STEMMUS:
Simultaneous Transfer of Energy, Mass and Momentum in Unsaturated Soil

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Contents

1 Introduction 1
   1.1 Motivation ........................................... 2
   1.2 Structures ........................................... 3
   1.3 How to use this manual ................................. 3
   1.4 Bibliography ........................................... 3

2 Brief Review of Previous Work 7
   2.1 Bibliography ........................................... 9

3 STEMMUS: Governing Equations and Constitutive Equations 13
   3.1 Governing Equations .................................. 14
   3.2 Constitutive Equations ................................ 19
   3.3 Simplification of Governing Equations ................. 26
   3.4 Bibliography ........................................... 32

4 STEMMUS: Finite Element Solution of Governing Equations 35
   4.1 Galerkin's Method of Weighted Residuals ............... 36
   4.2 Integrals' Calculation ................................ 37
   4.3 Finite Difference Time-Stepping Scheme ............... 40
   4.4 MATLAB Implementation ................................. 44
   4.5 Bibliography ........................................... 46

5 STEMMUS: Structures, Subroutines and Input Data 49
   5.1 Structure of STEMMUS: Overview .................... 50
   5.2 Initial and Boundary Conditions ..................... 53
   5.3 List of STEMMUS Variables ............................ 54
   5.4 How to Run STEMMUS ................................ 57
   5.5 Bibliography ........................................... 63
Introduction
1. Introduction

1.1 Motivation

STEMMUS (Simultaneous Transfer of Energy, Mass and Momentum in Unsaturated Soil) is a program for simulating coupled liquid water, water vapor, dry air and heat transfer in unsaturated soil. The program numerically solves the Richards equation with modification made by Milly [1]. The main driving factors are discussed as below:

A traditional conceptual model for water flow in unsaturated soil neglects the flow-of-gas phase, as can be seen in the statement: "Unsaturated flow . . . is nothing but a special case of simultaneous flow of two immiscible fluids, where the nonwetting fluid is assumed to be stagnant" [2]. According to this statement, air always remains at atmospheric pressure and is free to escape from or enter into the vadose zone. This assumption is widely used in the traditional coupled moisture and heat flow model, based on the theory by Philip and de Vries [3] (hereafter PdV model, referring to this traditional model), even when water vapor movement is considered. However, the flow in porous media is actually a two-phase flow problem [4], in need of complicated mathematical analysis of the response of soil to atmospheric forcing, caused by nonlinearities, moisture retention hysteresis, soil heterogeneity, as well as by multiple length and time scales [1]. The usual approach to solving the numerical model of water flow in soil involves the above cited assumption, which is often called the Richards approximation [5]. Although successful application of this assumption has been demonstrated in many cases, there are situations where the air phase can significantly retard or speed up infiltration [6, 7]. To properly describe these gas influenced infiltrations, a two-phase model must be used.

To improve the model representation of multiphase systems, there have been continuous efforts to build comprehensive multiphase models. At present, the modern two-phase heat and mass flow models have generally overcome most of the above mentioned difficulties [8, 9], and the weaknesses of the single-phase approach have been systematically discussed in these studies. Some of the existing comprehensive multiphase models, e.g., CODE_BRIGHT [8] and TOUGH2 [9], have been mainly applied to geothermal problems [10], without paying attention to the soil-atmosphere interacting mechanisms mentioned in section 1.1. Such comprehensive multiphase models (e.g., fluid flow in the deformable porous media) do not make including a two-phase heat and mass flow model into the land surface model straightforward. It is also not easy to understand why a two-phase flow mechanism is better than the traditional PdV model in the context of soil-atmosphere interaction. The PdV model has been widely used in many unsaturated flow simulators [11, 12, 13, 14], and subsequently adopted as sub-model in hydrological integration models [15, 16] and land surface models [17, 18, 19, 20]. Therefore, in aiming to understand the need to include a two-phase flow mechanism in the PdV model, it is necessary to know how the airflow influences the performance of the PdV model when simulating soil moisture and soil temperature.
On the other hand, the isothermal two-phase fluid flow in unsaturated soil, excluding heat flow and transport (e.g. considering air-water flow only), has seen an increase in development because of its indispensable role in simulating, modeling and studying waste storage, geological storage, underground natural resource recovery and environmental remediation etc. [21, 22]. However, most development has been focusing on multiscale problems or numerical formulations and solutions [23, 24], and very little attention has been paid to investigating how heat flow can affect the isothermal two-phase flow (air-water flow only) in unsaturated soil.

Therefore, to understand how airflow interact with coupled moisture and heat flow in soil, it’d better to develop a two-phase mass and heat transfer model (e.g. the STEMMUS Model) to investigate the interactions between them. This technical manual introduces the main physics behind the STEMMUS model, the numerical method the model uses, the program structure and the input data (e.g. boundary & initial condition) for running the model.

1.2 Structures

In the following chapter, a brief review on previous works is discussed. Chapter 3 shows the governing equations for STEMMUS, and the physics behind them. How the constitutive equations were chosen to have a closure for the model is briefly discussed. Chapter 4 introduces the finite element method used for solving the model. The structure of the model is presented in Chapter 5. How individual subroutine is designed to serve the main program and how to generate the boundary and initial condition for the model were also introduced.

1.3 How to use this manual

This technical manual is a documentation helping users to understand how STEMMUS is build and how to make it running. The application of the model is limited to very dry soil (e.g. in a desert environment) for the current version. The test of the model in other cases has not been made available at this stage. In future, the updated STEMMUS will be released regularly. Whenever you find there were any typos or errors or mistakes, please help us to improve the manual and the STEMMUS by dropping any line to yijian@itc.nl (/yijianzeng@gmail.com) or b_su@itc.nl.

1.4 Bibliography

1. Introduction


Brief Review of Previous Work
Under the Richards approximation (e.g. no gas phase transport in the soil), using practical or phenomenological approaches, common empirical constitutive relations (e.g. the laws of Darcy, Fick, Henry, Dalton and Kelvin) are directly incorporated in formulating the model for heat and mass transfer in a partially saturated porous medium, often called diffusion-based model with roots in Philip and de Vries [1]. The diffusion-based model has been adopted and extended by numerous authors [2, 3, 4, 5, 6]. Yet, unsatisfactory discrepancy is often found between theory prediction and field data. For example, Cahill and Parlange [7] demonstrated the significant underestimation of the magnitude as well as the incorrect direction predicted by the diffusion-based theory for vapor flux in their field experiments. Heitman et al. [8] revealed the noticeable differences between measured and calculated patterns of heat and moisture redistribution when the boundary temperature gradient was instantly reversed. As a result, both Cahill and Heitman suggested that to further develop the theory for better description of field conditions additional mechanisms need to be taken into consideration. Although no additional mechanism is pointed out specifically, the gas phase flow, which involves dry air and vapor flow, is an important mechanism that needs to be taken into account.

The gas phase flow in unsaturated soil has been studied for more than a century, since Buckingham [9] described the movement of air in soil in response to atmospheric pressure. However, not much attention was paid to this until the importance of gas flow in various engineering fields became apparent. Especially in environmental engineering, where gas flow is the major mechanism for assessing contaminant mass depletion due to volatilization and removing the volatile organic chemicals from the vadose zone by vapor extraction.

From a theoretical point of view, the gas phase flow problem has been analyzed using numerical or analytical approaches. Although many numerical simulators were developed to simulate gas flow problems in complex conditions [10, 11, 12], the capacity of analytical solutions to verify numerical codes led to the development of analytical solutions for soil gas flow in the vadose zone in the past two decades. For example, Massmann [13] and McWhorter [14] presented analytical solutions to solve one-dimensional radial gas flow with simple initial and boundary conditions; Shan [15, 16] developed analytical solutions for transient gas flow caused by barometric pumping in both one and two dimensions. These studies provided a good knowledge base on the induced gas flow field in soil, needed to successfully design a cleanup system for contaminated vadose zones.

At the same time, simultaneous flow of water and air through unsaturated porous media was intensively studied due to its vast applications in petroleum reservoir engineering, which also led to the development of either numerical or quasi-analytical solutions [17, 18, 19]. However, for the analysis of simultaneous flow of heat and mass through unsaturated porous media, a two phase flow model should also take the energy balance equation into account.
In nuclear or geothermal engineering, where an assessment of coupled liquid water, vapor, dry air and heat transport is required, the two-phase heat and mass flow model has been widely researched [20, 21, 22, 23, 24, 25]. Application of the two-phase heat and mass flow model is not limited to this. It is also important in the drying technology, where a precise thermo-hydro-mechanical model is highly recommended [26] for obtaining dried products of good quality, as well as being important in the storage of liquefied natural gas [27], where a comprehensive understanding of the processes of freezing and thawing is necessary for safety assessment, and in the CO2 sequestration system in a fault environment [28], where assessment of fault instability due to the impact of CO2 injection is a typical two-phase heat and mass flow problem, and so on. Although all these studies analyze the heat and mass transfer with a two-phase flow approach, which may fill the gap between theory and measurement pointed out by Cahill and Parlange [7] and Heitman et al. [8], further consideration of the coupled liquid, vapor, dry air and heat transport mechanism is needed.

From a mechanistic point of view, primary mechanisms of two phase heat and mass flow in unsaturated porous media include convection (movement with the bulk fluid) and hydrodynamic dispersion (mechanical dispersion and molecular diffusion) [29]. Mechanical dispersion, resulting from variations in fluid velocity at the micro pore scale, is the product of dispersion and convection. In most cases, the mechanical dispersion of gas phase is neglected due to its very small velocity compared to the dominant molecular diffusion [30]. This assumption is also applied in two-phase heat and mass flow models mentioned in the above paragraph. However, it has been argued that standard phenomenological approaches to modelling two-phase flow based on empirical constitutive relations (simplification of transport mechanisms) are not founded on an entirely sound physical basis [31]. Based on a series of work by Hassanizadeh and Gray [32, 33, 34], Niessner and Hassanizadeh [35, 36] presented a non-equilibrium two-phase heat and mass flow model including the interfacial area as state variable. The reliability of their physically-based model was made convincing by capturing additional physical processes (hysteresis) compared to the standard model. However, the focus of their research is on microscopic scale problems, which is not suitable for solving the field-scale problem yet.

2.1 Bibliography


2. Brief Review of Previous Work


2.1. Bibliography


2. Brief Review of Previous Work


STEMMUS: Governing Equations and Constitutive Equations
3. STEMMUS: Governing Equations and Constitutive Equations

3.1 Governing Equations

In this section, two main groups of equations (conservation equations and constitutive equations) have been used to describe the two-phase heat and mass flow model. The Milly’s equations [1], considering the predominantly vertical interactive process between atmosphere and soil, have been introduced first to describe the traditional coupled heat and mass flow model scheme. Then, the two-phase heat and flow model has been developed on this basis. Next, considering dry air as a single phase and the main component of the gaseous phase in soil, the balance equation of dry air was introduced, based on Thomas’ work [2]. Henry’s law has been used to express the equilibrium of dissolved air in liquid. In addition, the thermal equilibrium assumption between phases has been adopted and the equation for energy balance established taking into account the internal energy in each phase (liquid, vapor, and dry air).

3.1.1 Liquid Transfer

Soil water is present in a liquid and a gaseous phase, and following Milly [1], the total moisture balance is expressed as

\[ \frac{\partial}{\partial t}(\rho_L \theta_L + \rho_V \theta_V) = -\frac{\partial}{\partial z}(q_L + q_V) \] (3.1)

where \( \rho_L \) (kg m\(^{-3}\)) represents the density of liquid water; \( \rho_V \) (kg m\(^{-3}\)) the density of water vapor; \( \theta_L \) the volumetric water content; \( \theta_V \) the volumetric water vapor content; \( z \) (m) the vertical space coordinate, positive upwards; \( q_L \) and \( q_V \) the liquid mass flux and the vapor mass flux (kg m\(^{-2}\) s\(^{-1}\)). The liquid flux is expressed by a general form of Darcy’s flow

\[ q_L = -\rho_L K \frac{\partial h_w + z}{\partial z} \] (3.2)

where \( h_w \) (Pa) is the pore-water pressure; \( y_w \) (kg m\(^{-2}\) s\(^{-2}\)) the specific weight of water; and \( K \) (m s\(^{-1}\)) the unsaturated hydraulic conductivity. According to Groenevelt and Kay [3], the effect of the heat of wetting on the pressure field and the resulting flow is taken into account by Milly [1], which leads to an additional liquid flow term in equation (3.2) resulting in

\[ q_L = -\rho_L K \frac{\partial h_w + z}{\partial z} - \rho_L D_{Ta} \frac{\partial T}{\partial z} \] (3.3)

where \( D_{Ta} \) (m\(^2\) s\(^{-1}\) °C\(^{-1}\)) is the transport coefficient for adsorbed liquid flow due to temperature gradient; and \( T \) (°C) the temperature. According to the definition of capillary potential, \( h_w \) could be expressed as the
3.1. Governing Equations

The difference between the pore-air pressure and the pore-water pressure [4, 5, 2]

\[ h = \frac{h_w - P_g}{\gamma_w} \]  

(3.4)

where \( h \) (m) is the capillary pressure head; and \( P_g \) (Pa) the mixed pore-air pressure (e.g. including vapor and dry air pressure). Substituting equation (3.4) into equation (3.3) yields

\[ q_L = -\rho_L K \frac{\partial(h + \frac{P_g}{\gamma_w} + z)}{\partial z} - \rho_L D_{Ta} \frac{\partial T}{\partial z} \]  

(3.5)

Equation (3.5) can be rewritten [6] as

\[ q_L = -\rho_L \left[ K \frac{\partial(h + \frac{P_g}{\gamma_w})}{\partial z} + D_{Ta} \frac{\partial T}{\partial z} + K \right] \]  

(3.6)

in which \( q_{Lh} \) and \( q_{LT} \) are the isothermal and thermal liquid flux (kg m\(^{-2}\) s\(^{-1}\)); \( q_{La} (\rho_L K \frac{\partial P_g}{\partial z}) \) the advective liquid flux due to soil air pressure gradient (kg m\(^{-2}\) s\(^{-1}\)); and \( K_{La} \) (s) the advective liquid transport coefficient.

3.1.2 Vapor Transfer

The vapor flux is expressed by a generalized form of Fick’s law

\[ q_V = -D_V \frac{\partial \rho_V}{\partial z} \]  

(3.7)

where \( D_V \) (m\(^2\) s\(^{-1}\)) is the molecular diffusivity of water vapor in soil. When dry air is considered, the vapor flow is assumed to be induced in three ways: firstly diffusive transfer, driven by a vapor pressure gradient equation (3.7); secondly advective transfer, as part of the bulk flows of air (\( \rho_V q_{aa} \rho_{da} \)); and thirdly dispersive transfer, due to longitudinal dispersivity (\( -D_{Vg} \frac{\partial \rho_V}{\partial z} \)). Accordingly, equation (3.7) can be rewritten as

\[ q_V = -D_V \frac{\partial \rho_V}{\partial z} + \rho_V q_{aa} \frac{\partial \rho_V}{\partial z} - \theta_V D_{Vg} \frac{\partial \rho_V}{\partial z} \]  

(3.8)

where \( q_{aa} (=-\rho_{da} K_g \frac{\partial P_g}{\partial z}) \) is the advective dry air flux (kg m\(^{-2}\) s\(^{-1}\)); \( \rho_{da} \) (kg m\(^{-3}\)) the dry air density; \( D_{Vg} \) (m\(^2\) s\(^{-1}\)) the gas-phase longitudinal dispersion coefficient; and \( K_g \) the gas conductivity (m s\(^{-1}\)).

Considering vapor density to be a function of matric potential and temperature, the vapor flux can be divided into isothermal and thermal
components. According to the chain rule for partial derivatives, the vapor flux in equation (3.8) could be rewritten using the three state variables as

$$q_V = q_{Vh} + q_{VT} + q_{Va}$$

$$= - \left( \left( D_V + \theta_V D_{Vg} \right) \frac{\partial p_V}{\partial h} \frac{\partial h}{\partial z} + \frac{\partial}{\partial z} \left[ (D_V + \theta_V D_{Vg}) \frac{\partial T}{\partial z} + \rho_V K_g \frac{\partial P_g}{\partial z} \right] \right) \tag{3.9}$$

where $q_{Vh}$, $q_{VT}$, and $q_{Va}$ is the isothermal vapor flux, the thermal vapor flux, and the advective vapor flux ($kgm^{-2}s^{-1}$).

Combining the governing equations for liquid water (equation 3.6) and vapor flow (equation 3.9) leads to the governing differential equation for moisture transfer:

$$\frac{\partial}{\partial t} \left( \rho_L \theta_L + \rho_V \theta_V \right) = - \frac{\partial}{\partial z} \left( q_L + q_V \right)$$

$$= - \frac{\partial}{\partial z} \left( q_{Lh} + q_{LT} + q_{La} \right) - \frac{\partial}{\partial z} \left( q_{Vh} + q_{VT} + q_{Va} \right)$$

$$= \rho_L \frac{\partial}{\partial z} \left[ K \left( \frac{\partial h}{\partial z} + 1 \right) + D_{Ta} \frac{\partial T}{\partial z} + K \frac{\partial P_g}{\partial z} \right] \tag{3.10}$$

where, $D_{Vh} = (D_V + \theta_V D_{Vg}) \frac{\rho_v}{\rho_h}$ is the isothermal vapor diffusion coefficient ($kgm^{-2}s^{-1}$); $D_{VT} = (D_V + \theta_V D_{Vg}) \frac{\rho_v}{\theta_T}$ the thermal vapor diffusion coefficient ($kgm^{-1}s^{-1}°C^{-1}$); and $D_{Va} = \rho_v K_g$ the advective vapor transfer coefficient ($s$).

The terms within the square brackets in equation (3.6) represent the liquid flux. The term $(\frac{P}{\gamma_w})$ is the mixed soil air pressure expressed as the height of a water column. The terms within the square brackets in equation (3.8) represent the water vapor flux, with the first term representing the diffusive flux (Fick’s law), the second representing the advective flux (Darcy’s law) and the third the dispersive flux (Fick’s law).

Equation (3.3) shows clearly that only thermal (e.g. explicitly through the temperature dependence of $K$) and isothermal liquid advection and water vapor diffusion are considered in the traditional coupled heat and mass transport model (PdV model). However, equation (3.6) shows that dry air is considered to be a single phase. Thus not only diffusion, but also advection and dispersion become included in the water vapor transport mechanism. As for the liquid transport, the mechanism remains the same, but with atmospheric pressure acting as one of driving force gradients.

### 3.1.3 Dry Air Transfer

Dry air transport in unsaturated soil is driven by two main gradients, the dry air concentration or density gradient and the air pressure gradient. The first one diffuses dry air in soil pores, while the second one causes
3.1 Governing Equations

The governing equation for dry air may be presented [2] as

$$\frac{\partial}{\partial t} [\epsilon \rho_{da} (S_a + H_c S_L)] = - \frac{\partial q_a}{\partial z}$$

(3.11)

and the dry air flow $q_a$ ($kg \ m^{-2} \ s^{-1}$) is given by

$$q_a = -D_V \frac{\partial \rho_{da}}{\partial z} - \rho_{da} K_g \frac{\partial P_g}{\partial z} + H_c \rho_{da} \frac{q_L}{\rho_L} - \theta_a D_{Vg} \frac{\partial \rho_{da}}{\partial z}$$

(3.12)

where $H_c (= 0.02$ for air at $1 \ atm$ and $25 \ ^{\circ}C)$ Henry's constant; $S_a (= 1 - S_L)$ the degree of air saturation of soil; $S_L (= \theta_L / \epsilon)$ the degree of saturation of soil; and $\epsilon$ the porosity. In the right hand side (RHS) of equation (3.12), the first term depicts diffusive flux (Fick’s law), the second term advective flux (Darcy’s law), the third dispersive flux (Fick’s law), and the fourth advective flux due to dissolved air (Henry’s law).

Considering dry air density is a function of matric potential, temperature and air pressure, equation (3.12) could be rewritten with three state variables. Combining equation (3.12) with equation (3.11), the governing equation for dry air can be expressed as

$$\frac{\partial}{\partial t} [\epsilon \rho_{da} (S_a + H_c S_L)] = - \frac{\partial}{\partial z} (q_{ah} + q_{aT} + q_{aa})$$

$$= \frac{\partial}{\partial z} [K_{ah} \frac{\partial h}{\partial z} + K_{aT} \frac{\partial T}{\partial z} + K_{aa} \frac{\partial P_g}{\partial z} + V_{ah} \frac{\partial h}{\partial z} + V_{aT} \frac{\partial T}{\partial z} + V_{aa} \frac{\partial P_g}{\partial z} + H_c \rho_{da} \frac{\partial K}{\partial z}]$$

(3.13)

where $q_{ah}$, $q_{aT}$, and $q_{aa}$ are the isothermal air flux, the thermal air flux, and the advective flux ($kg \ m^{-2} \ s^{-1}$). Accordingly, the transport coefficients for air flux are

$$K_{ah} = (D_V + \theta_a D_{Vg}) \frac{\partial \rho_{da}}{\partial h} + H_c \rho_{da} K$$

$$K_{aT} = (D_V + \theta_a D_{Vg}) \frac{\partial \rho_{da}}{\partial T} + H_c \rho_{da} D_{Ta}$$

$$K_{aa} = (D_V + \theta_a D_{Vg}) \frac{\partial \rho_{da}}{\partial P_g} + \rho_{da} (K_g + H_c \frac{K}{\gamma_w})$$

(3.14)

where $V_{ah}$, $V_{aT}$ and $V_{aa}$ are introduced in section 3.3.2.

3.1.4 Energy Transfer

In the vadose zone, the mechanisms for energy transport include conduction and convection. The conductive heat transfer contains contributions...
from liquids, solids and gas. Conduction is the main mechanism for
heat transfer in soil and contributes to the energy conservation by solids,
liquids and air. Advective heat in soil is conveyed by liquid flux, vapor
flux, and dry air flux. On the other hand, heat storage in soil includes
the bulk volumetric heat content, the latent heat of vaporization and
a source term associated with the exothermic process of wetting of a
porous medium (integral heat of wetting) \[7\]. Accordingly, following
the general approach by de Vries \[7\], the energy balance equation in
unsaturated soil may be written as four parts

- **Solid:**
  \[
  \frac{\partial}{\partial t} \left[ \rho_s \theta_s c_s (T - T_r) \right] = \frac{\partial}{\partial z} \left( \lambda_s \theta_s \frac{\partial T}{\partial z} \right) \tag{3.15}
  \]

- **Liquid:**
  \[
  \frac{\partial}{\partial t} \left[ \rho_l \theta_l c_l (T - T_r) \right] = \frac{\partial}{\partial z} \left( \lambda_l \theta_l \frac{\partial T}{\partial z} \right) - \frac{\partial}{\partial z} \left[ q_l c_l (T - T_r) \right] \tag{3.16}
  \]

- **Air and Vapor:**
  \[
  \frac{\partial}{\partial t} \left[ (\rho_{da} c_a + \rho_V c_V) \theta_g (T - T_r) + \rho_V L_0 \theta_g \right] = \frac{\partial}{\partial z} \left( \lambda_g \theta_g \frac{\partial T}{\partial z} \right) - \frac{\partial}{\partial z} \left[ q_V (c_V (T - T_r) + L_0) + q_a c_a (T - T_r) \right] \tag{3.17}
  \]

- **Heat of Wetting:**
  \[
  H_w = -\rho L W \frac{\partial \theta_l}{\partial t} \tag{3.18}
  \]

where \(\lambda_s, \lambda_l, \lambda_g\) represent the thermal conductivities of solids, liquids and pore gas (= \(\lambda_a + \lambda_V\), including dry air and water vapor) respectively (\(W \text{ m}^{-1} \text{ c}^{-1}\)); \(\theta_s\) the volumetric content of solids in the soil; \(\theta_g\) the volumetric content of gas (= \(\theta_V = \theta_a\)) in the soil; \(c_s, c_l, c_a\) and \(c_V\) specific heat of solids, liquids, air and vapor, respectively (\(J \text{ kg}^{-1} \text{ c}^{-1}\)); \(T_r\) (\(^\circ\text{C}\)) the reference temperature; \(\rho_s\) the density of solids in the soil (\(\text{kg m}^{-3}\)); \(L_0\) the latent heat of vaporization of water at temperature \(T_r\) (\(J \text{ kg}^{-1}\)); and \(W\) the differential heat of wetting (the amount of heat released when a small amount of free water is added to the soil matrix) (\(J \text{ kg}^{-1}\)). The latent heat of vaporization varies with \(T\) according to
\[
L(T) = L_0 - (c_L - c_V)(T - T_r) \approx 2.501 \times 10^6 - 2369.2 \times T \tag{8}
\]
In accordance with equation (3.16) to equation (3.18), the conservation equation for energy transfer in the soil is given as

\[
\frac{\partial}{\partial t} \left[ (\rho_s \theta_s c_s + \rho_l \theta_l c_l + \rho_{da} \theta_a c_a + \rho_V \theta_V c_V) (T - T_r) + \rho_V L_0 \theta_g \right] - \rho L W \frac{\partial \theta_l}{\partial t} = \frac{\partial}{\partial z} \left( \lambda_{eff} \frac{\partial T}{\partial z} \right) - \frac{\partial}{\partial z} \left[ q_l c_l (T - T_r) + q_V (c_V (T - T_r) + L_0) + q_a c_a (T - T_r) \right] \tag{3.19}
\]
where $\lambda_{\text{eff}}$ is the effective thermal conductivity ($W m^{-1} K^{-1}$), combining the thermal conductivity of solid particles, liquid, vapor and dry air in the absence of flow. The parameters in the first term in the left hand side (LHS) of equation (3.19) and can be determined by de Vries' [7] scheme. Equation (3.10), (3.13) and (3.19) are solved jointly with the specified boundary and initial condition of the solution domain to obtain spatial and temporal variations of the three prime variables $h$, $T$ and $P_g$. If the advective flux conveyed by the dry air flux $(q_a c_a(T - T_r))$ and the bulk volumetric heat content of dry air $(\rho_a \theta_a c_a)$ were to be neglected, equation (3.19) would result in the heat balance equation of Milly [1].

### 3.2 Constitutive Equations

The constitutive equations link the independent state variables (unknowns) and the dependent variables. Each governing equation is solved for a single unknown (a state variable), for example, equation (3.10) for matric potential, equation (3.13) for atmospheric pressure and equation (3.19) for temperature. The closure of the model developed above requires all dependent variables to be computable from the set of unknowns. The governing equations are finally written in terms of the unknowns when the constitutive equations given below are substituted.

#### 3.2.1 Unsaturated Hydraulic Conductivity

The pore-size distribution model of Mualem [9] was used to predict the isothermal unsaturated hydraulic conductivity from the saturated hydraulic conductivity [10]:

$$K = K_s K_r = K_s S_e^{l \left[1 - \frac{1}{m} S_e \right]^m}$$

(3.20)

where $K_s$ is the saturated hydraulic conductivity (m s$^{-1}$); $K_r$, the relative hydraulic conductivity (m s$^{-1}$); $S_e$ (= $\frac{\theta_L - \theta_{res}}{\theta_{sat} - \theta_{res}}$) the effective saturation (unitless) (In STEMMUS, the $S_e$ is approximated as $S_L$); $\theta_{res}$, the residual water contents; and $l$ and $m$ empirical parameters ($l = 0.5$). The parameter $m$ is a measure of the pore-size distribution and can be expressed as $m = 1 - \frac{1}{n}$, which in turn can be determined by fitting van Genuchten's analytical model [10]

$$\theta(h) = \begin{cases} \theta_{res} + \frac{\theta_{sat} - \theta_{res}}{1 + (\alpha h)^m}, & h < 0 \\ \theta_{sat}, & h \geq 0 \end{cases}$$

(3.21)

where $\alpha (m^{-1})$ is related to the inverse air-entry pressure. According to equation (3.20), the unsaturated hydraulic conductivity is a function of $\theta_L$, which subsequently is a function of $h$ (e.g. from equation (3.21)). The $h$ is actually temperature dependence, $h_{\text{TempCorr}} = h e^{C_\psi(T - T_r)}$, where $\frac{\partial h}{\partial T} = C_\psi h$ and $C_\psi$ is assumed to be a constant ($= 0.0068 \ ^{\circ}c^{-1}$)[11]. Such temperature dependence is implied by the temperature dependence
3. STEMMUS: Governing Equations and Constitutive Equations

of surface tension and viscous flow [12]. Therefore, the temperature apparently has an effect on the unsaturated hydraulic conductivity, due to the temperature dependence of $h$, which is given by Milly [1] as

$$K(\theta, T) = K_s K_r(\theta) K_T(T)$$

(3.22)

and $K_T$ is given as

$$K_T = \frac{\mu_w(T_r)}{\mu_w(T)}$$

(3.23)

where $\mu_w$ is the viscosity of water. The dynamic viscosity of water is given [13] as

$$\mu_w = \mu_{w0} \exp\left(\frac{\mu_1}{R(T + 133.3)}\right)$$

(3.24)

where $\mu_{w0} = 2.4152 \times 10^{-2}$ the water viscosity at reference temperature (Pa s), $\mu_1 = 4.7428$ (kJ mol$^{-1}$), $R = 8.314472$ (J mol$^{-1}$ °c$^{-1}$), and $T$ is in °c.

3.2.2 Gas Conductivity [14]

In unsaturated soil, the pore space generally is occupied by gas and liquid. Under the ideal assumption that there is no interaction between the fluids (which is actually not the case in the reality), Darcy’s low is applied to determine the gas conductivity. When the pore space is filled gradually by a single fluid, the permeability with respect to the other fluid will decreased accordingly, because of the cross-sectional area available for the flow of that fluid (other than the fluid occupying the pore space) is less. According to Darcy’s law, the gas conductivity can be expressed as

$$K_g = \frac{K_{rg}(S_a)}{\rho_{l} \beta}$$

(3.25)

where $\beta$ is gas viscosity (kg m$^{-1}$ s$^{-1}$), and the air viscosity, $\mu = 1.846 \times 10^{-5}$ kg m$^{-1}$ s$^{-1}$); $K_{rg}$ the relative gas conductivity, which is a function of effective gas saturation and is defined by Van Genuchten-Mualem model as

$$K_{rg} = \left(1 - S_a^{0.5}\right)^{2} \left[1 - \left(1 - S_a^{1/m}\right)\right]^{0.5}$$

(3.26)

3.2.3 Gas-Phase Density

Gas phase density includes water vapor density and dry air density. The water vapor density is given by Philip and de Vries [6] as

$$\rho_V = \rho_{SV} H_r, \quad H_r = \exp\left(\frac{h g}{R_r T}\right)$$

(3.27)
where \( \rho_{SV} \) is the density of saturated water vapor \( \exp(31.3716 - 6014.79/T - 7.92495 \times 10^{-3}T) \) \( (kg \ m^{-3}) \); \( H_r \) the relative humidity; \( R_V \) the specific gas constant for vapor \( (= 461.5 \ J \ kg^{-1} \ K^{-1}) \); \( g \) the gravitational acceleration \( (m \ s^{-2}) \); and \( T \) in K. The gradient of the water vapor density with respect to \( z \) can be expressed as

\[
\frac{\partial \rho_V}{\partial z} = \rho_{SV} \frac{\partial H_r}{\partial T} \bigg|_h + \rho_{SV} \frac{\partial H_r}{\partial h} \bigg|_T + H_r \frac{\partial \rho_{SV}}{\partial T} \frac{\partial T}{\partial z} \tag{3.28}
\]

Assuming that pore-air and pore-vapor could be considered to be ideal gas, air and vapor density can be expressed as

\[
\rho_{da} = \frac{P_{da}}{R_{da} T}, \quad \text{and} \quad \rho_V = \frac{P_V}{R_V T} \tag{3.29}
\]

where \( R_{da} \) is the specific gas constant for dry air \( (= 287.1 \ J \ kg^{-1} \ K^{-1}) \); \( P_{da} \) (Pa) and \( P_V \) (Pa) are the dry air pressure and vapor pressure; and \( T \) is in K. According to Dalton's law of partial pressure, the mixed soil air pressure should be equal to the sum of the dry air pressure and the vapor pressure: \( P_g = P_{da} + P_V \). Therefore, the dry air density could be given as

\[
\rho_{da} = \frac{P_g}{R_{da} T} = \frac{P_{da} R_V}{R_{da} T} \tag{3.30}
\]

Differentiating equation (3.30) with respect to time and space yields

\[
\frac{\partial \rho_{da}}{\partial t} = X_{aa} \frac{\partial P_g}{\partial t} + X_{aT} \frac{\partial T}{\partial t} + X_{ah} \frac{\partial h}{\partial t} \tag{3.31}
\]

\[
\frac{\partial \rho_{da}}{\partial z} = X_{aa} \frac{\partial P_g}{\partial z} + X_{aT} \frac{\partial T}{\partial z} + X_{ah} \frac{\partial h}{\partial z} \tag{3.31}
\]

where

\[
X_{aa} = \frac{1}{R_{da} T} \]

\[
X_{aT} = - \left[ \frac{P_g}{R_{da} T^2} + \frac{R_V}{R_{da}} \left( H_r \frac{\partial \rho_{SV}}{\partial T} + \rho_{SV} \frac{\partial H_r}{\partial T} \right) \right] \tag{3.32}
\]

\[
X_{ah} = - \frac{\partial \rho_V}{\partial h} \tag{3.32}
\]

### 3.2.4 Vapor Diffusivity

The vapor diffusion described by Fick’s law in the atmosphere has been modified so as to apply in porous media by Rollins [15] as

\[
ad_V = -D_{atm} \nu \tau a \nabla \rho_V \tag{3.33}
\]

where \( D_{atm} \) is the molecular diffusivity of water vapor in air \( (m^2 \ s^{-1}) \); \( \tau \) a tortuosity factor allowing for the extra path length; \( a \) the volumetric air content of the medium \( (\theta_a = \theta_V = \theta_g = 1 - \theta_L) \); and \( \nu \) the 'mass-flow factor' introduced to allow for the mass flow of vapor arising from
3. STEMMUS: Governing Equations and Constitutive Equations

the difference in boundary conditions governing the air and the vapor components of the diffusion system. Equation (3.33) has been described as the 'simple theory' of vapor transfer by Philip and De Vries [6] and has been proven not enough to explain the vapor transfer in soil [6]. In equation (3.33), the vapor diffusivity in soil can be expressed as:

$$D_{V, Sim, h} = D_{atm} \nu \tau \theta_a,$$

which is called as isothermal vapor diffusivity for the 'simple theory'.

With the thermodynamic relationship between the vapor density and the relative humidity in soil, which is a function of temperature and capillary pressure [16], the thermal vapor diffusivity for the 'simple theory' can be expressed as

$$D_{V, Sim, \tau} = D_{atm} \nu \theta_a H \beta$$

(3.34)

where $\beta$ is for $\frac{\partial \rho_v}{\partial T}$, and $D_{V, Sim, \tau}$, the thermal vapor diffusivity for the 'simple theory'. In a single air-filled pore, $\tau$ equals to 1 and $\theta_a$ is considered as a unity as well, presuming similarity of temperature and vapor fields in the pore. Therefore, the vapor transfer due to the air temperature gradient ($\nabla T_a$) in the pore can be expressed as

$$q_V = -D_{atm} \nu H \beta (\nabla T)_a$$

(3.35)

On the other hand, Philip and De Vries [6] assumed that the vapor can transfer through 'liquid island' (i.e. the liquid capillary connecting soil particles) by condensing on the cold side of the island and evaporating on the warm side. With such assumption, the cross section available for vapor transfer is equal to that occupied by air and liquid. Now, assuming that the mean flux density in the connecting liquid island is equal to that in the air-filled pores, we can get

$$-(\theta_a + \theta_L) D_{atm} \nu H \beta (\nabla T)_a = -D_{V, pdV, \tau} \nabla T$$

(3.36)

where $D_{V, pdV, \tau}$ represents the thermal vapor diffusivity following Philip and De Vries' assumption on 'liquid island', which employs the concept of air temperature gradient in a single pore and increases cross-section for vapor transfer. The ratio of the thermal vapor diffusivity proposed by Philip and De Vries to that of 'simple theory' is expressed as

$$\eta = \frac{\theta_a + \theta_L (\nabla T)_a}{\tau \theta_a}$$

(3.37)

where $\eta$ is the ratio and called as the enhancement factor for thermal vapor transfer in soil.

According to the equations and concept described above, the isothermal vapor diffusivity is given as the same as the isothermal vapor diffusivity for the 'simple theory'

$$D_{iso, V} = D_{V} \frac{\partial \rho_v}{\partial h} = D_{atm} \nu \theta_a \frac{\partial \rho_v}{\partial h}$$

(3.38)

where $\nu$ is set as 1, $\tau = \theta_a^{2/3}$, and $D_{atm} = 0.229 \left(1 + \frac{T}{273}\right)^{1.75} \text{ (m}^2\text{ s}^{-1})$. 

22
While the thermal vapor diffusivity is given by considering the enhancement factor as

\[ D_{Noniso,V} = D_v \frac{\partial \rho_v}{\partial T} \]

\[ = D_{atm} (\theta_d + f(\theta_d)\theta_L) \frac{(\nabla T)_a}{\nabla T} \frac{\partial \rho_v}{\partial T} = D_{atm} \eta \frac{\partial \rho_v}{\partial T} \]  

Where \( f(\theta_d) \) is a factor introduced to account for decreasing cross-section due to increasing moisture content and increasing degree of liquid continuity, and is given by De Vries [7] as

\[ f(\theta_d) = \begin{cases} 1, & \theta_L \leq \theta_k \\ \frac{\theta_a}{\epsilon - \theta_k}, & \theta_k < \theta_L \end{cases} \]  

Substitute \( \theta_L = \epsilon - \theta_a \) into equation (3.39), the cross-section for vapor transfer will be equal to \( \theta_a + \frac{\theta_a}{\epsilon - \theta_k}(\epsilon - \theta_a) \), when \( \theta_k < \theta_L \). On the other hand, when the moisture content decreases till \( \theta_k (\theta_k = \theta_L) \), the cross sectional area equals to \( \theta_a + \theta_L = \theta_a + \theta_k \). At this every moment when \( \theta_k \) merely equal to \( \theta_L \) but less than \( \theta_L \), we can approximate that \( \theta_a + \frac{\theta_a}{\epsilon - \theta_k}(\epsilon - \theta_a) \approx \theta_a + \theta_k \approx \epsilon \). It is easy to know that \( \theta_a(\epsilon - \theta_a) = \theta_k(\epsilon - \theta_k) \), which means \( \theta_a \approx \theta_k \). This indicates that the cross sectional area reach maximum when \( \theta_a \approx \theta_L \approx \theta_k = 0.5\epsilon \). It means that at moderate moisture content, continuity of both liquid and vapor phases reaches maximum, together with islands of both phases.

In the enhancement factor, \( \frac{(\nabla T)_a}{\nabla T} \) is regarded as the local temperature gradient effect due to a higher average pore-air temperature gradient compared to the average temperature gradient of the bulk medium, and is given by Philip and De Vries [6] as

\[ \eta_T = \frac{(\nabla T)_a}{\nabla T} = (\nabla T)_a \left[ \sum_{i=1}^{5} (\nabla T)_i \theta_i \right]^{-1} \]

Where \( (\nabla T)_i \) is the thermal gradient in the \( i \)th constituent, and \( \theta_i \) the volumetric fraction of the \( i \)th constituent. Based on De Vries' approach [17], the ratio of the average temperature gradient in the \( i \)th constituent to the average temperature gradient of the bulk medium can be expressed by a conceptual model

\[ k_i = \frac{2}{3} \left[ 1 + \left( \frac{\lambda_i}{\lambda_1} - 1 \right) \theta_i \right]^{-1} + \frac{1}{3} \left[ 1 + \left( \frac{\lambda_i}{\lambda_1} - 1 \right) (1 - 2 \theta_i) \right]^{-1} \]

Where \( k_i \) is the ratio; \( \lambda_i \) the thermal conductivity of the \( i \)th constituent (\( J cm^{-1} S^{-1} °c^{-1} \)); and \( \theta_i \) the 'shape factor' of the \( i \)th constituent (see Table 3.1). For the solid particles, constant values for \( \theta_i \) as given in Table (3.1) are assumed. For liquid water, no value is needed since its
3. STEMMUS: Governing Equations and Constitutive Equations

coefficient is zero. The value of \( g_2 \) is considered a function of moisture content as follows \[18\]

\[
g_2 = \begin{cases} 
0.013 + \left( \frac{0.022}{\theta_{wilting} - 4.2} + \frac{0.298}{\theta} \right) \theta_L, & \theta_L < \theta_{wilting} \\
0.035 + \frac{0.298}{\theta} \theta_L, & \theta_L > \theta_{wilting}
\end{cases}
\]

(3.43)

By applying the definition of the \( k_i \) \[17\], equation (3.41) can be transformed as

\[
\eta_T = k_2 \left( \sum_{i=1}^{5} k_i \theta_i \right)
\]

(3.44)

The value of \( \eta_T \) is valid for \( \theta_L \) down to \( \theta_k \). For \( \theta_L = 0 \), \( \eta_T \) may be calculated using air as the continuous phase, and may be interpolated for \( \theta_L \) between 0 and \( \theta_k \) \[11\].

Table 3.1 Properties of Soil Constituents \[17\]

<table>
<thead>
<tr>
<th>Constituent</th>
<th>( i )</th>
<th>( \frac{C_i}{J \text{cm}^{-3} \text{c}^{-1}} )</th>
<th>( \frac{A_i}{J \text{cm}^{-1} \text{S}^{-1} \text{c}^{-1}} )</th>
<th>( \theta_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid Water</td>
<td>1</td>
<td>1.0</td>
<td>( 5.73 \times 10^{-3} )</td>
<td>...</td>
</tr>
<tr>
<td>Air</td>
<td>2</td>
<td>( 1.25 \times 10^{-3} )</td>
<td>( 2.5 \times 10^{-4} )</td>
<td>...</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>( +LD_i(\partial \rho V/\partial T)</td>
<td>_h )</td>
</tr>
<tr>
<td>Quartz</td>
<td>3</td>
<td>2.66</td>
<td>( 8.8 \times 10^{-2} )</td>
<td>0.125</td>
</tr>
<tr>
<td>Other Materials</td>
<td>4</td>
<td>2.66</td>
<td>( 2.9 \times 10^{-2} )</td>
<td>0.125</td>
</tr>
<tr>
<td>Other Materials</td>
<td>5</td>
<td>1.3</td>
<td>( 2.5 \times 10^{-3} )</td>
<td>0.5</td>
</tr>
</tbody>
</table>

3.2.5 Gas Dispersivity

The gas phase longitudinal dispersivity, \( D_{Vg} \), is given by Bear \[19\] as

\[
D_{Vg} = \alpha_{L,i} q_i, \quad i = \text{gas/liquid}
\]

(3.45)

where \( q_i \) is the pore fluid flux in phase \( i \), and \( \alpha_{L,i} \) the longitudinal dispersivity in phase \( i \). \( \alpha_{L,i} \) has been evaluated by various authors for different levels of soil saturation. Laboratory studies have shown that \( \alpha_{L,i} \) increases when the soil volumetric water content decreases. In this study, as done by Grifoll et al. \[20\], a correlation made from simulation results \[21\] and experimental data obtained by Haga et al. \[22\] is used:

\[
\alpha_{L,i} = \alpha_{L,Sat} \left[ 13.6 - 16 \times \frac{\theta}{\epsilon} + 3.4 \times \left( \frac{\theta}{\epsilon} \right)^5 \right]
\]

(3.46)

As Grifoll et al. \[20\] pointed out, the lack of dispersivity values led to, the saturation dispersivity, \( \alpha_{L,Sat} \), used in the above correlation to be set at 0.078 m, the Figure reported in the field experiments by Biggar and Nielsen \[23\] and shown to be a reasonable value in previous modeling studies \[24\].
3.2.6 Thermal Property [17]

3.2.6.1 Heat Capacity

The volumetric heat capacity of a soil is a weighted average of the capacities of its components

\[ C = \sum_{i=1}^{5} C_i \theta_i \]  
(3.47)

where \( \theta_i \) and \( C_i \) are the volumetric fraction and the volumetric heat capacity of the \( i \)th soil constituent \((J cm^{-3} \circ c^{-1})\). The five components are (1) water, (2) air, (3) quartz particles, (4) other minerals, and (5) organic matter (see Table (3.1)).

3.2.6.2 Thermal Properties

The effective thermal conductivity of a moist soil is given by

\[ \lambda_{eff} = \left( \frac{1}{\sum_{i=1}^{5} k_i \theta_i} \right) \left( \frac{1}{\sum_{i=1}^{5} k_i \theta_i} \right)^{-1} \]  
(3.48)

the unit of which is \((J cm^{-1} S^{-1} \circ c^{-1})\) (see Table (3.1)).

3.2.6.3 Differential Heat of Wetting

The differential heat of wetting, \( W \) \((J Kg^{-1})\), is the amount of heat released when a small amount of free water is added to the soil matrix and is original expressed by Edlefsen and Anderson [16] as

\[ W = -\rho_L (\psi - T \frac{\psi}{T}) = -0.01g(h + Ta h) = -0.01gh(1 + Ta) \]  
(3.49)

where \( \psi J kg^{-1} = 0.01gh \) \((cm)\) at \( T = 293K \) with the value of \( a = 0.0068 \) \((K^{-1})\) [25]. Thus, Prunty [26] expressed the differential heat of wetting as

\[ W = -0.2932h \]  
(3.50)

3.2.6.4 Transport Coefficient for Adsorbed Liquid Flow

The transport coefficient for adsorbed liquid flow due to temperature gradient is expressed by Groenevelt and Kay [3] as

\[ D_{Ta} = \frac{H_w \epsilon}{b \mu_w T} (1.5548 \times 10^{-15}) \]  
(3.51)

where \( H_w \) is the integral heat of wetting \((J m^{-2})\); \( b = 4 \times 10^{-8} \) \((m)\); \( T \) is in \(^\circ c\).
3. STEMMUS: Governing Equations and Constitutive Equations

3.3 Simplification of Governing Equations

The governing differential equations are derived to be in a simple form containing neatly the three state variables and their coefficients. This allows the conversion of the governing equations to the non-linear ordinary differential equations whose unknowns are the values of the prime variables at a finite number of nodes by using Galerkin’s method of weighted residuals, which will be explained in Chapter 4.

3.3.1 Soil Moisture Equation

The left hand side (LHS) of equation (3.10) can be expanded, considering the dependence of moisture content on matric potential and temperature as follows

\[
\frac{\partial}{\partial t} (\theta_L + \frac{\rho_V}{\rho_l} \theta_V) \\
= \left[ \frac{\partial \theta_L}{\partial t} + \frac{\rho_V}{\rho_l} \frac{\partial (e - \theta_L)}{\partial t} + \theta_V \frac{\partial}{\partial t} \left( \frac{\rho_V}{\rho_l} \right) \right] = \left[ \left( 1 - \frac{\rho_V}{\rho_l} \right) \frac{\partial \theta_L}{\partial h} + \frac{\theta_V}{\rho_l} \frac{\partial \rho}{\partial h} \right] \\
= C_{hh} \frac{\partial h}{\partial t} + C_{hT} \frac{\partial T}{\partial t}
\] (3.52)

where \( \rho_l \) associated with \( \theta_L \) has been eliminated by dividing \( \rho_l \) on the both sides of equation (3.10), the coefficients in above equation can be expressed accordingly as:

\[
C_{hh} = \left( 1 - \frac{\rho_V}{\rho_l} \right) \frac{\partial \theta_L}{\partial h} + \frac{\theta_V}{\rho_l} \frac{\partial \rho}{\partial h} \\
C_{hT} = \left( 1 - \frac{\rho_V}{\rho_l} \right) \frac{\partial \theta_L}{\partial T} + \frac{\theta_V}{\rho_l} \frac{\partial \rho}{\partial T}
\] (3.53)

In the right hand side (RHS) of equation (3.10), the term associated with \( D_{Va} \) should be expanded as

\[
\frac{\partial \left( D_{Va} \frac{\partial P_g}{\partial z} \right)}{\partial z} \\
= D_{Va} \frac{\partial \left( \frac{\partial P_g}{\partial z} \right)}{\partial z} + \frac{\partial D_{Va}}{\partial z} \frac{\partial P_g}{\partial z} \\
= D_{Va} \frac{\partial \left( \frac{\partial P_g}{\partial z} \right)}{\partial z} + K_g \frac{\partial P_g}{\partial z} \frac{\partial \rho}{\partial z} \\
= D_{Va} \frac{\partial \left( \frac{\partial P_g}{\partial z} \right)}{\partial z} + K_g \frac{\partial P_g}{\partial z} \left( \frac{\partial \rho}{\partial h} \frac{\partial h}{\partial z} + \frac{\partial \rho}{\partial T} \frac{\partial T}{\partial z} \right)
\] (3.54)
3.3. Simplification of Governing Equations

Accordingly, the last bracket in the RHS of equation (3.10) can be rewritten as

\[
\frac{1}{\rho_L} \frac{\partial}{\partial z} \left[ D_{Vh} \frac{\partial h}{\partial z} + D_{VT} \frac{\partial T}{\partial z} + D_{Va} \frac{\partial P_g}{\partial z} \right]
\]

\[= \frac{1}{\rho_L} \frac{\partial}{\partial z} \left[ D_{Vh} \frac{\partial h}{\partial z} + D_{VT} \frac{\partial T}{\partial z} \right] + \frac{1}{\rho_L} \left( D_{Va} \frac{\partial}{\partial z} \left( \frac{\partial P_g}{\partial z} \right) + K_g \frac{\partial P_g}{\partial z} \frac{\partial V}{\partial z} \right) \tag{3.55}\]

We can rewrite the RHS of equation (3.10) as

\[
\text{RHS} = \frac{\partial}{\partial z} \left[ K_{hh} \frac{\partial h}{\partial z} + K_{hT} \frac{\partial T}{\partial z} + K_{ha} \frac{\partial P_g}{\partial z} \right] + \frac{\partial K_{Lh}}{\partial z} + V_{Vh} \frac{\partial h}{\partial z} + V_{VT} \frac{\partial T}{\partial z} \tag{3.56}\]

where

\[
K_{hh} = K + \frac{D_{Vh}}{\rho_L} \quad V_{Vh} = -\frac{1}{\rho_L} V_a \frac{\partial V}{\partial h} \\
K_{hT} = \frac{D_{VT}}{\rho_L} \quad V_{VT} = -\frac{1}{\rho_L} V_a \frac{\partial V}{\partial T} \\
K_{ha} = \frac{K}{\gamma_w} + \frac{D_{Va}}{\rho_L} \quad V_a = -K_g \frac{\partial P_g}{\partial z} \tag{3.57}\]

Combining equation (3.52), (3.53), (3.56) and (3.57) yield the moisture equation in the form as below:

\[
C_{hh} \frac{\partial h}{\partial t} + C_{hT} \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left[ K_{hh} \frac{\partial h}{\partial z} + K_{hT} \frac{\partial T}{\partial z} + K_{ha} \frac{\partial P_g}{\partial z} \right] + \frac{\partial K_{Lh}}{\partial z} + V_{Vh} \frac{\partial h}{\partial z} + V_{VT} \frac{\partial T}{\partial z} \tag{3.58}\]

3.3.2 Dry Air Equation

The same procedure applied to equation (3.13), and recall that \(S_a = 1 - S_L\) and \(S_L = \theta_L / \epsilon\) we can have

\[
\frac{\partial}{\partial t} \left[ \epsilon \rho_{da} (S_a + H_c S_L) \right] = \frac{\partial}{\partial t} \left[ \epsilon \rho_{da} (1 - S_L + H_c S_L) \right] \\
= \epsilon \frac{\partial \rho_{da}}{\partial t} + (H_c - 1) \rho_{da} \frac{\partial \theta_L}{\partial t} + (H_c - 1) \theta_L \frac{\partial \rho_{da}}{\partial t} \\
= \left[ \epsilon + (H_c - 1) \theta_L \right] \left( X_{ah} \frac{\partial h}{\partial t} + X_{at} \frac{\partial T}{\partial t} + X_{aa} \frac{\partial P_g}{\partial t} \right) \\
+ (H_c - 1) \rho_{da} \left( \frac{\partial \theta_L}{\partial h} \frac{\partial h}{\partial t} + \frac{\partial \theta_L}{\partial T} \frac{\partial T}{\partial t} \right) \\
= C_{ah} \frac{\partial h}{\partial t} + C_{at} \frac{\partial T}{\partial t} + C_{aa} \frac{\partial P_g}{\partial t} \tag{3.59}\]

3. STEMMUS: Governing Equations and Constitutive Equations

where

\[
C_{ah} = [\epsilon + (H_c - 1)\theta_L]X_{ah} + (H_c - 1)\rho_d a\left|_{\frac{\partial h}{\partial h}}\right. \\
C_{aT} = [\epsilon + (H_c - 1)\theta_L]X_{aT} + (H_c - 1)\rho_d a\left|_{\frac{\partial T}{\partial T}}\right. \\
C_{aa} = [\epsilon + (H_c - 1)\theta_L]X_{aa} + (H_c - 1)\rho_d a\left|_{\frac{\partial P_g}{\partial P_g}}\right.
\]

(3.60)

The RHS of equation (3.13) can be rewritten as below

\[
\frac{\partial}{\partial z}\left[K_{ah} \left(\frac{\partial h}{\partial z} + H_c \rho_d aK + K_{aT} \frac{\partial T}{\partial z} + K_{aa} \frac{\partial P_g}{\partial z}\right)\right] \\
= \frac{\partial}{\partial z}\left[(D_V + \theta_a D_Vg) \left(\frac{\partial h}{\partial z} + X_{aT} \frac{\partial T}{\partial z} + X_{aa} \frac{\partial P_g}{\partial z}\right) + \rho_d aK_g \frac{\partial P_g}{\partial z}\right] \\
+ K_g \frac{\partial P_g}{\partial z} - H_c \frac{p_L}{\rho_L} \left(\frac{\partial h}{\partial z} + X_{aT} \frac{\partial T}{\partial z} + X_{aa} \frac{\partial P_g}{\partial z}\right) \\
+ H_c \rho_d a \frac{\partial}{\partial z}\left[K \frac{\partial}{\partial z}\left(h + p_L + z\right) + D_T \frac{\partial T}{\partial z}\right]
\]

(3.61)

The RHS of equation (3.13) can be rewritten as

\[
\text{RHS} = \frac{\partial}{\partial z}\left[K_{ah} \left(\frac{\partial h}{\partial z} + K_{aT} \frac{\partial T}{\partial z} + K_{aa} \frac{\partial P_g}{\partial z}\right)\right] \\
+ V_{ah} \frac{\partial h}{\partial z} + V_{aT} \frac{\partial T}{\partial z} + V_{aa} \frac{\partial P_g}{\partial z} + H_c \rho_d a \frac{\partial K}{\partial z}
\]

(3.62)
where

\[K_{ah} = (D_V + \theta_a D_V \theta_a) X_{ah} + H_c \rho_d a K\]
\[K_{aT} = (D_V + \theta_a D_V \theta_a) X_{aT} + H_c \rho_d a D_{Ta}\]
\[K_{aa} = (D_V + \theta_a D_V \theta_a) X_{aa} + \rho_d a (K_\theta + H_c \frac{K_{\gamma}}{Y_w})\]

\[V_{ah} = \left[ K_{\theta} \frac{\partial P_\theta}{\partial z} - H_c \frac{q_L}{\rho_L} \right] X_{ah} \quad (3.63)\]
\[V_{aT} = \left[ K_{\theta} \frac{\partial P_\theta}{\partial z} - H_c \frac{q_L}{\rho_L} \right] X_{aT}\]
\[V_{aa} = \left[ K_{\theta} \frac{\partial P_\theta}{\partial z} - H_c \frac{q_L}{\rho_L} \right] X_{aa}\]

Combining equation (3.59) and equation (3.62), the dry air mass equation can be represented as below:

\[\frac{C_{ah}}{\partial t} \frac{\partial h}{\partial t} + \frac{C_{aT}}{\partial t} \frac{\partial T}{\partial t} + \frac{C_{aa}}{\partial t} \frac{\partial \theta_T}{\partial t} = \frac{\partial}{\partial z} \left[ K_{ah} \frac{\partial h}{\partial z} + K_{aT} \frac{\partial T}{\partial z} + K_{aa} \frac{\partial \theta_T}{\partial z} \right] + V_{ah} \frac{\partial h}{\partial z} + V_{aT} \frac{\partial T}{\partial z} + V_{aa} \frac{\partial \theta_T}{\partial z} + H_c \rho_d a \frac{\partial K}{\partial z} \quad (3.64)\]

### 3.3.3 Energy Equation

Equation (3.19) can be rewritten in a brief form as:

\[\frac{\partial C_{unsat}(T - T_r)}{\partial t} + L_0 \frac{\partial \rho_V \theta_\theta}{\partial t} - \rho_L W \frac{\partial \theta_L}{\partial t} = \frac{\partial}{\partial z} \left( \lambda_{eff} \frac{\partial T}{\partial z} \right) \quad (3.65)\]

\[-\frac{\partial}{\partial z} \left[ q_T c_T (T - T_r) + q_V (c_V (T - T_r) + L_0) + q_a c_a (T - T_r) \right] \]

The LHS of equation (3.65) can be expressed as:

\[\frac{\partial}{\partial t} \left[ C_{unsat} (T - T_r) \right] + L_0 \frac{\partial \rho_V \theta_\theta}{\partial t} - \rho_L W \frac{\partial \theta_L}{\partial t} = \frac{\partial}{\partial t} \left[ C_{unsat} (T - T_r) \right] + L_0 \frac{\partial \rho_V (\epsilon - \theta_L)}{\partial t} - \rho_L W \frac{\partial \theta_L}{\partial t} \quad (3.66)\]

\[= \frac{\partial}{\partial t} \left[ C_{unsat} (T - T_r) \right] + L_0 (\epsilon - \theta_L) \frac{\partial \rho_V}{\partial t} - (L_0 \rho_V + \rho_L W) \frac{\partial \theta_L}{\partial t}\]
3. STEMMUS: Governing Equations and Constitutive Equations

Where \( \frac{\partial}{\partial t} C_{\text{unsat}}(T - T_r) \) can be expanded as:

\[
\frac{\partial}{\partial t} \left[ C_{\text{unsat}}(T - T_r) \right] = C_{\text{unsat}} \frac{\partial (T - T_r)}{\partial t} + (T - T_r) \frac{\partial C_{\text{unsat}}}{\partial t}
\]

\[
= C_{\text{unsat}} \frac{\partial T}{\partial t} + (T - T_r) \frac{\partial }{\partial t} \left[ \rho_c c_L \frac{\partial \theta}{\partial t} + (\epsilon - \theta_L)c_a \frac{\partial \rho_{da}}{\partial t} - \rho_{da} c_a \frac{\partial \theta}{\partial t} + (\epsilon - \theta_L)c_v \frac{\partial \rho_V}{\partial t} - \rho_V c_v \frac{\partial \theta}{\partial t} \right] \tag{3.67}
\]

After substituting equation (3.67) into equation (3.66) and rearrangement, we have the LHS of equation (3.65) as

\[
LHS = [(T - T_r)(\rho_c c_L - \rho_{da} c_a - \rho_V c_v) - (L_0 \rho_V + \rho_L W)] \frac{\partial \theta}{\partial t} + (T - T_r)(\epsilon - \theta_L)c_a \frac{\partial \rho_{da}}{\partial t} + [(T - T_r)(\epsilon - \theta_L)c_v + L_0(\epsilon - \theta_L)] \frac{\partial \rho_V}{\partial h}
\]

\[
+ [(T - T_r)(\epsilon - \theta_L)c_v + L_0(\epsilon - \theta_L)] \left( \frac{\partial \rho_V}{\partial h} \frac{\partial h}{\partial \theta} \right) + (T - T_r)(\epsilon - \theta_L)c_a \frac{\partial \rho_{da}}{\partial t} + (T - T_r)(\epsilon - \theta_L)c_v \frac{\partial \rho_V}{\partial t}
\]

\[
= C_{Th} \frac{\partial h}{\partial \theta} + C_{TT} \frac{\partial T}{\partial \theta} + C_{Ta} \frac{\partial p_g}{\partial \theta} \tag{3.68}
\]

where

\[
C_{Th} = [(T - T_r)(\rho_c c_L - \rho_{da} c_a - \rho_V c_v) - (L_0 \rho_V + \rho_L W)] \frac{\partial \theta}{\partial h} + (T - T_r)(\epsilon - \theta_L)c_a X_{gh} + [(T - T_r)(\epsilon - \theta_L)c_v + L_0(\epsilon - \theta_L)] \frac{\partial \rho_V}{\partial h}
\]

\[
C_{TT} = [(T - T_r)(\rho_c c_L - \rho_{da} c_a - \rho_V c_v) - (L_0 \rho_V + \rho_L W)] \frac{\partial \theta}{\partial T} + (T - T_r)(\epsilon - \theta_L)c_a X_{gT}
\]

\[
+ [(T - T_r)(\epsilon - \theta_L)c_v + L_0(\epsilon - \theta_L)] \frac{\partial \rho_V}{\partial T} + C_{unsat}
\]

\[
C_{Ta} = (T - T_r)(\epsilon - \theta_L)c_a X_{gT} \tag{3.69}
\]

Now, using relation of \( c_v(T - T_r) + L_0 = c_L(T - T_r) + L \) and \( q_m = q_L + q_V \), applying the same procedure above to the RHS of equation yields (3.65)

\[
\frac{\partial}{\partial z} \left( \lambda_{eff} \frac{\partial T}{\partial z} \right) = \frac{\partial}{\partial z} \left[ q_L c_L(T - T_r) + q_V(c_v(T - T_r) + L_0) + q_a c_a(T - T_r) \right] \tag{3.70}
\]

\[
= \frac{\partial}{\partial z} \left[ \lambda_{eff} \frac{\partial T}{\partial z} - (q_L c_L + q_a c_a)(T - T_r) - q_v(c_v(T - T_r) + L) \right]
\]

3.3. Simplification of Governing Equations

Substituting expressions of $q_L$, $q_V$ and $q_a$ into equation (3.70), we have the RHS as

$$RHS = \frac{\partial}{\partial z} \left[ \lambda_{eff} \frac{\partial T}{\partial z} - (q_m c_L + q_a c_a)(T - T_r) - q_V L \right]$$

$$= \frac{\partial}{\partial z} \left( \lambda_{eff} \frac{\partial T}{\partial z} \right)$$

$$+ c_L (T - T_r) \left[ \frac{\partial}{\partial z} \left( K_{hh} \frac{\partial h}{\partial z} + K_{hr} \frac{\partial T}{\partial z} + K_{ha} \frac{\partial P_a}{\partial z} \right) \right]$$

$$+ c_a (T - T_r) \left[ \frac{\partial}{\partial z} \left( K_{ah} \frac{\partial h}{\partial z} + K_{ar} \frac{\partial T}{\partial z} + K_{aa} \frac{\partial P_a}{\partial z} \right) \right]$$

$$+ V_{hh} \frac{\partial h}{\partial z} + V_{ht} \frac{\partial T}{\partial z} + \frac{\partial K}{\partial z}$$

$$+ V_{ha} \frac{\partial h}{\partial z} + V_{ht} \frac{\partial T}{\partial z} + V_{aa} \frac{\partial P_a}{\partial z} + H_c \rho a \frac{\partial K}{\partial z}$$

$$+ L \frac{\partial}{\partial z} \left[ \left( D_V + \theta_V D_{Vg} \right) \left( \frac{\partial \rho V}{\partial h} \frac{\partial T}{\partial z} + \frac{\partial \rho V}{\partial T} T \right) \right]$$

$$+ \left[ \left( D_V + \theta_V D_{Vg} \right) \frac{\partial P_a}{\partial z} + \rho_a K_g \frac{\partial P_a}{\partial z} \right] c \frac{\partial T}{\partial z}$$

$$+ \left[ \left( D_V + \theta_a D_{Vg} \right) \frac{\partial P_a}{\partial z} + \rho_a K_g \frac{\partial P_a}{\partial z} \right] c \frac{\partial T}{\partial z}$$

$$= \frac{\partial}{\partial z} \left( K_{hh} \frac{\partial h}{\partial z} + K_{hr} \frac{\partial T}{\partial z} + K_{ha} \frac{\partial P_a}{\partial z} \right)$$

$$+ V_{hh} \frac{\partial h}{\partial z} + V_{ht} \frac{\partial T}{\partial z} + V_{aa} \frac{\partial P_a}{\partial z} + c \frac{\partial T}{\partial z}$$

$$= \frac{\partial}{\partial z} \left( K_{hh} \frac{\partial h}{\partial z} + K_{hr} \frac{\partial T}{\partial z} + K_{ha} \frac{\partial P_a}{\partial z} \right)$$

$$+ V_{hh} \frac{\partial h}{\partial z} + V_{ht} \frac{\partial T}{\partial z} + V_{aa} \frac{\partial P_a}{\partial z} + c \frac{\partial T}{\partial z}$$

where

$$K_{hh} = c_L (T - T_r) K_{hh} + c_a (T - T_r) K_{ha} + L (D_V + \theta_V D_{Vg}) \frac{\partial \rho V}{\partial h}$$

$$K_{hr} = \lambda_{eff} + c_L (T - T_r) K_{hr} + c_a (T - T_r) K_{ar} + L (D_V + \theta_V D_{Vg}) \frac{\partial \rho V}{\partial T}$$

$$K_{ha} = c_L (T - T_r) K_{ha} + c_a (T - T_r) K_{aa} + L \rho V K_g$$

$$V_{hh} = c_L (T - T_r) V_{hh} + c_a (T - T_r) V_{ha} + (D_V + \theta_V D_{Vg}) \frac{\partial \rho V}{\partial h} + c_a (D_V + \theta_a D_{Vg}) X_{ah} + (c_L + H_c \rho da) \frac{ca}{\rho_L} K$$

$$V_{ht} = c_L (T - T_r) V_{ht} + c_a (T - T_r) V_{at} + (D_V + \theta_V D_{Vg}) \frac{\partial \rho V}{\partial T} + c_a (D_V + \theta_a D_{Vg}) X_{at} + (c_L + H_c \rho da) \frac{ca}{\rho_L} D_{Ta}$$

$$V_{aa} = c_L K_g \frac{\partial \rho V}{\partial h} + c_a (T - T_r) V_{aa}$$

$$+ c_a \left[ (D_V + \theta_a D_{Vg}) X_{aa} + \rho_a K_g \right] + (c_L + H_c \rho da) \frac{ca}{\rho_L} K$$

$$C_T = \left[ c_L (T - T_r) + c_a (T - T_r) H_c \rho da \right] \frac{\partial K}{\partial z} + (c_L + H_c \rho da) \frac{ca}{\rho_L} K$$
3. STEMMUS: Governing Equations and Constitutive Equations

Combing equation (3.68) and equation (3.71), the energy equation can be rewritten as

\[
C_{Th} \frac{\partial h}{\partial t} + C_{TT} \frac{\partial T}{\partial t} + C_{Ta} \frac{\partial P_g}{\partial t}
\]

\[
= \frac{\partial}{\partial z} \left( K_{Th} \frac{\partial h}{\partial z} + K_{TT} \frac{\partial T}{\partial z} + K_{Ta} \frac{\partial P_g}{\partial z} \right) + V_{Th} \frac{\partial h}{\partial z} + V_{TT} \frac{\partial T}{\partial z} + V_{Ta} \frac{\partial P_g}{\partial z} + C_{T\theta}
\]

3.4 Bibliography


3.4. Bibliography


STEMMUS: Finite Element Solution of Governing Equations
4. STEMMUS: Finite Element Solution of Governing Equations

4.1 Galerkin’s Method of Weighted Residuals

The governing differential equations are converted to non-linear ordinary differential equations whose unknowns are the values of the prime variables at a finite number of nodes by using Galerkin’s method of weighted residuals. Then, a finite-difference time-stepping scheme is applied to evaluate the time derivatives, which is solved by a successive linearization iterative scheme. To describe the spatial discretization and time stepping of the governing equations, an example of the derivation is presented below, using the moisture equation. For the dry air equation and the energy equation, the procedure is similar.

The standard piece-wise linear basis functions for approximation of the prime variables are expressed as

\[
\hat{h}(z,t) = h_1 \phi_1 + h_2 \phi_2 = \sum_{j=1}^{2} h_j(t) \phi_j(z)
\]

\[
\hat{T}(z,t) = T_1 \phi_1 + T_2 \phi_2 = \sum_{j=1}^{2} T_j(t) \phi_j(z)
\]

\[
\hat{P}_g(z,t) = P_{g1} \phi_1 + P_{g2} \phi_2 = \sum_{j=1}^{2} P_{gj}(t) \phi_j(z)
\]

where \(j\) is the node index, and \(\phi_j(z)\) the usual shape function defined element by element (\(\phi_1 = \frac{z-e}{\Delta}, \phi_2 = \frac{e-z}{\Delta}\)). If the approximations given by equation (4.1) are substituted into the equations (3.10), (3.13) and (3.19), residuals are obtained for each governing differential equation, which are then minimized using Galerkin’s method. Introducing the new notation for the coefficients in the moisture mass conservation equation, equation (3.10) becomes

\[
M_{moisture}(h, T) = c_1 \frac{\partial h}{\partial t} + c_2 \frac{\partial T}{\partial t} - \frac{\partial}{\partial z} \left( c_3 \frac{\partial h}{\partial z} + c_4 \frac{\partial T}{\partial z} + c_5 \frac{\partial P_g}{\partial z} + c_6 \right) - c_7 \frac{\partial h}{\partial z} - c_8 \frac{\partial T}{\partial z} \tag{4.2}
\]

where \(c_1\) to \(c_8\) are defined implicitly by equation (3.10) and (4.2). Following Galerkin’s method of weighted residuals [1] for each element, the residuals obtained by substituting \(\hat{h}, \hat{T}\) and \(P_g\) into equation (4.2) are required to be orthogonal to the set of trial functions:

\[
\int_z \left[ c_1 \frac{\partial \hat{h}}{\partial t} + c_2 \frac{\partial \hat{T}}{\partial t} - \frac{\partial}{\partial z} \left( c_3 \frac{\partial \hat{h}}{\partial z} + c_4 \frac{\partial \hat{T}}{\partial z} + c_5 \frac{\partial \hat{P}_g}{\partial z} + c_6 \right) - c_7 \frac{\partial \hat{h}}{\partial z} - c_8 \frac{\partial \hat{T}}{\partial z} \right] \phi_i \, dz = 0 \tag{4.3}
\]

where \(z\) is the solution domain, and \(i = 1, 2\). We apply integration by part (\(\int u dv = uv - \int v du\)) to the third, fourth and fifth term, which may
be recognized as the flux divergence.

\[
\int_z \left(c_1 \frac{\partial \hat{h}}{\partial t} + c_2 \frac{\partial \hat{T}}{\partial t}\right) \phi_i \, dz + \int_z \left(c_3 \frac{\partial \hat{h}}{\partial z} + c_4 \frac{\partial \hat{T}}{\partial z} + c_5 \frac{\partial \hat{p}_d}{\partial z} + c_6 \right) \phi_i \, dz + \int_z c_7 \hat{h} \phi_i' \, dz + \int_z c_8 \hat{T} \phi_i' \, dz = \left[\left(c_3 \frac{\partial \hat{h}}{\partial z} + c_4 \frac{\partial \hat{T}}{\partial z} + c_5 \frac{\partial \hat{p}_d}{\partial z} + c_6 \right) + c_7 \hat{h} + c_8 \hat{T}\right] \phi_i \bigg|_{z_1}^{z_2} = [-Q_m \phi_i]_{z_1}^{z_2}
\]  

where \( z_1 \) and \( z_2 \) are two points in one element and subscripted according to a local numbering system. According to the definition of \( c_3, c_4, c_5, c_6, c_7 \) and \( c_8 \), \( Q_m \) is implicitly seen as the sum of liquid and vapor mass flux. Now, substituting from equation (4.1) into equation (4.4) yields

\[
\sum_{j=1}^2 h_j \int c_1 \phi_j \phi_i \, dz + \sum_{j=1}^2 T_j \int c_2 \phi_j \phi_i \, dz + \sum_{j=1}^2 h_j \int c_3 \phi_j' \phi_i' \, dz + \sum_{j=1}^2 T_j \int c_4 \phi_j' \phi_i' \, dz + \sum_{j=1}^2 p_{hj} \int c_5 \phi_j' \phi_i' \, dz + \int c_6 \phi_i' \, dz + \sum_{j=1}^2 h_j \int c_7 \phi_j \phi_i' \, dz + \sum_{j=1}^2 T_j \int c_8 \phi_j \phi_i' \, dz = [-Q_m \phi_i]_{z_1}^{z_2}
\]  

4.2 Integrals’ Calculation

In equation (4.5), the primed state variables are time derivatives. Equation (4.5) can be interpreted as approximate mass conservation relations for node 1 and 2. Their sum is a mass conservation condition for the element. The ‘\( c \)’ coefficients are assumed to vary linearly within the element. Their values at the nodes could be given by

\[
c_{m1} = c_m(h_1, T_1) \\
c_{m2} = c_m(h_2, T_2)
\]  

where \( m = 1, 2, \ldots, 8 \). If \( c \) is discontinuous at a node, it is evaluated as the limit of \( c \) that is approached from inside the element. Given this form for the variation of the coefficient, we may proceed to evaluate the integrals in equation (4.5), using the definitions from equation (4.1). Taking the first item in equation (4.5) as an example, we have

\[
\int c_1 \phi_j \phi_i \, dz = \int c_{11} \phi_j \phi_i \, dz + \int c_{12} \phi_j \phi_i \, dz
\]  

where in general, we can get \( \int \phi_k \phi_j \phi_i \, dz \) for equation (4.7). Recall that, \( \phi_1 \) equals to \( \frac{z_2 - z}{\Delta z} \) and \( \phi_2 \) equals to \( \frac{z - z_1}{\Delta z} \).
When \( i = j = k \):

\[
\int \phi_k \phi_j \phi_i dz = \int_{z_e}^{z_{e+1}} \phi_1^3 dz \\
= \int_{z_e}^{z_{e+1}} \left( \frac{z_e+1-z}{\Delta} \right)^3 dZ = \left[ -\frac{\Delta}{4} \left( \frac{z_e+1-z}{\Delta} \right)^4 \right]_{z_e}^{z_{e+1}} = \frac{\Delta}{4}
\]

\[
\int \phi_k \phi_j \phi_i dz = \int_{z_e}^{z_{e+1}} \phi_j^3 dz \\
= \int_{z_e}^{z_{e+1}} \left( \frac{z - z_e}{\Delta} \right)^3 dz = \left[ -\frac{\Delta}{4} \left( \frac{z - z_e}{\Delta} \right)^4 \right]_{z_e}^{z_{e+1}} = \frac{\Delta}{4}
\]

(4.8)

when otherwise:

\[
\int \phi_k \phi_j \phi_i dz = \int_{z_e}^{z_{e+1}} \phi_1^3 \phi_2^3 dz \\
= \int_{z_e}^{z_{e+1}} \left( \frac{z_e+1-z}{\Delta} \right)^2 \left( \frac{z - z_e}{\Delta} \right)^3 dZ \\
= -\frac{\Delta}{3} \int_{z_e}^{z_{e+1}} \frac{z - z_e}{\Delta} \phi (\frac{z_e+1-z}{\Delta})^3 dz \\
= -\frac{\Delta}{3} \int_{z_e}^{z_{e+1}} \left( \frac{z - z_e}{\Delta} \right)^3 \frac{z_e+1-z}{\Delta} dz + \frac{\Delta}{3} \int_{z_e}^{z_{e+1}} \left( \frac{z - z_e}{\Delta} \right)^3 dz \\
= \frac{1}{3} \int_{z_e}^{z_{e+1}} \left( \frac{z_e+1-z}{\Delta} \right)^3 = \frac{1}{3} \int_{z_e}^{z_{e+1}} \left[ -\frac{\Delta}{4} \left( \frac{z_e+1-z}{\Delta} \right)^4 \right]_{z_e}^{z_{e+1}} = \frac{\Delta}{12}
\]

Above result is the same for the integrals containing \( C_2 \), which could be defined as the first type of integrals. As for the second type of integrals related to \( c_3, c_4 \) and \( c_5 \), we have

\[ c_3 \phi_j' \phi_i' dz = c_31 \phi_j' \phi_i' dz + c_32 \phi_i' \phi_i' dz \]

(4.10)

The general form for the above integrals is \( \int \phi_k \phi_j' \phi_i' dz \). Accordingly,

When \( i = j \):

\[
\int \phi_k \phi_j' \phi_i' dz = \int_{z_e}^{z_{e+1}} \phi_1 \phi_i' \phi_i' dz \\
= \int_{z_e}^{z_{e+1}} \left( \frac{z - z_e}{\Delta} \right)^2 dZ = \left( -\frac{1}{\Delta} \right)^2 \int_{z_e}^{z_{e+1}} \frac{1}{\Delta} \left( \frac{z - z_e}{\Delta} \right)^2 dZ = \frac{1}{2\Delta}
\]

(4.11)

when \( i \neq j \):

\[
\int \phi_k \phi_j' \phi_i' dz = \int_{z_e}^{z_{e+1}} \phi_2 \phi_i' \phi_i' dz \\
= \int_{z_e}^{z_{e+1}} \left( \frac{z - z_e}{\Delta} \right)^2 dZ = \left( -\frac{1}{\Delta} \right)^2 \int_{z_e}^{z_{e+1}} \frac{1}{\Delta} \left( \frac{z - z_e}{\Delta} \right)^2 dZ = -\frac{1}{2\Delta}
\]

(4.12)
4.2. Integrals’ Calculation

The same method applied to the integrals associated with $c_6$:

$$\int c_6 \phi'_idz = c_{61} \int \phi_1 \phi'_idz + c_{62} \int \phi_2 \phi'_idz$$  \hspace{1cm} (4.13)

where in general, we can get $\int \phi_k \phi'_idz$.

When $i = 1$:

$$\int \phi_k \phi'_idz = \int_{z_e}^{z_{e+1}} \phi_1 \phi'_idz$$  \hspace{1cm} (4.14)

$$= \int_{z_e}^{z_{e+1}} \left( \frac{z_{e+1} - z}{\Delta} \right) \left( -\frac{1}{\Delta} \right) \, dz = -\frac{1}{\Delta} \left[ \frac{z_{e+1} - z}{\Delta} \right]_{z_e}^{z_{e+1}} = -\frac{1}{2}$$

when $i = 2$:

$$\int \phi_k \phi'_idz = \int_{z_e}^{z_{e+1}} \phi_1 \phi'_idz$$  \hspace{1cm} (4.15)

$$= \int_{z_e}^{z_{e+1}} \left( \frac{z - z_e}{\Delta} \right) \left( \frac{1}{\Delta} \right) \, dz = \frac{1}{\Delta} \left[ \frac{(z - z_e)}{\Delta} \right]_{z_e}^{z_{e+1}} = \frac{1}{2}$$

For the integrals associated with $c_7$ and $c_8$, we have

$$\int c_7 \phi_j \phi'_idz = c_{71} \int \phi_1 \phi_j \phi'_idz + c_{72} \int \phi_2 \phi_j \phi'_idz$$  \hspace{1cm} (4.16)

where in general, we can get $\int \phi_k \phi_j \phi'_idz$. The integrals associated with $c_7$ and $c_8$ are more complicated than the integrals mentioned above.

When $k = j$ and $i = 1$:

$$\int \phi_k \phi_j \phi'_idz$$

$$= \int_{z_e}^{z_{e+1}} \left( \frac{z_{e+1} - z}{\Delta} \right) \left( \frac{z - z_e}{\Delta} \right) \left( -\frac{1}{\Delta} \right) \, dz$$

$$= -\frac{1}{\Delta} \int_{z_e}^{z_{e+1}} \frac{\Delta}{2} \left( \frac{z_{e+1} - z}{\Delta} \right) \, dz = -\frac{1}{\Delta} \left[ \frac{\Delta}{3} \left( \frac{z_{e+1} - z}{\Delta} \right)^3 \right]_{z_e}^{z_{e+1}} = -\frac{1}{3}$$  \hspace{1cm} (4.17)

when $k \neq j$ and $i = 1$:

$$\int \phi_k \phi_j \phi'_idz$$

$$= \int_{z_e}^{z_{e+1}} \left( \frac{z_{e+1} - z}{\Delta} \right) \left( \frac{z - z_e}{\Delta} \right) \left( -\frac{1}{\Delta} \right) \, dz$$

$$= -\frac{1}{\Delta} \int_{z_e}^{z_{e+1}} \frac{\Delta}{2} \left( \frac{z_{e+1} - z}{\Delta} \right) \, dz$$

$$= -\frac{1}{\Delta} \left[ \frac{\Delta}{2} \left( \frac{z_{e+1} - z}{\Delta} \right)^2 \right]_{z_e}^{z_{e+1}} + \frac{1}{\Delta} \int_{z_e}^{z_{e+1}} \frac{\Delta}{2} \left( \frac{z - z_e}{\Delta} \right)^2 \, dz$$

$$= -\frac{1}{\Delta^2} \left[ \frac{\Delta}{2} \left( \frac{z_{e+1} - z}{\Delta} \right)^2 \right]_{z_e}^{z_{e+1}} + \frac{1}{\Delta^2} \left[ \frac{\Delta}{3} \left( \frac{z - z_e}{\Delta} \right)^3 \right]_{z_e}^{z_{e+1}} = -\frac{1}{6}$$  \hspace{1cm} (4.18)
when \( k = j \) and \( i = 2 \):

\[
\int \phi_k \phi_j \phi_i' dz = \int_{z_e}^{z_{e+1}} \left( \frac{z - z_e}{\Delta} \right)^2 \left( \frac{1}{\Delta} \right) dz = \frac{1}{\Delta} \left[ -\frac{\Delta}{3} \left( \frac{z_{e+1} - z}{\Delta} \right)^3 \right]_{z_e}^{z_{e+1}} = \frac{1}{3}
\]

and

\[
\int \phi_k \phi_j \phi_i' dz = \int_{z_e}^{z_{e+1}} \left( \frac{z - z_e}{\Delta} \right)^2 \left( \frac{1}{\Delta} \right) dz = \frac{1}{\Delta} \left[ \frac{\Delta}{3} \left( \frac{z - z_e}{\Delta} \right)^3 \right]_{z_e}^{z_{e+1}} = \frac{1}{3}
\]  

when \( k \neq j \) and \( i = 2 \):

\[
\int \phi_k \phi_j \phi_i' dz = \int_{z_e}^{z_{e+1}} \left( \frac{z_{e+1} - z}{\Delta} \right) \left( \frac{z - z_e}{\Delta} \right) \left( \frac{1}{\Delta} \right) dz = \frac{1}{\Delta} \int_{z_e}^{z_{e+1}} \frac{\Delta}{2} \left( \frac{z_{e+1} - z}{\Delta} \right) d \left( \frac{z - z_e}{\Delta} \right)^2 \\
= \frac{1}{\Delta^2} \int_{z_e}^{z_{e+1}} \frac{\Delta}{2} \left( \frac{z - z_e}{\Delta} \right)^2 \left[ \frac{\Delta}{3} \left( \frac{z - z_e}{\Delta} \right)^3 \right]_{z_e}^{z_{e+1}} = \frac{1}{6}
\]  

We may evaluate the right-hand-side term of equation (4.5) as:

\[
[-Q_m \phi_i]_{z_e}^{z_{e+1}} = \begin{cases} 
Q_m \bigg|_{z_e}, & i = 1 \\
-Q_m \bigg|_{z_{e+1}}, & i = 2 
\end{cases}
\]

### 4.3 Finite Difference Time-Stepping Scheme

Having evaluated the coefficients in equation (4.5), we now rewrite that equation system in matrix form:

\[
\begin{bmatrix}
A_{11} & A_{12} & h_1' \hline
A_{21} & A_{22} & h_2'
\end{bmatrix}
\begin{bmatrix}
h_1' \\
h_2'
\end{bmatrix}
+ 
\begin{bmatrix}
B_{11} & B_{12} & T_1' \\
B_{21} & B_{22} & T_2'
\end{bmatrix}
\begin{bmatrix}
T_1' \\
T_2'
\end{bmatrix}
+ 
\begin{bmatrix}
C_{11} & C_{12} & h_1 \\
C_{21} & C_{22} & h_2
\end{bmatrix}
\begin{bmatrix}
h_1 \\
h_2
\end{bmatrix}
+ 
\begin{bmatrix}
D_{11} & D_{12} & T_1 \\
D_{21} & D_{22} & T_2
\end{bmatrix}
\begin{bmatrix}
T_1 \\
T_2
\end{bmatrix}
+ 
\begin{bmatrix}
E_{11} & E_{12} & P_1 \\
E_{21} & E_{22} & P_2
\end{bmatrix}
\begin{bmatrix}
P_1 \\
P_2
\end{bmatrix}
+ 
\begin{bmatrix}
F_1 \\
F_2
\end{bmatrix}
= 
\begin{bmatrix}
Q_m \bigg|_{z_1} \\
-Q_m \bigg|_{z_2}
\end{bmatrix}
\] (4.22)
where

\[
A_{ij} = c_1 \int \phi_j \phi_i dz, \quad B_{ij} = c_2 \int \phi_j \phi_i dz \\
C_{ij} = c_3 \int \phi_j' \phi'_i dz + c_7 \int \phi_j \phi_i dz \\
D_{ij} = c_4 \int \phi_j' \phi_i dz + c_8 \int \phi_j \phi_i dz \\
E_{ij} = c_5 \int \phi_j' \phi_i dz, \quad F_{ij} = c_6 \int \phi'_i dz
\]

(4.23)

Now, considering that the boundaries separating individual elements are points at which discontinuities may occur, coupling will be accomplished through the matching of boundary conditions at the discontinuities. The coupling conditions give us

\[
\begin{align*}
A_{ij} & = B_{ij} = C_{ij} = D_{ij} = E_{ij} = F_{ij} = 0 \\
T_1 & = T_2 \\
p_{ij} & = p_{ij}
\end{align*}
\]

(4.24)

Expanding equation (4.22) from one element to two elements, introducing the global index for the coordinate \( z \) and for the state variables (i.e. superscript takes on values of \( 1 \) and \( 2 \)), and remembering the element indices increase in the positive upward \( z \) direction, we get

\[
\begin{pmatrix}
A_{11}^1 & A_{12}^1 & 0 & h_1' & B_{11}^1 & B_{12}^1 & 0 & T_1' \\
A_{21}^1 & A_{22}^1 + A_{11}^2 & A_{12}^2 & h_2' & B_{21}^1 & B_{22}^1 + B_{11}^2 & B_{12}^2 & T_2'
\end{pmatrix}
\]

\[
+ \begin{pmatrix}
C_{11}^1 & C_{12}^1 & 0 & h_1 & D_{11}^1 & D_{12}^1 & 0 & T_1 \\
C_{21}^1 & C_{22}^1 + C_{11}^2 & C_{12}^2 & h_2 & D_{21}^1 & D_{22}^1 + D_{11}^2 & D_{12}^2 & T_2
\end{pmatrix}
\]

\[
+ \begin{pmatrix}
E_{11}^1 & E_{12}^1 & 0 & p_{g1} & F_{11}^1 & F_{12}^1 & 0 & Q_m^1 |_{z1} \\
E_{21}^1 & E_{22}^1 + E_{11}^2 & E_{12}^2 & p_{g2} & F_{21}^1 & F_{22}^1 & F_{12}^2 & -Q_m^1 |_{z3}
\end{pmatrix}
\]

(4.25)

From equation (4.25) we know that the extension of this procedure will cover \( N \) nodes (\( N-1 \) elements) straightforward. The final pair of matrix equation for moisture balance equation is

\[
A_k h' + B_k T' + C_k h + D_k T + E_k p_{\theta} + F_k = Q_k
\]

(4.26)

Where \( k = 1, 2 \) and \( 3 \). To obtain the temporal solution to above equation, a fully implicit, backward difference scheme is used. This means that all terms other than the time derivative are evaluated at the end of the time step

\[
A_k \frac{h^k - h^{k-1}}{\Delta t} + B_k \frac{T^k - T^{k-1}}{\Delta t} + C_k h^k + D_k T^k + E_k p^k_{\theta} + F_k = Q_m^k
\]

(4.27)
where $\Delta t$ is the time increment. An implicit integration scheme is usually much more stable than an explicit one. Considering $h^k$ to be unknown yields

$$\left( \frac{A^k}{\Delta t} + C^k \right) h^k = \frac{A^k}{\Delta t} h^{k-1} - \left( \frac{B^k}{\Delta t} + D^k \right) T^k + \frac{B^k}{\Delta t} T^{k-1} - E^k P_g^k - F^k + Q_m^k$$

(4.28)

where $k$ is a time index and $\Delta t$ is the length of the time step. The coefficient matrices in equation (4.27) are to be evaluated at the new time level with an iterative scheme, which updates the coefficient matrices at each iteration until desired convergence criteria are achieved. The iterative solution strategy is implemented in STEMMUS [2]:

1. Extrapolate the solutions for the last two time steps ($k - 2$ and $k - 1$) forward to obtain an estimate of $h^k$, $T^k$ and $P_g^k$ (If this is the first time stop, only the $k - 1$ 'solution' is available - it is the initial condition. In this case, we can assume $h^k$ and $T^k$ are given by the initial conditions for a first guess.);
2. Use the estimated states to evaluate all components (except $h^k$) in equation (4.27). Solve the resulting tridiagonal matrix equation for $h^k$;
3. Use the latest estimates of $h^k$, $T^k$ and $P_g^k$ to evaluate and solve for $P_g^k$ in air equation similar to equation (4.27);
4. Use the latest estimates of $h^k$, $T^k$ and $P_g^k$ to evaluate and solve for $T^k$ in energy equation similar to equation (4.27);
5. Repeat steps 2 and 4 until some convergence criterion is met.

With this algorithm, we never need to solve a matrix equation any more complex than one in which the matrix is tridiagonal. A very fast procedure exists for the solution of such equations (e.g. Thomas algorithm). Note that it is possible to incorporate any of the boundary conditions, including the non-linear ones, into this iterative procedure, using the methods shown below:

In a problem where flux boundary conditions are prescribed, the relevant $Q'$s are substituted into the right-hand-side vector, and the four unknown states are found by integrating the system. On the other hand, if one or more of the states is fixed at a node (first-type boundary condition), the equations containing the unknown flux through that node is eliminated from the system of equations, keeping the solution uniquely determined. After solution, the neglected equations may be used to determine boundary fluxes [2].

Most of investigators have found that the form of the storage matrices generated by the Galerkin method often lead to numerical difficulties. A commonly accepted means of overcoming these problems is to diagonalize, or lump the storage matrix. Consider the first matrix of equation...
4.3. 

Finite Difference Time-Stepping Scheme

(4.22), we obtain

\[
\frac{1}{h} \sum_{j=1}^{2} c_1 \phi_j \phi_1 \, dz = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} h'_1 \\ h'_2 \end{bmatrix} = \begin{bmatrix} c_{11} \phi_1 \phi_1 (1 + c_{12} \phi_2 \phi_1) + c_{11} \phi_1 \phi_2 (1 + c_{12} \phi_2 \phi_1) \\ c_{11} \phi_1 \phi_2 (1 + c_{12} \phi_2 \phi_1) + c_{11} \phi_1 \phi_2 (1 + c_{12} \phi_2 \phi_1) \end{bmatrix} \begin{bmatrix} h'_1 \\ h'_2 \end{bmatrix} = \Delta \begin{bmatrix} \frac{1}{4}c_{11} + \frac{1}{12}c_{12} & \frac{1}{12}c_{11} + \frac{1}{12}c_{12} \\ \frac{1}{12}c_{11} + \frac{1}{12}c_{12} & \frac{1}{12}c_{11} + \frac{1}{12}c_{12} \end{bmatrix} \begin{bmatrix} h'_1 \\ h'_2 \end{bmatrix} = \Delta \begin{bmatrix} \frac{1}{7}c_{11} + \frac{1}{7}c_{12} & 0 \\ 0 & \frac{1}{7}c_{11} + \frac{1}{7}c_{12} \end{bmatrix} \begin{bmatrix} h'_1 \\ h'_2 \end{bmatrix}
\]

In the above storage matrix, the modification is made with the \( c_{11} = c_{12} \), which leads to the final form of the storage matrix shown as below

\[
\frac{1}{h_j} \sum_{j=1}^{2} c_1 \phi_j \phi_1 \, dz = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} h'_1 \\ h'_2 \end{bmatrix} = \Delta \begin{bmatrix} \frac{1}{7}c_{11} + \frac{1}{7}c_{12} & 0 \\ 0 & \frac{1}{7}c_{11} + \frac{1}{7}c_{12} \end{bmatrix} \begin{bmatrix} h'_1 \\ h'_2 \end{bmatrix}
\]

The same procedure applied to the terms related to \( C_{ij} \) and \( D_{ij} \), we have

\[
\frac{1}{h_j} \sum_{j=1}^{2} c_3 \phi_j' \phi_1' \, dz + \frac{1}{h_j} \sum_{j=1}^{2} c_7 \phi_j \phi_1 \, dz = \begin{bmatrix} \frac{1}{4}c_{11} + \frac{1}{12}c_{12} & -\frac{1}{12}c_{11} - \frac{1}{12}c_{12} \\ \frac{1}{12}c_{11} + \frac{1}{12}c_{12} & \frac{1}{12}c_{11} + \frac{1}{12}c_{12} \end{bmatrix} \begin{bmatrix} h'_{11} \\ h'_{12} \end{bmatrix} = \Delta \begin{bmatrix} \frac{1}{7}c_{11} + \frac{1}{7}c_{12} & 0 \\ 0 & \frac{1}{7}c_{11} + \frac{1}{7}c_{12} \end{bmatrix} \begin{bmatrix} h'_{11} \\ h'_{12} \end{bmatrix}
\]

Applying the same procedures to the terms associated with \( E_{ij} \) and \( F_{ij} \) and combining the lumped storage assumptions for equation (4.27),
Through the discretization scheme introduced in above sections, we now can translate these equations into MATLAB. Be aware of that, the examples shown above is only for soil moisture balance equation, the similar procedure can be applied for dry air equation and energy equation. In STEMMUS, the subroutines for implementing the task explained above include: “hPARM.m”, “h_MAT.m” and “h_EQ.m” (see Chapter 5).

In “hPARM.m”, the parameters related to matrix coefficients (e.g. c₁-c₈) are evaluated. The code is shown in figure 4.1. The subroutine in STEMMUS is coded as a function. It is not necessary to code in this way (i.e. to build a subroutine as a function instead of a ‘script’ file). However, one advantage to build subroutine as a function is that it is easy to check the code with Matlab, which automatically detects errors, warnings and so on by using different font color. One disadvantage of building subroutines as functions is that the variables claimed before in “Constants.m” have to be claimed again in the subroutine, as figure 4.1 shows.

As described above, the first part of “hPARM.m” includes the name of ‘function’, which is the same as the file name, followed by the global variable claiming. The first “for” loop is for calculating the derivative of soil moisture content with respect to matric potential (DTheta_LLh, \( \frac{\partial \theta}{\partial \eta} \)) and temperature (DTheta_LLT, \( \frac{\partial \theta}{\partial T} \)). The second “for” loop is to calculate the matrix coefficients: Chh, ChT, Khh, KhT, Kha, Vvh, VvT and Chg, expressions of which can be found in equation (3.53) and equation (3.57).

After the evaluation of the matrix coefficients, “h_MAT.m” assembles the coefficient matrices of the Galerkin expressions for the conservation equations. It uses a functional coefficient scheme to evaluate the matrix elements (see figure 4.2).
4.4. MATLAB Implementation

With all the coefficient matrices of the Galerkin expressions available, now we can proceed to perform the finite difference of the time derivatives of the matrix equation as equation (4.32) shows. The subroutine of “h_EQ.m” is employed for this purpose (see figure 4.3).

The same implementation procedures are applied to solve dry air equation and energy equation (see Chapter 5). After these three subroutines, we can get a trigonal matrix for each balance equation. To solve these trigonal matrices, the Thomas algorithm is employed.

```matlab
function hPARM
global ML MN ND NL nD RHOL Gamma_w DTheta_L_Lh DTheta_L_LT
global Cht Cyt Kht Cyt Vth Vth Chg Thmnlsc;
global Theta_L_Theta_LT_h h h T TT Theta_v ETA_V A
global RHOV DRHOVh DRHOVT KL_h D_Ta KL_T D_V D_Vg
global COR Dhu Itshr ml Beta_g Gamma_a0 Kla_Switch Dva_Switch

MN=0;
for ND=1:ND
    for NL=1:NL
        for ML=1:ML
            Chh(ML,ND)=(1-RHOV(MN)/RHOL)*DTheta_L_Lh(ML,ND);
            Khth(ML,ND)=(D_Vh(ML,ND)+D_Vg(ML,ND))*DRHOV(MN)/RHOL+
                        KL_h(ML,ND);
            Chg(ML,ND)=KL_h(ML,ND);
            if Thmnlsc==1
                Cyt(ML,ND)=(1-RHOV(MN)/RHOL)*DTheta_L_LT(ML,ND);
            end
            if Klau_Switch==1
                Kha(ML,ND)=RHOV(MN)*Beta_g(ML,ND)/RHOL+KL_h(ML,ND)/Gamma_w;
                Kha(ML,ND)=0;
            end
            if Dva_Switch==1
                Vth(ML,ND)=V_A(ML)*DRHOVh(MN)/RHOL;
                Vth(ML,ND)=V_A(ML)*DRHOVT(MN)/RHOL;
            else
                Vth(ML,ND)=0;
                Vth(ML,ND)=0;
            end
        end
    end
end
```

**Figure 4.1** Matlab code of hPARM.m in STEMMUS
4.5 Bibliography


4.5. Bibliography

Figure 4.2 Matlabe code of h_MAT.m in STEMMUS

```matlab
function h_MAT
global C1 C2 C4 C3 C4_a C5 C6 C7 C4ARG1 C4ARG2_1 C4ARG2_2 C5ARG1
global C6ARG C7ARG C5ARG2_1 C5ARG2_2 C5_a
global ML NL NN ND Chg DelT Z Chh Chlh Kht Khv Vh Vv T

for MN=1:NN
% Clean the space in C1-7 every iteration, otherwise, in *.PARM files,
% for ND=1-2 % C1-7 will be mixed up with pre-stored data, which will cause
% extremely crazy for computation, which exactly results in NAN.
    C1(MN,ND)=0;
    C7(MN)=0;
    C4(MN,ND)=0;
    C4_a(MN)=0;
    C5_a(MN)=0;
    C2(MN,ND)=0;
    C3(MN,ND)=0;
    C5(MN,ND)=0;
    C6(MM,ND)=0;
end

for ML=1:ML
    C1(ML,1)=C1(ML,1)+Chh(ML,1)*DelT(ML)/2;
    C1(ML+1,1)=C1(ML+1,1)+Chh(ML,2)*DelT(ML)/2;
    C2(ML,1)=C2(ML,1)+Chh(ML,1)*DelT(ML)/2;
    C2(ML+1,1)=C2(ML+1,1)+Chh(ML,2)*DelT(ML)/2;
    C4ARG1=(Kh(ML,1)+Kh(ML,2))/2*DelT(ML)
    C4ARG2_1=VVh(ML,1)+VVh(ML,2)/2;
    C4ARG2_2=VVh(ML,1)+VVh(ML,2)/2;
    C4(ML,1)=C4(ML,1)+C4ARG1+C4ARG2_1;
    C4(ML,2)=C4(ML,2)-C4ARG1-C4ARG2_2;
    C4(ML+1,1)=C4(ML+1,1)+C4ARG1+C4ARG2_2;
    C4(ML+1,2)=C4(ML+1,2)-C4ARG1-C4ARG2_2;
    C5ARG1=Kh(ML,1)+Kh(ML,2))/2*DelT(ML)
    C5ARG2_1=VVh(ML,1)+VVh(ML,2)/2;
    C5ARG2_2=VVh(ML,1)+VVh(ML,2)/2;
    C5(ML,1)=C5(ML,1)+C5ARG1+C5ARG2_1;
    C5(ML,2)=C5(ML,2)-C5ARG1-C5ARG2_2;
    C5(ML+1,1)=C5(ML+1,1)+C5ARG1+C5ARG2_2;
    C5(ML+1,2)=C5(ML+1,2)-C5ARG1-C5ARG2_2;
    C6ARG=(Khn(ML,1)+Khn(ML,2))/2*DelT(ML));
    C6(ML,1)=C6(ML,1)+C6ARG;
    C6(ML,2)=C6(ML,2)-C6ARG;
    C6(ML+1,1)=C6(ML+1,1)+C6ARG;
    C6(ML+1,2)=C6(ML+1,2)-C6ARG;
    C7ARG=(Chg(ML,1)+Chg(ML,2))/2;
    C7(ML)=C7(ML)+C7ARG;
    C7(ML+1)=C7(ML+1)+C7ARG;
end
```

47
4. STEMMUS: Finite Element Solution of Governing Equations

```matlab
function h_EQ
global ARG1 ARG2 ARG3 C1 C2 C4 C5 C6 C7 C5_a
global MN ML ND NL NN Det_t RHS T T hh P_gg SAVE Thmrefc Soliarefc
if Thmrefc & & Soliarefc
    RHS(1) = C7(1) + C1(1,1)*h(1) + C1(1,2)*h(2))/Det_t ...
    -C2(1,1)/Det_t + C5(1,1)*T(T1)-C2(1,2)/Det_t + C5(1,2)*T(T2) ...
    +C(2,1,1)/Det_t + C(2,1,2)/Det_t)*T(T2);
for ML=2:NL;
    ARG1=C2(ML-1,2)/Det_t;
    ARG2=C2(ML,1)/Det_t;
    ARG3=C2(ML,2)/Det_t;
    RHS(ML)=C7(ML)+(C(ML-1,2)*h(ML-1)+C1(ML,1)*h(ML) ...
    +C1(ML,2)*h(ML-1))/Det_t ...
    -C(ML-1,2)/Det_t + C5(ML,1)*T(T1)-C(ML,2)/Det_t + C5(ML,2)*T(T2) ...
    +C(ML,1,1)/Det_t + C(ML,1,2)/Det_t)*T(T2);
end
end
RHS(NN)=C7(NN)+(C1(NN,1)*h(NN)+C1(NN,1)*h(NN))/Det_t ...
    -C2(NN,1,2)/Det_t + C5(NN,1)*T(T(NN)) ...
    +C2(NN,1,2)/Det_t + C5(NN,1)*T(T(NN));
else
    if Thmrefc & & Soliarefc
        RHS(1) = C7(1) + C1(1,1)*h(1) + C1(1,2)*h(2))/Det_t ...
        -C6(1,1)*P_gg(1)-C6(1,2)*P_gg(2);
        for ML=2:NL;
            RHS(ML)=C7(ML)+(C(ML-1,2)*h(ML-1)+C1(ML,1)*h(ML) ...
                +C1(ML,2)*h(ML-1))/Det_t ...
                -C6(ML-1,1)*P_gg(1)-C6(ML,1)*P_gg(2) ...
                +C6(ML,2)*P_gg(ML+1);
        end
        if NN=1:NN;
            RHN=2:NN;
            for MN=1:NN;
                C4(MN,ND)=C1(MN,ND)/Det_t + C4(MN,ND);
            end
            SAVE(1,1)=RHS(1);
            SAVE(1,2)=C4(1,2);
            SAVE(1,3)=C4(1,2);
            SAVE(2,1)=RHS(2);
            SAVE(2,2)=C4(2,2);
            SAVE(2,3)=C4(2,3);
    end
end
end
end
```

Figure 4.3 Matlab code of h_EQ.m in STEMMUS
STEMMUS: Structures, Subroutines and Input Data
This chapter provides documentation of the computer code for solving STEMMUS theoretical equations outlined in Chapter 3 & 4. The framework of STEMMUS will be present with a flowchart, which is defined by the main program of the code. Accordingly, each subroutine will be introduced with its specific role in the algorithm. The execution of STEMMUS requires the determination of input data including the system parameters, initial conditions and boundary conditions. The format of such input data can be easily perceived in the specific subroutines which will be indicated in this section. An extensive list of definitions of the MATLAB variables used in STEMMUS is also given.

5.1 Structure of STEMMUS: Overview

Figure 5.1 illustrates the main program of STEMMUS. After initial input and computations, STEMMUS code starts to loop through the subroutines following the flowchart. Inside a given simulation period, which includes many time steps, a time step loop is executed as many times as necessary to reach the end of the simulation period, given the constraints on time step size. For a given time step, the balance equations for soil moisture, temperature and dry air are solved alternatively to obtain successive estimates of three independent state variables: \( h \), \( T \), and \( P_g \).

In a time step, a specified maximum iteration number is given to consider “accuracy” and numerical “convergence”. It is also given to balance the simulation “accuracy” and the computation cost. During a simulation, the maximum iteration number is rarely reached unless the change of state variables (e.g \( h \), \( T \), or \( P_g \)) exceeds the predefined constrains. In that case, the time step will be adjusted (e.g usually be reduced with a given factor), and the current time step will be repeated, with a set of new updated state variables. The maximum changes of state variables in one time step are usually predefined with a value, within which the STEMMUS estimates of \( h \), \( T \), and \( P_g \) in one time step are accepted for producing “converged” successive estimates.

The subroutines can be divided into four groups playing different roles in the main program: Initialization Group, Parameterization Group, Processing Group and Post-Process Group. One caution here is that some subroutines can be involved in more than one single group and will be called during looping by different groups.

[The Initialization Group]:

MainLoop.m: The main routine of STEMMUS;

Constants.m: All constants needed for STEMMUS;

Dtrmn_Z.m:

Determination of nodal space \( \Delta z \);

StartInit.m: Initialization for a specific simulation period;

SOIL2.m:

Calculation of soil moisture \( \theta_L \);
5.1. Structure of STEMUS: Overview

Figure 5.1 Flowchart of STEMUS Main Program

Forcing_PARM.m: Generating forcing data.

[The Parameterization Group]:
Condl_h.m: Calculation of $K$ considering temperature dependence;
Condl_T.m: Calculation of $K_{LT}$ (Disabled, reasons to be discussed);
Density_V.m: Calculation of vapor density $\rho_V$;
Condl_Tdisp.m: Calculation of transport coefficient for adsorbed liquid flow due to temperature gradient $D_{Ta}$;
Latent.m: Calculation of latent heat $L$;
Density_DA.m: Calculation of dry air density $\rho_{da}$;
CondT_coeff.m & EfeCapCond.m: Calculation of thermal properties $\lambda_{eff}$, $C$, and $\eta$;
Condg_k_g.m: Calculation of gas conductivity $k_g$;
5. STEMMUS: Structures, Subroutines and Input Data

**CondV_DE.m:** Calculation of vapor diffusivity $D_v$;

**CondV_DVg.m:** Calculation of vapor dispersivity $D_{Vg}$, and $q_{aa}$;

**Evap_Cal.m:** Calculation of evaporation.

[The Processing Group]:

**SOIL1.m:** Updating the wetting history;

**h_sub.m:** Solve liquid equation for a new estimate of $hh$, which means the matric potential at the end of time step, while $h$ means the matric potential at the end of last time step;

**hPARM.m:**
Calculation of coefficient matrices for liquid equation;

**h_MAT.m:**
Assembles the global coefficient matrices of the Galerkin expressions for liquid equation;

**h_EQ.m:**
Performs the finite difference of the time derivatives in the matrix equation;

**h_BC.m:**
Determines the boundary condition for solving liquid equation;

**h_Solve.m:**
Using Thomas Algorithm to solve the matrix equation;

**h_Bndry_Flux.m:**
Calculation of liquid flux on the boundary node;

**Air_sub.m:** Solve dry air equation for a new estimate of $P_{gg}$, which means the mixed soil air pressure at the end of time step, while $P_g$ means the mixed soil air pressure at the end of last time step;

**AirPARM.m:**
Calculation of coefficient matrices for dry air equation;

**Air_MAT.m:**
Assembles the global coefficient matrices of the Galerkin expressions for dry air equation;

**Air_EQ.m:**
Performs the finite difference of the time derivatives in the matrix equation;

**Air_BC.m:**
Determines the boundary condition for solving dry air equation;

**Air_Solve.m:**
Using Thomas Algorithm to solve the matrix equation;

**Energy_sub.m:** Solve energy equation for a new estimate of $TT$, which means the soil temperature at the end of time step, while $T$ means the soil temperature at the end of last time step;
5.2 Initial and Boundary Conditions

Initial conditions include soil moisture content ($\theta_L$), soil temperature ($T$), atmospheric pressure ($P_g$) (there is no different symbol for this variable, with respect to mixed soil air pressure. It is assumed as the main forcing for soil air flow), air temperature ($T_a$), relative humidity ($H_{ra}$), wind speed ($U$), precipitation ($P$), and soil surface temperature ($T_s$).

The initial soil moisture content profile and soil temperature profile are built by linearly extrapolating or interpolating from the point measurement at different depths. The time step in STEMMUS is adjusted automatically during computing (1 to 1800 s). Accordingly, the time interval of the meteorological inputs need to be adjusted to match each new time step. However, in the field measurement, the time interval for recording data is fixed with half of an hour. To match this requirement of flexible time step, the Fourier transform method need to be applied for producing the successive forcing data, through approximating the frequency domain representation of the meteorological forcing data. After the transformation, the parameters for producing meteorological forcing data should be put in the subroutine of “Constants.m”.

Considering the aerodynamic resistance and soil surface resistance to water vapor transfer from soil to atmosphere, the evaporation is
expressed as [1]

\[ E = \frac{\rho_{VS} - \rho_{Va}}{r_a + r_s} \]  \hspace{1cm} (5.1)

where \( \rho_{VS} \) (\( kg \) \( m^{-3} \)) is the water vapor density at the soil surface; \( \rho_{Va} \) (\( kg \) \( m^{-3} \)) the atmospheric vapor density; \( r_s \) (\( s \) \( m^{-1} \)) the soil surface resistance to water vapor flow; and \( r_a \) (\( s \) \( m^{-1} \)) the aerodynamic resistance. Equation (5.1) forms the surface boundary condition for moisture transport. Without taking ponding and surface runoff into consideration, soil surface is open to the atmosphere and the measured atmospheric pressure is adopted as the surface boundary condition for dry air transport in the soil. The measured soil surface temperature is set as the boundary condition for heat transport. The surface energy balance equation also can be used for this purpose, which can be implemented in STEMMUS by introducing a specific subroutine for that.

Following van de Griend and Owe [2], the aerodynamic resistance \( (r_a) \) and soil surface resistance \( (r_s) \) was expressed as

\[ r_a = \frac{1}{k^2 U} \left[ \ln \left( \frac{Z_m - d - Z_{om}}{Z_{om}} \right) - \psi_{sm} \right] \left[ \ln \left( \frac{Z_m - d - Z_{oh}}{Z_{oh}} \right) - \psi_{sh} \right] \]
\[ r_s = r_{sl} e^{a (\theta_{min} - \theta_{sur})} \]  \hspace{1cm} (5.2)

where \( k \) is the von Karman constant (= 0.41); \( U \) (\( m \) \( s^{-1} \)) the measured wind speed at certain height; \( Z_m \) (\( m \)) the height of wind-speed measurement; \( d \) (\( m \)) the zero plane displacement (= 0 for bare soil); \( Z_{om} \) (= 0.001 \( m \)) the surface roughness length for momentum flux; \( \psi_{sm} \) the atmospheric stability correction factor for momentum flux; \( Z_{oh} \) (= 0.001 \( m \)) the surface roughness length for heat flux; \( \psi_{sh} \) the atmospheric stability correction factor for heat flux; \( r_{sl} \) (= 10 \( s \) \( m^{-1} \)) the resistance to molecular diffusion across the water surface itself; \( a \) (= 35.63) the fitted parameter; \( \theta_{min} \) (= 0.15 \( m^{-3} \)) the empirical minimum value above which the soil is able to deliver vapor at a potential rate; and \( \theta_{sur} \) the soil water content in the topsoil layer.

The above description of the boundary condition is far from complete. However, it shows the boundary condition used currently in STEMMUS for the case in the Badain Jaran Desert [3]. A comprehensive boundary condition description should consider water movement in soils occurs under both saturated and unsaturated conditions, which will be discussed in next version of STEMMUS manual.

5.3 List of STEMMUS Variables

All variables used in STEMMUS have been commented in the code. The list here is for the description of the most often used variables. The column of “Alias” indicates how the variables expressed in STEMMUS code.
### 5.3. List of STEMMUS Variables

**Table 5.1: Most often used notations in STEMMUS**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Alias</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\theta_L)</td>
<td>Theta_L</td>
<td>Volumetric moisture content at the start of current time step</td>
</tr>
<tr>
<td>(\theta_{LL})</td>
<td>Theta_LL</td>
<td>Volumetric moisture content at the end of current time step</td>
</tr>
<tr>
<td>(\frac{\partial \theta_L}{\partial h})</td>
<td>DTheta_LLh</td>
<td>Partial derivative of (\theta_L) with respect to (h)</td>
</tr>
<tr>
<td>(\frac{\partial \theta_L}{\partial T})</td>
<td>DTheta_LLTT</td>
<td>Partial derivative of (\theta_L) with respect to (T)</td>
</tr>
<tr>
<td>(\theta_{sat})</td>
<td>Theta_s</td>
<td>Saturated moisture content</td>
</tr>
<tr>
<td>(\theta_{res})</td>
<td>Theta_r</td>
<td>Residual moisture content</td>
</tr>
<tr>
<td>(\epsilon)</td>
<td>POR</td>
<td>Porosity</td>
</tr>
<tr>
<td>(S_e)</td>
<td>Se</td>
<td>Effective saturation, (= \frac{\theta_L - \theta_{res}}{\theta_{sat} - \theta_{res}} \approx S_L = \frac{\theta_L}{\epsilon}).</td>
</tr>
<tr>
<td>(S_a)</td>
<td>Sa</td>
<td>Degree of air saturation, (= 1 - S_L = \frac{\theta_g}{\epsilon}).</td>
</tr>
<tr>
<td>(\rho_L)</td>
<td>RHOL</td>
<td>Density of liquid water</td>
</tr>
<tr>
<td>(\rho_V)</td>
<td>RHOV</td>
<td>Density of vapor</td>
</tr>
<tr>
<td>(\frac{\partial \rho_V}{\partial h})</td>
<td>DRHOVh</td>
<td>Partial derivative of (\rho_V) with respect to (h)</td>
</tr>
<tr>
<td>(\frac{\partial \rho_V}{\partial T})</td>
<td>DRHOVT</td>
<td>Partial derivative of (\rho_V) with respect to (T)</td>
</tr>
<tr>
<td>(\rho_{SV})</td>
<td>RHOV_s</td>
<td>Density of saturated water vapor</td>
</tr>
<tr>
<td>(\frac{\partial \rho_{SV}}{\partial T})</td>
<td>DRHOV_sT</td>
<td>Partial derivative of (\rho_{SV}) with respect to (T)</td>
</tr>
<tr>
<td>(\rho_{VS})</td>
<td>RHOV_sur</td>
<td>Vapor density in the top soil layer</td>
</tr>
<tr>
<td>(\rho_{VA})</td>
<td>RHOV_A</td>
<td>Vapor density in air at certain height</td>
</tr>
<tr>
<td>(\rho_{da})</td>
<td>RHOVDA</td>
<td>Density of dry air</td>
</tr>
<tr>
<td>(E)</td>
<td>Evap</td>
<td>Evaporation rate</td>
</tr>
<tr>
<td>(r_a)</td>
<td>Resis_a</td>
<td>Aerodynamic resistance for evaporation</td>
</tr>
<tr>
<td>(r_s)</td>
<td>Resis_s</td>
<td>Surface resistance for evaporation</td>
</tr>
<tr>
<td>(P)</td>
<td>Precip</td>
<td>Precipitation rate</td>
</tr>
<tr>
<td>(k_{ah})</td>
<td>Kah</td>
<td>Isothermal air transfer coefficient</td>
</tr>
<tr>
<td>(k_{st})</td>
<td>KaT</td>
<td>Thermal air transfer coefficient</td>
</tr>
<tr>
<td>(k_{aa})</td>
<td>Kaa</td>
<td>Advective air transfer coefficient</td>
</tr>
</tbody>
</table>

Continued on next page
5. STEMMUS: Structures, Subroutines and Input Data

Table 5.1 – continued from previous page

<table>
<thead>
<tr>
<th>Variables</th>
<th>Alias</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_{Ta}$</td>
<td>D_Ta</td>
<td>Transport coefficient for adsorbed liquid flow due to temperature gradient</td>
</tr>
<tr>
<td>$D_V$</td>
<td>D_V</td>
<td>Vapor diffusivity in soil</td>
</tr>
<tr>
<td>$D_a$</td>
<td>D_a</td>
<td>Vapor diffusivity in air</td>
</tr>
<tr>
<td>$D_{Vg}$</td>
<td>D_Vg</td>
<td>Longitudinal dispersion coefficient</td>
</tr>
<tr>
<td>$\tau$</td>
<td>f0</td>
<td>Tortuosity factor</td>
</tr>
<tr>
<td>$\gamma_{w}$</td>
<td>Gamma_w</td>
<td>Specific weight of water</td>
</tr>
<tr>
<td>$\mu_{w}$</td>
<td>MU_W</td>
<td>Dynamic viscosity of water</td>
</tr>
<tr>
<td>$\mu_{a}$</td>
<td>MU_a</td>
<td>Dynamic viscosity of air</td>
</tr>
<tr>
<td>$h$</td>
<td>h</td>
<td>Matric potential at the start of current time step</td>
</tr>
<tr>
<td>hh</td>
<td></td>
<td>Matric potential at the end of current time step</td>
</tr>
<tr>
<td>$h_{TemCorr}$</td>
<td>hCor</td>
<td>Temperature corrected matric potential</td>
</tr>
<tr>
<td>$e^{\psi(T-T_r)}$</td>
<td>Cor</td>
<td>Temperature correction factor for matric potential</td>
</tr>
<tr>
<td>$\frac{1}{\tau} \frac{\partial h_{TemCorr}}{\partial t}$</td>
<td>DhU</td>
<td>Rate of change of temperature corrected matric potential with respect to temperature, with no change of moisture content</td>
</tr>
</tbody>
</table>

\[
= \frac{1}{\tau} (hh_{TemCorr} - h_{TemCorr}) = \frac{hCor}{T} + hh \frac{\partial Cor}{\partial T} = Cor \frac{hh-h}{T} + hh \frac{\partial Cor}{\partial T} + hh Cor (-C_T) \Rightarrow DhU = Cor (hh - h - hh C_T) 
\]

<table>
<thead>
<tr>
<th>Variables</th>
<th>Alias</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$</td>
<td>T</td>
<td>Soil temperature at the start of current time step</td>
</tr>
<tr>
<td>TT</td>
<td>T_T</td>
<td>Soil temperature at the end of current time step</td>
</tr>
<tr>
<td>$P_\beta$</td>
<td>Pg</td>
<td>Soil air pressure at the start of current time step</td>
</tr>
<tr>
<td>$P_{gg}$</td>
<td>Pg</td>
<td>Soil air pressure at the end of current time step</td>
</tr>
</tbody>
</table>
5.4 How to Run STEMMUS

To run the STEMMUS in MATLAB is straightforward in “MainLoop.m”. When you finished all numerical set-up and gave all input data to STEMMUS, please open “MainLoop.m” in MATLAB and press 'F5' to run the model (or press the green arrow “run” button shown on the tool bar in MATLAB). Typically, there are 5 steps to prepare before running the model.

1. Setting time information and domain information;
2. Setting soil properties;
3. Setting observation information and initialization;
4. Setting meteorological forcing information;
5. Setting boundary conditions;
6. Running “MainLoop.m”;

5.4.1 Time and Domain Information

The time information setting includes the determination of maximum iteration number (i.e. ‘NIT’) in one time step, duration of simulation period (i.e. ‘DURTN’), initial time step (i.e. ‘Delt_t’), maximum desirable change of state variables (i.e. ‘xERR’, ‘hERR’, ‘TERR’ and ‘PERR’), total depth of the domain of interest (i.e. ‘Tot_Depth’) AND the determination of how to discrete the domain (e.g. equal spaces for elements or finer discretization on the top layer) by the subroutine of “Dtrmn_Z.m”. Figure 5.2 shows how the code for setting time and domain information looks like.

For the maximum desirable change of state variables, PERR is not in use yet by the subroutine of “TimestepCHK.m”. The different choices of xERR and TERR sometime can give different outputs. The bigger the maximum change value, faster the STEMMUS running. However, this may cost the accuracy of the prediction by STEMMUS in regards to reality. It’d be better to tune this parameter to optimize the balance between the computation cost and accuracy. Considering the example which will be shown latter in this chapter the STEMMUS running only takes about 30 secs to finish, this indicates that the computation cost will not be a big problem for STEMMUS.

5.4.2 Soil Properties

The setting of soil properties includes saturated hydraulic conductivity (i.e. ‘SaturatedK’), saturated moisture content (i.e. ‘SaturatedMC’), residual moisture content (i.e. ‘ResidualMC’), soil porosity (i.e. ‘porosity’), parameters of soil water retention curve (i.e. ‘Coefficient_n’ & ‘Coefficient_Alpha’). In STEMMUS, the Van Genuchten-Mualem model is adopted (see section 3.2.1). In practically, residual moisture content is difficult to be detected in laboratory, and is usually determined by fitting the
experimental data to Van Genuchten model. Figure 5.3 shows how the code for setting soil properties information looks like.

In STEMMUS, the heterogeneity of soil is considered by assigning values to 'IS', which is defined as the index of soil type. The hysteresis is considered by detecting 'IH' in every time step. The 'IH' is defined as the index of wetting history of soil which would be assumed as dry at the first with the value of 1. Be aware of that 'IS' and 'IH' need to be defined in “StartInit.m”. There are other two important parameters in “StartInit.m”: one is the 'XK' that is associated with $\theta_k$ in equation (3.40) and is defined as $1/2\epsilon$; the other is the 'XWILT' that is defined as wilting point associated with a low matric potential of $-1.5 \times 10^4 \text{ cm}$.

The treatment of hysteresis and soil heterogeneity follows Milly and Eagleson's work [4]. As for the soil wetting history, 'XWRE' is a critical parameter, which is calculated in subroutine of “SOIL2” and defined as the value of the main wetting function evaluated at the effective reversal value of temperature-corrected matric potential 'h'.

5.4.3 Observation Information and Initialization

Observation information can be directly copied and pasted in the last block in “Constants.m” as figure 5.4 shows. 'Msr_Mois', 'Msr_Temp' and 'Msr_Time' represent respectively the measurement of moisture content, soil temperature and the measurement intervals (unit of seconds). Except for the measurement data, the information about what the depth the
5.4. How to Run STEMMUS

Measurement is taken need to be listed. Figure 5.5 shows how to input the information about the measurement depth and so on into STEMMUS for generating initial soil moisture and soil temperature profile.

To generate the initial soil moisture and temperature profile, we need to input the observation positions/depths (i.e. ‘InitND1’, …, ‘InitND5’), measured soil moisture content and temperature at ‘InitND?’ depth at the start of simulation period (i.e. ‘InitX1’, …, ‘BtmX’, and ‘InitT1’, …, ‘BtmT’ respectively). With these inputs, in “StartInit.m”, STEMMUS automatically interpolate these information to generate initial profile information as figure 5.6 shows. The measured soil matric potential can be input as well with minor changes in the code shown on figure 5.6.

5.4.4 Meteorological Forcing Information

The treatment of meteorological forcing data is a bit complicated compared to other inputs. The meteorological forcing data include mainly air temperature (i.e. ‘Ta’), air relative humidity (i.e. HRa), wind speed (i.e. ‘U’), surface temperature (i.e. ‘Ts’), atmospheric pressure (i.e. ‘TopPg’) and precipitation (i.e. Precip).

As stated above, the time step in STEMMUS is adjusted automatically during computing (1 to 1800 s). Accordingly, the time interval of the meteorological inputs need to be adjusted to match the new time step (1 to 1800 s). However, the recording interval of meteorological forcing data is usually fixed (e.g. half of an hour). To match this requirement of flexible time steps, the Fourier transformation is employed to capture the variation of meteorological variables. This is done outside of

Figure 5.3 Soil properties information block
5. STEMMUS: Structures, Subroutines and Input Data

Figure 5.4 Measurement information block

| %%%%/%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-%-% 
 | %The measured soil moisture and temperature data here% 
 | %The measured soil moisture and temperature data here% 
 | %The measured soil moisture and temperature data here% 

Figure 5.5 Observation information input

STEMMUS. One note here is appropriate, as long as you can express the meteorological data continuously by using a function of time, unit of which is second, it does not matter what kind of method you use to do that (e.g. methods other than Fourier transformation). In the current version of STEMMUS, the meteorological data is reproduced by Fourier transformation. The related parameters for this are shown in figure 5.7.
5.4.5 Boundary Conditions

The surface and bottom boundary conditions can be grouped according to different governing equations. For soil moisture balance equation, the surface boundary conditions (i.e. 'NBCh') include specified matric head (i.e. 'NBCh'=1), specified potential moisture flux (i.e. 'NBCh'=2) and specified atmospheric forcing (i.e. 'NBCh'=2), while the bottom boundary conditions (i.e. 'NBChB') include specified matric head (i.e. 'NBChB'=1), specified moisture flux(i.e. 'NBChB'=2) and zero matric head gradient (or gravity drainage, i.e. 'NBChB'=3). For dry air equation (e.g. 'NBCP' and 'NBCPB') and energy equation (e.g. 'NBCT' and 'NBCTB'), we can find similar description of the surface and bottom boundary conditions. All the boundary conditions are implemented by subroutines with an affix of “_BC”, for example “h_BC.m”, “Enrgy_BC.m” or “Air_BC.m”. Figure 5.8 shows how the code for setting boundary conditions looks like.

For the example shown in Zeng and coauthors’ work [3, 5], the surface boundary condition for soil moisture balance equation (‘NBCh’) is set as 3 for taking meteorological data into account, while the bottom condition (‘NBChB’) is set as gravity drainage. For dry air equation, the NBCP is set as 3 to use the measured atmospheric pressure as the surface boundary condition, and the NBCPB is set as 2 to use the specified soil air pressure at the bottom. For energy equation, the NBCT is set as 1 to adopt the measure surface temperature as the driving force for heat transport, and

```plaintext
if =1;  
if =1;  
if =1;  
end
for (i=1; i<nx; i++)  
    if =1;  
end
for (i=1; i<nx; i++)  
    if =1;  
end
for (i=1; i<nx; i++)  
    if =1;  
end
```

Figure 5.6 Automatic interpolation of observation information
5. STEMMUS: Structures, Subroutines and Input Data

Figure 5.7 Fourier transformation parameters for meteorological forcing data

NBCTB is set as 1 to assume a zero temperature gradient at the bottom.

There is a note for NBCh though, in the subroutine of "h_BC.m" the precipitation is evaluated by using a fixed amount of rainfall, which is evenly distributed during a certain period. For the case in Zeng et al.'s study, a fixed amount of rainfall ('Precip(KT)=0.35/3600,cms⁻¹')

Figure 5.8 Boundary conditions setting parameters
is used for the period spanning from 22nd hour to 27th hour (i.e. time released since the simulation started). This is in total about 1.2 cm precipitation for the recorded event. However, in reality, the precipitation recorded in the field is less and unevenly distributed during this span of time. The adjustment of the precipitation (e.g. in a certain range) sometime is needed for getting behavioral performance (e.g. not only the precipitation, but also other parameters like XERR, TERR and so on) of the STEMMUS model in representing reality. This is needed because the elimination of all the measurement error from device we used in the field is impossible if any. For example, the placement of the device is not at the exact depth as the STEMMUS describes numerically and the measurement error of the device itself. Although the measurement error of the device can be determined in the laboratory, it can not be eliminated completely. We do can quantify these uncertainties by running the STEMMUS using different patterns of driving forces (e.g. by adopting data assimilation technique).

5.4.6 Running STEMMUS

After all these steps, we now can run STEMMUS by running the main routine, “MainLoop.m”, which links all subroutines in sequence to solve the governing equations as figure 5.1 shows. There were several manners to run the "MainLoop.m":

1. Push the green “run” button after opening "MainLoop.m" in MATLAB;
2. Click “F5” after opening “MainLoop.m” in MATLAB;
3. Click “F9” without opening “MainLoop.m” in MATLAB, but with selecting "MainLoop.m" in the 'current folder' navigator in MATLAB.

All are convenient normal commands used in MATLAB to run a '*.m' script.

5.5 Bibliography


5. STEMMUS: Structures, Subroutines and Input Data