

A Model for Dehydration and Moisture Flow in Concrete at High Temperature

by

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Signature of Author.....

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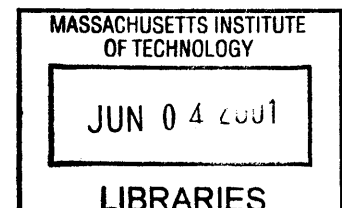
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BARKER



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ABSTRACT

This thesis presents a model for dehydration and moisture flow in concrete at temperatures below the critical point of water. The model is developed from Mainguy's isothermal model, which is presented in this work along with two other models as part of a literature review. Concrete is considered a porous material composed of an undeformable skeleton and three fluid phases (liquid, vapor and dry air) saturating the pore space. The water vapor and dry air form an ideal gas mixture called wet air. The model accounts for the mass conservation of water (liquid and vapor), mass conservation of dry air, entropy balance and liquid-vapor balance. State equations and conduction laws are used as required. In particular, a dehydration law is introduced as a linear relation between the degree of dehydration and the temperature rise. The set of equations is solved in cylindrical coordinates using the finite volume method with time discretization. The results indicate a slight increase in liquid water saturation where dehydration took place and a decrease in capillary pressure. However, due to the phase distinction, the model in its present form is restricted to a temperature range below the critical point of water. Beyond this point, conventional liquids do not exist and the model needs to be refined.

Thesis Supervisor: Franz-Josef Ulm

Title: Associate Professor of Civil and Environmental Engineering

A mis padres, mis hermanos y al 'ese' por todo el apoyo que me han dado.

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Introduction

Recent fires in European tunnels have highlighted the vulnerability of concrete structures subjected to high temperatures. A typical failure pattern observed under these conditions is known as ‘thermal spalling’ (a brittle failure with most fracture planes parallel to the heated surface [1]), and there are several hypotheses about the underlying mechanisms that lead to this type of failure. Some hypotheses include pressure buildup due to the low permeability of concrete and the drained conditions at the heated surface [2], and loss of material strength (thermal decohesion) and of elastic stiffness (thermal damage) [1].

High temperatures do not only affect tunnels in a fire situation but can also affect structures such as nuclear reactors, in which case a failure of the structure would be catastrophic. Therefore, it is important to predict a concrete structure’s performance under high temperatures in order to be able to design it properly and ensure the structure’s integrity under such conditions.

Even though there is no agreement on the physical origin of thermal spalling, there is some basic knowledge of the multiple phenomena involved in the process. It starts with a temperature above normal conditions which will affect not only the moisture content of the structure, but also the mechanical properties of it. As it can be seen in Figure 3 these two processes are not independent of each other because there is a coupling caused by the dehydration. However, in this

work this coupling will not be considered as a first approach, and we bear in mind its importance in the overall process.



Figure 1: Thermal spalling effects on The Chunnel tunnel after the Nov. 1996 fire.
(photo courtesy of The i-Center for Infrastructure Science and Technology, MIT)

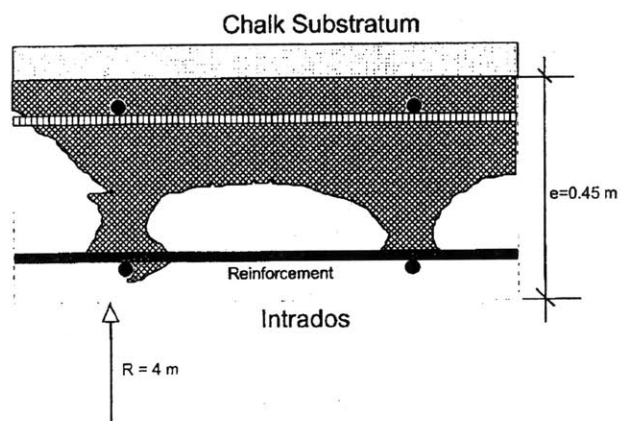


Figure 2: Typical damage pattern in reinforced concrete tunnel rings observed after The Chunnel fire [3]

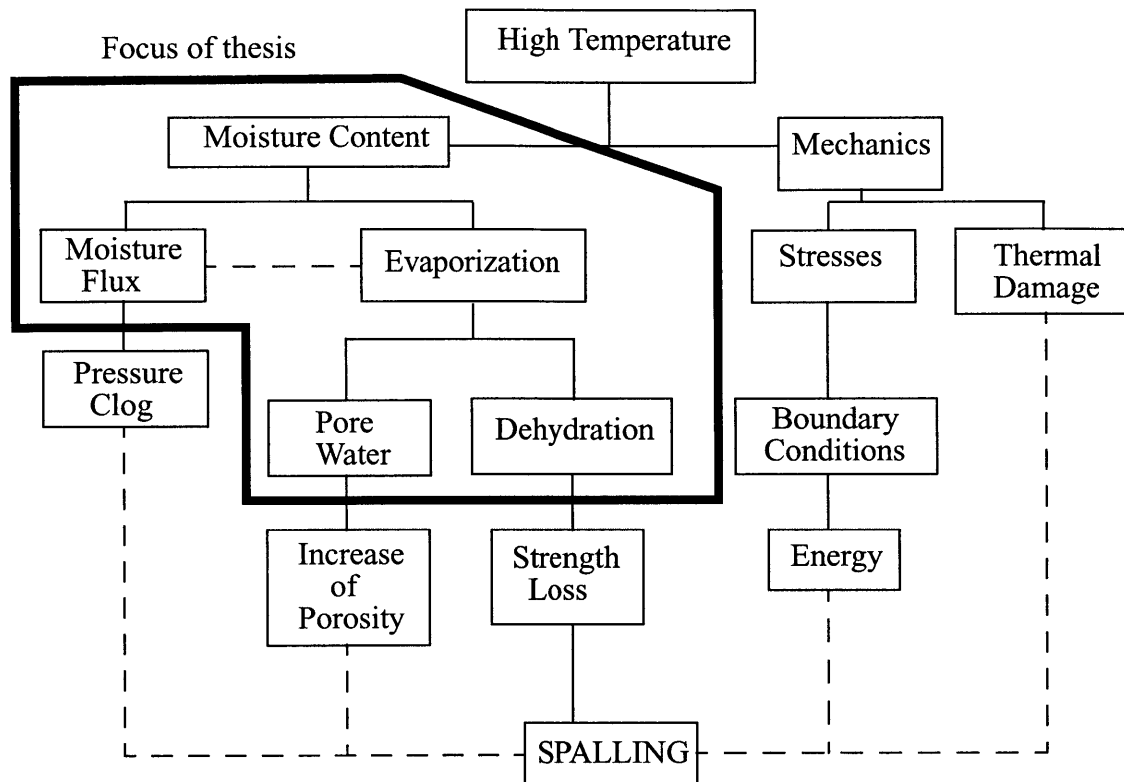


Figure 3: Overview

Moisture content is defined as the evaporable water, in liquid or vapor form, that is present in the material, including the bound water. Bound water results from the hydration process in concrete and is chemically or physically bound to the skeleton. By contrast, the free water fills the pore space of the structure and is free to evaporate or flow through the porous medium. Bound water becomes free water in the process of dehydration. Therefore, the amount of pore water is reduced by its evaporization and increased by dehydration of the skeleton.

This thesis focuses on the moisture flux and the effects of dehydration on the pore water content and on pore pressures. To this end, the first chapter of this work will focus on a literature review and a comparison of different models. The intent is to provide some overview of the different approaches and interpretations of these phenomena. Also, a comparison of these different approaches gives some insight into the various parameters that govern the processes above.

The second chapter is devoted to the development of a new model for the moisture flow in concrete that will include the dehydration of the concrete matrix and will be useful under non-isothermal conditions. The model is an extension of Mainguy's isothermal model [4] to non-isothermal situations while including dehydration.

The third chapter develops the numerical method to solve the model's system of equations. The method used is a finite volume scheme in cylindrical coordinates with time discretization. This facilitates its use in geometries such as tunnels. The numerical model is validated for isothermal conditions and applied considering a temperature rise and dehydration effects in a concrete structure. The results allow us to evaluate the effects of dehydration on pore pressure build up and saturation.

Finally, conclusions are drawn regarding the results, procedure and limitations of the model.

Chapter I

Literature Review

This chapter provides a brief summary and comparison of three different models for the moisture transfer in concrete:

- Bazant and Thonguthai's model for moisture diffusion and pore pressure [5]
- Mainguy's isothermal model for drying of cement based materials [4]
- Gawin et al's hygro-thermal behavior of concrete at high temperature [6]

The notation used in the articles has been altered from its original version in order to facilitate cross referencing and comparison among the models.

The dimensions of all parameters are presented in a length (L), mass (M), time (T), temperature (Θ), and moles (Mol) base dimension system.

I . 1 Bazant and Thonguthai's (1978) Model for Moisture Diffusion and Pore Pressure

Bazant and Thongutahi's (1978) model [5] was one of the first attempts to predict, mathematically, the behavior of concrete exposed to temperatures above 100 °C . Of the models presented in this literature review, this model can be considered to be the most macroscopic one, because it does not differentiate between water phases (liquid, vapor), and it does not explicitly refer to the porous nature of concrete.

I . 1 . 1 Governing Equations

The model considers two main variables: the moisture content and the temperature. They depend only on the gradients of temperature and pressure. Any coupling that could exist between moisture content and temperature is assumed negligible on the basis of data fits.

The model is based on two conservation laws, related to the free water mass content and the balance of heat.

Conservation of Mass

The mass conservation equation accounts for water consumed during hydration and water released during dehydration due to heating. The bound water depends on the amount of hydrated water before heating (which depends on the degree of hydration). It has a strong influence on the pore pressure and its release depends on the rate of heating.

The conservation of mass reads as follows:

$$\frac{\partial w}{\partial t} = -\text{div} \underline{J} + \frac{\partial w_d}{\partial t} \quad (\text{I.1})$$

where,

w = Free water (evaporable, not chemically bound), ($L^{-3}M$)

w_d = Mass of chemically bound (hydrate) water released to the pores, ($L^{-3}M$)

\underline{J} = Moisture flux, ($L^{-2}MT^{-1}$)

Equation (I.1) accounts for a correction in the normal conservation of mass due to the dehydration of the skeleton (loss of bound water, w_d) at high temperatures which adds water to the pores. The term w represents only the moisture in the pores, and does not distinguish water in form of vapor or liquid.

Conservation of Heat

The balance of heat in the model is written in the form:

$$\rho C \frac{\partial \theta}{\partial t} - C_a \frac{\partial w}{\partial t} - C_w \underline{J} \nabla \theta = -\text{div} \underline{q} \quad (\text{I.2})$$

where,

- ρ = Mass density of concrete, ($L^{-3}M$)
 C = Isobaric heat capacity of concrete, ($L^2T^{-2}\Theta^{-1}$)
 C_a = Heat of sorption of free water, (L^2T^{-2})
 C_w = Isobaric heat capacity of bulk (liquid) water, ($L^2T^{-2}\Theta^{-1}$)

Both the mass density and the heat capacity of concrete include the chemically combined water (bounded water) but exclude the free water (i.e. evaporable). Therefore, ρ and C refer to the concrete matrix.

Flux equations

The model analyzes the moisture and heat flux separately. As mentioned before, any coupling is assumed negligible on the basis of data fits.

The fluxes are written in the following form:

$$\underline{J} = -\frac{a}{g}\nabla p \quad (I.3)$$

$$\underline{q} = -k\nabla\theta \quad (I.4)$$

where,

- \underline{q} = Heat flux, (MT^{-3})
 k = Heat conductivity of concrete, ($LMT^{-3}\Theta^{-1}$)
 θ = Temperature, (Θ)
 \underline{J} = Moisture flux, ($L^{-2}MT^{-1}$)
 a = Permeability of concrete, (LT^{-1})
 g = Acceleration of gravity, (LT^{-2})
 p = Pore water pressure, ($L^{-1}MT^{-2}$)

To reduce uncertainty introduced by material properties into the state equation of pore water, constitutive relations between pore pressure, water content, and temperature are introduced. It is assumed that at all times there is a thermodynamic equilibrium between all phases of the pore water.

These relations are developed for three distinct stages of concrete saturation below the critical point of water¹:

- Non-saturated concrete
- Saturated concrete
- Saturation transition

The permeability of heated concrete was found to increase by two orders of magnitude for temperatures exceeding 100 °C. A permeability function is introduced and it illustrates the evo-

1. The critical point of water is where conventional liquids cease to exist. It occurs at a temperature of approximately 647 K.

lution of the permeability as well as the transition, which occurs between temperatures of 95 °C and 105 °C.

The heat conductivity is assumed to be constant in all computations, but the heat capacity is not because of its dependence on the amount of heat lost in dehydration and vaporization. The authors showed that the effects of these two heats are quite small because water is a small portion of the total concrete mass.

I.1.2 Boundary conditions

There are two types of boundary conditions imposed at the surface of concrete in contact with the environment. They both assume a linear relation between either flux and the environmental boundary conditions.

The moisture flux is assumed to be linearly dependent on the pressure difference, and the heat flux is assumed to be linearly dependent on both the temperature and pressure differences. This coupling of temperature and pressure is because of the loss of heat due to latent heat of moisture vaporization. The boundary conditions read as follows:

$$\underline{n} \cdot \underline{J} = B_w(p - p_{en}) \quad (1.5)$$

$$\underline{n} \cdot \underline{q} = B_T(\theta - \theta_{en}) + C_v B_w(p - p_{en}) \quad (1.6)$$

where,

\underline{n} = Unit outward normal at the surface, $[n] = 1$

B_w = Surface emissivity of water, $(L^{-1}T)$

p = Pore pressure just under the surface, $(L^{-1}MT^{-2})$

p_{en} = Water vapor pressure in the environment, $(L^{-1}MT^{-2})$

B_T = Surface emissivity of heat, $(MT^{-3}\Theta^{-1})$

C_v = Isobaric heat of vaporization of water, (L^2T^{-2})

θ = Temperature at the surface, (Θ)

θ_{en} = Environmental temperature, (Θ)

I . 2 Mainguy's Isothermal Model for Drying of Cement Based Materials

The next model considered is the isothermal model developed by Mainguy [4] for drying of cement based materials. This model is the basis for the non-isothermal model with dehydration effects developed in the next chapter.

I . 2 . 1 Porous Material Model

On a macroscopic scale, concrete is a porous material that can be represented as a superposition of different phases, as sketched in Figure I.1 (where a homogeneous distribution of porosity and liquid and gas phases may be assumed). The following partial volumes are considered:

V_w = volume occupied by the liquid phase, (L^3)

V_g = volume occupied by the gas phase, (L^3)

V_s = volume occupied by the solid phase, (L^3)

V_t = total volume of the material, (L^3)

Using the previous definitions we can obtain the following macroscopic quantities:

Pore space of phase i (water, w , gas, g , and solid, s):

$$\phi_i = \frac{V_i}{V_t} \quad (I.7)$$

Total porosity ($[\phi] = 1$):

$$\phi = \phi_w + \phi_g = \frac{V_w + V_g}{V_t} \quad (I.8)$$

Saturation of phase i ($[S] = 1$):

$$S_i = \frac{\phi_i}{\phi} = \frac{V_i}{V_w + V_g} \quad (I.9)$$

$$S_w + S_g = 1 \quad (I.10)$$

Water mass content ($[w] = 1$):

$$w = \frac{m_w}{m_s} = \frac{\rho_w}{\rho_s} \phi_w \quad (I.11)$$

where,

m_s = dry mass of material, (M)

ρ_s = apparent volumetric mass of the material, ($L^{-3}M$)

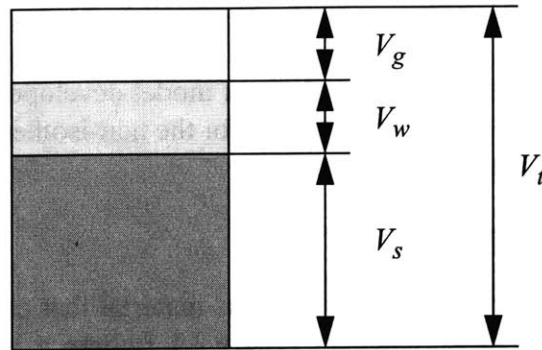


Figure I.1 Superposition of different phases

Mainguy's model is based on thermodynamics of porous media [7]. The porous medium is idealized as the superposition of a liquid, a gas and a skeleton. The solid matrix can contain an occluded porosity. The interesting part of this approach is the expression of any physical quantity as the sum of three different quantities. The result is the ability to use traditional thermodynamics for the porous medium.

The following model assumptions are made:

- The skeleton is considered undeformable. This simplifies the model because the fluid velocities compared to the skeleton become absolute and non-relative.
- The liquid phase, which is also regarded as incompressible, gathers liquid water present in many ways, and it is likely to evaporate. It is regarded as pure water in spite of the presence of various ionic species in the interstitial solution (where water is the main component).
- The gas phase is an ideal mixture of dry air and water vapor, and therefore obeys the law of perfect gases. The gas pressure is not constant and is not equal to the atmospheric pressure. The overpressures or depressions generated within the medium can become significant because of the low permeability of the porous material.
- The forces of gravity are small in comparison with the capillary forces, and therefore are neglected. This assumption is not relevant for the gas phase, and it is particularly true for the liquid phase with weak saturation. In the case where the saturation is close to unity, the capillary forces are quasi-null; at this point the permeability to water is at its maximum, and therefore the gravity forces, which are small in comparison with the pressures of liquid at strong saturation, can still be neglected.
- The temperature in Mainguy's original model is uniform and constant within the media. For drying, this assumption of isothermal drying seems accurate because the strong thermal conductivity, compared to the low permeability of the cement based materials, ensures that the characteristic time associated with the restoration of the temperature is much smaller than the characteristic time associated with the transport of moisture.

I . 2 . 2 Governing Equations

The model can be summarized in form of four equations. The equations come from the conservation of masses (liquid water, water vapor, and dry air) and the liquid-vapor balance of water (governed by the equality of the Gibbs mass potentials).

Conservation of Mass

The equations for the different water phases are the following:

$$\frac{\partial m_w}{\partial t} = -\text{div}\underline{w}_w - \mu^w_{l \rightarrow g} \quad (\text{I.12})$$

$$\frac{\partial m_v}{\partial t} = -\text{div}\underline{w}_v + \mu^w_{l \rightarrow g} \quad (\text{I.13})$$

$$\frac{\partial m_a}{\partial t} = -\text{div}\underline{w}_a \quad (\text{I.14})$$

where,

$m_i d\Omega$ = mass of each component contained in the elementary volume $d\Omega$ (M)

w_i = mass flux of each constituents, (L^2MT^{-1})

$\mu^w_{l \rightarrow g} dt d\Omega$ = mass of water that passes from the liquid phase to gas phase in the elementary volume, $d\Omega$, during time dt . The positive case being evaporation, the negative one condensation and the equilibrium situation represented as a zero value.

Using equations (I.7) to (I.11) the following relations can be derived between the mass and mass flow terms, the total porosity, ϕ , liquid water saturation, S_w , and volumetric mass, ρ_i , of each component:

$$m_w = \phi_w \rho_w = \phi S_w \rho_w \quad (\text{I.15})$$

$$m_v = \phi_g \rho_v = \phi(1 - S_w) \rho_v \quad (\text{I.16})$$

$$m_a = \phi_g \rho_a = \phi(1 - S_w) \rho_a \quad (\text{I.17})$$

In addition, the mass flux vectors in (I.12) to (I.14) can be written in the form:

$$\underline{w}_w = \phi_w \rho_w \underline{v}_w = \phi S_w \rho_w \underline{v}_w \quad (\text{I.18})$$

$$\underline{w}_v = \phi_g \rho_v \underline{v}_v = \phi(1 - S_w) \rho_v \underline{v}_v \quad (\text{I.19})$$

$$\underline{w}_a = \phi_g \rho_a \underline{v}_a = \phi(1 - S_w) \rho_a \underline{v}_a \quad (\text{I.20})$$

The conservation equations are complemented by equations of state for each fluid. The density of water ρ_w is assumed to be constant, i.e. incompressible or independent of the liquid pressure p_w . The remaining densities are connected to partial pressures p_i by the law of perfect gases:

$$p_i M_i = R \theta \rho_i \quad (I.21)$$

where,

ρ_i = volumetric mass of each component, ($L^{-3}M$)

R = constant for perfect gases, ($LM^2T^{-2}\Theta^{-1}Mol$) = 8314.41 ($J kmol^{-1}K^{-1}$)

θ = temperature, (Θ)

M_i = molar mass of each constituent, ($M Mol^{-1}$)

p_i = partial pressure of the constituent, ($L^{-1}MT^{-2}$)

Also, because dry air and water vapor are assumed to form an ideal mixture, the total gas pressure p_g is the sum of the partial dry air and water vapor pressures.

$$p_g = p_a + p_v \quad (I.22)$$

For an ideal mixture the molar fractions of gas, C_i , can be defined by ($[C_i] = 1$):

$$C_i = \frac{P_i}{P_g} \quad (I.23)$$

The flux terms are further developed into two separate terms: Darcean transport and Fickian transport. This results in the following expressions:

$$\underline{w}_w = -\rho_w \frac{k}{\eta_w} k_{ri}(S_w) grad(p_w) \quad (I.24)$$

$$\underline{w}_v = -\frac{M_v}{R\theta} p_v \frac{k}{\eta_g} k_{rg}(S_w) grad(p_g) - \frac{M_v}{R\theta} d_{va} f(\phi, S_w) grad\left(\frac{p_v}{p_g}\right) \quad (I.25)$$

$$\underline{w}_a = -\frac{M_a}{R\theta} p_a \frac{k}{\eta_g} k_{rg}(S_w) grad(p_g) - \frac{M_a}{R\theta} d_{va} f(\phi, S_w) grad\left(\frac{p_a}{p_g}\right) \quad (I.26)$$

where,

k = absolute or intrinsic permeability of the material (L^2)

η_i = dynamic viscosity of the corresponding phase, ($L^{-1}MT^{-1}$)

$k_{ri}(S_w)$ = permeability relative to the phase i , which is a function of the liquid water saturation, ($[k_{ri}] = 1$). The following expressions were used by Mainguy in his model [4]:

- Permeability relative to liquid phase ¹

$$k_{rl}(S_w) = \sqrt{S_w} \left[1 - \left(1 - S_w^{\frac{1}{m}} \right)^{m-2} \right] \quad (I.27)$$

- Permeability relative to gas phase ²

$$k_{rg}(S_w) = \sqrt{S_g} \left(1 - S_w^{\frac{1}{m}} \right)^{2m} \quad (I.28)$$

where,

m = material property

d_{va} = factor related to the diffusion coefficient of water vapor in air, D_{va}

$$d_{va} = D_{va}(p_g, \theta) p_g \quad [d_{va}] = LMT^{-3} \quad (I.29)$$

$$D_{va}(p_g, \theta) = 0.217 \frac{P_{atm}}{p_g} \left(\frac{\theta}{\theta_0} \right)^{1.88} \quad [D_{va}] = L^2T^{-1} \quad (I.30)$$

$f(\phi, S_w)$ = resistance to diffusion factor. It takes into account the reduction of the space available to gas to diffuse and the effects of tortuosity, through the form:

$$f(\phi, S_w) = \phi^{\frac{4}{3}} (1 - S_w)^{\frac{10}{3}} \quad (I.31)$$

Liquid-Vapor Balance

The liquid-vapor balance equation needs to be integrated and related to a state of reference, where variables are known (assuming incompressibility of the liquid). The chosen state of reference is a thermodynamic liquid-vapor balance without capillary action and under atmospheric pressure. The water vapor pressure is assumed to depend on temperature and to be equal to the saturation vapor pressure for a liquid pressure equal to atmospheric pressure.

The thermodynamic equilibrium is written in the form:

$$\rho_w \frac{R\theta}{M_v} d(\ln(p_v)) = d(p_w) \quad (I.32)$$

On the macroscopic scale the capillary pressure is defined as the difference between the macroscopic pressure of water and gas. In the case of an isotropic medium with an undeformable matrix, in isothermal evolution and in the absence of hysteresis phenomena, the capillary pressure is a function of only the liquid water saturation. i.e

$$p_g - p_w = p_c(S_w) \quad (I.33)$$

where,

-
1. Van Genuchten [8] showed that the permeability to water can be estimated by (I.27). Savage and Janssen [9] showed that this last equation can be applied to materials containing cement.
 2. Parker et al. [10] proposed (I.28) as an expression for the relative permeability to gas based on an extension of the model of Mualem to the non-moistured phase [11].
-

$$p_c(S_w) = a(S_w^{-b} - 1)^{1 - \frac{1}{b}} \quad (I.34)$$

with a and b being material properties.

I.2.3 Initial Conditions

The gas pressure at the beginning of drying is assumed to be uniform within the material and equal to the atmospheric pressure, p_{atm} :

$$p_{g_0} = p_{atm} \quad (I.35)$$

Providing values for both the relative humidity, h_r , and gas pressure has the same effect as imposing pressures for vapor water and dry air within the sample:

$$p_{v_0} = h_r p_{vs} \quad (I.36)$$

$$p_{a_0} = p_{g_0} - p_{v_0} \quad (I.37)$$

The initial hydrous state represents a thermodynamic balance with the atmospheric pressure. Therefore, the initial water saturation of the samples can be calculated from Kelvin's law:

$$\rho_w \frac{RT}{M_v} \ln(h_r) = -p_c(S_{w_0}) \quad (I.38)$$

I.2.4 Boundary Conditions

During drying the conditions imposed at the boundaries are the relative humidity and a total gas pressure equal to the atmospheric pressure. Similar to the initial conditions, these boundary conditions have the same effect as imposing pressures for water vapor and dry air:

$$h_r = h_r^b \quad (I.39)$$

$$p_g^b = p_{atm} \quad (I.40)$$

$$p_v^b = h_r^b p_{vs} \quad (I.41)$$

$$p_a^b = p_g^b - p_v^b \quad (I.42)$$

The thermodynamic balance also applies at the edge of the material and the liquid water saturation at the boundary, S_w^b , can also be calculated from Kelvin's law (I.38).

I.3 Gawin et al.'s Hygro-Thermal Behavior Of Concrete At High Temperature

High temperatures produce several non-linear phenomena in concrete structures. The model proposed by Gawin et al. [6] provides a computational analysis of hygro-thermal and mechanical behavior of concrete structures at high temperatures. Heat and mass transfers are simulated in a coupled fashion where non-linearities due to high temperatures are accounted for. Isotropic damage effects are taken into account in the model but will not be included in this literature review. Gawin et al.'s model is also based on the theory of porous media, but applies some different assumptions.

I.3.1 Introduction

In order to account for the different phenomena that affect concrete at high temperatures, Gawin et al.'s model considers the following:

- Heat Conduction
- Vapor diffusion
- Liquid water flow (caused by pressure gradients, capillary effects, and adsorbed water content gradients)
- Latent heat effects due to evaporation and desorption

In order to fully model moisture transport at high temperatures, phase changes and related thermal effects are included. The authors suggest that a purely diffusive uncoupled model is not appropriate. At high temperatures, the formulation of the governing equations for heat and mass transfers must be adapted because the pore structure of concrete and its physical properties change. These depend on the hydration and aging processes, but are also highly influenced by the loading and hygro-thermal conditions. For example, at high temperatures the following are affected:

- Permeability
- Physical properties of fluids filling the pores
- Amount of heat released or adsorbed (hydration or dehydration)

The physical mechanisms behind the liquid and gas transport in the pores relate to gradients. The capillary water and gas flow are triggered by pressure gradients, adsorbed water surface diffusion by saturation gradients, and air and vapor diffusion by density gradients.

For the numerical application the authors propose a finite element scheme which allows simulation of the evolution of

- Temperature
- Moisture content
- Global process kinetics
- Stress and strain behavior

I.3.2 Governing Equations

Concrete is idealized as a multiphase material. The pores of the skeleton are filled by a liquid and a gas phase. The liquid phase here is composed of bound water (adsorbed) and capil-

lary water (free and evaporable). The latter appears when the saturation exceeds the solid saturation point S_{SSP} .

Depending on the saturation degree, S , the liquid phase has different origins. Below saturation the liquid phase (l) is the bound water (b). While for the capillary region it is assumed that only capillary water (w) can move. Then,

$$S \leq S_{SSP}: \quad l = b \quad ; \quad \Delta h_{phase} = \Delta h_{adsorp}$$

$$S > S_{SSP}: \quad l = w \quad ; \quad \Delta h_{phase} = \Delta h_{vap}$$

where Δh is the enthalpy of the corresponding process, (L^2T^{-2}).

The gas phase is a mixture of dry air (non-condensable) and water vapor (condensable) and, like in Mainguy's model, the mixture is assumed to behave like an ideal gas.

The mathematical model consists of the following balance equations:

- Conservation of mass for
 - solid skeleton
 - dry air
 - water species (liquid and gas state, taking phase changes into account)
- Energy conservation
- Linear momentum of the multiphase system

Conservation of Mass

The first mass conservation equation is the solid mass conservation equation:

$$\frac{\partial}{\partial t}[(1 - \phi)\rho_s] + \nabla \cdot [(1 - \phi)\rho_s \underline{v}_s] = \frac{\partial}{\partial t}(\Delta m_{hydr}) \quad (1.43)$$

where,

ϕ = total porosity (pore volume / total volume), ($[\phi] = 1$)

ρ_s = solid phase density, ($L^{-3}M$)

\underline{v}_s = velocity of solid phase, (LT^{-1})

m_{hydr} = mass source term related to hydration-dehydration, ($L^{-3}MT^1$)

The dry air conservation equation accounts not only for mass changes but also for porosity changes, resulting from the dehydration of concrete, and the displacement of the solid matrix. The conservation law is given by:

$$\phi \frac{\partial}{\partial t} [(1-S)\rho_{ga}] + (1-S)\rho_{ga} \frac{\partial \phi_{hydr}}{\partial t} + \alpha(1-S)\rho_{ga} \frac{\partial}{\partial t} (\nabla \cdot \underline{u}) + \nabla \cdot (\rho_{ga} \underline{v}_g) + \nabla \cdot (\rho_{ga} \underline{v}_{ga}^d) = 0 \quad (I.44)$$

where,

ρ_{ga} = mass concentration of dry air in gas phase, ($L^{-3}M$)

ϕ_{hydr} = part of porosity resulting from dehydration of concrete, ($[\phi] = 1$)

α = Biot's constant, ($[\alpha] = 1$)

\underline{u} = displacement vector of solid matrix, (L)

\underline{v}_g = velocity of gaseous phase, (LT^{-1})

\underline{v}_{ga}^d = relative average diffusion velocity of dry air species, (LT^{-1})

The water species (liquid - vapor) conservation equation also takes into account porosity changes from dehydration and displacement of the solid matrix, in addition to the different mass terms:

$$\begin{aligned} \phi \frac{\partial}{\partial t} [(1-S)\rho_{gw}] + (1-S)\rho_{gw} \frac{\partial \phi_{hydr}}{\partial t} + \alpha(1-S)\rho_{gw} \frac{\partial}{\partial t} (\nabla \cdot \underline{u}) + \nabla \cdot (\rho_{gw} \underline{v}_g) + \nabla \cdot (\rho_{gw} \underline{v}_{gw}^d) \\ = -\phi \frac{\partial}{\partial t} (S\rho_w) - S\rho_w \frac{\partial \phi_{hydr}}{\partial t} - \alpha S\rho_w \frac{\partial}{\partial t} (\nabla \cdot \underline{u}) - \nabla \cdot [\rho_w \underline{v}_l] - \frac{\partial}{\partial t} (\Delta m_{hydr}) \end{aligned} \quad (I.45)$$

where,

ρ_{gw} = mass concentration of water vapor in gas phase, ($L^{-3}M$)

\underline{v}_{gw}^d = relative average diffusion velocity of water vapor species, (LT^{-1})

\underline{v}_l = velocity of liquid phase, (LT^{-1})

The volume-averaged velocities of capillary water and gaseous phase relative to the solid phase are obtained by using Darcy's law as a constitutive equation:

$$\underline{v}_w = -\frac{\underline{k}k_{rl}}{\eta_w}(\nabla p_g - \nabla p_c - \rho_w \underline{b}) \quad (I.46)$$

$$\underline{v}_g = -\frac{\underline{k}k_{rg}}{\eta_g}(\nabla p_g) \quad (I.47)$$

where,

\underline{k} = intrinsic permeability tensor, (L^2)

k_{rg}, k_{rl} = relative permeabilities of the gaseous and liquid phases, ($[k_i] = 1$)

η_g, η_w = dynamic viscosity of the gas and liquid phases, ($L^{-1}MT^{-1}$)

For the bound water flow, the following generalized constitutive law is applied

$$\underline{v}_b = -\underline{D}_b \nabla S_b \quad (I.48)$$

where,

$\underline{D}_b = \underline{D}_b(S_b)$ = water bound water diffusion tensor, (L^2T^{-1})

S_b = degree of saturation with adsorbed water, given by ($[S_b] = 1$)

$$S_b = \begin{cases} S & \text{for } S \leq S_{SSP} \\ S_{SSP} & \text{for } S > S_{SSP} \end{cases} \quad (I.49)$$

According to adsorption theory, S_b depends upon the partial vapor pressure (or the relative humidity of the moist air) or the capillary pressure, p_c :

$$S_b = S_b(p_{gw}) = S_b(p_c) \quad (I.50)$$

For the description of the diffusion process of the binary gas species mixture (dry air and water vapor), Fick's law is applied

$$v_{ga}^d = -\frac{M_a M_w}{M_g^2} D_{eff} \nabla \left(\frac{p_{ga}}{p_g} \right) \quad (I.51)$$

$$v_{gw}^d = -\frac{M_a M_w}{M_g^2} D_{eff} \nabla \left(\frac{p_{gw}}{p_g} \right) \quad (I.52)$$

where,

D_{eff} = effective diffusion coefficient of gas mixture, ($L^2 T^{-1}$)

M_i = molar mass of phase i , ($M Mol^{-1}$)

$$\frac{1}{M_g} = \frac{\rho_{gw}}{\rho_g} \frac{1}{M_w} + \frac{\rho_{ga}}{\rho_g} \frac{1}{M_a} \quad (I.53)$$

For all gaseous constituents (dry air, ga ; water vapor, gw ; and moist air, g) the Clapeyron equation of state of perfect gases and Dalton's law are used as state equations:

$$p_i = \frac{\rho_i \theta R}{M_i} \quad (I.54)$$

$$p_g = p_{ga} + p_{gw} \quad (I.55)$$

Linear Momentum Balance

In terms of total stresses, neglecting inertial effects, the momentum balance equation for the whole porous material is given by:

$$\nabla \cdot \frac{\partial}{\partial t} \underline{\sigma} + \frac{\partial \rho}{\partial t} \underline{b} = 0 \quad (I.56)$$

where,

$\underline{\sigma}$ = stress tensor, ($L^{-1} M T^{-2}$)

\underline{b} = specific body force term (normally corresponding to the gravity vector),
($L M T^{-2}$)

ρ = averaged density of the multiphase medium ($L^{-3} M$), given by

$$\rho = (1 - \phi) \rho_s + \phi S \rho_l + \phi (1 - S) \rho_g \quad (I.57)$$

If this last expression was derived for Mainguy's model, the only difference would be the distinction between the components of the gas phase. In Gawin et al.'s model the gas phase, g , is treated as a whole, whereas in Mainguy's model the gas phase is a mixture of dry air, a , and water vapor, v . On the other hand, both models assume the gaseous phase to be an ideal gas.

Conservation of Energy

The energy conservation in this model is presented in the form:

$$\begin{aligned} \rho C_p \frac{\partial \theta}{\partial t} + [C_{pw} \rho_w \underline{v}_l + C_{pg} \rho_g \underline{v}_g] \nabla \theta - \nabla \cdot (\lambda_{eff} \nabla \theta) \\ = \Delta h_{phase} \left[\phi \frac{\partial}{\partial t} (S \rho_w) + S \rho_w \frac{\partial \phi_{hydr}}{\partial t} + \alpha S \rho_w \frac{\partial}{\partial t} (\nabla \cdot \underline{u}) + \nabla \cdot [\rho_w \underline{v}_l] \right] + \Delta h_{hydr} \frac{\partial}{\partial t} (\Delta m_{hydr}) \end{aligned} \quad (I.58)$$

where,

ρ = apparent density of porous media, ($L^{-3}M$)

C_p = effective specific heat of porous media, ($L^2T^{-2}\Theta^{-1}$)

θ = temperature, (Θ)

C_{pw} = specific heat of water in liquid phase, ($L^2T^{-2}\Theta^{-1}$)

C_{pg} = specific heat of gas mixture, ($L^2T^{-2}\Theta^{-1}$)

ρ_g = gas phase density, ($L^{-3}M$)

\underline{v}_g = velocity of gaseous phase, (LT^{-1})

λ_{eff} = effective thermal conductivity, ($LMT^{-3}\Theta$)

I.3.3 Initial conditions

At $t = 0$ the initial conditions specify the full fields of gas pressure, capillary pressure, temperature and displacements:

$$p_g = p_g^0 \quad (I.59)$$

$$p_c = p_c^0 \quad (I.60)$$

$$\theta = \theta^0 \quad (I.61)$$

$$\underline{u} = \underline{u}^0 \quad (I.62)$$

I . 3 . 4 Boundary Conditions

The boundary conditions¹ can be of the first kind or Dirichlet's boundary conditions on Γ_i^1 ,

$$p_g = \hat{p}_g \text{ on } \Gamma_g^1 \quad (I.63)$$

$$p_c = \hat{p}_c \text{ on } \Gamma_c^1 \quad (I.64)$$

$$\theta = \hat{\theta}^0 \text{ on } \Gamma_\theta^1 \quad (I.65)$$

$$\underline{u} = \hat{u} \text{ on } \Gamma_u^1 \quad (I.66)$$

1. The boundary conditions can also be of the second kind or Neumanns condition on Γ_i^2 ,

$$\begin{aligned} -(\rho_{ga}v_g - \rho_g v_{gw}^d) \cdot \underline{n} &= q_{ga} \text{ on } \Gamma_g^2 & -(\rho_{ga}v_g + \rho_w v_l + \rho_g v_{gw}^d) \cdot \underline{n} &= q_{gw} + q_l \text{ on } \Gamma_c^2 \\ -(\rho_w v_l \Delta h_{phase} - \lambda_{eff} \nabla \theta) \cdot \underline{n} &= q_T \text{ on } \Gamma_\theta^2 & \underline{\sigma} \cdot \underline{n} &= t \text{ on } \Gamma_u^2 \end{aligned}$$

and of the third kind or Cauchy's (mixed) boundary conditions on Γ_i^3

$$\begin{aligned} (\rho_{gw}v_g + \rho_w v_w + \rho_g v_{gw}^d) \cdot \underline{n} &= \beta_c (\rho_{gw} - \rho_{gw\infty}) \text{ on } \Gamma_c^3 \\ (\rho_w v_l \Delta h_{phase} - \lambda_{eff} \nabla \theta) \cdot \underline{n} &= \alpha_c (\theta - \theta_\infty) + e \sigma_0 (\theta^4 - \theta_\infty^4) \text{ on } \Gamma_\theta^3 \end{aligned}$$

Where the boundary $\Gamma = \Gamma_i^1 \cup \Gamma_i^2 \cup \Gamma_i^3$, \underline{n} is the unit normal vector, pointing toward the surrounding gas, q_{ga} , q_{gw} , q_l and q_T are, respectively, the imposed dry air flux, the imposed vapor flux, the imposed liquid flux, and the imposed heat flux, t is the imposed traction, $\rho_{gw\infty}$ and θ_∞ are the mass concentration of water vapor and the temperature in the far field of undisturbed gas phase, e is the emissivity of the interface, σ_0 is the Stefan-Boltzmann constant, while α_c and β_c are convective heat and mass transfer coefficients.

The convective boundary conditions usually occur at the interface between the porous media and the surrounding fluid. In the case of heat transfer they correspond to the Newton's law of cooling. When concrete behavior at high temperatures is analyzed, the radiative boundary conditions are usually of importance.[6]

I.4 Comparison of Models

Table I.1 compares the three models that were reviewed in this chapter. This comparison is made in terms of the equations they use and the approach taken with the water mass conservation.

	Bazant	Mainguy	Gawin et al.
Solid Mass Conservation			X
Dry Air Conservation		X	X
Water Conservation	X (only distinguishes between bound and free)	X (liquid and vapor separately)	X (liquid and vapor together)
Energy	X		X
Linear Momentum Balance			X
Heat Flux	X		
Moisture Flux	X		
Liquid Vapor Balance		X	

Table I.1: Model Equations

With regard to the very nature of the problem, it is evident that the mass conservation equations must be included regardless of any other assumption made in the model. However, the way this mass is interpreted may well differ between models. Bazant's model deals with this in what seems to be the most simple way: all water phases are treated as one component and only free and bound water are distinguished. Mainguy's model goes one step further by separating the water into three phases: liquid water, water vapor, and dry air (these last two forming an ideal mixture which constitutes the gas phase). Finally, Gawin et al.'s model considers in addition a solid mass conservation (the model is also the only one that accounts for mechanical behavior such as strain and stress). However, in contrast to Mainguy's model, Gawin et al.'s model does not separate the conservation equations for liquid and vapor phases: there is only one conservation equation for water species. On the other hand, this model differentiates between the origin of the liquid phase. If the saturation state is above the saturation point the water is said to come from the capillary pores, whereas below saturation the water is said to come from the skeleton itself (i.e. bound water).

Obviously, when temperature is one of the variables, conservation of energy has to be included as one of the conservation equations. This is also true for the non-isothermal extension of Mainguy's model proposed by Heukamp [12]. As a matter of fact, the equation for conservation of energy is the only additional equation required for Mainguy's isothermal model to become temperature dependent.

Chapter II

Non-Isothermal Model with Dehydration Effects

In this chapter we propose an extension of Mainguy's isothermal model to non isothermal evolution with dehydration effects. This extension requires the consideration of entropy conservation, following developments proposed by Heukamp [12]. However, in addition, we will consider the dehydration phenomenon which affects concrete behavior at high temperature. This dehydration term needs to be integrated in the mass conservation equation of the liquid water.

First, a brief introduction to the model is given, and the conservation and state equations for the model are developed. The conduction laws are then presented, and finally the initial and boundary conditions are introduced. At all times, comparisons with the isothermal model are made in order to identify the new terms which account for both dehydration and temperature changes.

II.1 Introduction

The porous medium is still considered to be composed of an undeformable skeleton and three fluid phases saturating the pore space (see Figure I.1). The fluid phases are:

- liquid water, w
- vapor water, v
- dry air, a

The last two phases, v and a , are assumed to form an ideal mixture, the wet air (the gas phase, g), which is assumed to behave like an ideal gas.

The total porosity, ϕ ($[\phi] = 1$), is filled by the liquid water, of partial porosity ϕ_w , and by the wet air mixture, of partial porosity ϕ_g . From [I.7] to [I.10] it follows that:

$$\phi = \phi_w + \phi_g = S_w \phi + \phi_g \quad (\text{II. 1})$$

with $S_w =$ liquid saturation ($[S_w] = 1$)

Based on the previous notation the masses in an elementary volume $d\Omega$ are given by [I.15] to [I.17], which we recall:

- Liquid water

$$m_w = \phi S_w \rho_w \quad (\text{II. 2})$$

- Water vapor

$$m_v = \phi(1 - S_w) \rho_v \quad (\text{II. 3})$$

- Dry air

$$m_a = \phi(1 - S_w) \rho_a \quad (\text{II. 4})$$

with $\rho_i =$ volume mass density of phase i , ($L^{-3}M$)

II.2 Conservation Equations

The mass conservation equations in this model are almost identical to those in the isothermal model. The only difference is the dehydration term, which is added to the liquid water mass conservation. This term accounts for the water that leaves the skeleton (dehydration) and enters the pore space.

In addition, to account for non-isothermal conditions, the entropy conservation equation is introduced.

II . 2 . 1 Mass Conservation

The three mass conservation equations [I.12] to [I.14] become:

- Liquid water conservation

$$\Phi \rho_w \frac{\partial}{\partial t} S_w + \nabla \underline{w}_w = -\mu^{w_{l \rightarrow g}} - \mu_{s \rightarrow l} \quad (\text{II. 5})$$

- Water vapor conservation

$$\phi \frac{M_v}{R} \frac{\partial}{\partial t} \left((1 - S_w) \frac{p_v}{\theta} \right) + \nabla \underline{w}_v = \mu^{w_{l \rightarrow g}} \quad (\text{II. 6})$$

- Dry air conservation

$$\phi \frac{M_a}{R} \frac{\partial}{\partial t} \left((1 - S_w) \frac{p_a}{\theta} \right) + \nabla \underline{w}_a = 0 \quad (\text{II. 7})$$

where,

$\mu^{w_{l \rightarrow g}}$ = formation rate from liquid water to vapor, ($L^{-3}MT^{-1}$)

$\mu^{w_{l \rightarrow g}} dt d\Omega$ = amount of liquid water which transforms, in the elementary volume $d\Omega$ over a time interval dt , into vapor (M).

$\mu_{s \rightarrow l}$ = dehydration mass rate, ($L^{-3}MT^{-1}$)

\underline{w}_i = mass flux vectors of the corresponding fluid phase, ($L^{-2}MT^{-1}$)

Note here that the fluxes are related to the relative velocities (v_i) in the same way as for the isothermal model (i.e. equations (I.18), to (I.20)).

The liquid water mass conservation equation (II. 5) contains the dehydration term, $\mu_{s \rightarrow l}$, which represents the dehydration phase change of chemically or physically bound water (part of the skeleton), that goes into the free (evaporable) liquid phase. This term can be expressed in the following way [1]:

$$\mu_{s \rightarrow l} = -m^b_{l_o} \frac{\partial \xi}{\partial t} \quad (\text{II. 8})$$

where,

$m^b_{l_o}$ = combined (bound) water mass involved in the dehydration process, ($L^{-3}M$)

$\xi(t)$ = hydration degree, ($[\xi] = 1$)

- reference configuration, $\xi \equiv 1$
- complete dehydration, $\xi \equiv 0$

The hydration degree depends on a kinetics law. However, since the characteristic time of dehydration is very small compared to the time scales of the transport of heat and fluid masses, it can be assumed that the dehydration process is permanently at thermodynamic equilibrium [1]. This leads to a relation linking the hydration degree to the temperature:

$$\xi = \xi(\theta) = 1 - \Pi(\theta - \theta_0) \quad (\text{II. 9})$$

where,

Π = constant that linearly relates temperature and hydration degree ($[\Pi] = \Theta^{-1}$).

This dehydration function is shown in Figure II.1.

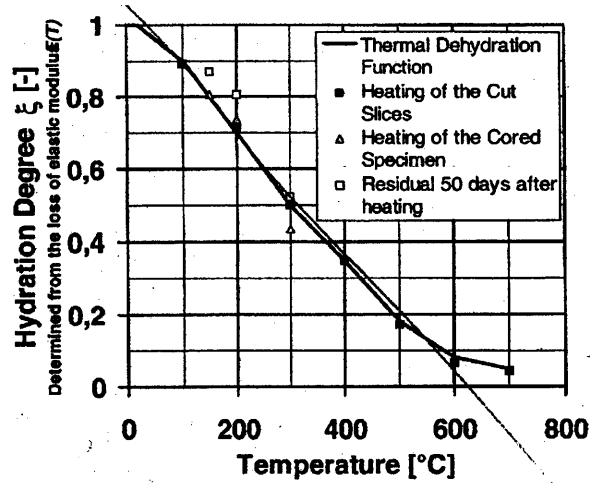


Figure II.1: Thermal dehydration function $\xi(\theta)$ (cited by Ulm et al [1] from Fasseu [13])

II.2.2 Entropy Conservation

As part of the extension to non-isothermal conditions, the entropy balance for the elementary volume is considered. Neglecting volume heat sources this equation reads as follows:

$$\left(\frac{\partial S}{\partial t} + \sum_{i=w,v,a} s_i \underline{w}_i \right) = -\nabla \cdot \frac{\underline{q}}{\theta} \quad (\text{II. 10})$$

where,

s_i = specific entropy per unit mass of the corresponding fluid phase ($i = w, v, a$)

$$([s_i] = L^2 T^{-2} \Theta^{-1})$$

$s_i \underline{w}_i \cdot \underline{n} da$ = efflux of entropy of the fluid flux, \underline{w}_i , through an infinitesimal surface da oriented by unit normal \underline{n} (the boundary)

\underline{q} = heat flux vector, ($[q] = MT^{-3}$)

$-(\underline{q} \cdot \underline{n}) da dt$ = heat supplied from the outside through the boundary in time dt

$\frac{\underline{q}}{\theta}$ = efflux of entropy by heat through the boundary

S = total internal entropy of all matter contained within the elementary volume $d\Omega$,
 ($[S] = L^{-1}MT^{-2}\Theta^{-1}$); it reads:

$$S = S_s + \sum_{i=w,v,a} m_i s_i \quad (\text{II. 11})$$

where,

m_i = mass content of fluid phase, (M)

Both, the entropy of the solid phase, S_s , and the one of the fluid phases, s_i , need to be specified by the solid phase and liquid phase state equations, respectively.

II . 3 State Equations

Use of the entropy balance equations requires the definition of state equations related to the entropy of the fluid and of the solid phases.

II . 3 . 1 Fluid State Equations

Before deriving the equations for each phase, some common terms need to be defined:

- Specific free energy of the fluid phase (ψ_i)

$$\psi_i = u_i - \theta s_i \quad (\text{II. 12})$$

where u_i = specific internal energy, (L^2T^{-2})

- Specific free enthalpy of a fluid phase ($g_i(p_i, \theta)$), Gibbs potential)

$$g_i(p_i, \theta) = \psi_i + \frac{p_i}{\rho_i} \quad (\text{II. 13})$$

where p_i = thermodynamic pressure of the fluid phase, ($L^{-1}MT^{-2}$)

From the potential we obtain the fluid state equations:

$$\frac{\partial g_i}{\partial p_i} = \frac{1}{\rho_i} \quad (\text{II. 14})$$

$$\frac{\partial g_i}{\partial \theta} = -s_i \quad (\text{II. 15})$$

- Enthalpy h_i , (L^2T^{-2})

$$h_i = u_i + \frac{p_i}{\rho_i} = g_i + \theta s_i \quad (\text{II. 16})$$

The enthalpy allows derivation of the specific heat of fluid phase i (at constant pressure p_i):

$$C_{pi} = \left. \frac{\partial h_i}{\partial \theta} \right|_{p_i} \quad (\text{II. 17})$$

II.3.2 Incompressible Water Phase

The incompressibility of the liquid water phase implies that the specific free energy depends only on temperature:

$$\psi_i = \psi_i(\theta) \rightarrow s_w = \frac{\partial \psi_w}{\partial \theta} = s_{w_0} + C_{pw} \ln\left(\frac{\theta}{\theta_0}\right) \quad (\text{II. 18})$$

where,

s_{w_0} = reference specific entropy (at temperature θ_0 and pressure p_{w_0})

C_{pw} = specific heat of liquid water phase (at constant pressure), ($L^2T^{-2}\Theta^{-1}$)

Using (II. 18), the total differential Gibbs potential (II. 13) reads:

$$dg_w = -s_w(\theta)d\theta + \frac{dp_w}{\rho_w} \quad (\text{II. 19})$$

where p_w = fluid pressure, ($L^{-1}MT^{-2}$)

Integrations of the last two equations, (II. 18) and (II. 19), result in:

$$g_w = g_{w_0} + \frac{p_w - p_{w_0}}{\rho_w} - s_{w_0}(\theta - \theta_0) - C_{pw} \left[\theta \ln\left(\frac{\theta}{\theta_0}\right) - (\theta - \theta_0) \right] \quad (\text{II. 20})$$

II.3.3 Vapor as an Ideal Gas

The ideal gas state equation reads as follows:

$$\frac{\partial g_v}{\partial p_v} = \frac{1}{\rho_v} = \frac{R\theta}{M_v p_v} \quad (\text{II. 21})$$

and the specific entropy:

$$s_v = \frac{\partial}{\partial \theta}(g_v) = s_{v_0} + C_{pv} \ln\left(\frac{\theta}{\theta_0}\right) - \frac{R}{M_v} \ln\left(\frac{p_v}{p_{v_0}}\right) \quad (\text{II. 22})$$

Integration leads to

$$g_v = g_{v_0} + \int_{p_{i_0}}^{p_i} \frac{dp_v}{\rho_v} - \int_{\theta_0}^{\theta} s_v d\theta \quad (\text{II. 23})$$

$$g_v = g_{v_0} + \frac{R\theta}{M_v} \ln\left(\frac{p_v}{p_{v_0}}\right) - s_{v_0}(\theta - \theta_0) - C_{pv} \left[\theta \ln\left(\frac{\theta}{\theta_0}\right) - (\theta - \theta_0) \right] \quad (\text{II. 24})$$

The same procedure can be applied to the dry air. In this case the specific entropy reads:

$$s_a = -\frac{\partial g_a}{\partial \theta} = s_{a_o} + C_{pa} \ln\left(\frac{\theta}{\theta_0}\right) - \frac{R}{M_a} \ln\left(\frac{p_a}{p_{a_0}}\right) \quad (\text{II. 25})$$

II.3.4 Thermodynamic Equilibrium Water-Vapor

The equilibrium state is defined by the equality of the Gibbs potentials:

$$g_w(p_w, \theta) = g_v(p_v, \theta) \quad (\text{II. 26})$$

Assuming that the reference state corresponds to a state of thermodynamic equilibrium it is apparent that:

$$g_{w_o} - g_{v_o} \equiv 0 \quad (\text{II. 27})$$

In addition, the latent heat of vaporization in the reference state is given by:

$$L^0_{l \rightarrow g} = \theta_0(s_{v_o} - s_{w_o}) \quad (\text{II. 28})$$

Using the previous expressions together with equations (II. 20) and (II. 24) we arrive at:

$$\frac{p_v}{p_{vs}(\theta)} = \exp\left[\frac{M_v}{R\theta\rho_w}(p_w - p_{w_o})\right] \quad (\text{II. 29})$$

where,

$$p_{vs}(\theta) = p_{v_o} \exp\left[\frac{M_v}{R\theta}\left(\frac{L^0_{l \rightarrow g}}{\theta_0}(\theta - \theta_0) - (C_{pw} - C_{pv})\left(\theta \ln\left(\frac{\theta}{\theta_0}\right) - (\theta - \theta_0)\right)\right)\right] \quad (\text{II. 30})$$

$$\frac{p_v}{p_{vs}} = \text{relative humidity relative to the saturating vapor pressure}$$

II.4 Mixture State Equations and Capillary Pressure

We recall that the total pressure of the mixture, p_g , is the sum of the partial pressures of the mixture components (water vapor, v , and dry air, a):

$$p_g = p_v + p_a \quad (\text{II. 31})$$

We also note that the volume mass is related to the molar volume density c_v and c_a by:

$$\rho_v = M_v c_v \quad (\text{II. 32})$$

$$\rho_a = M_a c_a \quad (\text{II. 33})$$

This in hand, the ideal fluid state equation (II. 21) together with (II. 31), (II. 32) and (II. 33) yields:

$$p_v = R\theta c_v = C_v p_g \quad (\text{II. 34})$$

$$p_a = R\theta c_a = C_a p_g \quad (\text{II. 35})$$

where,

C_v = molar fraction of vapor in the mixture, ($[C_v] = 1$)

C_a = molar fraction of dry air in the mixture, ($[C_a] = 1$), defined by:

$$C_v = \frac{c_v}{c_v + c_a} = \frac{p_v}{p_g} \quad (\text{II. 36})$$

$$C_a = \frac{c_a}{c_v + c_a} = \frac{p_a}{p_g} \quad (\text{II. 37})$$

$$C_v + C_a = 1 \quad (\text{II. 38})$$

Finally, in this model the capillary pressure is the difference between the wet air pressure and the liquid pressure:

$$p_c = p_g - p_w \quad (\text{II. 39})$$

II. 5 Solid State Equation

The solid state equation refers to the skeleton and the interface [14]:

$$S_s = S - \sum_{i=w,v,a} m_i s_i = S_m + S_c \quad (\text{II. 40})$$

where,

S_m = entropy of the solid matrix, ($L^{-1}MT^{-2}\Theta^{-1}$)

S_c = entropy associated with capillary actions at the liquid-gas interface,

($L^{-1}MT^{-2}\Theta^{-1}$)

II. 5. 1 Entropy of the Solid Matrix and Dehydration

If the material was chemically inert in addition to being incompressible, the entropy would only depend on the temperature [12]:

$$S_m = \frac{\partial \Psi_s}{\partial \theta} = C_s \ln\left(\frac{\theta}{\theta_0}\right) \quad (\text{II. 41})$$

where,

Ψ_s = free energy of the skeleton, (L^2T^{-2})

C_s = volume heat capacity of the skeleton (per unit of porous volume $d\Omega$)

$C_s = m_s c_s$, ($L^2T^{-2}\Theta^{-1}$).

m_s = skeleton mass (solid matrix + combined water), (M)

$$m_s = (1 - \phi)\rho_s$$

ρ_s = associated mass density of the skeleton, ($L^{-3}M$)

c_s = specific heat capacity of the skeleton, ($L^2T^{-2}\Theta^{-1}$)

On the other hand, due to dehydration, the entropy S_m depends not only on the temperature, θ , but also on the hydration degree ξ :

$$dS_m = C_s \frac{d\theta}{\theta} + m_{s_0} s_s d\xi \quad (\text{II. 42})$$

where,

s_s = specific entropy which is released during dehydration $d\xi < 0$

We should note that the specific entropy, s_s , may well depend on temperature, θ . If that is the case, then Maxwell symmetries would require:

$$m_{s_0} \frac{\partial s_s}{\partial \theta} = \frac{1}{\theta} \frac{\partial C_s}{\partial \xi} = \frac{\partial^2 \Psi_s}{\partial \theta \partial \xi} \quad (\text{II. 43})$$

which leads to,

$$s_s = \left[s_{s_0} + C_{s_0} \ln\left(\frac{\theta}{\theta_0}\right) \right] \quad (\text{II. 44})$$

$$C_s = c_{s_0} m_{s_0} \xi \quad (\text{II. 45})$$

where,

c_{s_0} = specific heat capacity of the skeleton in the reference state

s_{s_0} = specific entropy of the skeleton in the reference state.

The reference state is defined by: $m_{s_0} = (1 - \phi)\rho_{s_0}$ and θ_0

In a first approximation, we will assume that there is no coupling between specific heat and dehydration, and between specific entropy and temperature. This assumption means that (II. 43) is equal to zero, thus:

$$C_s \neq C_s(\xi) \Rightarrow C_s = C_{s_0} \quad (\text{II. 46})$$

$$s_s \neq s_s(\theta) \Rightarrow s_s = s_{s_0} \quad (\text{II. 47})$$

Assumptions (II. 48) and (II. 49) allow writing an analytical approximation for the entropy of the solid matrix, which is linear in ξ :

$$S_m = C_{s_0} \ln\left(\frac{\theta}{\theta_0}\right) + m_{s_0} s_{s_0} \xi \quad (\text{II. 48})$$

II . 5 . 2 Entropy of the Gas-Liquid Interface

The gas-liquid phase entropy is given by [12]:

$$S_c = -\phi \frac{\partial}{\partial \theta} \left[\gamma(\theta) \int_0^{p_c/\gamma(\theta)} S_w(x) dx \right] \quad (\text{II. 49})$$

where,

$$S_w = \text{liquid mass saturation, } ([S_w] = 1)$$

Heukamp [12] proposed the following function for non-isothermal evolution (valid only when the liquid phase is continuous within the porous medium):

$$S_w = \left[1 + \left(\frac{\gamma(\theta_0) p_c}{\gamma(\theta) a} \right)^{n-m} \right]^{-m} \quad (\text{II. 50})$$

where,

$n, m = \text{material constants}^1$

$\gamma(\theta) = \text{capillary surface tension at the liquid-gas phase interface formed by a meniscus.}$

Heukamp [12] suggested the following dependence in temperature:

$$\gamma(\theta) = \gamma(\theta_0)[1 - c_0(\theta - \theta_0)] \quad (\text{II. 51})$$

$$c_0 = 3 \times 10^{-3} K^{-1} \quad (\text{II. 52})$$

1. Assuming that $m = 1 - 1/n$, we often find that: $m = \frac{1}{b}$ and $n = \frac{b}{b-1}$

II.6 Conduction Laws

The conduction laws are needed for the fluid fluxes (in all phases) and the heat conduction in the entropy balance.

II.6.1 Fluid Conduction Laws

Similarly to Mainguy's [4] and Gawin et al.'s [6] model, Darcy's law is used to describe the flux of liquid water and wet air, and Fick's law is used for the gaseous phases.

Darcy's Law

For the wet air, Darcy's law reads:

$$\phi(1 - S_w)v_g = -\frac{k}{\eta_g}k_{rg}(S_w)grad(p_g) \quad (\text{II. 53})$$

and for the liquid phase,

$$\phi S_w v_w = -\frac{k}{\eta_w}k_{rl}(S_w)grad(p_w) \quad (\text{II. 54})$$

where,

k = intrinsic permeability of the porous material (independent of the fluid phase)

$$([k] = L^2)$$

$k_{ri}(S_w)$ = relative permeability of phase i ($[k_{ri}] = 1$).

We will assume that [I.27] and [I.28] remain valid also for high temperatures:

$$k_{rl}(S_w) = \sqrt{S_w}[1 - (1 - S_w^b)^{1/b}]^2 \quad (\text{II. 55})$$

$$k_{rg}(S_w) = \sqrt{(1 - S_w)}(1 - S_w^b)^{2/b} \quad (\text{II. 56})$$

b = material constant

η_i = dynamic viscosity of phase i , ($L^{-1}MT^{-1}$).

The dynamic viscosity for the liquid phase depends strongly on temperature, but the one for the gas phase varies little with it.

Use of Darcy's Law for the liquid phase with the ideal gas law, allows us to write the final equations for the liquid water flux in the form:

$$w_w = -\rho_w \frac{k}{\eta_w} k_{rl}(S_w) grad(p_w) \quad (\text{II. 57})$$

Fick's Law

The average molar velocity of the wet air (v_g , convective transport of vapor and dry air) is defined as:

$$v_g = C_v v_v + C_a v_a \quad (\text{II. 58})$$

where,

$$C_v, C_a = \text{molar fractions of the mixture (II. 36) and (II. 37)}$$

The conduction laws of the gas phase read:

$$C_v(v_v - v_g) = -D \text{grad}(C_v) \quad (\text{II. 59})$$

$$C_a(v_a - v_g) = -D \text{grad}(C_a) \quad (\text{II. 60})$$

where,

D = diffusion coefficient,

$$D = \tau \frac{d_{va}}{p_g} = \tau D_{va}$$

with,

$$d_{va} = d_{va_0} p_{atm} \left(\frac{\theta}{\theta_0} \right)^{1.88} \quad (\text{II. 61})$$

p_g = wet air pressure defined by (II. 31)

$$d_{va_0} = 0.217 \text{ cm}^2/\text{s}$$

$$\theta_0 = 273 \text{ K}$$

p_{atm} = atmospheric pressure

τ = tortuosity coefficient (accounts for effects of pore size and shapes in the diffusion process).

Combination of Conduction Laws to Obtain Gas Fluxes

Using Darcy's law for the gas phase (II. 53) in the previous definitions of the gas conduction laws (II. 59) and (II. 60) leads to the final expression for the water vapor and dry air fluxes.

Indeed, if we rewrite the conduction laws in the form

$$v_v = -\frac{D}{C_v} \text{grad}(C_v) + v_g = -\tau \frac{d_{va}(\theta)}{p_v} \text{grad}(C_v) + v_g \quad (\text{II. 62})$$

$$v_a = -\frac{D}{C_a} \text{grad}(C_a) + v_g = -\tau \frac{d_{va}(\theta)}{p_a} \text{grad}(C_a) + v_g \quad (\text{II. 63})$$

we can now combine them with Darcy's law:

$$\frac{w_v}{\rho_v} = \phi(1 - S_w)v_v = -\phi(1 - S_w)\tau\frac{d_{va}(\theta)}{p_v}\text{grad}(C_v) - \frac{k}{\eta_g}k_{rg}(S_w)\text{grad}(p_g) \quad (\text{II. 64})$$

$$\frac{w_a}{\rho_a} = \phi(1 - S_w)v_a = -\phi(1 - S_w)\tau\frac{d_{va}(\theta)}{p_a}\text{grad}(C_a) - \frac{k}{\eta_g}k_{rg}(S_w)\text{grad}(p_g) \quad (\text{II. 65})$$

For numerical calculations the resistance to diffusion factor, $f(\phi, S_w)$, will be used instead of the tortuosity. These are related in the following way [4]:

$$\tau(\phi, S_w) = \phi^{1/3}(1 - S_w)^{7/3} \quad (\text{II. 66})$$

$$f(\phi, S_w) = \phi^{4/3}(1 - S_w)^{10/3} = \tau(\phi, S_w)[\phi(1 - S_w)] \quad (\text{II. 67})$$

Finally, taking advantage of the ideal gas law the final version of the flux equations for the water vapor and dry air are obtained:

$$w_v = -f(\phi, S_w)\frac{M_v}{R\theta}d_{va}(\theta)\text{grad}\left(\frac{p_v}{p_g}\right) - \frac{M_v}{R\theta}p_v\frac{k}{\eta_g}k_{rg}(S_w)\text{grad}(p_g) \quad (\text{II. 68})$$

$$w_a = -f(\phi, S_w)\tau\frac{M_a}{R\theta}d_{va}(\theta)\text{grad}\left(\frac{p_a}{p_g}\right) - \frac{M_a}{R\theta}p_a\frac{k}{\eta_g}k_{rg}(S_w)\text{grad}(p_g) \quad (\text{II. 69})$$

II . 6 . 2 Heat Conduction Law

For heat conduction Fourier's law is applied. It reads:

$$\underline{q} = -\aleph \text{grad}(\theta) \quad (\text{II. 70})$$

where,

\aleph = heat conductivity, which can be expressed as the weighed sum of the different components ($MT^{-3}\Theta^{-1}$):

$$\aleph = \aleph_s + \phi S_w \aleph_w + \phi(1 - S_w) \aleph_g \quad (\text{II. 71})$$

\aleph_s = thermal conductivity of the skeleton

\aleph_w = thermal conductivity of the liquid water

\aleph_g = thermal conductivity of the wet air

II . 7 Boundary and Initial Conditions

The boundary and initial conditions are the same as for the isothermal model, which are defined in section I.2.3 and I.2.4.

II . 8 Summary

The model developed in this chapter is an extension of Mainguy's isothermal model. The dehydration term is added to the liquid water mass conservation equation (II. 5) and, in order to account for the non-isothermal situation, the conservation of entropy equation (II. 10) is integrated into the model. The liquid vapor balance equation is still used, but the temperature changes introduce some modifications to Mainguy's version (I.32).

The entropy conservation equation requires the use of an additional state equation for the liquid and solid phases. These state equations allow us to write the entropy of the different phases.

Finally, the conduction laws were written in a similar way to Mainguy's but with the addition of the heat conduction law.

Chapter III

Numerical Application by Means of the Finite Volume Method

In order to solve the set of equations developed in the previous chapter, the finite volume method is used. This is the same method used by Mainguy in his model [4], but here it will be developed in cylindrical coordinates (contrary to Mainguy's cartesian coordinates). This type of coordinate system facilitates the use of the model in geometries such as tunnels (see Figure II.1).

First, a brief review of the finite volume scheme is provided, and then the geometrical characteristics of the model are explained. Finally, a summary of the differences between the cartesian and cylindrical coordinates formulation is presented.

III . 1 Finite Volume

The basic principle of the finite volume method is to integrate the balance equations over each control volume, Ω_i , of the mesh. The control volume Ω_i starts at point x_i and goes to point x_{i+1} . In addition to this space integration, a time discretization has to be considered (because

this is an evolution problem). This is done by introducing discrete values of time $t^n = n(dt)$, for all integers n and time step dt , which we consider to be constant. The analysis is now restricted to a grid which is uniform in both space x and time t , and therefore the integration of the set of equations must be done over the control volume Ω_i and time step dt [15].

The solution at the i -th grid point at time t^n is given by:

$$\{u\}_i^n = u(t^n, x_i) \quad (\text{III. 1})$$

Using the equations of the non-isothermal model with dehydration effects, the finite volume scheme is written as:

Liquid water conservation

$$\int_{\Omega} \int_t^{t^{n+1}} \left(\phi \rho_w \frac{\partial S_w}{\partial t} \right) dt d\Omega + \int_{\Omega} \int_t^{t^{n+1}} \text{div}(\underline{w}_w) dt d\Omega = \int_{\Omega} \int_t^{t^{n+1}} (-\mu_{l \rightarrow g}) dt d\Omega + \int_{\Omega} \int_t^{t^{n+1}} \left(-m_{l_o}^b \frac{\partial \xi}{\partial t} \right) dt d\Omega \quad (\text{III. 2})$$

Water vapor conservation

$$\phi \frac{M_v}{R\theta} \int_{\Omega} \int_t \frac{\partial}{\partial t} (1 - S_w) p_v dt d\Omega + \int_{\Omega} \int_t \text{div}(\underline{w}_v) dt d\Omega = \int_{\Omega} \int_t \mu_{l \rightarrow g} dt d\Omega \quad (\text{III. 3})$$

Dry air conservation

$$\phi \frac{M_a}{R\theta} \int_{\Omega} \int_t \frac{\partial}{\partial t} (1 - S_w) p_a dt d\Omega + \int_{\Omega} \int_t \text{div}(\underline{w}_a) dt d\Omega = 0 \quad (\text{III. 4})$$

Liquid-vapor balance

$$\int_{\Omega} \int_t \frac{R\theta}{M_v} \ln\left(\frac{p_v}{p_{v0}}\right) dt d\Omega = \int_{\Omega} \int_t \left\{ \frac{p_w - p_{w0}}{\rho_w} + \frac{l_0}{\theta_0} (\theta - \theta_0) + (C_{pl} - C_{pv}) \left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right) \right] \right\} dt d\Omega \quad (\text{III. 5})$$

Entropy conservation

$$\int_{\Omega} \int_t \phi \left[\frac{\partial}{\partial t} \left(S_s + \sum_{i=w, v, a} m_i s_i \right) + \sum_{i=w, v, a} s_i \underline{w}_i \right] dt d\Omega = \int_{\Omega} \int_t [-\text{div}(\underline{q})] dt d\Omega \quad (\text{III. 6})$$

III . 2 Geometrical Characteristics

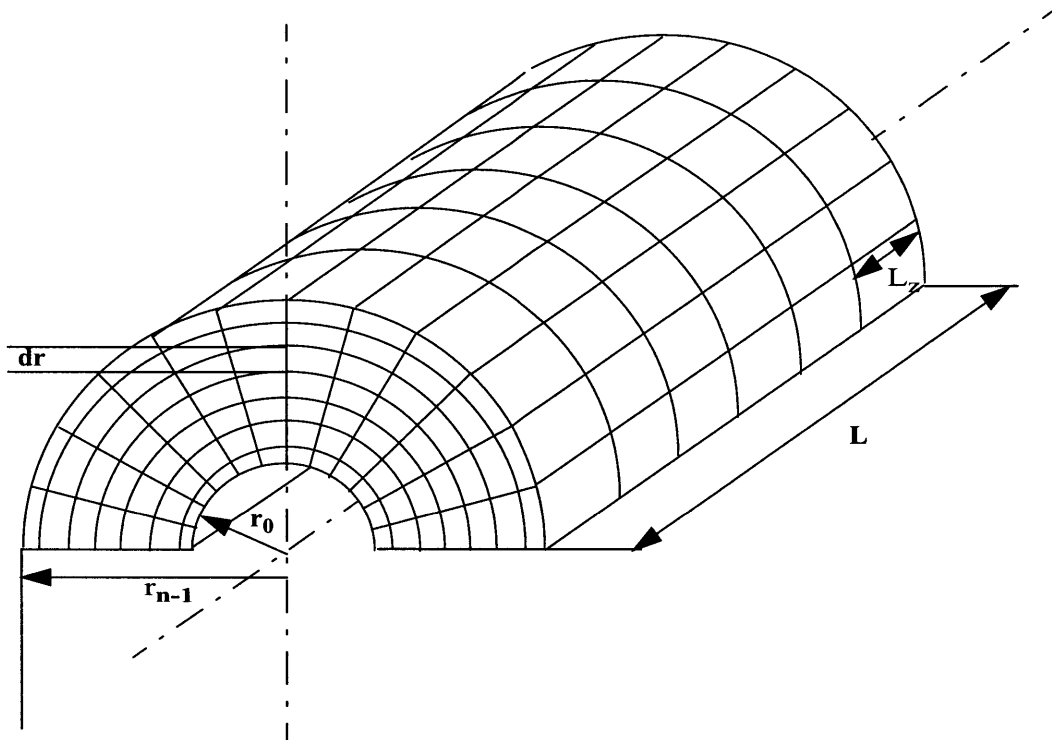


Figure II.1: Tunnel Shape

The consequences of changing the coordinate system from cartesian to cylindrical have not only an effect on the numerical methods, but also affect the shape and position of the elementary volume under consideration (see Figure II.2).

The elementary volume is a ring defined by its inner and outer radii. Its thickness is assumed to be of unit length in the z direction (L_z). The position of the volume values, however, are located in the middle of the elementary volume (see Figure II.2); therefore, we define the following:

- r_0^i = inner radius of elementary volume i
- r_1^i = outer radius of elementary volume i
- r_i = radial position of the middle of elementary volume i

The radial spacing, dr , can be determined in two ways: it can be assumed constant or its value can change so that the volume remains constant. This choice of spacing will mainly affect expressions for the volume integrals.

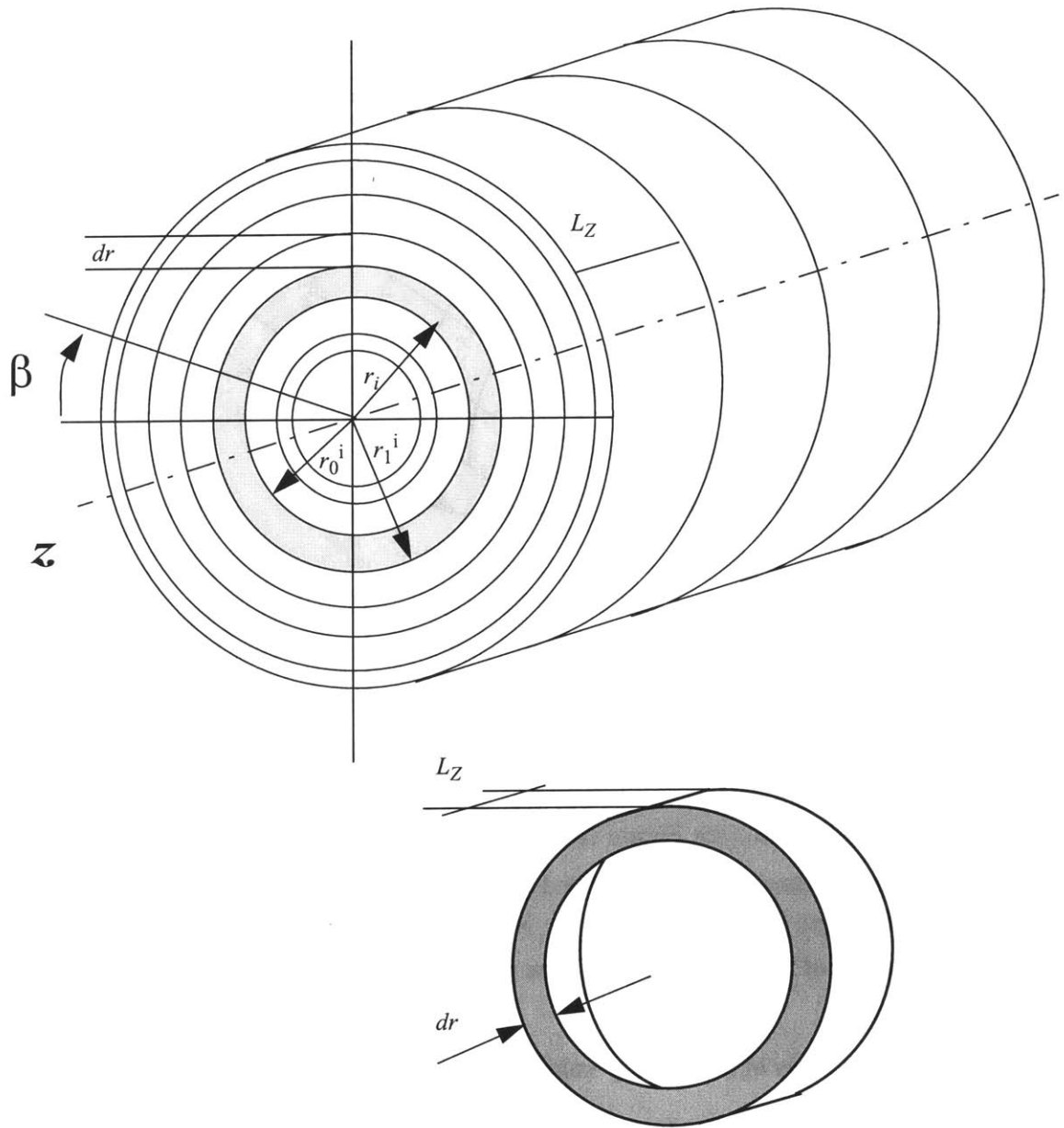


Figure II.2: Typical Elementary Volume

III . 3 Parameters Affected by Change of Coordinates

Equations (III. 2) to (III. 6) can be used in either the cartesian or cylindrical coordinate system. However, the volume and area integrals will introduce some differences in the resulting expressions for the discretized equations.

In order to simplify the approach, the discretization of the equations is limited to the one-dimensional case, i.e. nothing changes along the β or z direction (see Figure II.2).

The first difference that the change in coordinate system introduces is the resulting volume integral. It was determined in the derivations (Appendix A) that the differences in volume integrals resulting from the coordinate system change can be summarized in one variable called $m(K)$.

For either coordinate system, the approximation of the volume integral in the one dimensional case is given by the same expression:

$$\int_{\Omega} a d\Omega = m(K) \{a\}_k^n \quad (\text{III. 7})$$

Therefore, the discretized equations obtained can be adapted by changing the value of $m(K)$ for their use in either coordinate system.

Also, for the cylindrical coordinates case, the value of $m(K)$ is the only parameter affected when changing from a constant to a varied spacing.

Another difference in the discretized results is given by the area integral, $\int_A a dA$, resulting from the use of the divergence theorem to simplify the volume integrals of the divergence operators in equations (III. 2) to (III. 6).

Details for all these derivations are given in Appendix A. A summary of the different expressions in both coordinate systems is given in Table III. 1.

Appendix B provides detailed derivations of the discretized equations, for both isothermal and non-isothermal model with dehydration effects. They are derived in the one-dimensional case for both the cartesian and cylindrical coordinate systems.

	Cartesian	Cylindrical
$d\Omega$	$dx dy dz$	$r dr d\beta dz$
Ω	$\Omega = L_x L_y L_z$	$\Omega = \pi L_z \left\{ (r_1)^2 - (r_0)^2 \right\}$
$m(K)$	L_x	$\frac{r_1^2 - r_0^2}{2}$
dA	$dy dz$	$d\beta dz$
A	$L_y L_z$	$2\pi L_z$

Table III. 1: Summary of changes resulting from coordinate system modification (1-D case)

Chapter IV

Applications

This chapter presents the results obtained with the model developed in Chapter II and also verifies the accuracy of the development from cartesian to cylindrical coordinates. After the verification is performed, results obtained using the non-isothermal model, with and without dehydration effects, are presented and discussed. Finally, remarks regarding the extension of the model to temperatures beyond the critical point of water are developed.

IV . 1 Finite Volume Mesh

The mesh used for the cartesian and cylindrical coordinate models have similar characteristics. The distance x_i , or r_i for cylindrical coordinates, locates the middle of the control volumes, K_i . These midpoints are separated from each other by a constant ‘spacing’, dx for cartesian and dr for cylindrical coordinates. The first and last control volumes, K_0 and K_{n-1} , are of half the length of the other ones and their ‘mid-point’ position is located at the beginning and end of the control volume, respectively. There are n control volumes in the mesh. This is illustrated in Figure IV.1.

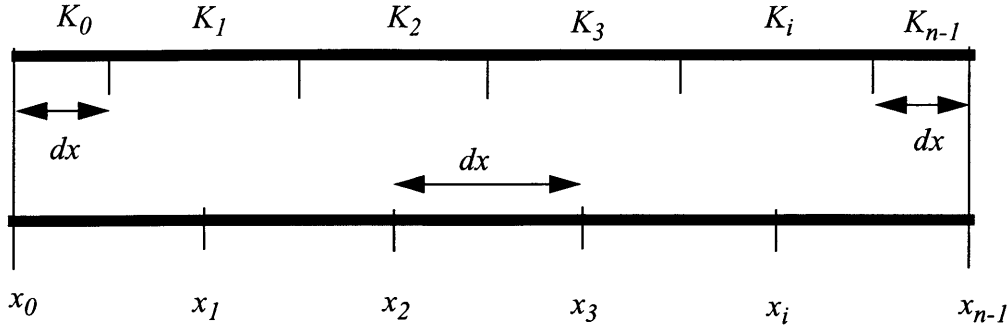


Figure IV.1: Typical mesh for cartesian coordinates (for cylindrical coordinates replace ‘ dx ’ with ‘ dr ’ and ‘ x ’ with ‘ r ’)

IV . 2 Verification of Model

First, the theory behind the verification is explained and then the conditions under which the simulations were performed are described. Finally, the results are presented.

IV . 2 . 1 Large Radius Verification

The extension to cylindrical coordinates is verified by using a large inner radius which theoretically will give a cartesian response. To illustrate this we use the liquid water mass conservation equation from the isothermal model (I.12):

$$\frac{\partial m_w}{\partial t} = -\text{div} \underline{w}_w - \mu^w_{l \rightarrow g} \quad (\text{IV. 1})$$

The only difference between the cartesian and cylindrical coordinates version of the previous equation is the divergence operator. For the one-dimensional case in cartesian coordinates this is given by [16]:

$$\text{div}(\underline{b}) = \frac{\partial b_x}{\partial x} \quad (\text{IV. 2})$$

where,

$$\underline{b} = \text{vector field}, \underline{b}(\underline{x}, t) = b_i(\underline{x}, t)e_i$$

For the cylindrical coordinates case the divergence operator is given by [16]:

$$\text{div}(\underline{b}) = \frac{1}{R} \frac{\partial}{\partial R} (R b_R) = \frac{1}{R} \left[b_R + R \frac{\partial b_R}{\partial R} \right] = \frac{b_R}{R} + \frac{\partial b_R}{\partial R} \quad (\text{IV. 3})$$

From (IV. 3) it appears that if the radius, R , becomes large, then the divergence operator has the same form as (IV. 2), corresponding to 1-D cartesian coordinates:

$$R \rightarrow \infty \quad \Rightarrow \quad \text{div}(\underline{b}) \approx \frac{\partial b_R}{\partial R} \quad (\text{IV. 4})$$

IV . 2 . 2 Simulation Conditions

The conditions and parameters attempt to simulate the isothermal drying of concrete for a period of 730 days.

Initial Conditions

At time $t = 0$ the following values are prescribed to all control volumes [4]:

$$\{p_v\}_i^0 = h_r p_{vs_0}$$

$$\{p_g\}_i^0 = \overline{p_{atm}}$$

$$\{\theta\}_i^0 = 293K$$

where,

$$h_r = \text{relative humidity, } ([h_r] = 1) = 0.85$$

$$p_{vs_0} = \text{saturation vapor pressure, } (L^{-1}MT^{-2}) = 2333Pa$$

$$p_{atm} = \text{atmospheric pressure, } (L^{-1}MT^{-2}) = 10.13MPa$$

Boundary Conditions

At the inner boundary, similar conditions to the ones prescribed initially are imposed. The only difference is now the value for the relative humidity:

$$h_r^b = 0.5$$

Geometrical and Time Parameters

In this simulation there are 201 control volumes ($n = 201$) and the total thickness, e , of the sample is 1 meter. The spacing is determined by:

$$\text{spacing} = \frac{e}{n - 1}$$

The total time for the simulation is 730 days and the time step, dt , is 0.1 seconds.

The initial inner radius, r_0^0 , is 50 meters.

IV.2.3 Comparison of Results

The results from the original isothermal model in cartesian coordinates were compared to a modified version of it in cylindrical coordinates. The results obtained with a large R were similar to those obtained with the cartesian model. Therefore, we conclude that the coordinate modifications are accurate.

Figure IV.2 and Figure IV.3 contain the results for the cartesian and cylindrical coordinates, respectively. They contain graphs for the variations along the specimen length of: (a) pressure, (b) concentrations, (c) capillary pressure and (d) liquid-vapor exchange rate. Boundary conditions were only imposed at the inner surface, i.e. left side of the graphs.

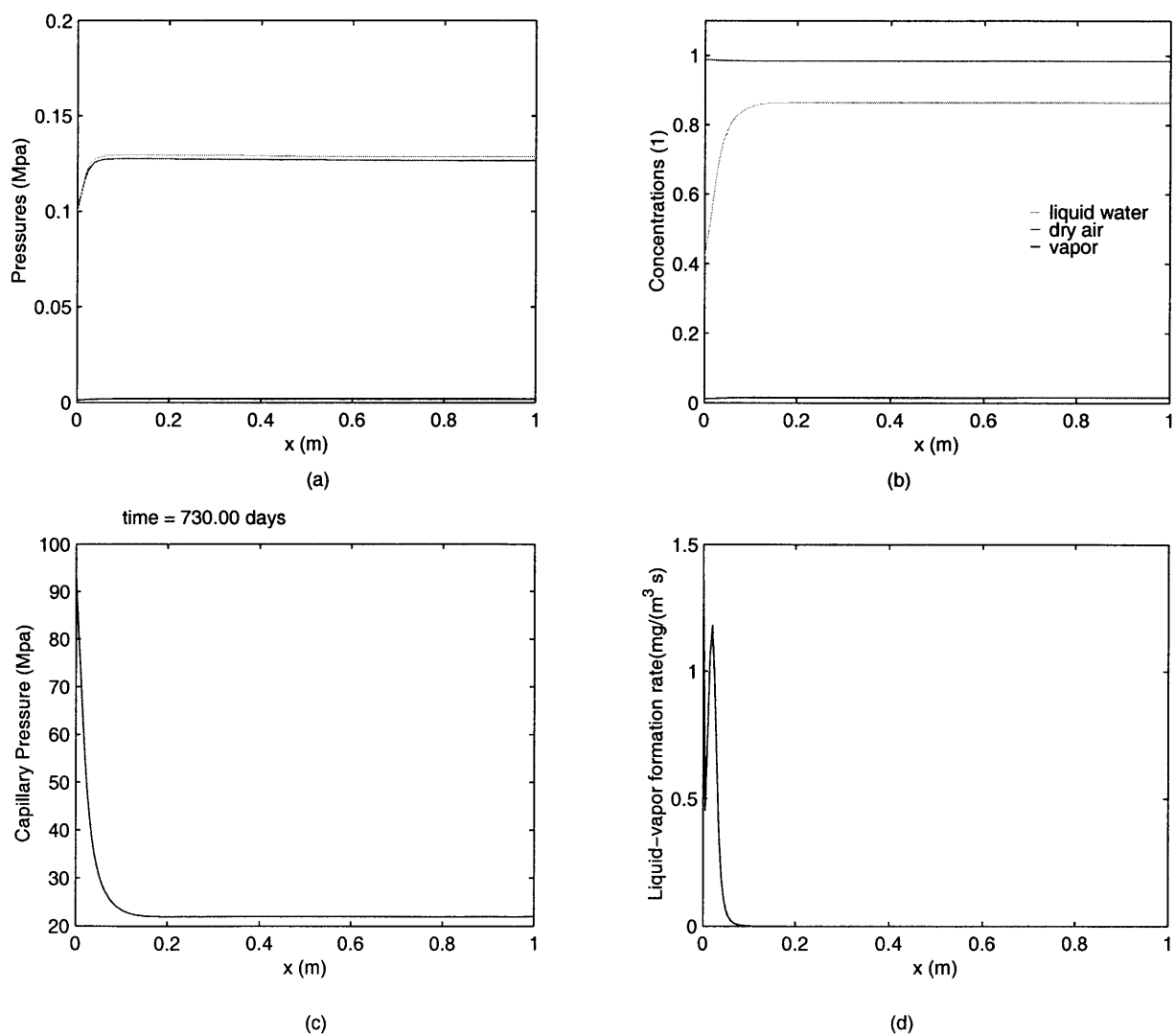


Figure IV.2: Results with the isothermal model in CARTESIAN coordinates

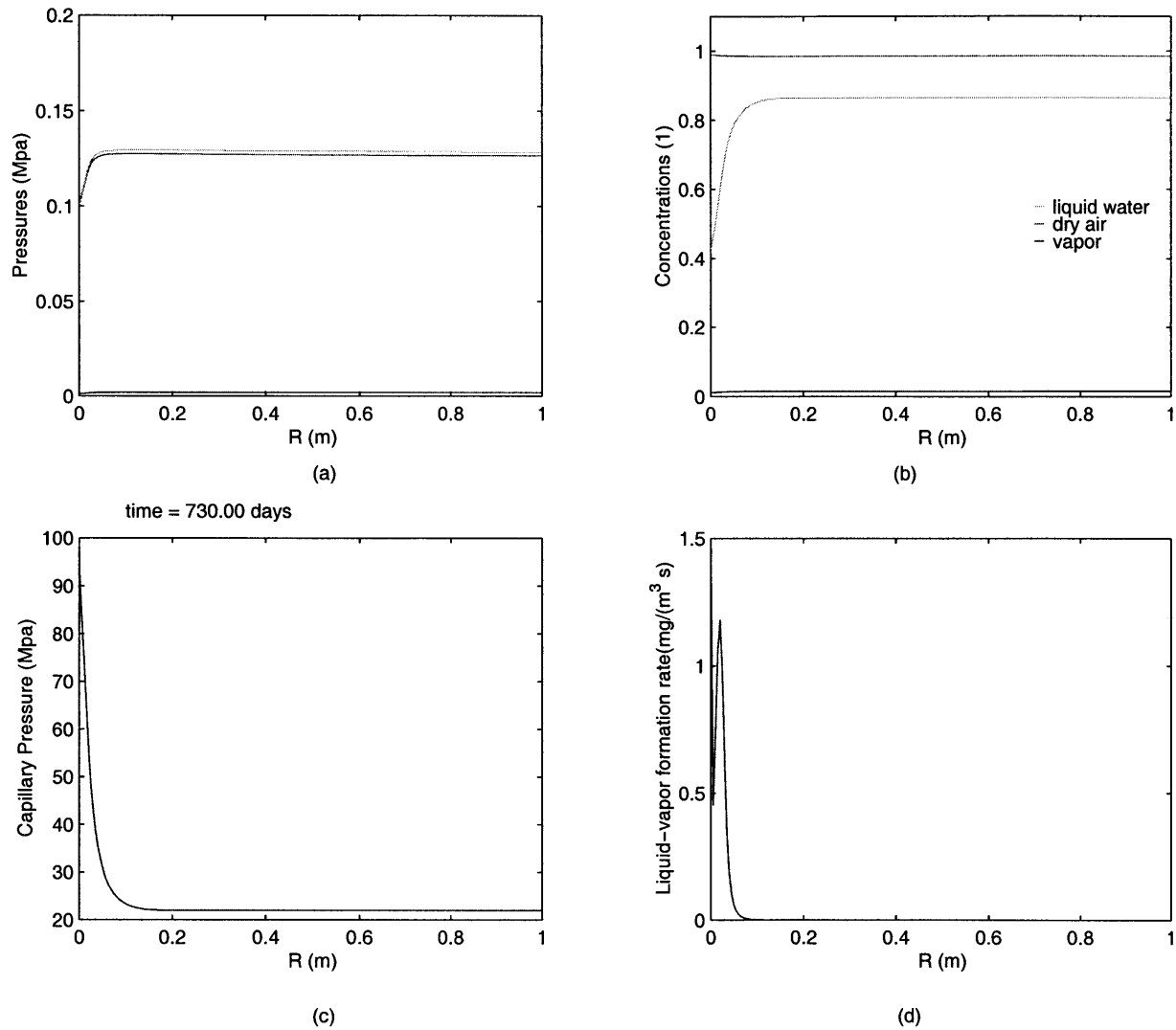


Figure IV.3: Results with the isothermal model in CYLINDRICAL coordinates for R large.

IV . 3 Results of the Non-Isothermal Model with and without Dehydration Effects

The following section provides the results obtained using the non-isothermal model with and without dehydration effects. The results presented in this section correspond to a temperature rise to 600 K for a period of 12 hours. First, the initial and boundary conditions plus the geometrical and time parameters used in the simulations are presented. Finally, the results are presented and compared.

IV . 3 . 1 Simulation Conditions

The conditions attempt to simulate a typical tunnel structure with an imposed temperature at the inner surface, i.e. a fire inside the tunnel.

Initial Conditions

The initial conditions prescribed to all control volumes are the same ones used for the verification of the model. The only difference is the value for the relative humidity:

$$h_r = 0.95$$

Boundary Conditions

At the inner boundary, moisture and temperature conditions are prescribed:

- Relative humidity, $h_r^b = 0.63$
- Temperature, θ^b

The temperature rises according to the following expression [3]:

$$\theta_{imp}(t) = \theta_0 + 345 \log(8t + 1) \leq \theta_{imp}^{max} \quad (IV. 5)$$

where,

t = time in minutes, (T)

θ_0 = initial temperature, (Θ)

θ_{imp}^{max} = maximum imposed temperature, (Θ)

It has been shown [3] that the time scale of heating is much smaller than the time scale of heat conduction for typical characteristics. The temperature rise takes approximately 12 minutes to be complete.

The outer boundary has no imposed temperature and no fluxes exit to the outside.

Geometrical and Time Parameters

There are 101 control volumes in this simulation, $n = 101$. The inner radius and total thickness, e^1 , have the following values:

- $r_0^0 = 4m$
- $e = 0.5m$

The total time is 12 hours and the time step, dt , is 0.01 seconds.

IV . 3 . 2 Results

Figure IV.4 illustrates the results for the non-isothermal model including dehydration effects. Figure IV.5 contains all the graphs for the case where the dehydration effects were not considered. Therefore, the dehydration degree does not only remain constant at a value of one, but also does not affect any of the equations used in the model.

Both figures are the results of a simulation performed under identical conditions with the only difference being the dehydration term. The graphs included are: (a) pressure variations, (b) dehydration degree, (c) temperature changes and (d) liquid water saturation degree. Boundary conditions were only imposed at the inner surface, i.e. left side of the graphs, at $R = 0$.

Results Including Dehydration Effects

As expected [4], the capillary pressures are quite high at the boundary due to its dependence on the liquid water saturation (which is quite low in this area). The vapor pressures reaches a peak not far from the surface. Throughout the evolution of the diffusion process, this peak tends to move toward the inside of the structure. The same occurs with the dry air pressure but with the difference that it has two peak points. It still moves toward the inside of the structure.

The dehydration degree is linearly dependant on the temperature (II. 9). Therefore, when the temperature reaches its maximum the dehydration degree will no longer change.

The liquid water saturation also behaves as expected, having low values close to the heated surface and going through large jump to reach the initial saturation state. The jump appears as a front.

Results Without Dehydration Effects

With the exception of the dehydration degree, most of the graphs have similar shapes as those obtained when the dehydration effects were included. However, there are some variations in the orders of magnitude of the different parameters.

$$1.e = r_1^n - r_0^0 = \text{final outer radius minus the initial inner radius}$$

Comparison of Results

Even though the results in both figures (Figure IV.4 and Figure IV.5) look quite similar there are some interesting changes in the parameters they represent.

The water liquid saturation slightly increases in those areas where the dehydration degree has changed. This is expected, because the dehydration of the skeleton releases liquid water into the pores. This increase in saturation results in a decrease of the capillary pressure. The increase of the pore water also could have an effect on the temperature propagation because there is more mass to counterbalance temperature changes; however, the temperature did not change as the other parameters did.

Figure IV.6 illustrates the variations for: (a) capillary pressures, (b) dehydration degree, (c) temperature and (d) liquid water saturation.

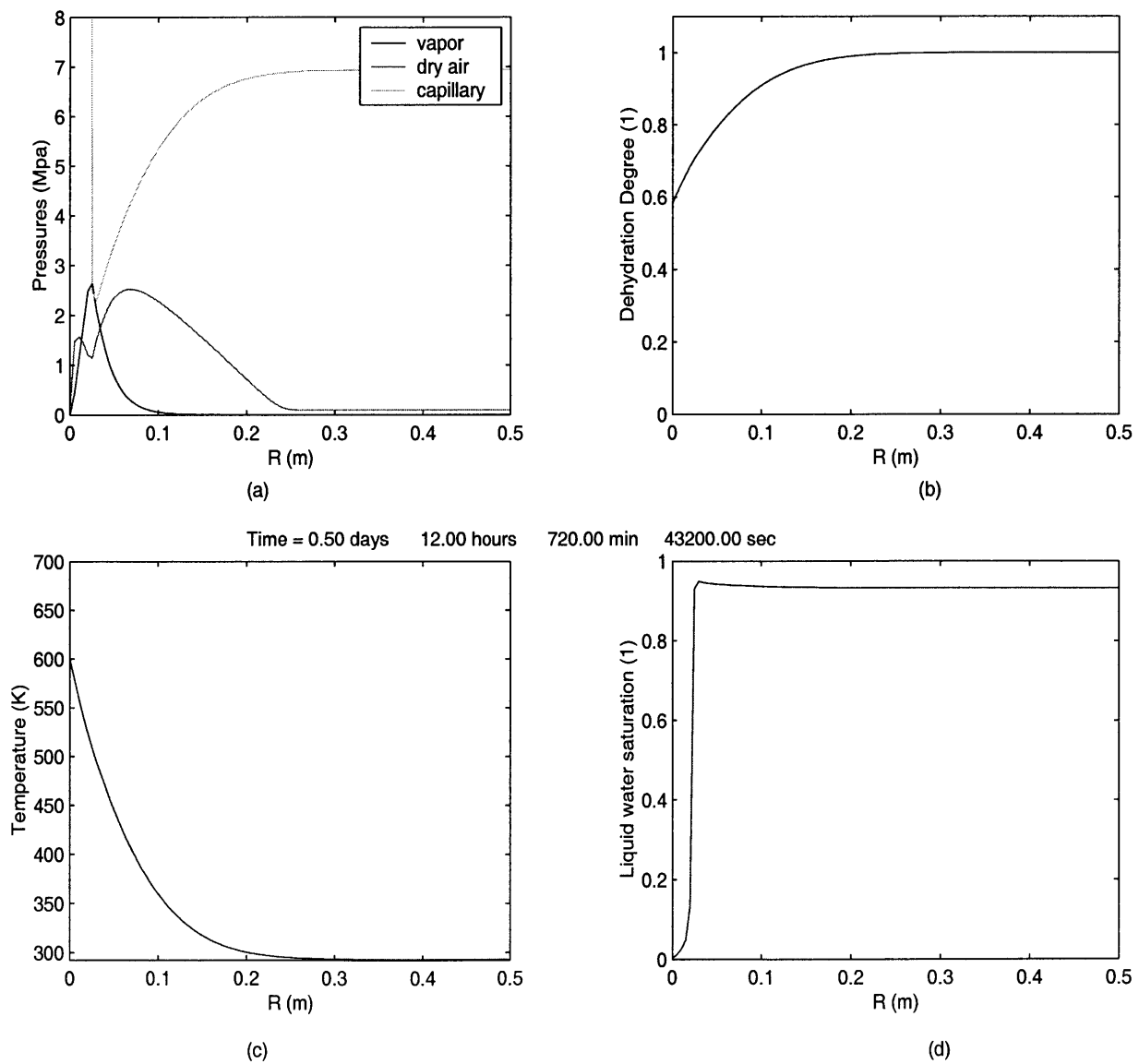


Figure IV.4: Results after 12 hour exposure to a 600 K temperature WITH dehydration effects.

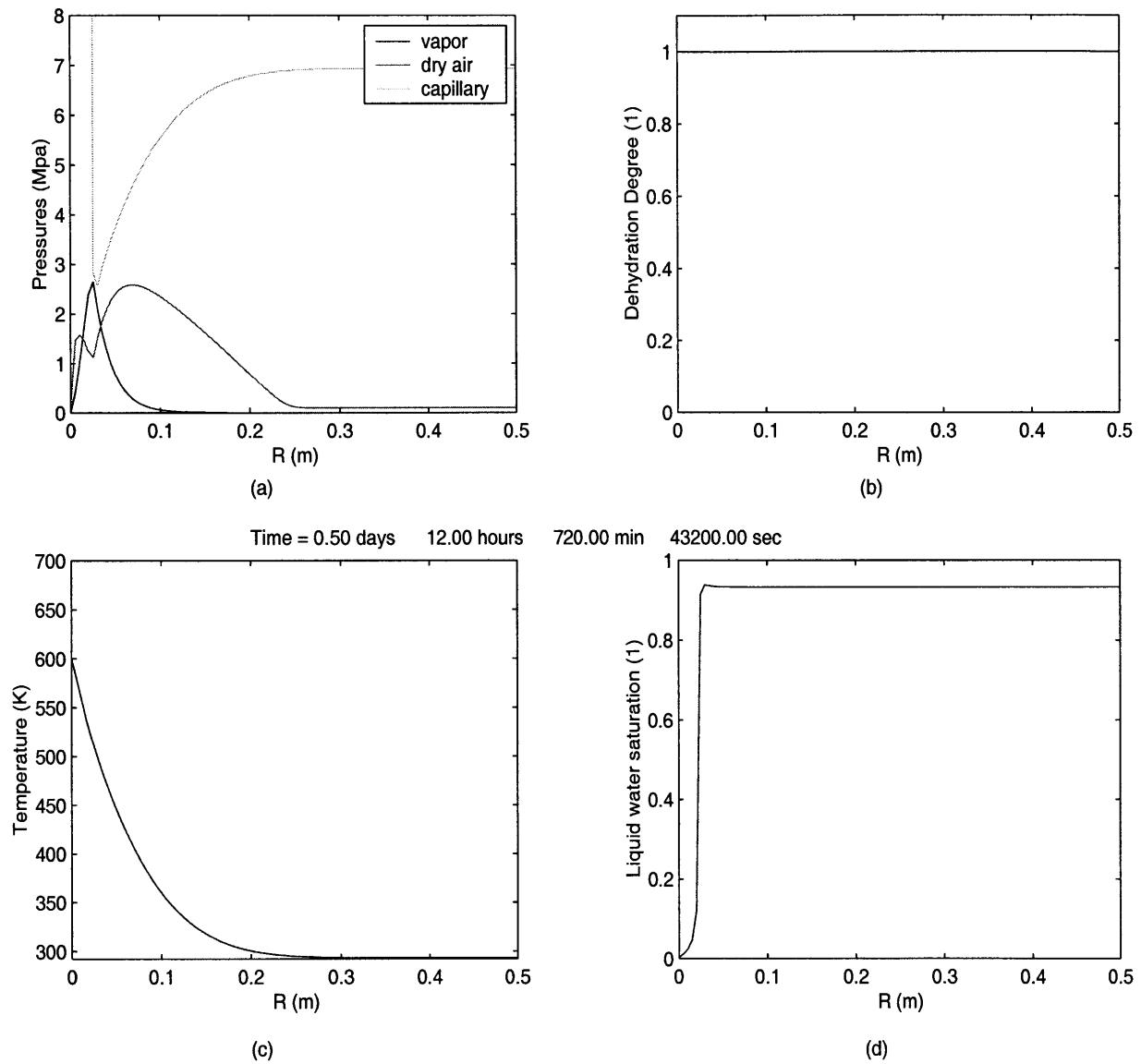


Figure IV.5: Results after 12 hour exposure to a 600 K temperature WITHOUT dehydration effects

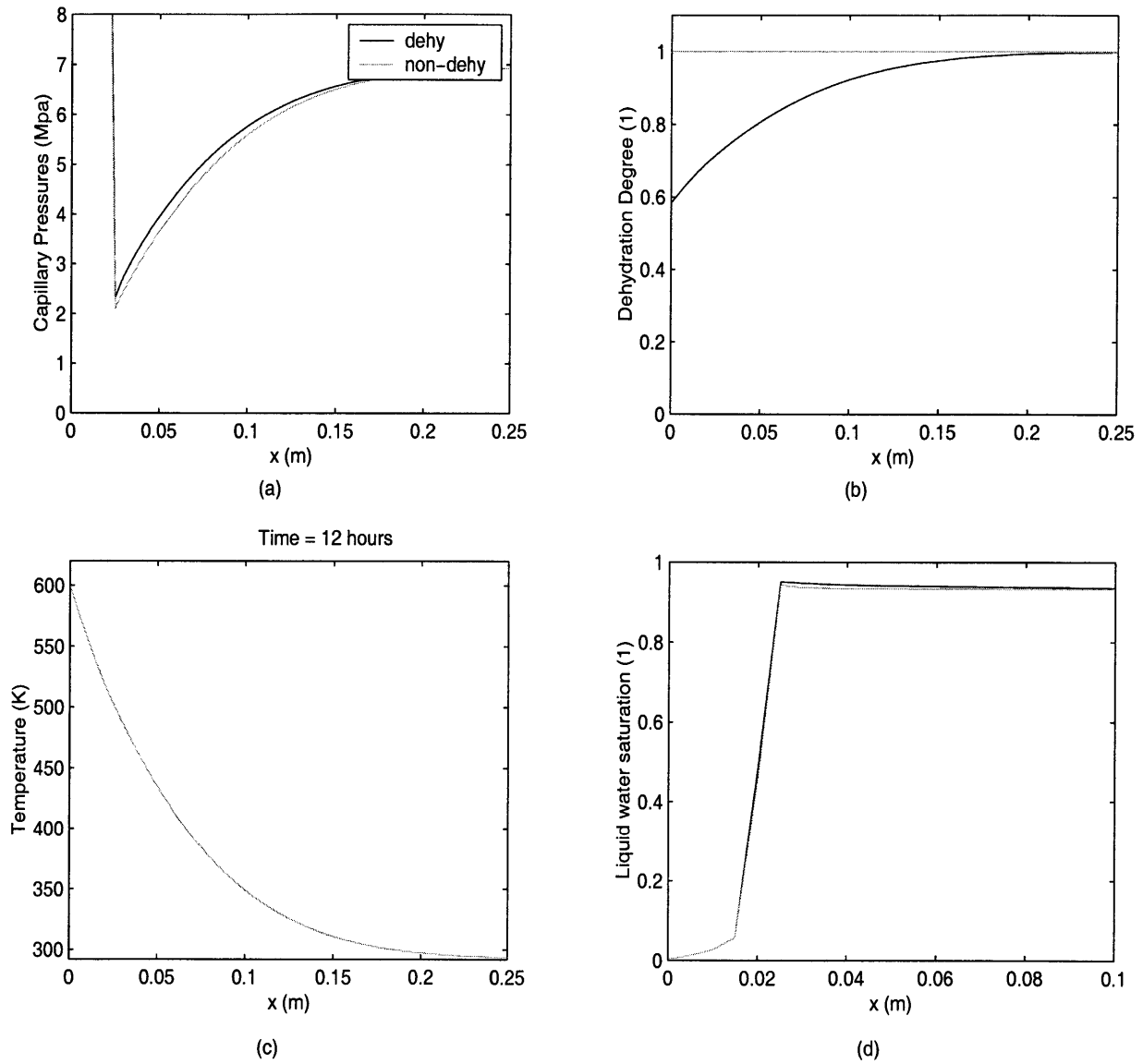


Figure IV.6: Comparison of results for model with dehydration and without dehydration

IV . 4 Beyond Critical Temperature

While the model performed accurately in temperature ranges below the critical temperature, it does not perform well beyond this point. This problem may well be related to the physical phenomena that occur beyond this point.

“...the critical point is the point where the curve of vapor pressure versus temperature comes to an abrupt halt. The temperature at which this occurs is the critical temperature and the corresponding vapor pressure is the critical pressure. The significance of this point is that, if the temperature exceeds the critical one, all the liquid molecules have sufficient kinetic energy to separate from one another, regardless of the pressure, and a conventional liquid no longer exists. Instead the substance is called a supercritical gas. A supercritical gas is one at a pressure so high that its density resembles a liquid's, while its viscosity (ability to flow) remains close to that of a gas... in the supercritical state, certain fluids, such as water and carbon dioxide, take on unexpected properties, such as the ability to dissolve normally insoluble materials”.[17]

Hence, beyond the specific temperature, the water phases that were differentiated in our model can no longer be separated from one another. This restricts the model in its present form to temperature below the critical temperature.

Conclusion

This thesis proposes a non-isothermal model for the moisture flow in concrete including dehydration effects, and uses a finite volume scheme in cylindrical coordinates to solve the system of equations. The model is an extension of Mainguy's isothermal model.

The porous material, concrete, is composed of a skeleton with three fluid phases saturating the pore space. The three water phases are liquid water, vapor water, and dry air. The equations that define the model are the mass conservation of the three different phases, the conservation of entropy, and the liquid-vapor balance equation. Also, the necessary state equation and conduction laws are used.

Numerical methods need to be implemented in order to solve the set of equations. To this end, the finite volume scheme in time and space is used with the discretized version of the equations in cylindrical coordinates. The coordinate modification from cartesian to cylindrical reference system shows a high accuracy. The choice of cylindrical coordinates allows the use of the model for structures such as tunnels.

The model shows that, due to dehydration, the liquid water content in the pore space is slightly increased, resulting in a small reduction of the capillary pressures. The temperature, however, did not change considerably.

Changes with respect to the non-dehydrated approximation are quite small because the additional mass that enters the pores due to dehydration is quite small, too. The temperature only reached 600 K, meaning a dehydration degree of 0.6 for that small part of the structure where this temperature is reached. If the temperature was allowed to reach real life fire type of temperatures of 900 K or more, then not only the dehydration degree would be higher but the portion of the total structure affected by this temperature would increase too. In this case, the liquid water mass added to the pores would most likely play a bigger role in the results, and the differences with the non-dehydrated model would be more pronounced.

It is important to note that the small differences between the results are only limited to the moisture content and pore pressures. Dehydration also affects other properties of concrete structures, such as strength (chemoplastic softening) [3]. These effects on material properties are not accounted for in the model developed.

Because of the phase distinctions used (liquid water, vapor water and dry air), the model in its present form is restricted to temperatures below the critical point of water. Beyond this point, a conventional liquid no longer exists and a reformulation of the model may be required. The development of a model without this limitation seems to be the most appropriate next step to acquire a better understanding of the behavior of concrete structures at high temperatures.

Appendix A

Numerical Approximations

Divergence Theorem

$$\int_K (\nabla \cdot \mathbf{w}) d\Omega = \int_{\partial K} (\mathbf{w} \cdot \mathbf{n}) d\gamma \approx \sum_{L \in N(K)} \int_{e_{K,L}} (\mathbf{w} \cdot \mathbf{n}) d\gamma$$

Where

N = Neighbor of K

$e_{K,L}$ = Common interface between 2 volumes

Volume Integral

Average Value at time t^n

$$\{a\}_k^n = \frac{1}{\Omega_K} \int_K a d\Omega$$

Cartesian coordinates:

$$d\Omega = dx dy dz$$

$$\Omega = L_x L_y L_z$$

$$\{a\}_k^n = \frac{1}{\Omega_K} \int_K a d\Omega = \frac{1}{\Omega_K} \int_K a dx dy dz$$

In the one-dimensional case where only x is the controlling variable we have,

$$\{a\}_k^n = \frac{1}{L_x L_y L_z} \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x a dx = \frac{L_y L_z}{L_x L_y L_z} \int_x a dx = \frac{1}{L_x} \int_x a dx$$

Then,

$$\int_x a dx = m(K) \{a\}_k^n$$

where,

$$m(K) = L_x$$

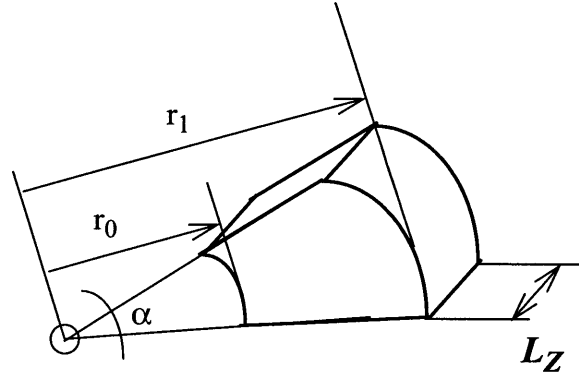
Cylindrical coordinates:

$$d\Omega = r dr d\beta dz$$

$$\int_K d\Omega = \int_0^\alpha d\beta \int_0^{L_z} dz \int_{r_0}^{r_1} r dr$$

$$\Omega = \frac{\alpha L_z}{2} \left\{ (r_1)^2 - (r_0)^2 \right\}$$

$$\{a\}_k^n = \frac{1}{\Omega_K} \int_K a d\Omega = \frac{1}{\Omega_K} \int_K a r dr d\beta dz$$



In the one-dimensional case, where only r is the controlling variable,

$$\{a\}_k^n = \frac{2}{\alpha L_z \left\{ (r_1)^2 - (r_0)^2 \right\}} \int_{\theta=0}^{\alpha} d\beta \int_{z=0}^{L_z} dz \int_{r=r_0}^{r_1} a r dr = \frac{2\alpha L_z}{\alpha L_z \left\{ (r_1)^2 - (r_0)^2 \right\}} \int_{r=r_0}^{r_1} a r dr$$

$$\{a\}_k^n = \left(\frac{2}{r_1^2 - r_0^2} \right) \int_{r=r_0}^{r_1} a r dr$$

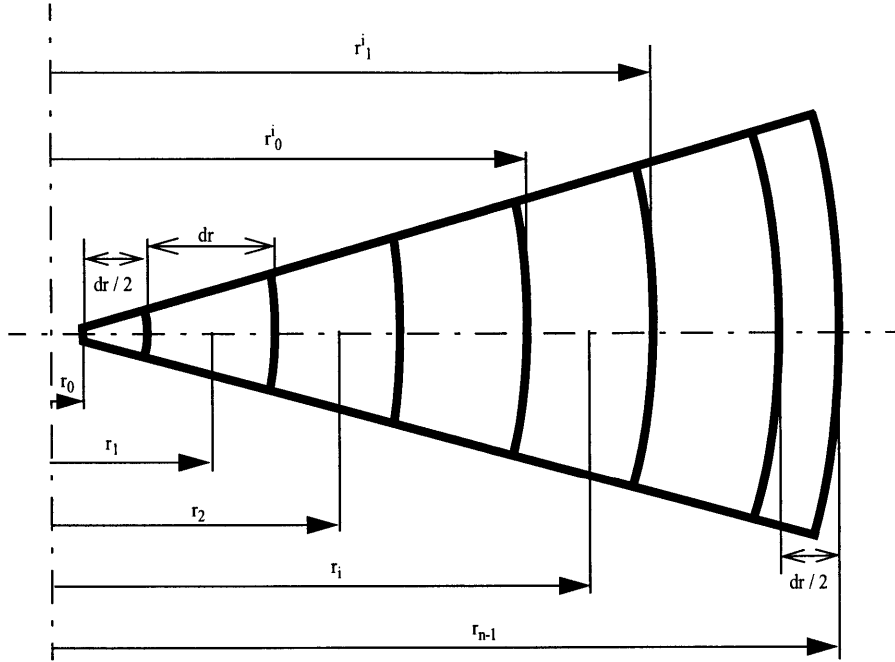
Then,

$$\int_{r=r_0}^{r_1} a r dr = \left(\frac{r_1^2 - r_0^2}{2} \right) \{a\}_k^n = m(K) \{a\}_k^n$$

where,

$$m(K) = \frac{r_1^2 - r_0^2}{2}$$

Constant Spacing (dr):



In this case the radial positions can be determined directly from the spacing:

$$\left. \begin{array}{l} r_0 = r_0 \\ r_1 = r_0 + dr \\ r_{n-1} = r_0 + (n-1)dr \end{array} \right\} r[i] = r_0 + idr$$

For $i(0, n-1)$

$$r_0^i = r_i - \frac{dr}{2} = r_0 + idr - \frac{dr}{2} = r_0 + dr\left(i - \frac{1}{2}\right)$$

$$r_1^i = r_i + \frac{dr}{2} = r_0 + idr + \frac{dr}{2} = r_0 + dr\left(i + \frac{1}{2}\right)$$

Then,

$$m(K_i) = \frac{(r_1^i)^2 - (r_0^i)^2}{2} = \frac{1}{2} \left\{ \left[r_0 + dr\left(i + \frac{1}{2}\right) \right]^2 - \left[r_0 + dr\left(i - \frac{1}{2}\right) \right]^2 \right\}$$

$$m(K_i) = \frac{1}{2} \left\{ (r_0)^2 + 2r_0dr\left(i + \frac{1}{2}\right) + \left[dr\left(i + \frac{1}{2}\right) \right]^2 - (r_0)^2 - 2r_0dr\left(i - \frac{1}{2}\right) - \left[dr\left(i - \frac{1}{2}\right) \right]^2 \right\}$$

$$m(K_i) = \frac{1}{2} \left\{ 2r_0dr \left[i + \frac{1}{2} - i + \frac{1}{2} \right] + (dr)^2 \left[\left(i + \frac{1}{2}\right)^2 - \left(i - \frac{1}{2}\right)^2 \right] \right\} = \frac{1}{2} \left\{ 2r_0dr + (dr)^2 \left[i^2 + i + \frac{1}{4} - i^2 + i - \frac{1}{4} \right] \right\}$$

$$m(K_i) = \frac{1}{2} \{ 2r_0dr + 2i(dr)^2 \} = dr(r_0 + idr) = dr \cdot r[i]$$

For $i = 0$

$$r_0^0 = r_0 \text{ and } r_1^0 = r_0 + \frac{dr}{2}$$

Then,

$$m(K_0) = \frac{(r_1^0)^2 - (r_0^0)^2}{2} = \frac{1}{2} \left\{ \left(r_0 + \frac{dr}{2} \right)^2 - (r_0)^2 \right\} = \frac{1}{2} \left\{ (r_0)^2 + r_0 dr + \frac{(dr)^2}{4} - (r_0)^2 \right\} = \frac{dr}{4} (2r_0 + dr)$$

For $i = n-1$

$$r_0^{n-1} = r_{n-1} - \frac{dr}{2} = r_0 + (n-1)dr - \frac{dr}{2} = r_0 + dr \left(n - \frac{3}{2} \right)$$

$$r_1^{n-1} = r_{n-1} = r_0 + (n-1)dr$$

Then,

$$m(K_{n-1}) = \frac{(r_1^{n-1})^2 - (r_0^{n-1})^2}{2} = \frac{1}{2} \left\{ [r_0 + (n-1)dr]^2 - \left[r_0 + dr \left(n - \frac{3}{2} \right) \right]^2 \right\}$$

$$m(K_{n-1}) = \frac{1}{2} \left\{ (r_0)^2 + 2(n-1)dr + (dr)^2(n-1)^2 - (r_0)^2 - 2 \left(n - \frac{3}{2} \right) dr - (dr)^2 \left(n - \frac{3}{2} \right)^2 \right\}$$

$$m(K_{n-1}) = \frac{1}{2} \left\{ 2dr \left[n - 1 - n + \frac{3}{2} \right] + (dr)^2 \left[(n-1)^2 - \left(n - \frac{3}{2} \right)^2 \right] \right\} = \frac{1}{2} \left\{ dr + (dr)^2 \left[n^2 - 2n + 1 - n^2 + 3n - \frac{9}{4} \right] \right\}$$

$$m(K_{n-1}) = \frac{dr}{2} \left\{ 1 + dr \left(n - \frac{5}{4} \right) \right\}$$

Constant Volume (Ω)

We already know the volume expression,

$$\Omega = \frac{\alpha L_z}{2} \left\{ (r_1)^2 - (r_0)^2 \right\}$$

Assuming the value for r_0 is given, the following scheme can be derived:

$$r_1^i = \left[\left(\frac{2\Omega}{\alpha L_z} \right) + r_0^i \right]^{\frac{1}{2}}$$

The the spacing dr is given by:

$$dr(i) = r_1^i - r_0^i$$

which leads us to the expression for the radius of the midpoint:

$$r_i = r_1^i - \frac{dr(i)}{2} = r_1^i - \left(\frac{r_1^i - r_0^i}{2} \right) = \frac{r_1^i + r_0^i}{2}$$

Using the previous expressions we derive the $m(K)$ values:

For $i(0, n-1)$

$$r_0^i = r_1^{i-1}$$

$$r_1^i = \left[\left(\frac{2\Omega}{\alpha L_z} \right) + r_1^{i-1} \right]^{1/2}$$

Then,

$$m(K_i) = \frac{(r_1^i)^2 - (r_0^i)^2}{2} = \frac{1}{2} \left[\frac{2\Omega}{\alpha L_z} + r_1^{i-1} - (r_1^{i-1})^2 \right]$$

For $i = 0$

$$r_0^0 = r_0$$

$$r_1^0 = \left[\left(\frac{2\Omega}{\alpha L_z} \right) + r_0 \right]^{1/2}$$

Then,

$$m(K_0) = \frac{(r_1^0)^2 - (r_0^0)^2}{2} = \frac{1}{2} \left[\frac{2\Omega}{\alpha L_z} + r_0 - (r_0)^2 \right]$$

For $i = n-1$

$$r_0^{n-1} = r_1^{n-2}$$

$$r_1^{n-1} = \left[\left(\frac{2\Omega}{\alpha L_z} \right) + r_1^{n-2} \right]^{1/2}$$

Then,

$$m(K_0) = \frac{(r_1^{n-1})^2 - (r_0^{n-1})^2}{2} = \frac{1}{2} \left[\frac{2\Omega}{\alpha L_z} + r_1^{n-2} - (r_1^{n-2})^2 \right]$$

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Appendix B

Discretization of Equations

Useful Relations

The following expression will be used to approximate the partial derivative of the pressure of phase i with respect to the distance in the j direction:

$$\{p_i\}_{K+1}^n = \{p_i\}_K^n + \frac{\partial}{\partial j} \{p_i\}_K^n d_j \quad (\text{C.1})$$

$$\frac{\partial}{\partial j} \{p_i\}_K^n = \frac{\{p_i\}_{K+1}^n - \{p_i\}_K^n}{d_j} \quad (\text{C.2})$$

The following expression will help to separate the discretized values of the liquid water saturation, s_w , and vapor water or dry air pressure, p_w or p_a :

$$\{p_v(1 - s_w)\}^n = \{p_v\}^n \{1 - s_w\}^n \quad (\text{C.3})$$

$$\{p_a(1 - s_w)\}^n = \{p_a\}^n \{1 - s_w\}^n \quad (\text{C.4})$$

The following expression will accumulate pressure and saturation values, they represent the mass of phase i :

$$\{m_w\}_K^n = \phi \rho_w \{s_w\}_K^n \quad (\text{C.5})$$

$$\{m_v\}_K^n = \phi \frac{M_v}{R} \left(\{p_v\}_K^n \{1 - s_w\}_K^n \right) \quad (\text{C.6})$$

$$\{m_a\}_K^n = \phi \frac{M_a}{R} \left(\{p_a\}_K^n \{1 - s_w\}_K^n \right) \quad (\text{C.7})$$

Isothermal Model

For the isothermal model the governing equations are the following:

Liquid water conservation:

$$\phi \rho_w \frac{\partial S_w}{\partial t} + \text{div}(\underline{w}_w) = -\mu_{l \rightarrow g}^w \quad (\text{C.8})$$

Vapor water conservation:

$$\phi \frac{M_v}{R\theta} \frac{\partial [p_v(1 - S_w)]}{\partial t} + \text{div}(\underline{w}_v) = \mu_{l \rightarrow g}^w \quad (\text{C.9})$$

Dry air conservation:

$$\phi \frac{M_a}{R\theta} \frac{\partial [p_a(1 - S_w)]}{\partial t} + \text{div}(\underline{w}_a) = 0 \quad (\text{C.10})$$

Liquid-Vapor balance:

$$\frac{R\theta}{M_v} d(\ln p_v) - \frac{1}{\rho_w} d[p_g - p_c(S_w)] = 0 \quad (\text{C.11})$$

and the flux equations are defined as follows:

Liquid water Flux:

$$\underline{w}_w = -\rho_w \frac{k}{\eta_w} k_{rl}(S_w) \text{grad}[p_g - p_c(s_w)] \quad (\text{C.12})$$

Vapor water flux:

$$\underline{w}_v = -\frac{M_v}{R\theta} p_v \frac{k}{\eta_g} k_{rg}(S_w) \text{grad}(p_g) - \frac{M_v}{R\theta} d_{va} f(\phi, S_w) \text{grad}\left(\frac{p_v}{p_g}\right) \quad (\text{C.13})$$

Dry air flux:

$$\underline{w}_a = -\frac{M_a}{R\theta} p_a \frac{k}{\eta_g} k_{rg}(S_w) \text{grad}(p_g) - \frac{M_a}{R\theta} d_{va} f(\phi, S_w) \text{grad}\left(\frac{p_a}{p_g}\right) \quad (\text{C.14})$$

Cartesian Coordinates

Liquid water conservation

$$\phi \rho_w \frac{\partial}{\partial t} S_w + \text{div}(\underline{w}_w) = -\mu_{l \rightarrow g}^w \quad (\text{C.15})$$

Integration on volume K from (t^n, t^{n+1})

$$\phi \rho_w \int_K \int_{t^n}^{t^{n+1}} \left(\frac{\partial S_w}{\partial t} \right) dt d\Omega + \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_w) dt d\Omega = - \int_K \int_{t^n}^{t^{n+1}} (\mu_{l \rightarrow g}^w) dt d\Omega \quad (\text{C.16})$$

Developing each term individually:

$$\begin{aligned} & \bullet \phi \rho_w \int_K \int_{t^n}^{t^{n+1}} \left(\frac{\partial S_w}{\partial t} \right) dt d\Omega \\ &= \phi \rho_w \int_K [S_w(t^{n+1}) - S_w(t^n)] d\Omega = \phi \rho_w \int_{y=0}^{L_y} \int_{z=0}^{L_z} \int_x [S_w(t^{n+1}) - S_w(t^n)] dx \quad (\text{C.17}) \end{aligned}$$

$$= \phi \rho_w (L_y L_z) m(K) \left(\{S_w\}_K^{n+1} - \{S_w\}_K^n \right) \quad (\text{C.18})$$

$$\begin{aligned} & \bullet \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_w) dt d\Omega \\ &= \Delta t \int_{\partial K} (\underline{w}_w \cdot \underline{n}) d\gamma = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_w \cdot \underline{n}) d\gamma \quad (\text{C.19}) \end{aligned}$$

$$= \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} \left[\left(-\rho_w \frac{k}{\eta_w} k_{rl}(S_w) \frac{\partial}{\partial x} [p_w] \underline{e}_x \right) \cdot \underline{e}_x \right] d\gamma \quad (\text{C.20})$$

$$= \Delta t \sum_{L \in N(K)} \rho_w \frac{k}{\eta_w} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right]_{e_{K,L}} \int \frac{\partial}{\partial x} [p_w] dy dz \quad (\text{C.21})$$

$$= \Delta t \sum_{L \in N(K)} \rho_w \frac{k}{\eta_w} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\frac{\{p_w\}_L^n - \{p_w\}_K^n}{d_x} \right] \int_{y=0}^{L_y} \int_{z=0}^{L_z} dy dz \quad (\text{C.22})$$

$$= \Delta t (L_y L_z) \sum_{L \in N(K)} \rho_w \frac{k}{\eta_w} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\frac{\{p_w\}_L^n - \{p_w\}_K^n}{d_x} \right] \quad (\text{C.23})$$

$$\bullet - \int_K \int_{t^n}^{t^{n+1}} (\mu_{l \rightarrow g}^w) dt d\Omega$$

$$= -\Delta t \int_K \mu_{l \rightarrow g}^w d\Omega = -\Delta t \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x \mu_{l \rightarrow g}^w dx \quad (C.24)$$

$$= -m(K) \Delta t (L_y L_z) \{\mu_{l \rightarrow g}^w\}_K^{n+1} \quad (C.25)$$

Putting all terms into the equation we derive the liquid water mass conservation in cartesian coordinates for the isothermal model:

$$m(K) \frac{\{m_w\}_K^{n+1} - \{m_w\}_K^n}{\Delta t} - \sum_{L \in N(K)} \rho_w \frac{k}{\eta_w} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\frac{\{p_w\}_L^n - \{p_w\}_K^n}{d_x} \right] = -m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1} \quad (C.26)$$

Vapor water conservation

$$\phi \frac{M_v}{R\theta} \frac{\partial}{\partial t} [p_v(1-S_w)] + \text{div}(\underline{w}_v) = \mu_{l \rightarrow g}^w \quad (\text{C.27})$$

Integration on volume K from (t^n, t^{n+1})

$$\phi \frac{M_v}{R\theta} \int_K \int_{t^n}^{t^{n+1}} \frac{\partial}{\partial t} [p_v(1-S_w)] dt d\Omega + \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_v) dt d\Omega = \int_K \int_{t^n}^{t^{n+1}} \mu_{l \rightarrow g}^w dt d\Omega \quad (\text{C.28})$$

Developing each term individually:

$$\begin{aligned} & \bullet \phi \frac{M_v}{R\theta} \int_K \int_{t^n}^{t^{n+1}} \frac{\partial}{\partial t} [p_v(1-S_w)] dt d\Omega \\ &= \phi \frac{M_v}{R\theta} \int_K (\{p_v(1-S_w)\}^{n+1} - \{p_v(1-S_w)\}^n) d\Omega \end{aligned} \quad (\text{C.29})$$

$$= \phi \frac{M_v}{R\theta} \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x (\{p_v\}^{n+1} \{1-S_w\}^{n+1} - \{p_v\}^n \{1-S_w\}^n) dx \quad (\text{C.30})$$

$$= \phi \frac{M_v}{R\theta} (L_y L_z) m(K) \left[\{p_v\}_K^{n+1} \{1-S_w\}_K^{n+1} - \{p_v\}_K^n \{1-S_w\}_K^n \right] \quad (\text{C.31})$$

$$\begin{aligned} & \bullet \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_v) dt d\Omega \\ &= \Delta t \int_{\partial K} (\underline{w}_v \cdot \underline{n}) d\gamma = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_v \cdot \underline{n}) d\gamma \end{aligned} \quad (\text{C.32})$$

$$= -\frac{M_v}{R\theta} \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} \left[p_v \frac{k}{\eta_g} k_{rg} S_w \frac{\partial p_g}{\partial x} - d_{va} f(\phi, S_w) \frac{\partial}{\partial x} \left(\frac{p_v}{p_g} \right) \right] \underline{e}_x \cdot \underline{e}_x dy dz \quad (\text{C.33})$$

$$\begin{aligned} &= -\frac{M_v}{R\theta} \Delta t \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial x} p_g dy dz \right. \\ &\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial x} \left(\frac{p_v}{p_g} \right) dy dz \right] \end{aligned} \quad (\text{C.34})$$

$$\begin{aligned} &= -\frac{M_v}{R\theta} \Delta t (L_y L_z) \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \cdot \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \cdot \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \cdot \left(\frac{\{p_g\}_{K+1}^n - \{p_g\}_K^n}{d_x} \right) \right. \\ &\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n}{\{p_g\}_L^n} - \frac{\{p_v\}_K^n}{\{p_g\}_K^n} \right) \frac{1}{d_x} \right] \end{aligned} \quad (\text{C.35})$$

The formation rate from liquid water to vapor has the same form as before. Therefore, the discretized expression of the water vapor mass conservation equation for the isothermal model in cartesian coordinates is:

$$\begin{aligned}
 m(K) \left[\frac{\{m_v\}_K^{n+1} - \{m_v\}_K^n}{\Delta t} \right] \\
 - \frac{M_v}{R\theta} \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \cdot \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \cdot \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \cdot \left(\frac{\{p_g\}_{K+1}^n - \{p_g\}_K^n}{d_x} \right) \right. \\
 \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n}{\{p_g\}_L^n} - \frac{\{p_v\}_K^n}{\{p_g\}_K^n} \right) \frac{1}{d_x} \right] = m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1}
 \end{aligned} \tag{C.36}$$

Dry Air Conservation

$$\phi \frac{M_a}{R\theta} \frac{\partial}{\partial t} [p_a(1-S_w)] + \text{div}(\underline{w}_a) = 0 \quad (\text{C.37})$$

Integration on volume K from (t^n, t^{n+1})

$$\phi \frac{M_a}{R\theta} \int_K \int_{t^n}^{t^{n+1}} \frac{\partial}{\partial t} [p_a(1-S_w)] dt d\Omega + \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_a) dt d\Omega = 0 \quad (\text{C.38})$$

Developing each term individually:

$$\begin{aligned} & \bullet \phi \frac{M_a}{R\theta} \int_K \int_{t^n}^{t^{n+1}} \frac{\partial}{\partial t} [p_a(1-S_w)] dt d\Omega \\ &= \phi \frac{M_a}{R\theta} \int_K (\{p_a(1-S_w)\}^{n+1} - \{p_a(1-S_w)\}^n) d\Omega \end{aligned} \quad (\text{C.39})$$

$$= \phi \frac{M_a}{R\theta} \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x (\{p_a\}^{n+1} \{1-S_w\}^{n+1} - \{p_a\}^n \{1-S_w\}^n) dx \quad (\text{C.40})$$

$$= \phi \frac{M_a}{R\theta} (L_y L_z) m(K) \left[\{p_a\}_K^{n+1} \{1-S_w\}_K^{n+1} - \{p_a\}_K^n \{1-S_w\}_K^n \right] \quad (\text{C.41})$$

$$\begin{aligned} & \bullet \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_a) dt d\Omega \\ &= \Delta t \int_{\partial K} (\underline{w}_a \cdot \underline{n}) d\gamma = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_a \cdot \underline{n}) d\gamma \end{aligned} \quad (\text{C.42})$$

$$= -\frac{M_a}{R\theta} \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} \left[p_a \frac{k}{\eta_g} k_{rg}(S_w) \frac{\partial}{\partial x} (p_g) - d_{va} f(\phi, S_w) \frac{\partial}{\partial x} \left(\frac{p_a}{p_g} \right) \right] \underline{e}_x \cdot \underline{e}_x dy dz \quad (\text{C.43})$$

$$\begin{aligned} &= -\frac{M_a}{R\theta} \Delta t \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial x} p_g d\gamma \right. \\ &\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial x} \left(\frac{p_a}{p_g} \right) d\gamma \right] \end{aligned} \quad (\text{C.44})$$

Using the expressions for each term in the conservation equation, we obtain the dry air mass conservation equation in cartesian coordinates for the isothermal model:

$$\begin{aligned}
 m(K) \left[\frac{\{m_a\}_K^{n+1} - \{m_a\}_K^n}{\Delta t} \right] \\
 - \frac{M_a}{R\theta} \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \cdot \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \cdot \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \cdot \left(\frac{\{p_g\}_{K+1}^n - \{p_g\}_K^n}{d_x} \right) \right. \\
 \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n}{\{p_g\}_L^n} - \frac{\{p_a\}_K^n}{\{p_g\}_K^n} \right) \frac{1}{d_x} \right] = 0
 \end{aligned} \tag{C.45}$$

Liquid-Vapor Water Equilibrium

$$\frac{R\theta}{M_v} d_v(\ln p_v) - \frac{1}{\rho_w} d[p_g - p_c(S_w)] = 0 \quad (C.46)$$

Integration on volume K from (t^n, t^{n+1})

$$\frac{R\theta}{M_v} \iint_{\Omega} \int_{t^n}^{t^{n+1}} d_v(\ln p_v) dt d\Omega - \frac{1}{\rho_w} \iint_{\Omega} \int_{t^n}^{t^{n+1}} d[p_g - p_c(S_w)] dt d\Omega = 0 \quad (C.47)$$

Developing each term individually:

$$\begin{aligned} & \bullet \frac{R\theta}{M_v} \iint_{\Omega} \int_{t^n}^{t^{n+1}} d_v(\ln p_v) dt d\Omega \\ &= \frac{R\theta}{M_v} \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x [\{\ln(p_v)\}^{n+1} - \{\ln(p_v)\}^n] dx \\ & \quad (C.48) \end{aligned}$$

$$= m(K)(L_y L_z) \frac{R\theta}{M_v} \left[\{\ln(p_v)\}_K^{n+1} - \{\ln(p_v)\}_K^n \right] \quad (C.49)$$

$$\begin{aligned} & \bullet \frac{1}{\rho_w} \iint_{\Omega} \int_{t^n}^{t^{n+1}} d[p_g - p_c(S_w)] dt d\Omega \\ &= \frac{1}{\rho_w} \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x [\{p_w\}^{n+1} - \{p_w\}^n] dx \\ & \quad (C.50) \end{aligned}$$

$$= \frac{m(K)}{\rho_w} (L_y L_z) \left[\{p_w\}_K^{n+1} - \{p_w\}_K^n \right] \quad (C.51)$$

Simplification finally leads us to the following discretized version of the liquid-vapor water equilibrium in cartesian coordinates for the isothermal model:

$$\frac{1}{\rho_w} \left[\{p_w\}_K^{n+1} - \{p_w\}_K^n \right] = \frac{R\theta}{M_v} \ln \left[\frac{(p_v)_K^{n+1}}{(p_v)_K^n} \right] \quad (C.52)$$

Summary of Discretized Equations for the One-Dimension Isothermal Model in Cartesian Coordinates

Liquid water conservation:

$$m(K) \frac{\{m_w\}_K^{n+1} - \{m_w\}_K^n}{\Delta t} - \sum_{L \in N(K)} \rho_w \frac{k}{\eta_w} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\frac{\{p_w\}_L^n - \{p_w\}_K^n}{d_x} \right] = -m(K) \{\mu^w\}_K^{n+1} \quad (C.53)$$

Water vapor conservation:

$$m(K) \left[\frac{\{m_v\}_K^{n+1} - \{m_v\}_K^n}{\Delta t} \right] - \frac{M_v}{R\theta} \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \cdot \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \left(\frac{\{p_g\}_{K+1}^n - \{p_g\}_K^n}{d_x} \right) \right. \\ \left. + \frac{d_{va}}{d_x} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n}{\{p_g\}_L^n} - \frac{\{p_v\}_K^n}{\{p_g\}_K^n} \right) \right] = m(K) \{\mu^w\}_K^{n+1} \quad (C.54)$$

Dry air conservation:

$$m(K) \left[\frac{\{m_a\}_K^{n+1} - \{m_a\}_K^n}{\Delta t} \right] - \frac{M_a}{R\theta} \sum_{L \in NK} \left[\frac{k}{\eta_g} \cdot \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \cdot \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \cdot \left(\frac{\{p_g\}_{K+1}^n - \{p_g\}_K^n}{d_x} \right) \right. \\ \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n}{\{p_g\}_L^n} - \frac{\{p_a\}_K^n}{\{p_g\}_K^n} \right) \frac{1}{d_x} \right] = 0 \quad (C.55)$$

Liquid-vapor balance:

$$\frac{1}{\rho_w} \left[\{p_w\}_K^{n+1} - \{p_w\}_K^n \right] = \frac{R\theta}{M_v} \ln \left[\frac{(p_v)_K^{n+1}}{(p_v)_K^n} \right] \quad (C.56)$$

Cylindrical Coordinates

Liquid water conservation

$$\phi \rho_w \frac{\partial}{\partial t} S_w + \text{div}(\underline{w}_w) = -\mu_{l \rightarrow g}^w \quad (\text{C.57})$$

Integration on volume K from (t^n, t^{n+1})

$$\phi \rho_w \int_K \int_{t^n}^{t^{n+1}} \frac{\partial S_w}{\partial t} dt d\Omega + \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_w) dt d\Omega = - \int_K \int_{t^n}^{t^{n+1}} \mu_{l \rightarrow g}^w dt d\Omega \quad (\text{C.58})$$

Developing each term individually:

$$\begin{aligned} \bullet \phi \rho_w \int_K \int_{t^n}^{t^{n+1}} \frac{\partial S_w}{\partial t} dt d\Omega \\ = \phi \rho_w \int_K [S_w(t^{n+1}) - S_w(t^n)] d\Omega \end{aligned} \quad (\text{C.59})$$

$$= \phi \rho_w \int_{\beta=0}^{2\pi} \int_{z=0}^{L_z} dz \int_r [S_w(t^{n+1}) - S_w(t^n)] r dr \quad (\text{C.60})$$

$$= \phi \rho_w (2\pi L_z) m(K) \left(\{S_w\}_K^{n+1} - \{S_w\}_K^n \right) \quad (\text{C.61})$$

$$\begin{aligned} \bullet \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_w) dt d\Omega \\ = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_w \cdot \underline{n}) r d\beta dz = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_w \cdot \underline{n}) d\gamma \end{aligned} \quad (\text{C.62})$$

$$= \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} \left[\left(-\rho_w \frac{k}{\eta_w} k_{rl}(S_w) \frac{\partial}{\partial r} [p_w] \underline{e}_r \right) \cdot \underline{e}_r \right] r d\beta dz \quad (\text{C.63})$$

$$= \Delta t \sum_{L \in N(K)} \rho_w \frac{k}{\eta_w} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \int_{e_{K,L}} \frac{\partial}{\partial r} [p_w] r d\beta dz \quad (\text{C.64})$$

$$= \left\{ \Delta t \rho_w \frac{k}{\eta_w} \sum_{L \in N(K)} (r) \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\frac{\{p_w\}_L^n - \{p_w\}_K^n}{d_r} \right] \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \right\} \quad (\text{C.65})$$

$$= \left\{ \Delta t (2\pi L_z) \rho_w \cdot \frac{k}{\eta_w} \sum_{L \in N(K)} \left(\frac{r}{d_r} \right) \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\{p_w\}_L^n - \{p_w\}_K^n \right] \right\} \quad (\text{C.66})$$

$$\begin{aligned} & \bullet - \int_K \int_{t^n}^{t^{n+1}} \mu_{l \rightarrow g}^w dt d\Omega \\ & = -\Delta t \int_K \mu_{l \rightarrow g}^w d\Omega \end{aligned} \quad (\text{C.67})$$

$$= -\Delta t \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \int_r \mu_{l \rightarrow g}^w r dr \quad (\text{C.68})$$

$$= -m(K) \Delta t (2\pi L_z) \left\{ \mu_{l \rightarrow g}^w \right\}_K^{n+1} \quad (\text{C.69})$$

Putting all terms in the conservation equation plus simplification of terms, we obtain the one-dimensional discretized version of the liquid water mass conservation in cylindrical coordinates for the isothermal model:

$$m(K) \frac{\{m_w\}_K^{n+1} - \{m_w\}_K^n}{\Delta t} - \left\{ \rho_w \cdot \frac{k}{\eta_{wL}} \sum_{N(K)} \left(\frac{r}{d_r} \right) \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\{p_w\}_L^n - \{p_w\}_K^n \right] \right\} = -m(K) \left\{ \mu_{l \rightarrow g}^w \right\}_K^{n+1} \quad (\text{C.70})$$

Vapor water conservation

$$\phi \frac{M_v}{R\theta} \frac{\partial}{\partial t} [p_v(1-S_w)] + \text{div}(\underline{w}_v) = \mu_{l \rightarrow g}^w \quad (\text{C.71})$$

Integration on volume K from (t^n, t^{n+1})

$$\phi \frac{M_v}{R\theta} \int_K \int_{t^n}^{t^{n+1}} \frac{\partial}{\partial t} [p_v(1-S_w)] dt d\Omega + \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_v) dt d\Omega = \int_K \int_{t^n}^{t^{n+1}} \mu_{l \rightarrow g}^w dt d\Omega \quad (\text{C.72})$$

Developing each term individually:

$$\begin{aligned} & \bullet \phi \frac{M_v}{R\theta} \int_K \int_{t^n}^{t^{n+1}} \frac{\partial}{\partial t} [p_v(1-S_w)] dt d\Omega \\ &= \phi \frac{M_v}{R\theta} \int_K (\{p_v(1-S_w)\}^{n+1} - \{p_v(1-S_w)\}^n) d\Omega \end{aligned} \quad (\text{C.73})$$

$$= \phi \frac{M_v}{R\theta} \int_{\beta=0}^{2\pi} \int_{z=0}^{L_z} \int_x dz (\{p_v\}^{n+1} \{1-S_w\}^{n+1} - \{p_v\}^n \{1-S_w\}^n) r dr \quad (\text{C.74})$$

$$= \phi \frac{M_v}{R\theta} (2\pi L_z) m(K) \left[\{p_v\}_K^{n+1} \{1-S_w\}_K^{n+1} - \{p_v\}_K^n \{1-S_w\}_K^n \right] \quad (\text{C.75})$$

$$\begin{aligned} & \bullet \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_v) dt d\Omega \\ &= \Delta t \int_{\partial K} (\underline{w}_v \cdot \underline{n}) d\gamma = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_v \cdot \underline{n}) d\gamma \end{aligned} \quad (\text{C.76})$$

$$= -\frac{M_v}{R\theta} \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} \left[p_v \frac{k}{\eta_g} k_{rg} S_w \frac{\partial p_g}{\partial r} - d_{va} f(\phi, S_w) \frac{\partial (p_v)}{\partial r} \right] \underline{e}_r \cdot \underline{e}_r r d\beta dz \quad (\text{C.77})$$

$$= -\frac{M_v}{R\theta} \Delta t \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \right] \int_{e_{K,L}} \frac{\partial}{\partial r} (p_g) r d\beta dz \quad (\text{C.78})$$

$$\begin{aligned} &= -\frac{M_v}{R\theta} \Delta t (2\pi L_z) \sum_{L \in N(K)} \left(\frac{r}{d_r} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \right] \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) \\ &\quad + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n}{\{p_g\}_L^n} - \frac{\{p_v\}_K^n}{\{p_g\}_K^n} \right) \end{aligned} \quad (\text{C.79})$$

We finally obtain the one-dimensional discretized version of the water vapor mass conservation equation for the isothermal model in cylindrical coordinates:

$$\begin{aligned}
 m(K) \left[\frac{\{m_v\}_K^{n+1} - \{m_v\}_K^n}{\Delta t} \right] \\
 - \frac{M_v}{R\theta} \sum_{L \in N(K)} \left(\frac{r}{d_r} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) \right. \\
 \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n}{\{p_g\}_L^n} - \frac{\{p_v\}_K^n}{\{p_g\}_K^n} \right) \right] = m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1}
 \end{aligned} \tag{C.80}$$

Dry Air Conservation

$$\phi \frac{M_a}{R\theta} \frac{\partial}{\partial t} [p_a(1 - S_w)] + \text{div}(\underline{w}_a) = 0 \quad (\text{C.81})$$

Integration on volume K from (t^n, t^{n+1})

$$\phi \frac{M_a}{R\theta} \int_K \int_{t^n}^{t^{n+1}} \frac{\partial}{\partial t} [p_a(1 - S_w)] dt d\Omega + \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_a) dt d\Omega = 0 \quad (\text{C.82})$$

Developing each term individually:

$$\begin{aligned} & \bullet \phi \frac{M_a}{R\theta} \int_K \int_{t^n}^{t^{n+1}} \frac{\partial}{\partial t} [p_a(1 - S_w)] dt d\Omega \\ &= \phi \frac{M_a}{R\theta} \int_K (\{p_a(1 - S_w)\}^{n+1} - \{p_a(1 - S_w)\}^n) d\Omega \end{aligned} \quad (\text{C.83})$$

$$= \phi \frac{M_a}{R\theta} \int_{\beta=0}^{2\pi} \int_{z=0}^{L_z} \int_r dz (\{p_a\}^{n+1} \{1 - S_w\}^{n+1} - \{p_a\}^n \{1 - S_w\}^n) r dr \quad (\text{C.84})$$

$$= \phi \frac{M_a}{R\theta} (2\pi L_z) m(K) \left[\{p_a\}_K^{n+1} \{1 - S_w\}_K^{n+1} - \{p_a\}_K^n \{1 - S_w\}_K^n \right] \quad (\text{C.85})$$

$$\begin{aligned} & \bullet \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_a) dt d\Omega \\ &= \Delta t \int_{\partial K} (\underline{w}_a \cdot \underline{n}) d\gamma = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_a \cdot \underline{n}) d\gamma \end{aligned} \quad (\text{C.86})$$

$$= -\frac{M_a}{R\theta} \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} \left[p_a \frac{k}{\eta_g} k_{rg}(S_w) \frac{\partial}{\partial r} (p_g) - d_{va} f(\phi, S_w) \frac{\partial}{\partial r} \left(\frac{p_a}{p_g} \right) \right] \underline{e}_r \cdot \underline{e}_r r d\beta dz \quad (\text{C.87})$$

$$\begin{aligned} &= -\frac{M_a}{R\theta} \Delta t \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial r} p_g r d\beta dz \right. \\ &\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial r} \left(\frac{p_a}{p_g} \right) r d\beta dz \right] \end{aligned} \quad (\text{C.88})$$

$$\begin{aligned} &= -\frac{M_a}{R\theta} \sum_{L \in N(K)} \left(\frac{r}{d_r} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) \right. \\ &\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n}{\{p_g\}_L^n} - \frac{\{p_a\}_K^n}{\{p_g\}_K^n} \right) \right] \end{aligned} \quad (\text{C.89})$$

Using the previous expressions in the conservation equation, we obtain the one-dimensional discretized version of the dry air mass conservation equation in cylindrical coordinates for the isothermal model:

$$\begin{aligned}
 m(K) \left[\frac{\{m_a\}_K^{n+1} - \{m_a\}_K^n}{\Delta t} \right] \\
 - \frac{M_a}{R\theta} \sum_{L \in N(K)} \left(\frac{r}{d_r} \right) \left[\frac{k}{\eta_g} \cdot \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \cdot \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \cdot (\{p_g\}_{K+1}^n - \{p_g\}_K^n) \right. \\
 \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n}{\{p_g\}_L^n} - \frac{\{p_a\}_K^n}{\{p_g\}_K^n} \right) \right] = 0
 \end{aligned} \tag{C.90}$$

Liquid-Vapor Water Equilibrium

$$\frac{R\theta}{M_v} d_v(\ln p_v) - \frac{1}{\rho_w} d[p_g - p_c(S_w)] = 0 \quad (\text{C.91})$$

Integration on volume K from (t^n, t^{n+1})

$$\frac{R\theta}{M_v} \int_{\Omega} \int_{t^n}^{t^{n+1}} d_v(\ln p_v) dt d\Omega - \frac{1}{\rho_w} \int_{\Omega} \int_{t^n}^{t^{n+1}} d[p_g - p_c(S_w)] dt d\Omega = 0 \quad (\text{C.92})$$

Developing each term individually:

$$\begin{aligned} & \bullet \frac{R\theta}{M_v} \int_{\Omega} \int_{t^n}^{t^{n+1}} d_v(\ln p_v) dt d\Omega \\ &= \frac{R\theta}{M_v} \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \int_r [\{\ln(p_v)\}^{n+1} - \{\ln(p_v)\}^n] dr \end{aligned} \quad (\text{C.93})$$

$$= m(K)(2\pi L_z) \frac{R\theta}{M_v} \left[\{\ln(p_v)\}_K^{n+1} - \{\ln(p_v)\}_K^n \right] \quad (\text{C.94})$$

$$\begin{aligned} & \bullet \frac{1}{\rho_w} \int_{\Omega} \int_{t^n}^{t^{n+1}} d[p_g - p_c(S_w)] dt d\Omega \\ &= \frac{1}{\rho_w} \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \int_r [\{p_w\}^{n+1} - \{p_w\}^n] dr \end{aligned} \quad (\text{C.95})$$

$$= \frac{m(K)}{\rho_w} (2\pi L_z) \left[\{p_w\}_K^{n+1} - \{p_w\}_K^n \right] \quad (\text{C.96})$$

Simplification finally leads us to the following one-dimensional discretized version of the liquid-vapor water equilibrium in cylindrical coordinates for the isothermal model:

$$\frac{1}{\rho_w} \left[\{p_w\}_K^{n+1} - \{p_w\}_K^n \right] = \frac{R\theta}{M_v} \ln \left[\frac{(p_v)_K^{n+1}}{(p_v)_K^n} \right] \quad (\text{C.97})$$

Summary of the Discretized Equations for the One-Dimension Isothermal Model in Cylindrical Coordinates

Liquid water conservation:

$$m(K) \frac{\{m_w\}_K^{n+1} - \{m_w\}_K^n}{\Delta t} - \left\{ \rho_w \cdot \frac{k}{\eta_w} \sum_{L \in N(K)} \left(\frac{r}{d_r} \right) \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\{p_w\}_L^n - \{p_w\}_K^n \right] \right\} = -m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1} \quad (\text{C.98})$$

Water vapor conservation:

$$m(K) \left[\frac{\{m_v\}_K^{n+1} - \{m_v\}_K^n}{\Delta t} \right] - \frac{M_v}{R\theta} \sum_{L \in N(K)} \left(\frac{r}{d_r} \right) \left[\frac{k}{\eta_g} \cdot \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \cdot \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \cdot \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n - \{p_v\}_K^n}{\{p_g\}_L^n - \{p_g\}_K^n} \right) \right] = m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1} \quad (\text{C.99})$$

Dry air conservation:

$$m(K) \left[\frac{\{m_a\}_K^{n+1} - \{m_a\}_K^n}{\Delta t} \right] - \frac{M_a}{R\theta} \sum_{L \in N(K)} \left(\frac{r}{d_r} \right) \left[\frac{k}{\eta_g} \cdot \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \cdot \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \cdot \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n - \{p_a\}_K^n}{\{p_g\}_L^n - \{p_g\}_K^n} \right) \right] = 0 \quad (\text{C.100})$$

Liquid-vapor balance:

$$\frac{1}{\rho_w} \left[\{p_w\}_K^{n+1} - \{p_w\}_K^n \right] = \frac{R\theta}{M_v} \ln \left[\frac{(p_v)_K^{n+1}}{(p_v)_K^n} \right] \quad (\text{C.101})$$

Non-isothermal Model With Dehydration Effects

This model does not account for temperature changes in the mass conservation equations because we assume the mass density of the different phases not to depend on temperature. Temperature changes are only included in the entropy and flux calculations.

The governing equations for the model are:

Liquid Water Conservation

$$\phi \rho_w \frac{\partial}{\partial t} S_w + \text{div}(\underline{w}_w) = -\mu_{l \rightarrow g} - m_l^b \frac{\partial \xi}{\partial t} \quad (\text{C.102})$$

Vapor Water Conservation

$$\phi \frac{M_v}{R} \frac{\partial}{\partial t} \left((1 - S_w) \frac{p_v}{\theta} \right) + \text{div}(\underline{w}_v) = \mu_{l \rightarrow g} \quad (\text{C.103})$$

Dry Air Conservation

$$\phi \frac{M_a}{R} \frac{\partial}{\partial t} \left((1 - S_w) \frac{p_a}{\theta} \right) + \text{div}(\underline{w}_a) = 0 \quad (\text{C.104})$$

Liquid-Vapor Balance

$$\frac{R\theta}{M_v} \ln \left(\frac{p_v}{p_{v_0}} \right) = \frac{p_w - p_{w_0}}{\rho_w} + \frac{l_0}{\theta_0} (\theta - \theta_0) + (C_{pl} - C_{pv}) \left(\theta - \theta_0 - \theta \ln \left(\frac{\theta}{\theta_0} \right) \right) \quad (\text{C.105})$$

Entropy Balance

$$\phi \left[\frac{\partial}{\partial t} \left(S_s + \sum_{i=w,v,a} m_i s_i \right) + \sum_{i=w,v,a} s_i \underline{w}_i \right] = -\text{div}(\underline{q}) \quad (\text{C.106})$$

and the fluxes are defined by:

Liquid water flux:

$$\underline{w}_w = -\rho_w \frac{k}{\eta_w} k_{rl}(S_w) \text{grad}(p_w) \quad (\text{C.107})$$

Vapor water flux:

$$\underline{w}_v = -f(\phi, S_w) \frac{M_v}{R\theta} d_{va}(\theta) \text{grad} \left(\frac{p_v}{p_g} \right) - \frac{M_v}{R\theta} p_v \frac{k}{\eta_g} k_{rg}(S_w) \text{grad}(p_g) \quad (\text{C.108})$$

Dry air flux:

$$\underline{w}_a = -f(\phi, S_w) \tau \frac{M_a}{R\theta} d_{va}(\theta) \text{grad} \left(\frac{p_a}{p_g} \right) - \frac{M_a}{R\theta} p_a \frac{k}{\eta_g} k_{rg}(S_w) \text{grad}(p_g) \quad (\text{C.109})$$

Cartesian Coordinates

Liquid Water Conservation:

$$\phi \rho_w \frac{\partial}{\partial t} S_w + \text{div}(\underline{w}_w) = -\mu_{l \rightarrow g} - m_{l_o}^b \frac{\partial \xi}{\partial t} \quad (\text{C.110})$$

First we proceed to integrate over the volume K from (t, t^{n+1})

$$\int_{\Omega} \int_t^{t^{n+1}} \left(\phi \rho_w \frac{\partial S_w}{\partial t} \right) dt d\Omega + \int_{\Omega} \int_t^{t^{n+1}} \text{div}(\underline{w}_w) dt d\Omega = \int_{\Omega} \int_t^{t^{n+1}} (-\mu_{l \rightarrow g}) dt d\Omega + \int_{\Omega} \int_t^{t^{n+1}} \left(-m_{l_o}^b \frac{\partial \xi}{\partial t} \right) dt d\Omega \quad (\text{C.111})$$

We will now develop each term individually:

$$\bullet \int_{\Omega} \int_t^{t^{n+1}} \left(\phi \rho_w \frac{\partial S_w}{\partial t} \right) dt d\Omega$$

$$= \phi \rho_w \int_K [S_w(t^{n+1}) - S_w(t^n)] d\Omega = \phi \rho_w \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_r [S_w(t^{n+1}) - S_w(t^n)] dx \quad (\text{C.112})$$

$$= (L_y L_z) \phi \rho_w m(K) \left(\{S_w\}_K^{n+1} - \{S_w\}_K^n \right) \quad (\text{C.113})$$

$$\bullet \int_{\Omega} \int_t^{t^{n+1}} \text{div}(\underline{w}_w) dt d\Omega$$

$$= \Delta t \int_{\partial K} (\underline{w}_w \cdot \underline{n}) d\gamma = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_w \cdot \underline{n}) dy dz \quad (\text{C.114})$$

$$= \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} \left[\left(-\rho_w \frac{k}{\eta_w} k_{rl}(S_w) \frac{\partial}{\partial x} [p_w] \underline{e}_x \right) \cdot \underline{e}_x \right] dy dz \quad (\text{C.115})$$

$$= \Delta t \sum_{L \in N(K)} \rho_w \frac{k}{\eta_w} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right]_{e_{K,L}} \int \frac{\partial}{\partial x} [p_w] dy dz \quad (\text{C.116})$$

$$= \Delta t \rho_w \frac{k}{\eta_w} \sum_{L \in N(K)} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\frac{\{p_w\}_L^n - \{p_w\}_K^n}{\Delta x} \right] \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \quad (\text{C.117})$$

$$= \left(\frac{L_y L_z}{\Delta x} \right) \Delta t \rho_w \cdot \frac{k}{\eta_w} \sum_{L \in N(K)} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\{p_w\}_L^n - \{p_w\}_K^n \right] \quad (\text{C.118})$$

$$\begin{aligned}
& \bullet \int_{\Omega} \int_t^{t^{n+1}} (-\mu_{l \rightarrow g}) dt d\Omega \\
& = -\Delta t \int_K \mu_{l \rightarrow g}^w d\Omega = -\Delta t \int_{y=0}^{L_y} d\beta \int_{z=0}^{L_z} dz \int_r (\mu_{l \rightarrow g}^w) dx = \Delta t (L_y L_z) m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1} \quad (C.119)
\end{aligned}$$

$$\begin{aligned}
& \bullet \int_{\Omega} \int_t^{t^{n+1}} \left(-m_{l_o}^b \frac{\partial \xi}{\partial t} \right) dt d\Omega \\
& = -m_{l_o}^b \int_{\Omega} \int_t^{t^{n+1}} \left(\frac{\partial \xi}{\partial t} \right) dt d\Omega = -m_{l_o}^b \int_K [\xi(t^{n+1}) - \xi(t^n)] d\Omega = m_{l_o}^b \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_K [\xi(t^{n+1}) - \xi(t^n)] dx \quad (C.120)
\end{aligned}$$

$$= -m_{l_o}^b (L_y L_z) m(K) (\{\xi\}_K^{n+1} - \{\xi\}_K^n) \quad (C.121)$$

$$= -m_{l_o}^b (L_y L_z) m(K) \left[\left(1 - \frac{l/\theta_0}{km_{s_0}} (\{\theta\}_K^{n+1} - \theta_0) \right) - \left(1 - \frac{l/\theta_0}{km_{s_0}} (\{\theta\}_K^n - \theta_0) \right) \right] \quad (C.122)$$

$$= -m_{l_o}^b (L_y L_z) m(K) \left[1 - \frac{l/\theta_0}{km_{s_0}} \{\theta\}_K^{n+1} + \frac{l}{km_{s_0}} - 1 + \frac{l/\theta_0}{km_{s_0}} \{\theta\}_K^n - \frac{l}{km_{s_0}} \right] \quad (C.123)$$

$$= -m_{l_o}^b (L_y L_z) m(K) \left[-\frac{l/\theta_0}{km_{s_0}} \{\theta\}_K^{n+1} + \frac{l/\theta_0}{km_{s_0}} \{\theta\}_K^n \right] = m_{l_o}^b (L_y L_z) m(K) \left(\frac{l/\theta_0}{km_{s_0}} \right) [\{\theta\}_K^{n+1} - \{\theta\}_K^n] \quad (C.124)$$

Which leads to the following discretized version of the liquid water mass conservation in cartesian coordinates for the non-isothermal model with dehydration effects:

$$\begin{aligned}
& m(K) \frac{\{m_w\}_K^{n+1} - \{m_w\}_K^n}{\Delta t} - \left(\rho_w \frac{k}{\eta_w} \right) \sum_{L \in N(K)} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] [\{p_w\}_L^n - \{p_w\}_K^n] \\
& = -m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1} + \frac{m_{l_o}^b m(K)}{\Delta t} \left(\frac{l/\theta_0}{km_{s_0}} \right) [\{\theta\}_K^{n+1} - \{\theta\}_K^n] \quad (C.125)
\end{aligned}$$

Vapor Water Conservation:

$$\phi \frac{M_v}{R} \frac{\partial}{\partial t} \left((1 - S_w) \frac{p_v}{\theta} \right) + \text{div}(\underline{w}_v) = \mu_{l \rightarrow g} \quad (\text{C.126})$$

Ignoring temperature effects we can rewrite the equation in the following way:

$$\phi \frac{M_v}{R\theta} \frac{\partial}{\partial t} ((1 - S_w) p_v) + \text{div}(\underline{w}_v) = \mu_{l \rightarrow g} \quad (\text{C.127})$$

First we proceed to integrate over the volume K from (t, t^{n+1})

$$\phi \frac{M_v}{R\theta} \int_{\Omega_t} \int_{\partial t} \frac{\partial}{\partial t} (1 - S_w) p_v dt d\Omega + \int_{\Omega_t} \int_{\partial t} \text{div}(\underline{w}_v) dt d\Omega = \int_{\Omega_t} \int_{\partial t} \mu_{l \rightarrow g} dt d\Omega \quad (\text{C.128})$$

Developing each term individually:

$$\begin{aligned} & \bullet \phi \frac{M_v}{R\theta} \int_{\Omega_t} \int_{\partial t} \frac{\partial}{\partial t} (1 - S_w) p_v dt d\Omega \\ &= \phi \frac{M_v}{R\theta} \int_K (\{p_v(1 - S_w)\}^{n+1} - \{p_v(1 - S_w)\}^n) d\Omega \quad (\text{C.129}) \end{aligned}$$

$$= \phi \frac{M_v}{R\theta} \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x (\{p_v\}^{n+1} \{1 - S_w\}^{n+1} - \{p_v\}^n \{1 - S_w\}^n) dx \quad (\text{C.130})$$

$$= \phi \frac{M_v}{R\theta} (L_y L_z) m(K) \left[\{p_v\}_K^{n+1} \{1 - S_w\}_K^{n+1} - \{p_v\}_K^n \{1 - S_w\}_K^n \right] \quad (\text{C.131})$$

$$\begin{aligned} & \bullet \int_{\Omega_t} \int_{\partial t} \text{div}(\underline{w}_v) dt d\Omega \\ &= \Delta t \int_{\partial K} (\underline{w}_v \cdot \underline{n}) d\gamma = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_v \cdot \underline{n}) d\gamma \quad (\text{C.132}) \end{aligned}$$

$$= -\Delta t \frac{M_v}{R} \sum_{L \in NK} \int_{e_{K,L}} \left[\frac{p_v k_{rg}(S_w) \frac{\partial p_g}{\partial x} + d_{va} f(\phi, S_w) \frac{\partial (p_v)}{\partial x (p_g)}}{\theta} \right] \underline{e}_x \cdot \underline{e}_x dy dz \quad (\text{C.133})$$

$$\begin{aligned} &= -\Delta t \frac{M_v}{R} \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left[k \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial x} (p_g) dy dz \right. \\ &\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial x} \left(\frac{p_v}{p_g} \right) dy dz \right] \quad (\text{C.134}) \end{aligned}$$

$$\begin{aligned}
&= -\frac{M_v}{R} \Delta t (L_y L_z) \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \left(\frac{\{p_g\}_{K+1}^n - \{p_g\}_K^n}{\Delta x} \right) \right. \\
&\quad \left. + \frac{d_{va}}{\Delta x} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n - \{p_v\}_K^n}{\{p_g\}_L^n - \{p_g\}_K^n} \right) \right] \\
&\hspace{20em} (C.135)
\end{aligned}$$

Which leads us to the discretized version of the water vapor conservation in cartesian coordinates for the non-isothermal model with dehydration effects:

$$\begin{aligned}
&m(K) \left[\frac{\{m_v\}_K^{n+1} - \{m_v\}_K^n}{\Delta t} \right] \\
&\quad - \frac{1}{\Delta x} \frac{M_v}{R} \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) \right. \\
&\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n - \{p_v\}_K^n}{\{p_g\}_L^n - \{p_g\}_K^n} \right) \right] = m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1} \\
&\hspace{20em} (C.136)
\end{aligned}$$

Dry Air Conservation:

$$\phi \frac{M_a}{R} \frac{\partial}{\partial t} \left((1 - S_w) \frac{p_a}{\theta} \right) + \text{div}(\mathbf{w}_a) = 0 \quad (\text{C.137})$$

Ignoring temperature effects we can rewrite the equation in the following way:

$$\phi \frac{M_a}{R\theta} \frac{\partial}{\partial t} ((1 - S_w) p_a) + \text{div}(\mathbf{w}_a) = 0 \quad (\text{C.138})$$

First we proceed to integrate over the volume K from (t, t^{n+1})

$$\phi \frac{M_a}{R\theta} \int_{\Omega_t} \int_{\partial t} \frac{\partial}{\partial t} (1 - S_w) p_a dt d\Omega + \int_{\Omega_t} \text{div}(\mathbf{w}_a) dt d\Omega = 0 \quad (\text{C.139})$$

Developing each term individually:

$$\begin{aligned} & \bullet \phi \frac{M_a}{R\theta} \int_{\Omega_t} \int_{\partial t} \frac{\partial}{\partial t} (1 - S_w) p_a dt d\Omega \\ &= \phi \frac{M_a}{R\theta} \int_K (\{p_a(1 - S_w)\}^{n+1} - \{p_a(1 - S_w)\}^n) d\Omega \end{aligned} \quad (\text{C.140})$$

$$= \phi \frac{M_a}{R\theta} \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x (\{p_a\}^{n+1} \{1 - S_w\}^{n+1} - \{p_a\}^n \{1 - S_w\}^n) dx \quad (\text{C.141})$$

$$= \phi \frac{M_a}{R\theta} (L_y L_z) m(K) \left[\{p_a\}_K^{n+1} \{1 - S_w\}_K^{n+1} - \{p_a\}_K^n \{1 - S_w\}_K^n \right] \quad (\text{C.142})$$

$$\begin{aligned} & \bullet \int_{\Omega_t} \text{div}(\mathbf{w}_a) dt d\Omega \\ &= \Delta t \int_{\partial K} (\mathbf{w}_v \cdot \mathbf{n}) d\gamma = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\mathbf{w}_a \cdot \mathbf{n}) d\gamma \end{aligned} \quad (\text{C.143})$$

$$= -\Delta t \frac{M_a}{R} \sum_{L \in NK} \int_{e_{K,L}} \left[\frac{p_a \frac{k}{\eta_g} k_{rg}(S_w) \frac{\partial p_g}{\partial x} + d_{va} f(\phi, S_w) \frac{\partial}{\partial x} \left(\frac{p_a}{p_g} \right)}{\theta} \right] \mathbf{e}_x \cdot \mathbf{e}_x dy dz \quad (\text{C.144})$$

$$\begin{aligned} &= -\Delta t \frac{M_a}{R} \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial x} (p_g) dy dz \right. \\ &\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial x} \left(\frac{p_a}{p_g} \right) dy dz \right] \end{aligned} \quad (\text{C.145})$$

$$\begin{aligned}
&= -\frac{M_a}{R\theta} (L_y L_z) \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \left(\frac{\{p_g\}_{K+1}^n - \{p_g\}_K^n}{\Delta x} \right) \right. \\
&\quad \left. + \frac{d_{va}}{\Delta x} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n - \{p_a\}_K^n}{\{p_g\}_L^n - \{p_g\}_K^n} \right) \right] \\
&\hspace{20em} \text{(C.146)}
\end{aligned}$$

Which leads us to the discretized version of the dry air conservation equation for the non-isothermal model with dehydration effects in cartesian coordinates:

$$\begin{aligned}
&m(K) \left[\frac{\{m_a\}_K^{n+1} - \{m_a\}_K^n}{\Delta t} \right] \\
&-\frac{M_a}{R} \left(\frac{1}{\Delta x} \right) \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) \right. \\
&\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n - \{p_a\}_K^n}{\{p_g\}_L^n - \{p_g\}_K^n} \right) \right] = 0 \\
&\hspace{20em} \text{(C.147)}
\end{aligned}$$

Liquid - Vapor Balance:

$$\frac{R\theta}{M_v} \ln\left(\frac{p_v}{p_{v0}}\right) = \frac{p_w - p_{w0}}{\rho_w} + \frac{l_0}{\theta_0}(\theta - \theta_0) + (C_{pl} - C_{pv})\left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right] \quad (C.148)$$

First we proceed to integrate over the volume K from (t, t^{n+1})

$$\int_{\Omega_t} \frac{R\theta}{M_v} \ln\left(\frac{p_v}{p_{v0}}\right) dt d\Omega = \int_{\Omega_t} \left\{ \frac{p_w - p_{w0}}{\rho_w} + \frac{l_0}{\theta_0}(\theta - \theta_0) + (C_{pl} - C_{pv})\left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right] \right\} dt d\Omega \quad (C.149)$$

Developing each term individually:

$$\begin{aligned} & \bullet \int_{\Omega_t} \frac{R\theta}{M_v} \ln\left(\frac{p_v}{p_{v0}}\right) dt d\Omega \\ &= \frac{R}{M_v} \int_{\Omega_t} \theta \ln\left(\frac{p_v}{p_{v0}}\right) dt d\Omega = \Delta t \frac{R}{M_v} \int_{\Omega} \theta \ln\left(\frac{p_v}{p_{v0}}\right) d\Omega \quad (C.150) \end{aligned}$$

$$= \Delta t \frac{R}{M_v} \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x \theta \ln\left(\frac{p_v}{p_{v0}}\right) dx = \Delta t \frac{R}{M_v} (L_y L_z) m(K) \left\{ \theta \ln\left(\frac{p_v}{p_{v0}}\right) \right\} \Big|_K^n \quad (C.151)$$

$$= \Delta t \frac{R}{M_v} (L_y L_z) m(K) \left\{ \theta \right\} \Big|_K^n \left\{ \ln\left(\frac{p_v}{p_{v0}}\right) \right\} \Big|_K^n = \Delta t \frac{R}{M_v} (L_y L_z) m(K) \left\{ \theta \right\} \Big|_K^n \ln\left(\frac{\{p_v\}_K^n}{\{p_v\}_K^{n-1}}\right) \quad (C.152)$$

$$\begin{aligned} & \bullet \int_{\Omega_t} \left\{ \frac{p_w - p_{w0}}{\rho_w} + \frac{l_0}{\theta_0}(\theta - \theta_0) + (C_{pl} - C_{pv})\left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right] \right\} dt d\Omega \\ &= \Delta t \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x \left\{ \frac{p_w - p_{w0}}{\rho_w} + \frac{l_0}{\theta_0}(\theta - \theta_0) + (C_{pl} - C_{pv})\left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right] \right\} dx \quad (C.153) \end{aligned}$$

$$= \Delta t (L_y L_z) m(K) \left\{ \frac{p_w - p_{w0}}{\rho_w} + \frac{l_0}{\theta_0}(\theta - \theta_0) + (C_{pl} - C_{pv})\left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right] \right\} \Big|_K^n \quad (C.154)$$

$$= \Delta t (L_y L_z) m(K) \left\{ \left\{ \frac{p_w - p_{w0}}{\rho_w} \right\} \Big|_K^n + \left\{ \frac{l_0}{\theta_0}(\theta - \theta_0) \right\} \Big|_K^n + \left\{ (C_{pl} - C_{pv})\left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right] \right\} \Big|_K^n \right\} \quad (C.155)$$

$$= \Delta t (L_y L_z) m(K) \left\{ \frac{\{p_w\}_K^n - \{p_w\}_K^{n-1}}{\rho_w} + l_0 \frac{\{\theta\}_K^n - \{\theta\}_K^{n-1}}{\{\theta\}_K^{n-1}} + (C_{pl} - C_{pv}) \left[\{\theta\}_K^n - \{\theta\}_K^{n-1} - \{\theta\}_K^n \ln\left(\frac{\{\theta\}_K^n}{\{\theta\}_K^{n-1}}\right) \right] \right\} \quad (C.156)$$

Then the liquid-vapor balance equation for the non-isothermal model reduces to:

$$\frac{R}{M_v} \left\{ \theta \right\} \Big|_K^n \ln\left(\frac{\{p_v\}_K^n}{\{p_v\}_K^{n-1}}\right) = \frac{\{p_w\}_K^n - \{p_w\}_K^{n-1}}{\rho_w} + l_0 \frac{\{\theta\}_K^n - \{\theta\}_K^{n-1}}{\{\theta\}_K^{n-1}} + (C_{pl} - C_{pv}) \left[\{\theta\}_K^n - \{\theta\}_K^{n-1} - \{\theta\}_K^n \ln\left(\frac{\{\theta\}_K^n}{\{\theta\}_K^{n-1}}\right) \right] \quad (C.157)$$

Entropy Balance:

$$\phi \left[\frac{\partial}{\partial t} \left(S_s + \sum_{i=w,v,a} m_i s_i \right) + \sum_{i=w,v,a} s_i w_i \right] = -\text{div}(q) \quad (\text{C.158})$$

First we proceed to integrate over the volume K from (t, t^{n+1})

$$\iint_{\Omega_t} \phi \left[\frac{\partial}{\partial t} \left(S_s + \sum_{i=w,v,a} m_i s_i \right) + \sum_{i=w,v,a} s_i w_i \right] dt d\Omega = \iint_{\Omega_t} [-\text{div}(q)] dt d\Omega \quad (\text{C.159})$$

Developing each term individually:

$$\begin{aligned} & \bullet \iint_{\Omega_t} \phi \left[\frac{\partial}{\partial t} \left(S_s + \sum_{i=w,v,a} m_i s_i \right) + \sum_{i=w,v,a} s_i w_i \right] dt d\Omega \\ &= \iint_{\Omega_t} \phi \frac{\partial}{\partial t} \left(S_s + \sum_{i=w,v,a} m_i s_i \right) dt d\Omega + \iint_{\Omega_t} \phi \sum_{i=w,v,a} s_i w_i dt d\Omega \end{aligned} \quad (\text{C.160})$$

$$= \phi \int_{\Omega} \left\{ \left(S_s + \sum_{i=w,v,a} m_i s_i \right)^{n+1} - \left(S_s + \sum_{i=w,v,a} m_i s_i \right)^n \right\} d\Omega + \Delta t \int_{\Omega} \left(\phi \sum_{i=w,v,a} s_i w_i \right) d\Omega \quad (\text{C.161})$$

$$= \phi \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x \left\{ \left(S_s + \sum_{i=w,v,a} m_i s_i \right)^{n+1} - \left(S_s + \sum_{i=w,v,a} m_i s_i \right)^n \right\} dx + \phi \Delta t \int_{y=0}^{L_y} dy \int_{z=0}^{L_z} dz \int_x \left(\sum_{i=w,v,a} s_i w_i \right) dx \quad (\text{C.162})$$

$$= \phi L_y L_z m(K) \left\{ \left(S_s + \sum_{i=w,v,a} m_i s_i \right) \Big|_K^{n+1} - \left(S_s + \sum_{i=w,v,a} m_i s_i \right) \Big|_K^n + \Delta t \left\{ \sum_{i=w,v,a} s_i w_i \right\} \Big|_K^n \right\} \quad (\text{C.163})$$

$$= \phi L_y L_z m(K) \left\{ \{S_s\}_K^{n+1} - \{S_s\}_K^n + \left\{ \sum_{i=w,v,a} m_i s_i \right\}_K^{n+1} - \left\{ \sum_{i=w,v,a} m_i s_i \right\}_K^n - \Delta t \left\{ \sum_{i=w,v,a} s_i w_i \right\}_K^n \right\} \quad (\text{C.164})$$

$$\begin{aligned} &= \phi L_y L_z m(K) \left\{ \left(\{S_s\}_K^{n+1} - \{S_s\}_K^n \right) + \left(\{m_w s_w\}_K^{n+1} - \{m_w s_w\}_K^n \right) + \left(\{m_v s_v\}_K^{n+1} - \{m_v s_v\}_K^n \right) - \left(\{m_a s_a\}_K^{n+1} - \{m_a s_a\}_K^n \right) \right. \\ &\quad \left. - \Delta t \left(\{s_w w_w\}_K^n + \{s_v w_v\}_K^n + \{s_a w_a\}_K^n \right) \right\} \end{aligned} \quad (\text{C.165})$$

$$\begin{aligned} &= \phi L_y L_z m(K) \left\{ \left(\{S_s\}_K^{n+1} - \{S_s\}_K^n \right) + \left(\{m_w\}_K^{n+1} \{s_w\}_K^{n+1} - \{m_w\}_K^n \{s_w\}_K^n \right) \right. \\ &\quad \left. + \left(\{m_v\}_K^{n+1} \{s_v\}_K^{n+1} - \{m_v\}_K^n \{s_v\}_K^n \right) - \left(\{m_a\}_K^{n+1} \{s_a\}_K^{n+1} - \{m_a\}_K^n \{s_a\}_K^n \right) \right. \\ &\quad \left. - \Delta t \left(\{w_w\}_K^n \{s_w\}_K^n + \{w_v\}_K^n \{s_v\}_K^n + \{w_a\}_K^n \{s_a\}_K^n \right) \right\} \end{aligned} \quad (\text{C.166})$$

with,

$$\{S_s\}_K^n = \{S_m\}_K^n + \{S_c\}_K^n \quad (\text{C.167})$$

$$S_m = C_{s_0} \ln\left(\frac{\theta}{\theta_0}\right) + m_{s_0} s_{s_0} \xi(\theta) \quad (\text{C.168})$$

$$\{S_m\}_K^n = C_s \left\{ \ln\left(\frac{\theta}{\theta_0}\right) \right\}_K^n + m_{s_0} s_{s_0} \{\xi(\theta)\}_K^n = C_s \ln\left(\frac{\{\theta\}_K^n}{\theta_0}\right) + \left(1 - \frac{l/\theta_0}{km_{s_0}} (\{\theta\}_K^n - \theta_0)\right) \quad (\text{C.169})$$

$$S_c = -\phi \frac{\partial}{\partial \theta} \left[\gamma(\theta) \int_0^{p_c/\gamma(\theta)} S_w(x) dx \right] \quad (\text{C.170})$$

$$\gamma(\theta) = \gamma(\theta_0) [1 - c_o(\theta - \theta_0)] \quad (\text{C.171})$$

$$S_w = \left[1 + \left(\frac{\gamma(\theta_0) p_c}{\gamma(\theta) a} \right)^{n-m} \right] = \left[1 + \left(\frac{1}{[1 - c_o(\theta - \theta_0)] a} p_c \right)^{n-m} \right] \quad (\text{C.172})$$

then the integral can be solved numerically using Gaussian Quadrature:

$$\int_{-1}^1 f(t) dt \approx \sum_{i=1}^n w_i f(t_i) \quad (\text{C.173})$$

The entropy for the different phases is given by:

$$\{s_w\}_K^n = \left\{ s_{w_0} + C_{pw} \ln\left(\frac{\theta}{\theta_0}\right) \right\}_K^n = s_{w_0} + C_{pw} \ln\left(\frac{\{\theta\}_K^n}{\{\theta\}_K^{n-1}}\right) \quad (\text{C.174})$$

$$\{s_v\}_K^n = \left\{ s_{v_0} + C_{pv} \ln\left(\frac{\theta}{\theta_0}\right) - \frac{R}{M_v} \ln\left(\frac{p_v}{p_{v_0}}\right) \right\}_K^n = s_{v_0} + C_{pv} \ln\left(\frac{\{\theta\}_K^n}{\{\theta\}_K^{n-1}}\right) - \frac{R}{M_v} \ln\left(\frac{\{p_v\}_K^n}{\{p_{v_0}\}_K^{n-1}}\right) \quad (\text{C.175})$$

$$\{s_a\}_K^n = \left\{ s_{a_0} + C_{pa} \ln\left(\frac{\theta}{\theta_0}\right) - \frac{R}{M_a} \ln\left(\frac{p_a}{p_{a_0}}\right) \right\}_K^n = s_{a_0} + C_{pa} \ln\left(\frac{\{\theta\}_K^n}{\{\theta\}_K^{n-1}}\right) - \frac{R}{M_a} \ln\left(\frac{\{p_a\}_K^n}{\{p_{a_0}\}_K^{n-1}}\right) \quad (\text{C.176})$$

The mass for the different phases is given by (C.5), (C.6) and (C.7)

And the flux expressions in each control volume are expressed as:

$$\{\underline{w}_w\}_K^n = \frac{1}{m(K)} \int \underline{w}_w dx = \frac{1}{m(K)} \int \left(-\rho_w \frac{k}{\eta_w} k_{ri}(S_w) \text{grad}[p_w] \right) dx \quad (\text{C.177})$$

$$= -\frac{1}{m(K)} \rho_w \frac{k}{\eta_w} \left(\frac{\{k_{ri}(S_w)\}_K^n + 2\{k_{ri}(S_w)\}_K^n + \{k_{ri}(S_w)\}_K^n}{4} \right) \int \left(\frac{\partial p_w}{\partial x} \right) dx \quad (\text{C.178})$$

$$= -\frac{1}{m(K)} \rho_w \frac{k}{\eta_w} \sum_{L \in N(K)} \left(\frac{\{k_{ri}(S_w)\}_K^n + \{k_{ri}(S_w)\}_L^n}{2} \right) \left(\frac{\{p_w\}_K^n + \{p_w\}_L^n}{2} \right) \quad (\text{C.179})$$

$$\{\underline{w}_v\}_K^n = \frac{1}{m(K)} \int \underline{w}_v dx = \frac{1}{m(K)} \int \left(-\frac{M_v}{R\theta} p_v \frac{k}{\eta_g} k_{rg}(S_w) \text{grad}(p_g) - \frac{M_v}{R\theta} d_{va} f(\phi, S_w) \text{grad}\left(\frac{p_v}{p_g}\right) \right) dx \quad (\text{C.180})$$

$$= \frac{-1}{m(K) R\theta} \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \left(\frac{\{p_g\}_K^n - \{p_g\}_L^n}{2} \right) \right. \\ \left. + \frac{d_{va}}{2} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n}{\{p_g\}_L^n} - \frac{\{p_v\}_K^n}{\{p_g\}_K^n} \right) \right] \quad (\text{C.181})$$

$$\{\underline{w}_a\}_K^n = \frac{1}{m(K)} \int \underline{w}_a dx = \frac{1}{m(K)} \int \left(-\frac{M_a}{R\theta} p_a \frac{k}{\eta_g} k_{rg}(S_w) \text{grad}(p_g) - \frac{M_a}{R\theta} d_{va} f(\phi, S_w) \text{grad}\left(\frac{p_a}{p_g}\right) \right) dx \quad (\text{C.182})$$

$$= \frac{-1}{m(K) R\theta} \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \left(\frac{\{p_g\}_K^n - \{p_g\}_L^n}{2} \right) \right. \\ \left. + \frac{d_{va}}{2} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n}{\{p_g\}_L^n} - \frac{\{p_a\}_K^n}{\{p_g\}_K^n} \right) \right] \quad (\text{C.183})$$

$$\bullet \int_{\Omega} \int_t [-\text{div}(q)] dt d\Omega$$

$$= \Delta t \int_{\Omega} [-\text{div}(q)] d\Omega = -\Delta t \int_{\partial K} (q \cdot n) d\gamma = -\Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (q \cdot n) d\gamma \quad (\text{C.184})$$

$$= \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} [\mathfrak{K} \text{grad}(\theta) \cdot n] d\gamma = \Delta t \mathfrak{K} \sum_{L \in N(K)} \int_{e_{K,L}} \left[\frac{\partial \theta}{\partial x} e_x \cdot e_x \right] d\gamma \quad (\text{C.185})$$

$$= \Delta t \mathfrak{K} \sum_{L \in N(K)} \int_{e_{K,L}} \left(\frac{\partial \theta}{\partial x} \right) dy dz = \Delta t \mathfrak{K} (L_y L_z) m(K) \sum_{L \in N(K)} \left(\frac{\{\theta\}_{K+1}^n - \{\theta\}_K^n}{\Delta x} \right) \quad (\text{C.186})$$

The previous terms allow us to write the discretized version of the entropy balance equation in cartesian coordinates for the non-isothermal model including dehydration effects:

$$\begin{aligned}
& \phi \left\{ \left(\{S_s\}_K^{n+1} - \{S_s\}_K^n \right) + \left(\{m_w\}_K^{n+1} \{s_w\}_K^{n+1} - \{m_w\}_K^n \{s_w\}_K^n \right) \right. \\
& \quad + \left(\{m_v\}_K^{n+1} \{s_v\}_K^{n+1} - \{m_v\}_K^n \{s_v\}_K^n \right) - \left(\{m_a\}_K^{n+1} \{s_a\}_K^{n+1} - \{m_a\}_K^n \{s_a\}_K^n \right) \\
& \quad \left. - \Delta t \left(\{w_w\}_K^n \{s_w\}_K^n + \{w_v\}_K^n \{s_v\}_K^n + \{w_a\}_K^n \{s_a\}_K^n \right) \right\} \\
& \qquad \qquad \qquad = \Delta t \mathfrak{K} \sum_{L \in N(K)} \left(\frac{\{\theta\}_{K+1}^n - \{\theta\}_K^n}{\Delta x} \right) \quad (\text{C.187})
\end{aligned}$$

Summary of the Discretized Equations for the One-Dimension Non-Isothermal Model in Cartesian Coordinates

Liquid water conservation:

$$\begin{aligned}
 m(K) \frac{\{m_w\}_K^{n+1} - \{m_w\}_K^n}{\Delta t} - \left(\rho_w \frac{k}{\eta_w} \right) \sum_{L \in N(K)} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\{p_w\}_L^n - \{p_w\}_K^n \right] \\
 = -m(K) \{\mu_{l \rightarrow g}\}_K^{n+1} + \frac{m_l^b m(K) (l/\theta_0)}{\Delta t} \left(\frac{l}{km_{s_0}} \right) [\{\theta\}_K^{n+1} - \{\theta\}_K^n] \quad (C.188)
 \end{aligned}$$

Vapor water conservation:

$$\begin{aligned}
 m(K) \left[\frac{\{m_v\}_K^{n+1} - \{m_v\}_K^n}{\Delta t} \right] \\
 - \frac{1}{\Delta x} \frac{M_v}{R\theta} \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) \right. \\
 \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n - \{p_v\}_K^n}{\{p_g\}_L^n - \{p_g\}_K^n} \right) \right] = m(K) \{\mu_{l \rightarrow g}\}_K^{n+1} \quad (C.189)
 \end{aligned}$$

Dry air conservation:

$$\begin{aligned}
 m(K) \left[\frac{\{m_a\}_K^{n+1} - \{m_a\}_K^n}{\Delta t} \right] \\
 - \frac{M_a}{R\theta} \left(\frac{1}{\Delta x} \right) \sum_{L \in N(K)} \left[\frac{k}{\eta_g} \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) \right. \\
 \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n - \{p_a\}_K^n}{\{p_g\}_L^n - \{p_g\}_K^n} \right) \right] = 0 \quad (C.190)
 \end{aligned}$$

Liquid-vapor balance:

$$\frac{R}{M_v} \{\theta\}_K^n \ln \left(\frac{\{p_v\}_K^n}{\{p_v\}_K^{n-1}} \right) = \frac{\{p_w\}_K^n - \{p_w\}_K^{n-1}}{\rho_w} + l_0 \frac{\{\theta\}_K^n - \{\theta\}_K^{n-1}}{\{\theta\}_K^{n-1}} + (C_{pl} - C_{pv}) \left[\{\theta\}_K^n - \{\theta\}_K^{n-1} - \{\theta\}_K^n \ln \left(\frac{\{\theta\}_K^n}{\{\theta\}_K^{n-1}} \right) \right] \quad (C.191)$$

Entropy balance:

$$\begin{aligned}
& \Phi \left\{ \left(\{S_s\}_K^{n+1} - \{S_s\}_K^n \right) + \left(\{m_w\}_K^{n+1} \{s_w\}_K^{n+1} - \{m_w\}_K^n \{s_w\}_K^n \right) \right. \\
& \quad + \left(\{m_v\}_K^{n+1} \{s_v\}_K^{n+1} - \{m_v\}_K^n \{s_v\}_K^n \right) - \left(\{m_a\}_K^{n+1} \{s_a\}_K^{n+1} - \{m_a\}_K^n \{s_a\}_K^n \right) \\
& \quad \left. - \Delta t \left(\{w_w\}_K^n \{s_w\}_K^n + \{w_v\}_K^n \{s_v\}_K^n + \{w_a\}_K^n \{s_a\}_K^n \right) \right\} \\
& = \Delta t \mathfrak{K} \sum_{L \in N(K)} \left(\frac{\{\theta\}_K^{n+1} - \{\theta\}_K^n}{\Delta x} \right) \quad (\text{C.192})
\end{aligned}$$

Cylindrical Coordinates

Mass Conservation of Liquid Water

$$\phi \rho_w \frac{\partial}{\partial t} S_w + \text{div}(\underline{w}_w) = -\mu_{l \rightarrow g} - m_{l \rightarrow o}^b \frac{\partial \xi}{\partial t} \quad (\text{C.193})$$

First we proceed to integrate over the volume K from (t, t^{n+1})

$$\int_{\Omega} \int_t^{t^{n+1}} \left(\phi \rho_w \frac{\partial S_w}{\partial t} \right) dt d\Omega + \int_{\Omega} \int_t^{t^{n+1}} \text{div}(\underline{w}_w) dt d\Omega = \int_{\Omega} \int_t^{t^{n+1}} (-\mu_{l \rightarrow g}) dt d\Omega + \int_{\Omega} \int_t^{t^{n+1}} \left(-m_{l \rightarrow o}^b \frac{\partial \xi}{\partial t} \right) dt d\Omega \quad (\text{C.194})$$

We will now develop each term individually:

$$\bullet \int_{\Omega} \int_t^{t^{n+1}} \left(\phi \rho_w \frac{\partial S_w}{\partial t} \right) dt d\Omega$$

$$= \phi \rho_w \int_K [S_w(t^{n+1}) - S_w(t^n)] d\Omega = \phi \rho_w \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \int_r [S_w(t^{n+1}) - S_w(t^n)] r dr \quad (\text{C.195})$$

$$= (2\pi L_z) \phi \rho_w m(K) \left(\{S_w\}_K^{n+1} - \{S_w\}_K^n \right) \quad (\text{C.196})$$

$$\bullet \int_{\Omega} \int_t^{t^{n+1}} \text{div}(\underline{w}_w) dt d\Omega$$

$$= \Delta t \int_{\partial K} (\underline{w}_w \cdot \underline{n}) d\gamma = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_w \cdot \underline{n}) r d\beta dz \quad (\text{C.197})$$

$$= \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} \left[\left(-\rho_w \frac{k}{\eta_w} k_{rl}(S_w) \frac{\partial}{\partial r} [p_w] \underline{e}_r \right) \cdot \underline{e}_r \right] r d\beta dz \quad (\text{C.198})$$

$$= \Delta t \sum_{L \in N(K)} \rho_w \frac{k}{\eta_w} \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \int_{e_{K,L}} \frac{\partial}{\partial r} [p_w] r d\beta dz \quad (\text{C.199})$$

$$= \Delta t \rho_w \frac{k}{\eta_w} \sum_{L \in N(K)} (r) \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\frac{\{p_w\}_L^n - \{p_w\}_K^n}{d_r} \right] \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \quad (\text{C.200})$$

$$= (2\pi L_z) \Delta t \rho_w \cdot \frac{k}{\eta_w} \sum_{L \in N(K)} \left(\frac{r}{d_r} \right) \left[\frac{\{k_{rl}(S_w)\}_K^n + \{k_{rl}(S_w)\}_L^n}{2} \right] \left[\{p_w\}_L^n - \{p_w\}_K^n \right] \quad (\text{C.201})$$

$$\bullet \int_{\Omega} \int_t^{t^{n+1}} (-\mu_{l \rightarrow g}) dt d\Omega$$

$$= -\Delta t \int_K \mu_{l \rightarrow g}^w d\Omega = -\Delta t \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \int_r (\mu_{l \rightarrow g}^w) r dr = \Delta t (2\pi L_z) m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1} \quad (\text{C.202})$$

$$\bullet \int_{\Omega} \int_t^{t^{n+1}} \left(-m_{l \rightarrow o}^b \frac{\partial \xi}{\partial t} \right) dt d\Omega$$

$$= -m^b_{l_o} \int_{\Omega} \int_t^{t^{n+1}} \left(\frac{\partial \xi}{\partial t} \right) dt d\Omega = -m^b_{l_o} \int_K [\xi(t^{n+1}) - \xi(t^n)] d\Omega = m^b_{l_o} \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \int [\xi(t^{n+1}) - \xi(t^n)] r dr \quad (\text{C.203})$$

$$= -m^b_{l_o} (2\pi L_z) m(K) (\{\xi\}_K^{n+1} - \{\xi\}_K^n) \quad (\text{C.204})$$

$$= -m^b_{l_o} (2\pi L_z) m(K) \left[\left(1 - \frac{l/\theta_0}{km_{s_0}} (\{\theta\}_K^{n+1} - \theta_0) \right) - \left(1 - \frac{l/\theta_0}{km_{s_0}} (\{\theta\}_K^n - \theta_0) \right) \right] \quad (\text{C.205})$$

$$= -m^b_{l_o} (2\pi L_z) m(K) \left[1 - \frac{l/\theta_0}{km_{s_0}} \{\theta\}_K^{n+1} + \frac{l}{km_{s_0}} - 1 + \frac{l/\theta_0}{km_{s_0}} \{\theta\}_K^n - \frac{l}{km_{s_0}} \right] \quad (\text{C.206})$$

$$= -m^b_{l_o} (2\pi L_z) m(K) \left[-\frac{l/\theta_0}{km_{s_0}} \{\theta\}_K^{n+1} + \frac{l/\theta_0}{km_{s_0}} \{\theta\}_K^n \right] = m^b_{l_o} (2\pi L_z) m(K) \left(\frac{l/\theta_0}{km_{s_0}} \right) [\{\theta\}_K^{n+1} - \{\theta\}_K^n] \quad (\text{C.207})$$

Which leads to the following discretized version of the liquid water mass conservation in cylindrical coordinates for the non-isothermal model including dehydration effects:

$$m(K) \frac{\{\mu_w\}_K^{n+1} - \{\mu_w\}_K^n}{\Delta t} - \left\{ \rho_w \cdot \frac{k}{\bar{n}_{wL} \in N(K)} \sum \left(\frac{r}{d_r} \right) \left[\frac{\{\kappa_{ri}(S_w)\}_K^n + \{\kappa_{ri}(S_w)\}_L^n}{2} \right] [\{p_w\}_L^n - \{p_w\}_K^n] \right\} = -m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1} + \frac{m^b_{l_o} m(K)}{\Delta t} \left(\frac{l/\theta_0}{km_{s_0}} \right) [\{\theta\}_K^{n+1} - \{\theta\}_K^n] \quad (\text{C.208})$$

Mass Conservation of Water Vapor

$$\phi \frac{M_v}{R} \frac{\partial}{\partial t} \left((1 - S_w) \frac{p_v}{\theta} \right) + \text{div}(\underline{w}_v) = \mu_{l \rightarrow g} \quad (\text{C.209})$$

Assuming the temperature does not affect the mass density of the liquid water we can rewrite the equation in the following way:

$$\phi \frac{M_v}{R\theta} \frac{\partial}{\partial t} ((1 - S_w)p_v) + \text{div}(\underline{w}_v) = \mu_{l \rightarrow g} \quad (\text{C.210})$$

First we proceed to integrate over the volume K from (t, t^{n+1})

$$\phi \frac{M_v}{R\theta} \int_{\Omega_t} \int_{\partial t} \frac{\partial}{\partial t} (1 - S_w) p_v dt d\Omega + \int_{\Omega_t} \int_{\partial t} \text{div}(\underline{w}_v) dt d\Omega = \int_{\Omega_t} \mu_{l \rightarrow g} dt d\Omega \quad (\text{C.211})$$

Developing each term individually:

$$\begin{aligned} & \bullet \phi \frac{M_v}{R\theta} \int_{\Omega_t} \int_{\partial t} \frac{\partial}{\partial t} (1 - S_w) p_v dt d\Omega \\ &= \phi \frac{M_v}{R\theta} \int_K (\{p_v(1 - S_w)\}^{n+1} - \{p_v(1 - S_w)\}^n) d\Omega \quad (\text{C.212}) \end{aligned}$$

$$= \phi \frac{M_v}{R\theta} \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \int_x (\{p_v\}^{n+1} \{1 - S_w\}^{n+1} - \{p_v\}^n \{1 - S_w\}^n) r dr \quad (\text{C.213})$$

$$= \phi \frac{M_v}{R\theta} (2\pi L_z) m(K) \left[\{p_v\}_K^{n+1} \{1 - S_w\}_K^{n+1} - \{p_v\}_K^n \{1 - S_w\}_K^n \right] \quad (\text{C.214})$$

$$\begin{aligned} & \bullet \int_{\Omega_t} \int_{\partial t} \text{div}(\underline{w}_v) dt d\Omega \\ &= \Delta t \int_{\partial K} (\underline{w}_v \cdot \underline{n}) d\gamma = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_v \cdot \underline{n}) d\gamma \quad (\text{C.215}) \end{aligned}$$

$$= -\Delta t \frac{M_v}{R} \sum_{L \in NK} \int_{e_{K,L}} \left[\frac{p_v \frac{k}{\eta_g} k_{rg}(S_w) \frac{\partial p_g}{\partial r} + d_{va} f(\phi, S_w) \frac{\partial}{\partial r} \left(\frac{p_v}{p_g} \right)}{\theta} \right] \underline{e}_r \cdot \underline{e}_r r d\beta dz \quad (\text{C.216})$$

$$\begin{aligned} &= -\Delta t \frac{M_v}{R} \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left[\left(\frac{k}{\eta_g} \right) \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial r} (p_g) r d\beta dz \right. \\ &\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial r} \left(\frac{p_v}{p_g} \right) r d\beta dz \right] \quad (\text{C.217}) \end{aligned}$$

$$\begin{aligned}
&= -\frac{M_v}{R} \sum_{L \in N(K)} \left(\frac{2(2\pi L_z)}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left(\frac{r}{dr} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \right] \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) \\
&\quad + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n}{\{p_g\}_L^n} - \frac{\{p_v\}_K^n}{\{p_g\}_K^n} \right) \quad (C.218)
\end{aligned}$$

Which leads to the following discretized version of the vapor water mass conservation in cylindrical coordinates for the non-isothermal model including dehydration effects:

$$\begin{aligned}
&m(K) \left[\frac{\{m_v\}_K^{n+1} - \{m_v\}_K^n}{\Delta t} \right] \\
&\quad - \frac{M_v}{R} \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left(\frac{r}{dr} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \right] \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) \\
&\quad + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n}{\{p_g\}_L^n} - \frac{\{p_v\}_K^n}{\{p_g\}_K^n} \right) \right] = -m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1} \quad (C.219)
\end{aligned}$$

Mass Conservation of Dry air:

$$\phi \frac{M_a}{R} \frac{\partial}{\partial t} \left((1 - S_w) \frac{p_a}{\theta} \right) + \text{div}(\underline{w}_a) = 0 \quad (\text{C.220})$$

Ignoring temperature effects we can rewrite the equation in the following way:

$$\phi \frac{M_a}{R\theta} \frac{\partial}{\partial t} ((1 - S_w) p_a) + \text{div}(\underline{w}_a) = 0 \quad (\text{C.221})$$

First we proceed to integrate over the volume K from (t, t^{n+1})

$$\phi \frac{M_a}{R\theta} \int_{\Omega_t} \int_{t^n}^{t^{n+1}} \frac{\partial}{\partial t} (1 - S_w) p_a dt d\Omega + \int_{\Omega_t} \text{div}(\underline{w}_a) dt d\Omega = 0 \quad (\text{C.222})$$

Developing each term individually:

$$\begin{aligned} & \bullet \phi \frac{M_a}{R\theta} \int_K \int_{t^n}^{t^{n+1}} \frac{\partial}{\partial t} [p_a (1 - S_w)] dt d\Omega \\ &= \phi \frac{M_a}{R\theta} \int_K (\{p_a (1 - S_w)\}^{n+1} - \{p_a (1 - S_w)\}^n) d\Omega \end{aligned} \quad (\text{C.223})$$

$$= \phi \frac{M_a}{R\theta} \int_{\beta=0}^{2\pi} \int_{z=0}^{L_z} dz \int_r (\{p_a\}^{n+1} \{1 - S_w\}^{n+1} - \{p_a\}^n \{1 - S_w\}^n) r dr \quad (\text{C.224})$$

$$= \phi \frac{M_a}{R\theta} (2\pi L_z) m(K) \left[\{p_a\}_K^{n+1} \{1 - S_w\}_K^{n+1} - \{p_a\}_K^n \{1 - S_w\}_K^n \right] \quad (\text{C.225})$$

$$\begin{aligned} & \bullet \int_K \int_{t^n}^{t^{n+1}} \text{div}(\underline{w}_a) dt d\Omega \\ &= \Delta t \int_{\partial K} (\underline{w}_a \cdot \underline{n}) d\Upsilon = \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} (\underline{w}_a \cdot \underline{n}) d\Upsilon \end{aligned} \quad (\text{C.226})$$

$$= -\frac{M_a}{R} \Delta t \sum_{L \in N(K)} \int_{e_{K,L}} \left[\frac{p_a k_{rg}(S_w) \frac{\partial}{\partial r} (p_g) - d_{va} f(\phi, S_w) \frac{\partial}{\partial r} \left(\frac{p_a}{p_g} \right)}{\theta} \right] \underline{e}_r \cdot \underline{e}_r r d\beta dz \quad (\text{C.227})$$

$$\begin{aligned} &= -\frac{M_a}{R} \Delta t \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial r} p_g r d\beta dz \right. \\ &\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \int_{e_{K,L}} \frac{\partial}{\partial r} \left(\frac{p_a}{p_g} \right) r d\beta dz \right] \end{aligned} \quad (\text{C.228})$$

$$\begin{aligned}
&= -\frac{M_a}{R} \sum_{L \in N(K)} \left(\frac{2(2\pi L_z)}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left(\frac{r}{d_r} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \right] \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) \\
&\quad + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n - \{p_a\}_K^n}{\{p_g\}_L^n - \{p_g\}_K^n} \right) \\
&\hspace{15em} \text{(C.229)}
\end{aligned}$$

Which leads to the following discretized version of the dry air mass conservation in cylindrical coordinates for the non-isothermal model including dehydration effects:

$$\begin{aligned}
&m(K) \left[\frac{\{m_a\}_K^{n+1} - \{m_a\}_K^n}{\Delta t} \right] \\
&\quad - \frac{M_a}{R} \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left(\frac{r}{d_r} \right) \left[\frac{k}{\eta_g} \cdot \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \cdot \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \cdot \left(\{p_g\}_{K+1}^n - \{p_g\}_K^n \right) \right. \\
&\quad \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n - \{p_a\}_K^n}{\{p_g\}_L^n - \{p_g\}_K^n} \right) \right] = 0 \\
&\hspace{15em} \text{(C.230)}
\end{aligned}$$

Liquid - Vapor Balance:

$$\frac{R\theta}{M_v} \ln\left(\frac{p_v}{p_{v0}}\right) = \frac{p_w - p_{w0}}{\rho_w} + \frac{l_0}{\theta_0}(\theta - \theta_0) + (C_{pl} - C_{pv})\left(\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right) \quad (\text{C.231})$$

First we proceed to integrate over the volume K from (t, t^{n+1})

$$\int_{\Omega_t} \int \frac{R\theta}{M_v} \ln\left(\frac{p_v}{p_{v0}}\right) dt d\Omega = \int_{\Omega_t} \int \left\{ \frac{p_w - p_{w0}}{\rho_w} + \frac{l_0}{\theta_0}(\theta - \theta_0) + (C_{pl} - C_{pv})\left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right] \right\} dt d\Omega \quad (\text{C.232})$$

Developing each term individually:

$$\begin{aligned} & \bullet \int_{\Omega_t} \int \frac{R\theta}{M_v} \ln\left(\frac{p_v}{p_{v0}}\right) dt d\Omega \\ &= \frac{R}{M_v} \int_{\Omega_t} \int \theta \ln\left(\frac{p_v}{p_{v0}}\right) dt d\Omega = \Delta t \frac{R}{M_v} \int \theta \ln\left(\frac{p_v}{p_{v0}}\right) d\Omega \quad (\text{C.233}) \end{aligned}$$

$$= \Delta t \frac{R}{M_v} \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \int_x \theta \ln\left(\frac{p_v}{p_{v0}}\right) r dr = \Delta t \frac{R}{M_v} (2\pi L_z) m(K) \left\{ \theta \ln\left(\frac{p_v}{p_{v0}}\right) \right\} \Big|_K^n \quad (\text{C.234})$$

$$= \Delta t \frac{R}{M_v} (2\pi L_z) m(K) \left\{ \theta \right\} \Big|_K^n \left\{ \ln\left(\frac{p_v}{p_{v0}}\right) \right\} \Big|_K^n = \Delta t \frac{R}{M_v} (2\pi L_z) m(K) \left\{ \theta \right\} \Big|_K^n \ln\left(\frac{\{p_v\}_K^n}{\{p_v\}_K^{n-1}}\right) \quad (\text{C.235})$$

$$\begin{aligned} & \bullet \int_{\Omega_t} \int \left\{ \frac{p_w - p_{w0}}{\rho_w} + \frac{l_0}{\theta_0}(\theta - \theta_0) + (C_{pl} - C_{pv})\left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right] \right\} dt d\Omega \\ &= \Delta t \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \int_x \left\{ \frac{p_w - p_{w0}}{\rho_w} + \frac{l_0}{\theta_0}(\theta - \theta_0) + (C_{pl} - C_{pv})\left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right] \right\} r dr \quad (\text{C.236}) \end{aligned}$$

$$= \Delta t (2\pi L_z) m(K) \left\{ \frac{p_w - p_{w0}}{\rho_w} + \frac{l_0}{\theta_0}(\theta - \theta_0) + (C_{pl} - C_{pv})\left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right] \right\} \Big|_K^n \quad (\text{C.237})$$

$$= \Delta t (2\pi L_z) m(K) \left\{ \left\{ \frac{p_w - p_{w0}}{\rho_w} \right\} \Big|_K^n + \left\{ \frac{l_0}{\theta_0}(\theta - \theta_0) \right\} \Big|_K^n + \left\{ (C_{pl} - C_{pv})\left[\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right] \right\} \Big|_K^n \right\} \quad (\text{C.238})$$

$$= \Delta t (2\pi L_z) m(K) \left\{ \frac{\{p_w\}_K^n - \{p_w\}_K^{n-1}}{\rho_w} + l_0 \frac{\{\theta\}_K^n - \{\theta\}_K^{n-1}}{\{\theta\}_K^{n-1}} + (C_{pl} - C_{pv}) \left[\{\theta\}_K^n - \{\theta\}_K^{n-1} - \{\theta\}_K^n \ln\left(\frac{\{\theta\}_K^n}{\{\theta\}_K^{n-1}}\right) \right] \right\} \quad (\text{C.239})$$

Then the liquid-vapor balance equation for the non-isothermal model reduces to:

$$\frac{R}{M_v} \left\{ \theta \right\} \Big|_K^n \ln\left(\frac{\{p_v\}_K^n}{\{p_v\}_K^{n-1}}\right) = \frac{\{p_w\}_K^n - \{p_w\}_K^{n-1}}{\rho_w} + l_0 \frac{\{\theta\}_K^n - \{\theta\}_K^{n-1}}{\{\theta\}_K^{n-1}} + (C_{pl} - C_{pv}) \left[\{\theta\}_K^n - \{\theta\}_K^{n-1} - \{\theta\}_K^n \ln\left(\frac{\{\theta\}_K^n}{\{\theta\}_K^{n-1}}\right) \right] \quad (\text{C.240})$$

Entropy Balance:

$$\phi \left[\frac{\partial}{\partial t} \left(S_s + \sum_{i=w,v,a} m_i s_i \right) + \sum_{i=w,v,a} s_i w_i \right] = -\text{div}(q) \quad (\text{C.241})$$

First we proceed to integrate over the volume K from (t, t^{n+1})

$$\iint_{\Omega_t} \phi \left[\frac{\partial}{\partial t} \left(S_s + \sum_{i=w,v,a} m_i s_i \right) + \sum_{i=w,v,a} s_i w_i \right] dt d\Omega = \iint_{\Omega_t} [-\text{div}(q)] dt d\Omega \quad (\text{C.242})$$

Developing each term individually:

$$\begin{aligned} & \bullet \iint_{\Omega_t} \phi \left[\frac{\partial}{\partial t} \left(S_s + \sum_{i=w,v,a} m_i s_i \right) + \sum_{i=w,v,a} s_i w_i \right] dt d\Omega \\ &= \iint_{\Omega_t} \phi \frac{\partial}{\partial t} \left(S_s + \sum_{i=w,v,a} m_i s_i \right) dt d\Omega + \iint_{\Omega_t} \phi \sum_{i=w,v,a} s_i w_i dt d\Omega \end{aligned} \quad (\text{C.243})$$

$$= \phi \int_{\Omega} \left\{ \left(S_s + \sum_{i=w,v,a} m_i s_i \right)^{n+1} - \left(S_s + \sum_{i=w,v,a} m_i s_i \right)^n \right\} d\Omega + \Delta t \int_{\Omega} \left(\sum_{i=w,v,a} s_i w_i \right) d\Omega \quad (\text{C.244})$$

$$= \phi \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \int_x \left\{ \left(S_s + \sum_{i=w,v,a} m_i s_i \right)^{n+1} - \left(S_s + \sum_{i=w,v,a} m_i s_i \right)^n \right\} r dr + \phi \Delta t \int_{\beta=0}^{2\pi} d\beta \int_{z=0}^{L_z} dz \int_x \left(\sum_{i=w,v,a} s_i w_i \right) r dr \quad (\text{C.245})$$

$$= \phi (2\pi L_z) m(K) \left\{ \left[S_s + \sum_{i=w,v,a} m_i s_i \right]_K^{n+1} - \left[S_s + \sum_{i=w,v,a} m_i s_i \right]_K^n + \Delta t \left[\sum_{i=w,v,a} s_i w_i \right]_K^n \right\} \quad (\text{C.246})$$

$$= \phi (2\pi L_z) m(K) \left\{ \{S_s\}_K^{n+1} - \{S_s\}_K^n + \left[\sum_{i=w,v,a} m_i s_i \right]_K^{n+1} - \left[\sum_{i=w,v,a} m_i s_i \right]_K^n - \Delta t \left[\sum_{i=w,v,a} s_i w_i \right]_K^n \right\} \quad (\text{C.247})$$

$$\begin{aligned} &= \phi (2\pi L_z) m(K) \left\{ \left(\{S_s\}_K^{n+1} - \{S_s\}_K^n \right) + \left(\{m_w s_w\}_K^{n+1} - \{m_w s_w\}_K^n \right) + \left(\{m_v s_v\}_K^{n+1} - \{m_v s_v\}_K^n \right) - \left(\{m_a s_a\}_K^{n+1} - \{m_a s_a\}_K^n \right) \right. \\ & \quad \left. - \Delta t \left(\{s_w w_w\}_K^n + \{s_v w_v\}_K^n + \{s_a w_a\}_K^n \right) \right\} \end{aligned} \quad (\text{C.248})$$

$$\begin{aligned} &= \phi (2\pi L_z) m(K) \left\{ \left(\{S_s\}_K^{n+1} - \{S_s\}_K^n \right) + \left(\{m_w\}_K^{n+1} \{s_w\}_K^{n+1} - \{m_w\}_K^n \{s_w\}_K^n \right) \right. \\ & \quad + \left(\{m_v\}_K^{n+1} \{s_v\}_K^{n+1} - \{m_v\}_K^n \{s_v\}_K^n \right) - \left(\{m_a\}_K^{n+1} \{s_a\}_K^{n+1} - \{m_a\}_K^n \{s_a\}_K^n \right) \\ & \quad \left. - \Delta t \left(\{w_w\}_K^n \{s_w\}_K^n + \{w_v\}_K^n \{s_v\}_K^n + \{w_a\}_K^n \{s_a\}_K^n \right) \right\} \end{aligned} \quad (\text{C.249})$$

The terms involved in this last expression are the same as those derived for the cartesian coordinates one. The only changes are taken into account by the $m(K)$ term.

$$\bullet \iint_{\Omega_t} [-div(q)] dt d\Omega$$

$$= \Delta t \int_{\Omega} [-div(q)] d\Omega = -\Delta t \int_{\partial K} (q \cdot n) d\gamma = -\Delta t \sum_{L \in N(K)_{e_{K,L}}} \int (q \cdot n) d\gamma \quad (C.250)$$

$$= \Delta t \sum_{L \in N(K)_{e_{K,L}}} \int [\mathfrak{K} grad(\theta) \cdot n] d\gamma = \Delta t \mathfrak{K} \sum_{L \in N(K)_{e_{K,L}}} \int \left[\frac{\partial \theta}{\partial r} e_r \cdot e_r \right] d\gamma \quad (C.251)$$

$$\Delta t \mathfrak{K} \sum_{L \in N(K)_{e_{K,L}}} \int \left(\frac{\partial \theta}{\partial r} \right) r d\beta dz = \Delta t \mathfrak{K} (2\pi L_z)(r) m(K) \sum_{L \in N(K)} \left(\frac{\{\theta\}_{K+1}^n - \{\theta\}_K^n}{d_r} \right) \quad (C.252)$$

The previous terms allow us to write the discretized version of the entropy balance equation in cartesian coordinates for the non-isothermal model including dehydration effects:

$$\begin{aligned} & \phi \left\{ \left(\{S_s\}_K^{n+1} - \{S_s\}_K^n \right) + \left(\{m_w\}_K^{n+1} \{s_w\}_K^{n+1} - \{m_w\}_K^n \{s_w\}_K^n \right) \right. \\ & \quad + \left(\{m_v\}_K^{n+1} \{s_v\}_K^{n+1} - \{m_v\}_K^n \{s_v\}_K^n \right) - \left(\{m_a\}_K^{n+1} \{s_a\}_K^{n+1} - \{m_a\}_K^n \{s_a\}_K^n \right) \\ & \quad \left. - \Delta t \left(\{w_w\}_K^n \{s_w\}_K^n + \{w_v\}_K^n \{s_v\}_K^n + \{w_a\}_K^n \{s_a\}_K^n \right) \right\} \\ & = \Delta t \mathfrak{K} \sum_{L \in N(K)} \left(\frac{r}{d_r} \right) (\{\theta\}_{K+1}^n - \{\theta\}_K^n) \quad (C.253) \end{aligned}$$

Summary of the Discretized Equations for the One-Dimension Non-Isothermal Model in Cylindrical Coordinates

Liquid water conservation:

$$\begin{aligned}
 m(K) \frac{\{m_w\}_K^{n+1} - \{m_w\}_K^n}{\Delta t} & - \left\{ \rho_w \cdot \frac{k}{\eta_w} \sum_{L \in N(K)} \left(\frac{r}{dr} \right) \left[\frac{\{k_{ri}(S_w)\}_K^n + \{k_{ri}(S_w)\}_L^n}{2} \right] \left[\{p_w\}_L^n - \{p_w\}_K^n \right] \right\} \\
 & = -m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1} + \frac{m_l^b m(K)}{\Delta t} \left(\frac{l/\theta_0}{km_{s_0}} \right) [\{\theta\}_K^{n+1} - \{\theta\}_K^n]
 \end{aligned} \tag{C.254}$$

Water vapor conservation:

$$\begin{aligned}
 m(K) \left[\frac{\{m_v\}_K^{n+1} - \{m_v\}_K^n}{\Delta t} \right] & - \frac{M_v}{R} \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left(\frac{r}{dr} \right) \left[\frac{k}{\eta_g} \left(\frac{\{p_v\}_K^n + \{p_v\}_L^n}{2} \right) \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) (\{p_g\}_{K+1}^n - \{p_g\}_K^n) \right. \\
 & \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_v\}_L^n}{\{p_g\}_L^n} - \frac{\{p_v\}_K^n}{\{p_g\}_K^n} \right) \right] = -m(K) \{\mu_{l \rightarrow g}^w\}_K^{n+1}
 \end{aligned} \tag{C.255}$$

Dry air conservation:

$$\begin{aligned}
 m(K) \left[\frac{\{m_a\}_K^{n+1} - \{m_a\}_K^n}{\Delta t} \right] & - \frac{M_a}{R} \sum_{L \in N(K)} \left(\frac{2}{\{\theta\}_K^n + \{\theta\}_L^n} \right) \left(\frac{r}{dr} \right) \left[\frac{k}{\eta_g} \cdot \left(\frac{\{p_a\}_K^n + \{p_a\}_L^n}{2} \right) \cdot \left(\frac{\{k_{rg}(S_w)\}_K^n + \{k_{rg}(S_w)\}_L^n}{2} \right) \cdot (\{p_g\}_{K+1}^n - \{p_g\}_K^n) \right. \\
 & \left. + d_{va} \left(\frac{f(\phi, \{S_w\}_K^n) + f(\phi, \{S_w\}_L^n)}{2} \right) \left(\frac{\{p_a\}_L^n}{\{p_g\}_L^n} - \frac{\{p_a\}_K^n}{\{p_g\}_K^n} \right) \right] = 0
 \end{aligned} \tag{C.256}$$

Liquid-vapor balance

$$\frac{R}{M_v} \{\theta\}_K^n \ln \left(\frac{\{p_v\}_K^n}{\{p_v\}_K^{n-1}} \right) = \frac{\{p_w\}_K^n - \{p_w\}_K^{n-1}}{\rho_w} + l_0 \frac{\{\theta\}_K^n - \{\theta\}_K^{n-1}}{\{\theta\}_K^{n-1}} + (C_{pl} - C_{pv}) \left[\{\theta\}_K^n - \{\theta\}_K^{n-1} - \{\theta\}_K^n \ln \left(\frac{\{\theta\}_K^n}{\{\theta\}_K^{n-1}} \right) \right] \quad (\text{C.257})$$

Entropy balance:

$$\begin{aligned} \phi \left\{ \left(\{S_s\}_K^{n+1} - \{S_s\}_K^n \right) + \left(\{m_w\}_K^{n+1} \{s_w\}_K^{n+1} - \{m_w\}_K^n \{s_w\}_K^n \right) \right. \\ \left. + \left(\{m_v\}_K^{n+1} \{s_v\}_K^{n+1} - \{m_v\}_K^n \{s_v\}_K^n \right) - \left(\{m_a\}_K^{n+1} \{s_a\}_K^{n+1} - \{m_a\}_K^n \{s_a\}_K^n \right) \right. \\ \left. - \Delta t \left(\{w_w\}_K^n \{s_w\}_K^n + \{w_v\}_K^n \{s_v\}_K^n + \{w_a\}_K^n \{s_a\}_K^n \right) \right\} \\ = \Delta t \mathfrak{K} \sum_{L \in N(K)} \left(\frac{r}{d_r} \right) (\{\theta\}_{K+1}^n - \{\theta\}_K^n) \quad (\text{C.258}) \end{aligned}$$

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References

- [1] Ulm, F.-J., Coussy, O., and Bazant, Z.P., (1999). "The 'Chunnel' Fire. I: Chemoplastic Softening in Rapidly Heated concrete." *J.Engrg.Mech.*, ASCE, 125(3), 272-282.
- [2] Anderber, Y. (1997). "Spalling Phenomena of HPC and OC." Proc., Int. Workshop on Fire Performance of High Strength Concrete, NIST Spec. Publ. 919, L.T. Phan, N.J. Carino, D.Duthinh, and E. Garboczi, eds., National Institute of Standards and Technology, Gaithersburg, Md., 69-73.
- [3] Ulm, F.-J., Acker, P., and Levy, M., (1999). "The 'Chunnel' Fire. II: Analysis of Concrete Damage." *J.Engrg.Mech.*, ASCE, 125(3), 283-289.
- [4] Mainguy, Marc (1999). *Modeles de Diffusion non-Lineaires en Milieux Poreux. Applications a la Dissolution et au Sechage des Materiaux Cimentaires.* These de Doctorat. Ecole Nationale des Ponts et Chaussees, 1999 (in French).
- [5] Bazant, Z. P. and Thonguthai, W. (1978). 'Pore Pressures and drying of concrete at high temperature.' *J. Engrg.Mech.Div.*, ASCE 104, 1058-1080.
errata: *J.Engrg.Mech.Div.*, ASCE 105
- [6] Gawin, D., Majorana, C.E., and Schrefler, B.A. (1999). "Numerical Analysis of Hygro-Thermal Behaviour and Damage of Concrete at High Temperature". *Mech.Cohes.-Frict.Mater.* 4, 37-74.
- [7] Bazant, Z. P. and Kaplan, M. F. (1996). *Concrete at high Temperatures: Material Properties and Mathematical Models*, Longman Group Limited, England.
- [8] van Genuchten, M.Th. (1980). "A Closed -form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils". *Soil Science Society of America Journal*, 44:892-898.
- [9] Savage, B.M. and Janssen, D.J. (1997). "Soil Physics Principles Validated for Use in Predicting Unsaturated Moisture Movement in Portland Cement Concrete". *ACI Materials Journal*, 94(1):63-70.
- [10] Parker, J.C., Lenhard, R.J., and Kuppusamy, T. (1987). "A Parametric Model for Constitutive Properties Governing Multiphase Flow in Porous Media". *Water Res. Res.*, 23(4):618-624.
- [11] Luckner, L., van Genuchten, M.Th., and Nielsen, D.R. (1989). "A Consistent Set of Parametric Models for the Two-phase-flow of Immiscible Fluids in the Subsurface". *Water Res. Res.*, 25(10): 2187-2193.
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- [12] Heukamp, Franz-Hoyte (1999). *Modelisation Mecanique et Numerique du Sechage Non IsoTherme des Materiaux Tres peu Permeables a Base de Ciment*. Project de fin d'etudes. Ecole Nationale des Ponts et Chaussees (in French)
- [13] Fasseu, P. (1997). "Eurotunnel-Fire. Analysis of the effect of the fire on the concrete quality.: Res.Rep. No. 96.6002532 (April 1997), Laboratoire Regional des Ponts et Chaussees de Lille, Lille, France (in French).
- [14] Ulm, F.-J. and Heukamp, F.H. (2000). "Review of Mass and Heat Transport Under High Temperatures". Internal Note, MIT.
- [15] Ulm, F.-J. (2000). *Durability Mechanics - Class Notes 1.570*. MIT.
- [16] Ulm, F.-J. (1999). *Mechanics of Materials - Class Notes 1.57*. MIT.
- [17] Kotz., J.C., and Treichel, P. Jr. (1996). *Chemistry and Chemical Reactivity*. Saunders College Publishing. Third Edition.
- [18] American Society of Mechanical Engineers (2000). *ASME Steam Tables for Industrial Use*, ASME Press, New York, N.Y.
- [19] Nilson, Arthur H. (1997). *Design of Concrete Structures*, WCB/McGraw-Hill, USA.