric profiles of temperature, wind and humidity are calculated as well as soil temperature and moisture. The calculations refer to a latitude of 50°N and the autumnal equinox as well as cloud free conditions. The base temperature is taken from GEIGER (1961), the corresponding soil moisture profiles are located within the range of the field capacity. The air temperature at the upper boundary is taken from the US-standard atmosphere, the relative humidity is assumed to be 40% at this height. The frictional velocity for neutral conditions needed for the exchange formulation is taken from BLACKADAR (1962) as 0.23 and 0.44 m/s corresponding to a roughness height of 1 cm. Aerosol concentration is taken to be small enough such that its influence on the radiation field is almost negligible. All calculations are started at sunrise.

Figure 2, referring to a loamy soil, displays the daily course of temperature at shelter height and of the liquid water content in 0.5 cm depth below the surface of the earth. The liquid water content at a depth of 1 m was fixed at $\eta^2 = 0.2$ during the entire prediction periods; the initial value at the surface was taken as 0.15, linear interpolation for grid points in between was used initially. This range of values is commonly observed in field experiments as follows from GEIGER (1961). These particular soil moisture values were adopted for the reason of demonstrating the drying process of the soil and the decrease of the associated evaporation and the increase of the amplitude of the temperature wave. Calculations for this figure refer to a geostrophic wind of 7 m/s.
In addition to the daily course of temperature at shelter height, the envelopes of the daily run of the surface temperature are also shown. The extreme values are marked. For the geostrophic wind speed of 7 m/s, the temperature wave within the first three days remains almost constant. This is at least partly explained by the fact that the minimum value of $\eta^2 = 0.1$ in the early afternoon occurs only within a very thin layer which guarantees a sufficiently strong water supply from below. Because of non-existing evaporation at night, water accumulates in the upper soil layer at the expense of neighbouring layers just below. After the third day the uppermost soil layer dries out more completely and to a greater depth so that upward moisture transport becomes less efficient since the hydraulic conductivity decreases quickly with decreasing values of $\eta^2$. Thus the uppermost soil layer becomes an effective barrier to evaporation. A consequence of this process is that more solar energy is available for surface heating resulting in increased values of the temperature near the ground. Moreover, the thermal conductivity $\lambda$ of the soil decreases with $\eta^2$ so that heat conduction near the surface is not very efficient. Additional computations (not displayed) show that on the tenth day the temperature amplitude has reached its maximum value.

A similar situation is displayed in Figure 3 which again refers to a loamy soil but to a geostrophic wind speed of 12 m/s. Inspection of this figure shows that due to the higher wind speed the potential evaporation is increased so that the effects described in Figure 2 now start at an earlier time. For this larger wind speed the drying process of the uppermost soil layer is nearly completed on the seventh day for the same set of initial conditions used in the previous figure. The difference of maximum temperatures between the soil surface and shelter height is less at the greater geostrophic wind of 12 m/s due to the increased value of turbulent mixing.

The concept of evaporation barrier is fundamental to understand Figure 4 which displays the cumulative evaporation of two soil types. The evaporation includes both the transformation of liquid water and the direct water vapor transport through the surface of the earth. The values of all curves are in agreement with information given by GEIGER (1961) and, for example by HILLEL (1971) which are based on observational evidence. During the first few days the evaporation amounts to about 3–4 mm, the
Figure 3
The daily run of temperature at shelter height and liquid water content \(\eta^2\) at 0.5 cm below the surface; loam, \(v_g = 12\) m/s. The dashed lines represent the envelopes of the soil surface extreme temperatures. The crosses mark the time of the extreme temperatures.

Bild 3
Tagesgang der Temperatur \(T_d\) in Hüttengröße und des Flüssigwassergehaltes \(\eta^2\) 0.5 cm unter der Erdoberfläche für Lehm und \(v_g = 12\) m/s; die unterbrochenen Linien sind die Umhüllenden des Tagesganges der Erdbodentemperatur. Die Zeiten der Temperaturextrema sind durch Kreuze markiert.

Figure 4
Cumulative evaporation as function of time for loam and sand. Full lines refer to \(v_g = 7\) m/s, dashed lines to \(v_g = 12\) m/s.

Bild 4
Aufsummierte Verdunstung als Funktion der Zeit für Sand und Lehm. Die durchgezogenen Linien beziehen sich auf \(v_g = 7\) m/s, die unterbrochenen auf \(v_g = 12\) m/s.
computed value of nocturnal dew to values slightly less than one tenth of evaporation, in agreement with GEIGER (1961) and MONTEITH (1957). As expected, in the first few days the evaporation for the higher geostrophic wind exceeds the evaporation for the lower wind speed by about 3 mm in 72 hours. For the larger geostrophic wind of 12 m/s evaporation begins to decrease after 3 days due to the earlier formation of the evaporation barrier while for the lower geostrophic wind this decrease does not occur before the fifth day. The result is that the cumulative evaporation after 7 days is larger for the smaller wind speed.

Some remarks on the amount of global solar radiation consumed for evaporation appear to be of interest. For abbreviation a quantity \( r \) is defined as the ratio of latent heat flux \( \hat{t}_{21} \) for the global solar radiation after subtraction of ground reflected energy. The fraction \( r \) is largest during the noon hours at the beginning of the prediction period when the water supply is abundant. For loamy soil and \( v_g = 7 \) to 12 m/s \( r \) varies from .70 to .75. As the drying process proceeds maximum values of \( r \) are shifted to the morning hours. On the fifth day, \( v_g = 12 \) m/s, \( r_{max} \) is 0.50 at 9h. This \( r \)-value is observed at about the same time during the entire prediction period. The constancy of the \( r \)-value at this time of the day is caused by dew formation and accumulations of water near the surface during the night. After 10 h the \( r \)-value reduces to about 0.10 and remains constant for the rest of the day. This daily course is observed from the fifth day on. For \( v_g = 7 \) m/s the shift of \( r_{max} \) occurs about two days later.

To supplement the previous information for the loamy surface, vertical temperature profiles in the air and the soil, daily runs of relative humidity and vapor pressure, selected wind spirals was well as exchange coefficient profiles are displayed in Figures 5–10.
Figure 6
Air and soil temperature profiles for various times of the day; dried out loam near the end of the prediction period, $v_g = 7 \text{ m/s}$.

Bild 6
Temperaturprofile in der Luft und im Erdboden zu verschiedenen Tageszeiten; getrockneter Lehm gegen Ende der Vorhersagezeit, $v_g = 7 \text{ m/s}$.

Figure 7
Daily course of relative humidity $U$ and vapor pressure $p^v$ (dashed) at shelter height. The prediction time corresponds to Figure 5 and the loamy soil.

Bild 7
Tagesgang der relativen Feuchte $U$ (durchzogen) und des Dampfdruckes $p^v$ (unterbrochen) in Hüttenhöhe. Die Abbildung bezieht sich auf Lehm Boden und den gleichen Vorhersagezeitraum wie bei Bild 5.
During the first three days the liquid water availability at the surface is nearly constant for a given time so that the temperature profiles in the air and the soil are nearly identical. Results are shown in Figure 5 for various times of the day. Figure 6 shows the corresponding temperature profiles four days after the first increase of the soil surface maximum temperature (see Figure 2), i.e., on the seventh day. At the end of the prediction period the daily amplitude at shelter height is about 20 °C due to the much drier ground in contrast to the value of 15 °C at the beginning of the prediction when the upper soil layer still contains sufficient moisture. In case of the drier upper soil layer the inversion is more intense. Within the soil, the temperature wave penetrates to a depth of 50 cm in the prediction period.

Figure 7 shows the daily run of relative humidity and vapor pressure at shelter height and corresponds to Figure 5. Due to the rich moisture supply at the ground, the relative humidity, a function of vapor pressure and temperature, does not exhibit a strong variation during the day. The maximum vapor pressure amplitude is reached at about 18 hours. After this time, water vapor transport in downward direction leads to a fast decrease of the vapor pressure amplitude and to dew formation.

Figure 8 corresponds to the temperature distribution of Figure 6. In the morning hours the increase in vapor pressure occurs at about the same rate as in the situation of the moist soil due to the evaporation of the dew deposited during the night and the accumulated liquid water in the upper soil layer. Between 9 and 10 hours, the removal of water vapor due to increased vertical mixing begins to overcompensate the reduced moisture supply at the ground. This leads to the formation of the double wave as often observed in nature and described by GEIGER (1961). Therefore, the amplitude of the relative humidity in this case is more pronounced than in the previous situation. The larger amplitude is also partly due to the higher temperature.

In Figure 9 the wind spirals are shown for the rather moist and dried out soil at the beginning and the end of the prediction period at 13 hours. For the geostrophic wind of 7 m/s the wind spirals do not show any significant differences. The cross isobar angles of about 17 degrees are in agreement with expected observational values for the assumed roughness height.

The exchange coefficient profiles for the moist soil (II) and the dried out upper soil layer (III), corresponding to the wind profiles of the previous figure, are shown in Figure 10. For comparison the exchange profile for the stable atmosphere shortly before sunrise is shown as curve I. There is no essential difference between exchange profiles for dry and moist soil under stable conditions.

- **Figure 8**
  Daily course of relative humidity U and vapor pressure \( p^1 \) (dashed) at shelter height. The prediction time corresponds to Figure 6 and the loamy soil.

- **Bild 8**
  *Tagesgang der relativen Feuchte U (durchgezogen) und des Dampfdruckes \( p^1 \) (unterbrochen) in Hüttenhöhe. Die Abbildung bezieht sich auf Lehmboden und den gleichen Vorhersagezeitraum wie bei Bild 6.*

- **Figure 9**
  Wind spirals for the geostrophic wind of 7 m/s and the time of maximum surface temperatures for loamy soil. The full line refers to the beginning, the dashed line to the end of the prediction period when the soil has dried out.

- **Bild 9**
  Windspiralen für $v_g = 7$ m/s über Lehmboden zur Zeit der maximalen Oberflächentemperatur. Die durchgezogene Linie bezieht sich auf den Anfang des Vorhersagezeitraums, die unterbrochene auf das Ende, wenn der Boden getrocknet ist.

- **Figure 10**
  Profiles of the exchange coefficient for heat $K_h$ over loamy soil, $v_g = 7$ m/s. Curve I refers to stable conditions at sunrise, curve II to moist loam for unstable conditions at noon, and curve III refers to dried out loam for unstable conditions at noon.

- **Bild 10**
  Profile des Austauschkoefizienten für den sensiblen Wärmefluß ($K_h$) über Lehmboden, $v_g = 7$ m/s. Kurve I zeigt $K_h$ bei stabilen Bedingungen zu Sonnenaufgang, Kurve II zeigt $K_h$ bei instabilen Bedingungen zur Mittagszeit über feuchtem, und Kurve III über getrocknetem Lehmboden.
To demonstrate the influence of soil types, the calculations are repeated for sand. Since the sand has a lower field capacity than loam, smaller initial values of $\eta^2$ at a depth of 1 m (0.16) and at the surface (0.12) are assumed. Figure 11 corresponds to Figure 2. In this case the evaporation barrier is reached very quickly as follows from the increasing amplitudes and the decreasing liquid water content. The transition from moist to dry soil is much more abrupt than for the loam. Additional calculations (not shown) demonstrate that the increase of the maximum temperature of the air layer near the ground may occur several days later when a higher initial water content is selected but the slopes of the envelopes to ground and shelter height temperature remain nearly the same. For comparison the same situation is depicted in Figure 12 for a geostrophic wind of 12 m/s. Now the drying process is even more accelerated.

The previously defined quantity $r$ characterizing evaporation is nearly identical for sand and loam at the beginning of the prediction period due to a sufficiently large moisture supply. Since sand dries more rapidly than loam, $r_{max}$ is shifted to 9 h two days earlier for both geostrophic winds. At the end of the prediction period, the $r$-value for sand after 10 h is about .07 while for loam $r = 0.10$ is calculated.

At this point, a comparison of the cumulative evaporation for loam and sand may be of interest, refer to Figure 4. The effect of wind velocity is qualitatively the same for both soils. For the geostrophic wind of 12 m/s, the evaporation rate is the same for both soil types during the first 30 hours. The evaporation barrier for sand has formed at this time so that after 30 hours the cumulative evaporation of sand is strongly exceeded by that of loam, whose evaporation barrier will not form until several days later. For the lower geostrophic wind of 7 m/s the evaporation curves do not separate the first 3 days and a half since the evaporation barrier does not form so quickly. During the period of time that the curves for both soil types, for a given geostrophic wind speed, coincide the actual and potential evaporation are identical. Further inspection of Figure 4 shows that for loam the actual and potential evaporation coincide even for a somewhat longer period of time.
Finally, temperature profiles for sand are shown in Figure 13 which correspond to Figure 6, \( v_g = 7 \, \text{m/s} \). The daily amplitude of temperature (23 °C) at shelter height exceeds that of loam (19 °C) substantially. Furthermore, the temperature inversion in the air is much more intense for sand than for loam, the reason being the small evaporation as well as the low heat capacity and heat conduction for the rather dry sand.

### 4.3 Comparison with a conventional soil model

For comparison purposes, calculations with a simple conventional model were carried out for a loamy soil and a geostrophic wind speed of 7 m/s. In the simple model, the heat equation is reduced to

\[
\rho c_p \frac{\partial T}{\partial t} = - \frac{\partial}{\partial z} J^q_1 \quad \text{with} \quad J^q_1 = - \lambda \frac{\partial T}{\partial z}
\]

where \( \lambda \) is the thermal conductivity of the soil which depends on \( \eta^2 \). Transport equations for the water phases are omitted. The interface condition for heat (79) simplifies to

\[
F_N + J^q_A - J^q_1 + J^q_{A121} = 0.
\]

Following ATWATER (1972), the humidity at the soil surface is determined according to

\[
q(z = 0) = M q_{\text{sat}}(z = 0) + (1 - M) q(z_1)
\]

where \( z_1 = 1 \, \text{cm} \) is the height of the first atmospheric grid point. The HALSTEAD parameter \( M \) represents an efficiency factor for evaporation from the soil which cannot be calculated but must be specified according to experience. In the case of a water saturated soil or at the presence of dew \( M = 1 \), for a dried out soil \( M \to 0 \).

---

In the calculations with the simple model, for better comparison with the detailed model, not \( \lambda \) but \( \eta^2 \) was specified, and \( \lambda \) was calculated from \( \eta^2 \). A series of different \( M \) and \( \eta^2 \) was tried to find out the best combination.

Table 2 gives some comparing results for the case of a moist, a medium dry and a dried out soil, using those \( \eta^2, M \)-values that produced best agreement in relative humidity. For the detailed model, the three cases were represented by the result of the second, the fourth and the sixth day of the prediction period displayed in Figure 2.

It is striking that the detailed model produces higher maximum temperatures. The reason for this behavior is found in the fact that the daily course of \( \eta^2 \) exhibits minimum values in the early afternoon, resulting in a reduced thermal conductivity of the soil and also in a reduced evaporation. The depth of the dried out layer increases during the prediction period, and therefore the difference in maximum temperature produced by the two models increases with dryness of the soil. During the night, the \( \eta^2 \) and therefore the \( \lambda \) values are nearly the same for both models in all three cases. Nevertheless the models produce different temperatures at sunrise. These differences can be attributed to two facts. First, lower temperatures are produced by the simple model during the day time. Second, the rewetting of the upper soil layers during the night is not only caused by liquid water flow, but also by vapor transport from the inner soil to the surface with resulting condensation in the pores of the uppermost soil layers. This inner dew, as termed by GEIGER (1961), raises the minimum temperature. It is accounted for only in the detailed model.
Table 2  Comparison of the detailed and the simple soil model

<table>
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<tr>
<th></th>
<th>Moist Loam</th>
<th>Medium dry Loam</th>
<th>Dry Loam</th>
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<tr>
<td></td>
<td>detailed</td>
<td>simple</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2nd day</td>
<td>4th day</td>
<td>6th day</td>
</tr>
<tr>
<td>$\eta^2$ (z = 0, t = 6.00)</td>
<td>0.140</td>
<td>0.128</td>
<td>0.110</td>
</tr>
<tr>
<td>$\eta^2$ (z = 0, t = 12.00)</td>
<td>0.021</td>
<td>0.014</td>
<td>0.010</td>
</tr>
<tr>
<td>T(z = 0, t = 6.00)</td>
<td>-1.8</td>
<td>-1.8</td>
<td>-2.3</td>
</tr>
<tr>
<td>T(z = 0, t = 12.00)</td>
<td>15.6</td>
<td>18.0</td>
<td>25.8</td>
</tr>
<tr>
<td>U(z = 2m, t = 6.00)</td>
<td>98</td>
<td>98</td>
<td>95</td>
</tr>
<tr>
<td>U(z = 2m, t = 12.00)</td>
<td>65</td>
<td>58</td>
<td>42</td>
</tr>
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</table>

It may be concluded that no complete conformity can be produced between the simple and the detailed model. The main shortcoming of the simple model is that $\eta^2$ and M must be specified. Therefore the simple model is only capable to calculate the variables of state for a given wetness of the soil. In contrast to the detailed model it cannot simulate the daily drying out and rewetting of the soil as well as the drying out over a longer period.

5  Conclusion

The theory of irreversible thermodynamics has been used to derive a consistent set of transport equations for heat and moisture within the soil. Independent microscopic arguments verify the theoretical results obtained from the linear ONSAGER theory. The transport coefficients of the phenomenological laws derived from the entropy production equation were related to the coefficients appearing in well established empirical laws. Special consideration was given to the derivation of a rather complete equation of heat flow.

The theory which was developed for the soil has been applied to study the influence of two different soil types (loam, sand) on atmospheric profiles of temperatures, humidity and wind. Moreover, evaporation rates were investigated for these two soil types and for two geostrophic winds. It has been demonstrated that atmospheric temperature and humidity in the boundary layer depend strongly on the type of soil and its moisture content. The actual and the potential evaporation rate are the same as long as the lower limit of the field capacity is not reached in the soil layer adjacent to the earth’s surface. Even though the present investigation is restricted to bare soils, the system of equations may still be applied to various realistic situations. Future research will include the effects of plants in an approximate manner to increase the applicability of the model.

Appendix

Proof of Equation (29)

For the component k of a mixture of ideal gases the following equation is valid.

$$\mu_k = \dot{\mu}_k(T) + R_k T \ln p^k$$

where $\dot{\mu}_k(T)$ depends on temperature only. From

$$\rho_0 \ \nabla \mu_0 = \nabla p^0, \ \rho_1 \ \nabla \mu_1 = \nabla p^1$$

and from $p^0 + p^1 = p$ one obtains the required identity

$$\rho_0 \ \nabla \mu_0 + \rho_1 \ \nabla \mu_1 = \nabla p.$$
References


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