

Building Technology and Urban Systems Lawrence Berkeley National Laboratory

THERM 8 Technical Documentation – New Hygrothermal Modeling Functionality

D. Simon Vidanovic
D. Charlie Curcija
Mikael Salonvaara, Oak Ridge National Lab
Simon Pallin, Oak Ridge National Lab

11/18/2020



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Acknowledgements

This work was supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Building Technologies Program, of the U.S. Department of Energy, under Contract No. DE-AC02-05CH11231. And the California Energy Commission through its Electric Program Investment Charge (EPIC) Program on behalf of the citizens of California and

The authors thank these supporters: Amir Roth, U.S. Department of Energy and Karen Perrin, and Virginia Lew, California Energy Commission.

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D. Simon Vidanovic D. Charlie Curcija Mikael Salonvaara, Oak Ridge National Lab Simon Pallin, Oak Ridge National Lab

Ernest Orlando Lawrence Berkeley National Laboratory 1 Cyclotron Road, MS 90R4000 Berkeley CA 94720-8136

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Acronyms and Abbreviations

FEM	Finite Element Method
GUI	Graphical User's Interface

Nomenclature

Variable	Description	Units
а	Equation coefficients	-
Α	Area	m^2
С	Specific heat	$J/(kg \cdot K)$
D	Liquid transport coefficient	m^2 / s for l and kg / $(m^2 \cdot s)$ for φ
Ε	Diffusion coefficient for stagnant air	m^2/s
ġ	Mass flux density	$kg/(m^2 \cdot s)$
G	Gravity acceleration	m/s^2
G	Total discharge	m^3/s
h	Specific enthalpy	J / kg
Н	Enthalpy of the system	J
Ι	Transfer rate between states	$kg/(m^3 \cdot s)$
k	Intrinsic permeability of the medium	m^2
L	Length	m
М	Mass	kg
Р	Pressure	<i>Pa</i> or $kg/(m \cdot s^2)$
\vec{q}	Heat flux density	W/m^3 or $J/(m^2 \cdot s)$
Q	Heat source	$J/(m^3 \cdot s)$
\mathcal{Q}_p	Energy available for a potential phase change	J/m^3
R	Roughness factor	-
RH	Relative Humidity	-
S	Water source	$kg/(m^3 \cdot s)$
t	Time	S
Т	Temperature	K or $^{\circ}C$
v	Velocity	m/s
V	Volume	<i>m</i> ³
W	View factor	-
x	Humidity ratio	kg / kg
Ζ	Altitude	m

Greek-letter notation

Variable	Explanation	Units
α	Heat transfer coefficient	$W/(m^2 \cdot K)$ or $J/(m^2 \cdot K \cdot s)$
β	Water vapor transfer coefficient	<i>m / s</i>
γ	Material mass over given domain	kg/m^3
δ	Water vapor permeability	m^2/s
ε	emissivity	-
η	Dynamic viscosity	$Pa \cdot s$
λ	Thermal conductivity	$W/(m\cdot K)$ or $J/(m\cdot K\cdot s)$
μ	Water vapor transfer resistance factor	-
ξ	Sorption curve slope	kg/m^3 · –
ρ	Density	kg/m^3
σ	Stefan-Boltzmann constant (5.67·10 ⁻⁸ W/(m ² ·K ⁴)	$J/(m^2\cdot K^4\cdot s)$
ϕ	Porosity	-
φ	Relative humidity	-
К	Tilt angle	-
ω	Specific volume	m^3 / kg

Subscripts and other Symbols

Subscript	Description
adv	Advection
air	Moist air
atm	Atmospheric
boundary	Boundary
С	Celsius
conv	convective
d	Dry
diff	Diffusion
den	Density
eq	equivalent
ex	exterior
f	Forced
gnd	ground
i	Water (ice)
il	Ice to liquid
in	interior
k	State
l	Water (liquid)
gl	Liquid to gas
lw	Long wave

n	Direction	
р	Pore	
sat	saturation	
sky	sky	
surf	Surface	
SW	Short wave	
tot	total	
v	Vapor	
vent	Ventilation	
W	Water total	
w10	Reference at 10 m	
φ	Relative Humidity	
φs	Suction	
φr	Redistribution	
ð	Derivative	
∇	Nabla operator	

1. Introduction and Background

The DOE's and nation's goals for ZNE buildings, in order to mitigate the negative effects of accelerated global climate change, are leading to more and more buildings being built with highly insulated and very tight envelopes. By failing to account for the moisture characteristics in the thermal envelope, designers and builders can introduce moisture-related problems that endanger the health and safety of building occupants as well as the durability of the building itself. It is imperative that we solve the problems of designing and constructing building envelopes that are correctly detailed for ensuring excellent thermal performance without introducing moisture problems. Damage due to moisture problems is one of the leading causes of lawsuits in construction, and having the best tools for modeling moisture and thermal characteristics will help ensure that United States can meet its energy, comfort, health and durability goals in buildings. Because moisture research by itself doesn't save energy, it is rarely supported by energy agencies. But the development of an integrated thermal and moisture tool will make sure that we design for energy efficiency while avoiding collateral problems in our buildings.

Analysis of moisture migration through building structures is primarily done by engineers using 1-D simplified models (e.g., WUFI – software tool for analyzing moisture migration through the building structure). These models ignore or make crude assumptions about thermal bridges and non-homogeneities in building construction. Considering that such elements are primary pathways and causes for condensation and moisture buildups, it is important to properly consider them in thermal/moisture analysis. Thermal analysis of building structures, including thermal bridges, is often done with the software program THERM. The LBNL team developed THERM in the early 1990s in response to the need for a user-friendly 2-D heat transfer tool for the analysis of windows and thermal bridges in building envelopes. THERM is a freely available computer program in wide use, with 20,000 unique users downloading the program annually, and over 500,000 program launches. THERM is used for calculating two-dimensional (2-D) heat transfer in building components such as windows, walls, foundations, roofs, and doors, as well as appliances and other products where thermal bridges are of concern. THERM is based on the finite element numerical method (FEM) and incorporates sophisticated automated meshing and error estimation for rapid model generation that ensures accurate results. THERM is used by building component manufacturers, engineers, educators, students, architects, and others, but most prominently it is used as an official tool in NFRC (National Fenestration Rating Council). It is also used by PHIUS (Passive House Institute US) and will soon be used by AERC (Window Attachment Energy Rating Council). In addition to THERM, the LBNL team has developed several other software tools, widely used by industry, both nationally and internationally (i.e., WINDOW, OPTICS, RESFEN, COMFEN, RADIANCE) over the past 30+ years.

2. Theoretical Model

This chapter sets the theoretical background for the moisture and heat transfer model in porous media. Some general equations (laws) that are used as drivers for developing certain models are given in the Appendixes so it is easier to understand the limitations for which models are derived. The final result is a finite element model that will be able to calculate mass and temperature distribution within a given domain and within a given time.

The model calculates water, moisture and air transfer through the model along with the calculation of temperature distribution. Because water and air distribution depend on temperature and vice versa, the temperature field will depend on the water and air content, and thus these two cannot be observed and calculated separately. In addition, water content can change its phase during the process, which makes the model even harder to calculate. In order to perform calculations of such a complex physical model, the calculation must be simplified into several smaller models that will be calculated iteratively (see Figure 1) during each timestep.

The first model to be solved is <u>Air Pressure Distribution</u> which is a very important driver for water distribution and thus affects everything else in the domain. During the air pressure calculation, it is assumed that the mass of water, and the temperature of the domain, are not changing. After calculating air pressure within the domain, the next step is to calculate <u>Mass Distribution (Transfer)</u>. Again, in this step it is assumed that pressure and temperatures remain constant. Finally, the last step is to calculate <u>Temperature Distribution</u>, under the constant mass and pressure field. The newly calculated temperature field results in the amount of heat flux, and therefore allows the calculation of <u>Phase Change</u>. Since the re-calculated within iteration loops until the convergence criteria has been achieved (Figure 1).



Figure 1. Steps in Solving Coupled Heat, Air and Moisture Transport

Note: Convergence must be satisfied over all three fields (pressure, mass and temperature) before proceeding to the next timestep.

2.1 Coupled Heat, Air and Moisture Transport (HAM)

2.1.1 Heat Transfer (Energy) Equations

The change in enthalpy depends on the conductive heat transport, the mass transport of water and the air and enthalpy transport by water vapor transport as well as potential phase changes.

2.1.1.1 Conduction Heat Transfer

The heat flux density due to conduction can be described using Fourier's law, as seen in Equation (6.9) and (6.10).

$$\vec{q_c} = -\left[\left(k_x \frac{\partial T}{\partial x}\right) + \left(k_y \frac{\partial T}{\partial y}\right)\right]$$
(2.1)

Where

 \vec{q}_c = heat flux density [W/m²]

$$k =$$
 Thermal conductivity of material [W/(m·K)]

Since materials typically contains water, the resulting thermal conductivity is needed. One option is to calculate an equivalent thermal conductivity based on dry material thermal conductivity and water content. Values obtained this way are usually not precise and that is why the thermal conductivity of material with different water content is provided through a set of measurements.

Using Equation (6.10), the temperature can be solved as:

$$\rho_{eq} \cdot C_{eq} \frac{\partial T}{\partial t} = \\ = -\left[\frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right)\right] + C_l\left(g_{l,x} \cdot \frac{\partial T}{\partial x} + g_{l,y} \cdot \frac{\partial T}{\partial y}\right) \\ + C_v\left(g_{v,diff,x} \cdot \frac{\partial T}{\partial x} + g_{v,diff,y} \cdot \frac{\partial T}{\partial y}\right) + h_{lg}\left(\frac{\partial g_{v,x}}{\partial x} + \frac{\partial g_{v,y}}{\partial y}\right) + Q$$

$$(2.2)$$

Where

 h_{lg} = Enthalpy of Vaporization [J/kg]

 C_l = Heat capacity of water [J/K]

 C_v = Heat capacity of water vapor [J/K]

Q = Additional sensible heat source [J/(m³·s)]

NOTE: Reference point is zero Celsius.

Tomporatura	Water Liquid		lce	
Temperature	Conductivity	Density	Conductivity	Density
[C]	[W/(mK)]	[kg/dm³]	[W/(mK)]	[kg/dm³]
100	0.68	0.958		
90	0.68	0.965		
80	0.67	0.972		
70	0.67	0.978		
60	0.66	0.983		
50	0.65	0.988		
40	0.63	0.992		
30	0.62	0.996		
20	0.61	0.998		
10	0.59	1.000		
5	0.58	1.000		
0	0.57	1.000	2.050	916.2
-5			2.027	917.5
-10			2.000	918.9
-15			1.972	919.4
-20			1.943	919.4
-25			1.913	919.6
-30			1.882	920.0
-35			1.850	920.4
-40			1.818	920.8
-45			1.785	921.2
-50			1.751	921.6

Table 1. Thermal Conductivity of water liquid and ice, as a function of temperature.

2.1.1.2 Heat Transfer Summary

Heat transfer may also occur through advection. The total energy equation is defined as:

$$\rho_{eq} \cdot C_{eq} \frac{\partial T}{\partial t} + S \cdot h_{il} \cdot I_{il} =
= \frac{\partial}{\partial x} \left(k \cdot \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \cdot \frac{\partial T}{\partial y} \right) - h_{lg} \left(\frac{\partial \vec{g}_{v}}{\partial x} + \frac{\partial \vec{g}_{v}}{\partial y} \right)$$

$$-C_{l} \left(\vec{g}_{l,x} \cdot \frac{\partial T}{\partial x} + \vec{g}_{l,y} \cdot \frac{\partial T}{\partial y} \right) - C_{v} \left(\vec{g}_{v,x} \cdot \frac{\partial T}{\partial x} + \vec{g}_{v,y} \cdot \frac{\partial T}{\partial y} \right) - C_{air,d} \left(\vec{g}_{air,x} \cdot \frac{\partial T}{\partial x} + \vec{g}_{air,y} \cdot \frac{\partial T}{\partial y} \right) + Q$$

$$(2.3)$$

With

S = 0 for non-freezing conditions and 1 for freezing conditions

 H_{il} = Additional heat capacity due to heat of fusion [J/(m³·s)]

 $C_{air,d}$ = Heat capacity of dry air [J/K]

The above energy equation assumes

 ρ_{eq} = An equivalent density of all material components [kg/m³]

 C_{ea} = An equivalent specific heat of all material components [J/(kg·K)]

 ρ_{air} = Density of moist air, see Equation (2.52) [kg/m³]

 C_{air} = Specific heat of moist air [J/(kg·K)]

Bulk material dry density, as it is measured including pores is:

$$\rho_{bulk} = (1 - \phi) \cdot \rho_d + \phi \cdot \rho_{air}$$

 ρ_d = It is material density as it is measured without pores [kg/m³]

Equivalent density of moist material can be then calculated as:

 $\rho_{eq} = \rho_{bulk} + \phi_{ice} \cdot \rho_{ice} + \phi_l \cdot \rho_l - (\phi - \phi_{air}) \cdot \rho_{air}$

Since air influence is very small, approximated equation is to calculate the equivalent density of the material:

$$\rho_{eq} = \rho_{bulk} + \phi_{ice} \cdot \rho_{ice} + \phi_l \cdot \rho_l \tag{2.4}$$

The same approach can be used for equivalent capacitance:

$$C_{eq} = C_{bulk} + \phi_{ice} \cdot C_{ice} + \phi_l \cdot C_l \tag{2.5}$$

The moist air heat capacity is found using a relation between the dry air and water vapor capacities respectively.

$$C_{air} = (1 - x) \cdot C_{air,d} + x \cdot C_g \tag{2.6}$$

The humidity ratio, x, is given in Equation (2.46).

2.1.2 Mass Transfer (Moisture)

For the mass balance equation (6.19) the material must take into consideration phase change. For a given phase k (vapor, liquid or solid), a transient mass balance on the liquid/vapor/ice yields:

$$\frac{\partial \boldsymbol{M}_{k}}{\partial t} - \boldsymbol{\mathcal{G}}_{k} = -\nabla \left(\boldsymbol{M}_{k} \cdot \vec{\boldsymbol{v}}\right) + \boldsymbol{S}_{k}$$

Where:

M_k = Mass of water in phase state [kg]

 \mathcal{T}_k = Rate of water mass that is transforming into state k [kg/s]

$$\vec{v}$$
 = Velocity [m/s]

$$S_k$$
 = External source of water (state k) [kg/s]

t = time [s]

If we introduce content of mass per volume, the equation becomes:

$$\frac{\partial \gamma_{k}}{\partial t} + \nabla \left(\gamma_{k} \cdot \vec{v} \right) = I_{k} + S_{k}$$

$$\frac{\partial \gamma_{k}}{\partial t} + \nabla \vec{g}_{k} = I_{k} + S_{k}$$
Where:
(2.7)

Where:

 $\gamma_k = \frac{M_k}{V}$ = Moisture/water/ice content in given domain [kg/m³] $I_k = \frac{\mathcal{J}_k}{V}$ = transfer of water from the phase k due to phase change [kg/(m³·s)] $V = \text{Domain volume } [\text{m}^3]$ $S_{k,vol}$ = External volumetric source of water (state k) [kg/(m³·s)] g_k = flux density of water of state k [kg/(m²·s)]

In subsequent derivations, the subscript k is replaced with v for vapor, l for liquid water and i for ice. For vapor, the following equation results:

$$\frac{\partial \gamma_{v}}{\partial t} = -\left(\frac{\partial g_{v}}{\partial x} + \frac{\partial g_{v}}{\partial y}\right) + I_{v} + S_{v}$$
(2.8)

Where:

 g_v = water vapor flux [kg/(m²·s)]

 S_v = Water vapor source [kg/(m³·s)]

 I_v = Transfer from water liquid to water vapor phase [kg/(m³·s)]

For liquid water:

$$\frac{\partial \gamma_l}{\partial t} = -\left(\frac{\partial g_l}{\partial x} + \frac{\partial g_l}{\partial y}\right) + I_l + S_l$$

$$I_l = \frac{\partial \gamma_l}{\partial t} + \left(\frac{\partial g_l}{\partial x} + \frac{\partial g_l}{\partial y}\right)$$
(2.9)

Where

 g_l = water liquid flux [kg/(m²·s)]

S_l = Water liquid source [kg/(m³·s)]

 I_1 = Transfer from ice, or water vapor to liquid phase [kg/(m³·s)]

For ice, there is no ice flow, nor source:

$$\frac{\partial \gamma_i}{\partial t} = I_i \tag{2.10}$$

The summation of the above equations gives:

$$\frac{\partial (\gamma_{v} + \gamma_{l} + \gamma_{i})}{\partial t} = -\left(\frac{\partial (g_{v} + g_{l})}{\partial x} + \frac{\partial (g_{v} + g_{l})}{\partial y}\right) + \sum_{i,l,v} I_{k} + \sum_{l,v} S_{k}$$
(2.11)

However, the total change in phase state is equal to zero:

$$\sum_{i,l,\nu} I_k = 0 \tag{2.12}$$

Thus, the equation can be simplified to a total change in water content, γ_w , (independent of phase state).

$$\frac{\partial(\gamma_{v} + \gamma_{l} + \gamma_{i})}{\partial t} = \frac{\partial\gamma_{w}}{\partial t} = -\left(\frac{\partial(g_{v} + g_{l})}{\partial x} + \frac{\partial(g_{v} + g_{l})}{\partial y}\right) + S_{v} + S_{l}$$
(2.13)

The total change in water content, $\frac{\partial \gamma_w}{\partial t}$, can be found using the water liquid flux, g_l , the water

vapor flux, g_v , and the ice. A separation of the phase state is not required for the total water content.

Once, the total change in water content is found, the new water content can be found after a given time step, Δt , as:

$$\gamma_{w}(t + \Delta t) = \gamma_{w}(t) + \frac{\partial \gamma_{w}}{\partial t} \Delta t$$
(2.14)

There is a relation between the water content, γ_w , and the relative humidity, φ , that can be illustrated using a sorption isotherm (moisture storage function).



Figure 2. Water sorption isotherm of arbitrary porous material illustrating the relationship between water content and relative humidity.

Thus, using the sorption isotherm, the relative humidity is given.

$$\frac{\partial \gamma_{w}}{\partial t} = \frac{\partial \gamma_{w}}{\partial \varphi} \cdot \frac{\partial \varphi}{\partial t} = -\left(\frac{\partial (g_{v} + g_{l})}{\partial x} + \frac{\partial (g_{v} + g_{l})}{\partial y}\right) + S_{v} + S_{l}$$
(2.15)

Next, we need to express change of vapor and liquid water flow as functions of relative humidity.

Once the relative humidity is known, together with temperature, the water vapor content can be found using (2.49) and (2.50):

$$\gamma_{v} = \varphi \cdot \frac{e^{\left(77.345 + 0.0057 \cdot T - \frac{7235}{T}\right)}}{461.4 \cdot T^{9.2}} \cdot \phi_{air}$$

(2.16)

Where ϕ_{air} is given by (6.18).

Similarly, the water vapor pressure can be found using (2.48) and (2.51):

$$P_{v} = \varphi \cdot \frac{e^{\left(77.345 + 0.0057 \cdot T - \frac{7235}{T}\right)}}{T^{8.2}}$$

(2.17)

2.1.2.1 Water Liquid Transportation - Capillary Transport

If we have Darcy's velocity \vec{v} , the following relation is given:

$$v_l = \frac{g_l}{\gamma_l} \tag{2.18}$$

where

 V_l = Water liquid velocity [m/s]

 g_l = water liquid flux [kg/(m²·s)]

 γ_l = Liquid water content [kg/m³]

The water transport flux density is defined in accordance with (6.31) for Darcy's velocity:

$$v_{l} \cdot \gamma_{l} = \vec{g}_{l} = -\frac{\mathbf{k}_{l}\rho_{l}}{\eta_{l}} \left(\frac{\partial P_{p,x}}{\partial x} \cdot \vec{i} + \frac{\partial P_{p,y}}{\partial y} \cdot \vec{j} - \gamma_{l} \cdot G \cdot \vec{j} \right)$$

$$\vec{g}_{l} = -\frac{\mathbf{k}_{l}\rho_{l}}{\eta_{l}} \left(\nabla P_{p} - \gamma_{l} \cdot \vec{G} \right)$$
(2.19)

Where:

 \mathbf{k}_{l} = Water liquid permeability [m²]

 μ_l = Dynamic viscosity of liquid water [kg/m·s]

 P_p = Pore water pressure [Pa]

G = Gravity acceleration (9.81 m/s²) [m/s²]

The pore water pressure, P_l , will change with water content, γ_l . Therefore, the water liquid flux, can also be defined using a liquid transport coefficient in combination with the water content gradient (Fick's second law (6.23)):

$$\frac{\partial M}{\partial t} = D_f \nabla^2 M = D_f \left(\frac{\partial^2 M}{\partial x^2} + \frac{\partial^2 M}{\partial y^2} \right)$$

$$g_l = -D_l \nabla \gamma_l$$
(2.20)

where

 D_l = Liquid transport coefficient [m²/s]

Combining equations we find;

$$\nabla \gamma_l = -\frac{k_l \cdot \rho_l}{\eta_l \cdot D_l} \left(\nabla P_l - \gamma_l \cdot G \right)$$
(2.21)

Since gravitational forces only occur in vertical direction (y), and allows the water transport flux density to be defined as;

$$g_{l} = -D_{l} \left(\frac{\partial \gamma_{l}}{\partial x} \right) - D_{l} \left(\frac{\partial \gamma_{l}}{\partial y} - \frac{k_{l} \rho_{l}}{\eta_{l} D_{l}} \gamma_{l} \cdot G \right)$$
(2.22)

The resulting change in total water content due to liquid flow is given as:

$$\frac{\partial \gamma_{w}}{\partial t} = \frac{\partial g_{l}}{\partial x} + \frac{\partial g_{l}}{\partial y}$$

$$\frac{\partial \gamma_{w}}{\partial t} = -\frac{\partial}{\partial x} \left(D_{l} \left(\frac{\partial \gamma_{l}}{\partial x} \right) \right) - \frac{\partial}{\partial y} \left(D_{l} \left(\frac{\partial \gamma_{l}}{\partial y} - \frac{k_{l} \rho_{l}}{\eta_{l} D_{l}} \gamma_{l} \cdot G \right) \right)$$
(2.23)

The relationship between the liquid and relative humidity transport coefficients is;

$$D_{\varphi} = \xi \cdot D_l = \frac{\partial \gamma_w}{\partial \varphi} D_l \tag{2.24}$$

Where ξ is the slope of the sorption isotherm, also called moisture storage function.

The following equation is expressed as a function of relative humidity (ignoring the gravitational part):

$$\vec{g}_{l} = -D_{\varphi,x} \left(\frac{\partial \varphi}{\partial x} \right) - D_{\varphi,y} \left(\frac{\partial \varphi}{\partial y} \right)$$
(2.25)

where

 D_{φ} = Relative humidity transport coefficient [kg/(m·s)]

Thus, the resulting change in water liquid content is:

$$\frac{\partial \gamma_{w}}{\partial t} = \frac{\partial}{\partial x} \left(D_{\varphi, x} \left(\frac{\partial \varphi}{\partial x} \right) \right) + \frac{\partial}{\partial y} \left(D_{\varphi, y} \left(\frac{\partial \varphi}{\partial y} \right) \right)$$
(2.26)

On fully wetted surfaces, liquid water transport is dominated by larger capillaries, as they have lower flow resistance. When no new water is taken up, the redistribution of the water in the material is dominated by smaller capillaries with higher capillary tension. Therefore, two different transport coefficients, $D_{\omega s}$ and $D_{\omega r}$ are introduced according to Künzel (Künzel 1995).

$$D_{\varphi} = \begin{cases} D_{\varphi s} & \text{if (rain)} \\ D_{\varphi r} & \text{if (norain)} \end{cases}$$
(2.27)

 $D_{\varphi s}$, the liquid conduction coefficient for suction, is applied if liquid water from rain or source is present. $D_{\varphi r}$, the liquid conduction coefficient for redistribution, is applied if no liquid water from rain or source is present.

2.1.2.2 Water Vapor Transportation

Water vapor transportation can be divided into two components:

- Transportation from diffusion
- Transportation from advection (airflow)

Therefore, the change in vapor content is:

$$\frac{\partial \gamma_{\nu}}{\partial t} = \frac{\partial \gamma_{\nu,diff}}{\partial t} + \frac{\partial \gamma_{\nu,ad\nu}}{\partial t}$$
(2.28)

And the total vapor flux density \vec{g}_{v} is:

$$\vec{g}_{v} = \vec{g}_{v,diff} + \vec{g}_{v,adv}$$
(2.29)

2.1.2.2.1 Transportation from Diffusion

The vapor diffusion flux is derived from the first Fick law (see (6.22))

$$\vec{g}_{v,diff} = -\delta_x \frac{\partial \gamma_v}{\partial x} - \delta_y \frac{\partial \gamma_v}{\partial y}$$
(2.30)

Where:

 δ_n = Water vapor permeability in direction n [m²/s]

 γ_v = Humidity by volume [kg/m³]

The water vapor permeability δ_n in direction n, can be expressed as a quotient of the diffusion coefficient D for stagnant air and the resistance factor μ that describes the reduction of the diffusive flow in porous materials. This results is a diffusive flux according to the following equation :

$$\vec{g}_{\nu,diff} = -\frac{E}{\mu_x} \frac{\partial \gamma_\nu}{\partial x} - \frac{E}{\mu_y} \frac{\partial \gamma_\nu}{\partial y}$$
(2.31)

With

 $\vec{g}_{v,diff}$ = vapor diffusion flux [kg/(m²·s)]

E = diffusion coefficient for stagnant air [m²/s]

 μ = water vapor diffusion resistance factor [-]

Hagentoft (Hagentoft 2001) describes that the diffusion coefficient E for stagnant air can be calculated depending on the temperature with equation:

$$E = (22.2 + 0.14 \cdot T_c) \cdot 10^{-6} \tag{2.32}$$

With

 T_C = Temperature in Celsius [°C]

The resulting change in water content due to water vapor flow is given as:

$$\frac{\partial \gamma_{w}}{\partial t} = \frac{\partial}{\partial x} \left(\delta_{x} \frac{\partial \gamma_{v}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\delta_{y} \frac{\partial \gamma_{v}}{\partial y} \right)$$
(2.33)

Which can also be expressed as a function of relative humidity and the vapor diffusion resistance factor:

$$\frac{\partial \gamma_{w}}{\partial t} = \frac{\partial}{\partial x} \left(\frac{E}{\mu_{x}} \frac{\partial \varphi \gamma_{v_{sat}}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{E}{\mu_{y}} \frac{\partial \varphi \gamma_{v_{sat}}}{\partial y} \right)$$
(2.34)

where $\gamma_{v_{ref}}$ is found using (2.49).

2.1.2.2.2 Transportation from advection (airflow)

Using the air flow rate found in (2.54), the vapor flux density due to advection can be calculated with the following equation:

$$\vec{g}_{v,adv} = \vec{g}_{air} \cdot x \tag{2.35}$$

Where x is the humidity ratio given in Equation (2.46). The resulting change in water content due to advective vapor flow utilizing Equation (2.56) is:

$$\frac{\partial \gamma_{w}}{\partial t} = \frac{\partial}{\partial x} \left(\frac{k_{air,x} \cdot \varphi \gamma_{v_{sat}}}{\eta_{air}} \cdot \frac{\partial P_{air}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{k_{air,y} \cdot \varphi \gamma_{v_{sat}}}{\eta_{air}} \cdot \frac{\partial P_{air}}{\partial y} \right) - \frac{\partial}{\partial y} \left(\frac{k_{air,y} \cdot \varphi \gamma_{v_{sat}}}{\eta_{air}} \gamma_{air} G \right)$$
(2.36)

2.1.2.2.3 Water Vapor Transportation – Liquid Source

A water liquid source S_i may come from precipitation or water leakage. If this source exists, it will be added directly to the material.

There may also be a liquid source from air leakage (Section 2.1.4), if the dew-point temperature of the air is higher than that of the surface material. However, this phenomenon is accounted for in the overall equation for mass transfer.

2.1.2.3 Water Transfer Summary

There is a relationship between water content and relative humidity. In addition, there is also a phenomenon referred to as hysteresis. The hysteresis effect is illustrated in Figure 3 and is driven by whether the material is subject to dryer (desorption), or wetter (sorption) conditions.





Studies have shown that this phenomenon has, for most cases, insignificant effect on the water transportation (Zhang et al. 2016), and is thus neglected in the governing equations of mass transportation for this document.

The sorption isotherm illustrates how much moisture can be absorbed or released at any given temperature, due to both liquid and vapor transportation. In general, at a relative humidity below 50%, the main transportation mechanism is from the exchange of vapor. Once the pores inside the material are filled with water, more and more liquid transportation will occur, and this transportation mechanism will start to dominate. The hygroscopic range covers the interval of approximately 0 to 98% relative humidity. For a material to reach levels beyond the hygroscopic range, the material needs to be in direct contact with water.

Summarizing the total water transfer, but neglecting the gravitational effects yields the following equation:

$$\frac{\partial \gamma_{w}}{\partial \varphi} \frac{\partial \varphi}{\partial t} = \frac{\partial}{\partial x} \left(\frac{E}{\mu_{x}} \frac{\partial \varphi \gamma_{v_{sat}}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{E}{\mu_{y}} \frac{\partial \varphi \gamma_{v_{sat}}}{\partial y} \right) + \frac{\partial}{\partial y} \left(\frac{E}{\mu_{y}} \frac{\partial \varphi \gamma_{v_{sat}}}{\partial y} \right) + \frac{\partial}{\partial y} \left(\frac{k_{air,y} \cdot \varphi \gamma_{v_{sat}}}{\eta_{air}} \cdot \frac{\partial P_{air}}{\partial y} \right) + \frac{\partial}{\partial y} \left(\frac{k_{air,y} \cdot \varphi \gamma_{v_{sat}}}{\eta_{air}} \cdot \frac{\partial P_{air}}{\partial y} \right) + \frac{\partial}{\partial y} \left(D_{\varphi,y} \left(\frac{\partial \varphi}{\partial y} \right) \right) + S_{l} + S_{v}$$

$$(2.37)$$

Where γ_l can be calculated from sorption curves as:

$$\gamma_l = \gamma_w \left(\frac{\phi_l}{\phi_l + \phi_i} \right) \tag{2.38}$$

2.1.3 Air flow through Porous Materials

Air flow, or mass flow of air over time, is caused by an air pressure difference, and air mass body forces such as gravity. For air flow through materials, the air permeability of the material will affect the resulting air flow. Using Darcy's law, as presented in Appendix C, Section 6.7.2, the air flow rate can be defined as

$$\frac{\partial V_{air}}{\partial t} = \mathbf{\mathcal{G}}_{air} = -\frac{k_{air} \cdot A}{\eta_{air}} \cdot \frac{\partial P}{\partial L}$$
(2.39)

Where:

 V_{air} = Air volume [m³]

t = Time [s]

 \boldsymbol{G}_{air} = Total air discharge [m³/s]

 k_{air} = Intrinsic permeability of the medium [m²]

A = Cross-sectional area to flow [m²]

P = Total pressure [Pa]

 η_{air} = Dynamic viscosity of air [Pa·s]

In general, the air pressure gradient is induced by a combination of conditions, such as wind, buoyance, and ventilation forces. Wind is a surface phenomenon and will be further discussed in Section 2.1.7 for boundary conditions. Buoyance forces cause an air pressure gradient, induced by a density differential. Changes in density mainly exist due to variations in temperature and moisture conditions.

The resulting pressure gradient is defined as:

$$\frac{\partial P}{\partial L} = \frac{\partial P_{air}}{\partial L} + \frac{\partial P_{\rho}}{\partial L} + \frac{\partial P_{vent}}{\partial L}$$
(2.40)

Where:

 P_{air} = Forced air pressure differences, such as wind loads [Pa] P_{air} = Cravitational air pressure gradient by body (density) forces [Pa]

$$\rho = Gravitational all pressure gradient by body (density) forces [Fa]$$

 P_{vent} = Mechanical air pressure differences induced by ventilation system [Pa]

Assuming a balanced air ventilation system, and combining Equation (2.39) and (2.40), the air flow is defined as:

$$\boldsymbol{\mathcal{G}}_{air} = -\frac{k_{air} \cdot A}{\eta_{air}} \cdot \left(\frac{\Delta P_{air}}{\partial L} + \frac{\Delta P_{\rho}}{\partial L}\right)$$
(2.41)

Specifically, the forced air pressure difference can be calculate based on the loads from which it originates. The gravitational pressure gradient can be expressed using the air density, together with the gravity acceleration. Thus (2.41) becomes:

$$\boldsymbol{\mathcal{G}}_{air} = -\frac{k_{air} \cdot A}{\eta_{air}} \cdot \left(\frac{\Delta P_{air} - G \cdot \Delta \gamma_{air} \cdot \left(\frac{V_{air}}{A}\right)}{\partial L} \right)$$
(2.42)

Where:

G = Gravity acceleration (9.81)
$$[m/s^2]$$

$$\gamma_{air}$$
 = air content in given domain [kg/m³]

 $A = Area [m^2]$

In order to solve Equation (2.42), and thus the total air flow rate, both the forced air and the gravity driven pressure gradients must be found. Since the forced air pressure gradient is caused by wind loads, this gradient is solved under surface boundary condition, Section 2.1.7. The gravity driven pressure gradient, and thus the moist air density, is solved in Section 2.1.3.1 below.

2.1.3.1 Air Density of Moist Air

For air flow through porous materials, the air pressure gradient and the air permeability, k_{air} , of the materials govern the resulting air flow rate.

According to the *ASHRAE Handbook of Fundamentals* (American Society of Heating, Refrigerating and Air-Conditioning Engineers 2017), the density of moist air can be expressed as:

$$\rho_{air} = \frac{1}{\omega} (1+x) \tag{2.43}$$

Where

 ρ_{air} = density of moist air [kg/m³]

$$\omega$$
 = specific volume (...)

x = humidity ratio [kg/kg]

The specific volume, $\mathcal O$, can be defined as:

$$\omega = \frac{287.042(T + 273.15)(1 + 1.607858 \cdot x)}{P_{atm}}$$
(2.44)

in which the atmospheric air pressure, P_{atm} in Pa, can be given or calculated for a given altitude with:

$$P_{atm} = 101325 \cdot \left(1 - 2.25577 \cdot 10^{-5} Z\right)^{5.2559} , \qquad (2.45)$$

where

Z = Altitude [m],

and the humidity ratio, x:

$$x = 0.621945 \cdot \frac{P_{v}}{P_{atm} - P_{v}}$$
(2.46)

With

 P_{v} = Partial vapor pressure [Pa]

Further, per (Hagentoft 2001), the partial pressure of water vapor at saturation can be estimated as:

$$P_{v_{sat}} = 461.4 \cdot T \cdot \gamma_{v_{sat}} \tag{2.47}$$

Where

$$\gamma_{v} = \frac{M_{v}}{V}$$
 = Vapor content in given domain [kg/m³]
 T = Temperature [K]

$$P_{v_{sat}} = \frac{e^{\left(77.345 + 0.0057 \cdot T - \frac{7235}{T}\right)}}{T^{8.2}}$$
(2.48)

Using (2.47) and (2.48), the vapor content in a given domain at saturation is found accordingly:

$$\gamma_{v_{sat}} = \frac{e^{\left(77.345 + 0.0057 \cdot T - \frac{7235}{T}\right)}}{461.4 \cdot T^{9.2}}$$
(2.49)

With

 $\gamma_{v,sat}$ = saturation vapor content [kg/m³]

The relative humidity φ [-] of air can thus be expressed as:

$$\varphi = \frac{\gamma_{\nu}}{\gamma_{\nu_{sat}}} , \qquad (2.50)$$

or as;

$$P_{v} = \varphi \cdot P_{v_{vat}} \tag{2.51}$$

Utilizing Equation (2.43) based on Equations (2.44) through (2.50) gives:

$$\rho_{air} = \frac{P_{atm}(1+x)}{287.042(T+273.15)(1+1.607858x)} = P_{atm} \cdot K_1$$
(2.52)

And as a result, K_1 computes to:

$$K_1 = \frac{(1+x)}{287.042(T+273.15)(1+1.607858x)}$$
(2.53)

2.1.3.2 Resulting Air Flow

By applying Equation (6.27), the areal air flow rate, ignoring gravitational effects, can be found as

$$\vec{g}_{air} = \vec{v}_{air}\rho_{air} = -\rho_{air} \left(\frac{k_{air,x}}{\eta_{air}} \frac{\partial P_{air}}{\partial x} + \frac{k_{air,y}}{\eta_{air}} \frac{\partial P_{air}}{\partial y} \right)$$
(2.54)

where,

→

 \vec{g}_{air} = Areal air flow rate [kg/(m²·s)]

$$V_{air}$$
 = Air velocity [m/s]

Introducing γ_{air} as air content ($\gamma_{air} = \phi_{air} \cdot \rho_{air}$) in kg/m³, we can write the continuity equation for air in porous media:

$$\frac{\partial \gamma_{air}}{\partial t} + \nabla \cdot \vec{g}_{air} = 0$$
(2.55)

Where,

$$\gamma_{air}$$
 = Air content [kg/m³]

Finally, as seen in (6.32), the resulting air flow rate through a porous material is defined as:

$\frac{\partial \gamma_{air}}{\partial P_{air}} \frac{\partial P_{air}}{\partial P_{air}} = \frac{\partial P_{air}}{\partial P_{air}}$	$\left(\underline{k_{air}} \cdot \rho_{air} \cdot \frac{\partial P_{air}}{\partial P_{air}} \right)$	$+\frac{\partial}{\partial \left(\frac{k_{air}\cdot\rho_{air}}{\partial \rho_{air}},\frac{\partial P_{air}}{\partial \rho_{air}}\right)}$	(2.56)
$\partial P_{air} \partial t = \partial x$	$\left(\begin{array}{cc} \eta_{air} & \partial x \end{array} \right)$	$\int \partial y \left(\begin{array}{cc} \eta_{air} & \partial y \end{array} \right)$	(2.00)

2.1.4 Phase Change of Water

The phase change of water will either provide or consume energy, depending on which phase state the water is transforming into. There is a jump in specific enthalpy at 0° C, which must be accounted for in hygrothermal simulations.

Specific Enthalpy of Water [KJ/Kg]



Figure 4. Specific enthalpy of water as a function of temperature [°C]

As described in (Diachao Sheng 1993), the enthalpy of phase change can be evaluated through an averaging technique. Otherwise, this direct evaluation may run the risk of skipping the phase change interval in a single timestep.

2.1.4.1 Heat of fusion

If a phase change occurs in water between its liquid and solid form, the phase change is referred to as fusion. The enthalpy of fusion, h_{il} , which defines the amount of energy required to change the phase of water from solid, *i*, to liquid, *l*, is 333.55 kJ/Kg.

2.1.4.2 Heat of evaporation

Water, in its free form and at typical air pressure, evaporates at 100° C. However, a partial phase change, between available liquid, l, and gas, g, form of water occurs regardless of temperature change. With changing temperature, gradients in partial pressure exists, causing saturated humidity levels to change accordingly, as seen in (2.48). Since vaporization, or condensation, consumes or generates energy respectively, the enthalpy of vaporization is defined as:

$$h_{lg} = -\left(2500.8 - 2.36 \cdot T_c + 0.016 \cdot T_c^2 - 0.00006 \cdot T_c^3\right) [\text{KJ/kg}]$$
(2.57)

Here, T_c is given in degree Celsius.

2.1.5 Heat Transfer in Air Cavities

A frame cavity shall be treated as though it contains an opaque solid which is assigned an effective conductivity. This effective conductivity accounts for both radiative and convective heat transfer and shall be determined as follows.

$$\lambda_{\rm eff} = (h_{\rm c} + h_{\rm r}) \cdot d \tag{2.58}$$

where

 $\lambda_{\rm eff}$ = the effective conductivity;

 $h_{\rm c}$ = the convective heat transfer coefficient;

 h_r = the radiative heat transfer coefficient (h_r =0 in the case when detailed radiation procedure is used);

d = the thickness or width of the air cavity in the direction of heat flow.

The convective heat transfer coefficient, h_c , is calculated from the Nusselt number, Nu, which can be determined from various correlations, depending on aspect ratio, orientation and direction of heat flow.

$$h_{\rm c} = N u \frac{\lambda_{\rm air}}{d}$$
(2.59)

(2.60)

There are three different cases to be considered, depending on whether the heat flow is upward, downward, or horizontal.

2.1.5.1 Heat flow downward

Nu = 1.0



Figure 5. Illustration of rectangular frame cavity downward flow direction

2.1.5.2 Heat flow upward

This situation is inherently unstable and will yield a Nusselt number that is dependent on the height-to-width aspect ratio, L_V/L_h , where L_V and L_h are the largest cavity dimensions in the vertical and horizontal directions, as shown in Figure 6.



Figure 6. Illustration of rectangular frame cavity upward flow direction

a) for
$$\frac{L_{\rm v}}{L_{\rm h}} \le 1$$
 convection is restricted by wall friction, and

$$Nu = 1.0$$
 (2.61)

b) for
$$1 < \frac{L_v}{L_h} \le 5$$
 the Nusselt number is calculated according to the method given by

$$Nu = 1 + \left[1 - \frac{Ra_{\text{crit}}}{Ra}\right]^{+} \left[k1 + 2(k2)^{1 - \ln k2}\right] + \left[\left(\frac{Ra}{5380}\right)^{\frac{1}{3}} - 1\right]^{+} \left[1 - e^{-0.95\left(\left(\frac{Ra_{\text{crit}}}{Ra}\right)^{\frac{1}{3}} - 1\right)^{+}}\right]$$
(2.62)

where

$$k1 = 1.40$$
$$k2 = \frac{Ra^{\frac{1}{3}}}{450.5}$$

$$[x]^+ = \frac{x+|x|}{2}$$

 Ra_{crit} is a critical Rayleigh number, which is found by least squares regression of tabulated values.

$$Ra_{\rm crit} = e^{\left(0.721\frac{L_{\rm h}}{L_{\rm v}}\right) + 7.46}$$

Ra is the Rayleigh number for the air cavity:

$$Ra = \frac{\rho_{\text{air}}^2 L_v^3 g \beta C_{p,air} (T_{\text{hot}} - T_{\text{cold}})}{\mu_{\text{air}} \lambda_{\text{air}}}$$

c) for $\frac{L_v}{L_h} > 5$ the Nusselt number is:

$$Nu = 1 + 1.44 \left[1 - \frac{1708}{Ra} \right]^{+} + \left[\left(\frac{Ra}{5830} \right)^{\frac{1}{3}} - 1 \right]^{+}$$

2.1.5.3 Horizontal heat flow



Figure 7. Illustration of rectangular frame cavity horizontal flow direction

a) for $\frac{L_v}{L_h} < \frac{1}{2}$ the Nusselt number is:

$$Nu = 1 + \left\{ \left(2.756 \cdot 10^{-6} Ra^2 \left(\frac{L_v}{L_h} \right)^8 \right)^{-0.386} + \left(0.623 Ra^{\frac{1}{5}} \left(\frac{L_h}{L_v} \right)^{\frac{2}{5}} \right)^{-0.386} \right\}^{-2.59}$$
(2.63)

where *Ra* is Raleigh number and is defined as:

$$Ra = \frac{\rho_{\text{air}}^2 L_h^3 g \beta C_{\text{p,air}} (T_{\text{hot}} - T_{\text{cold}})}{\mu_{\text{air}} \lambda_{\text{air}}}$$

b) for $\frac{L_v}{L_h} > 5$ the following correlation, also the maximum *Nu* is gives as:

$$Nu_{\rm ct} = \left\{ 1 + \left[\frac{\left(0.104 Ra^{0.293} \right)}{\left(1 + \left(\frac{6310}{Ra} \right)^{1.36} \right)} \right]^3 \right\}^{\frac{1}{3}}$$
(2.64)

$$Nu_{1} = 0.242 \left(Ra \frac{L_{\rm h}}{L_{\rm v}} \right)^{0.273}$$
(2.65)

$$Nu_{\rm t} = 0.0605 Ra^{\frac{1}{3}} \tag{2.66}$$

Note: For more details, see Reference (Wright 1996).

c) for $\frac{1}{2} < \frac{L_v}{L_h} < 5$ the Nusselt number is found using a linear interpolation between the endpoints

of (a) and (b) above.

For jamb frame sections, frame cavities are oriented vertically and therefore the height of the cavity is in the direction normal to the plane of the cross section. For these cavities, it is assumed that the heat flow is always in horizontal direction with $L_v/L_h > 5$, and so correlations in Equations (2.64) to (2.66) in 6.6.3.b shall be used.

The temperatures T_{hot} and T_{cold} are not known in advance, so it is necessary to estimate them. From previous experience it is recommended to apply $T_{hot}=10^{\circ}$ C and $T_{cold}=0^{\circ}$ C. However, after the simulation is completed, it is necessary to update these temperatures from the results of the previous simulation. This procedure shall be repeated until the values of T_{hot} - T_{cold} from two consecutive simulations are within 1°C. Also, it is important to inspect the direction of heat flow after the initial simulation, because if the direction of the bulk of heat flow is different than initially specified, it will need to be corrected for the next simulation.

For an unventilated irregularly shaped frame cavity, the geometry shall be converted into equivalent rectangular cavity according to the procedure in ISO 10077-2 (see also Figure 8). For these cavities, the following procedure shall be used to determine which surfaces belong to vertical and horizontal surfaces of equivalent rectangular cavity (see also Figure 9).

If the shortest distance between two opposite surfaces is smaller than 5 mm then the frame cavity shall be split at this "throat" region. Also:

- a) any surface whose normal is between 315° and 45° is a left vertical surface
- b) any surface whose normal is between 45° and 135° is a bottom horizontal surface
- c) any surface whose normal is between 135° and 225° is a right vertical surface
- d) any surface whose normal is between 225° and 315° is a top horizontal surface



$$\frac{L_1}{H_1} = \frac{L_1}{H_1}$$
; $t \le 5mm$; and $\frac{L_2}{H_2} = \frac{L_2}{H_2}$

Figure 8. Illustration of the treatment of irregularly shaped frame cavities



Figure 9. Illustration of how to select surface orientation for frame cavities; dashed lines indicate the direction of the normal to the surface with cut of angles at 45°, 135°, 225° and 315°.

Temperatures of equivalent vertical and horizontal surfaces shall be calculated as the mean of the surface temperatures according to the classification shown above. The direction of heat flow shall be determined from the temperature difference between vertical and horizontal surfaces of the equivalent cavity. The following rule shall be used (see also Figure 10).

heat flow is horizontal if the absolute value of the temperature difference between vertical cavity surfaces is larger than between horizontal the cavity surfaces;

- a) heat flow is vertical heat flow up if the absolute temperature difference between horizontal cavity surfaces is larger than between vertical cavity surfaces, and the temperature difference between the top horizontal cavity surface and bottom horizontal cavity surface is negative;
- b) heat flow is vertical, heat flow down if the absolute temperature difference between horizontal cavity surfaces is larger than between vertical cavity surfaces and the temperature difference between the top horizontal cavity surface and bottom horizontal cavity surface is positive.



Figure 10. Illustration of how to select heat flow direction

2.1.5.4 Radiant heat flow

The radiative heat transfer can be calculated two ways: 1) a simplified approach utilizing the correlation for radiative surface heat transfer coefficient h_r , and 2) utilizing the detailed, view factor-based radiation heat transfer calculation 2-D grey body radiation theory.

2.1.5.4.1 Simplified Radiation Heat Transfer Calculation

 $h_{\rm r}$ shall be calculated using:

$$h_{\rm r} = \frac{4 \,\sigma \, T_{\rm ave}^3}{\frac{1}{\varepsilon_{\rm cold}} + \frac{1}{\varepsilon_{\rm hot}} - 2 + \frac{1}{\frac{1}{2} \left[\left[\left(1 + \left(\frac{L_{\rm h}}{L_{\rm v}} \right)^2 \right]^{\frac{1}{2}} - \frac{L_{\rm h}}{L_{\rm v}} + 1 \right]} \qquad \frac{W}{m^2 K}$$
(2.67)

where:

$$T_{\rm ave} = \frac{T_{\rm cold} + T_{\rm hot}}{2}$$

The above notation assumes radiant heat flow in the horizontal direction. If the heat flow direction is vertical then the inverse of the ratio L_h/L_v shall be used (i.e., L_v/L_h).

2.1.5.4.2 Detailed, View Factor-Based Radiation Heat Transfer Calculation

The net radiation heat transfer at any surface "*i*" is the difference between emitted radiation and the absorbed portion of incident radiation. The temperatures of the surfaces do not appreciably differ, so using Kirchhoff's law:

$$q_{\rm r,i} = \varepsilon_{\rm i} \sigma T_{\rm i}^4 - \varepsilon_{\rm i} G_{\rm i} \tag{2.68}$$

where, Gi is irradiance at surface *i* from all other surfaces.

$$G_{\mathrm{i}} = \sum_{\mathrm{j}}^{\mathrm{N}} F_{\mathrm{i-j}} J_{\mathrm{j}}$$

and F_{i-j} is the view factor from surface *i* to surface *j*. The radiosity of surface *j*, J_j , is given by:

$$J_{j} = \varepsilon_{j}\sigma T_{j}^{4} + \rho_{j}G_{j}$$
(2.69)

Assuming all surfaces are grey: $\rho_j = 1 - \varepsilon_j$. Substituting ρ_j and G_j and using subscript *i* for convenience, Equation (2.68) becomes:

$$J_{i} = \varepsilon_{i}\sigma T_{i}^{4} + (1 - \varepsilon_{i})\sum_{j=1}^{N} F_{i-j}J_{j}$$
(2.70)

Equation (2.70) represents a system of N linear algebraic equations for the N unknown radiosities, J_{j} , which are determined from the solution of this system of equations. The system of Equation (2.70) when expressed in matrix form becomes:

$$[C]{J} = {F}$$
(2.71)

where

$$C_{ij} = \frac{\delta_{ij} - (1 - \varepsilon_i)F_{i-j}}{\varepsilon_i}$$
(2.72)

$$F_{\rm i} = \sigma T_{\rm i}^{4} \tag{2.73}$$

 T_i in Equation (2.73) is the known temperature from the previous iteration k, (i.e., $T_i|^k$). For the first iteration, the values for T_i are initial guesses.

Temperatures are calculated from the solution to the conduction problem, while net radiation heat flow rate (see Equation(2.68)) is calculated using J_i values from Equation (2.70) and linearized term T_i^4 , by using the first two terms of its Taylor series expansion about $T_i|^k$.

$$T_{i}^{4} = 4 \left(T_{i} \right)^{k} T_{i}^{k+1} - 3 \left(T_{i} \right)^{k} \right)^{4}$$
(2.74)

This procedure is repeated until the following condition is satisfied:

$$\frac{\left\|T\right|^{k+1} \left\|-\left\|T\right|^{k}\right\|}{\left\|T\right|^{k+1}} \le tol$$
(2.75)

where *tol* is the solution tolerance, whose value is typically less than 10^{-3} . $\| \|$ denotes the norm or root mean square value of the temperature vector.

View factors $F_{i\cdot j}$ can be calculated using Hottel's cross-string rule, detailed below. If the view between two radiating surfaces is obstructed by a third surface, the effect of this obstruction shall be included, which is also detailed below.

2.1.5.4.3 View Factor Calculation

The view factor is defined as the fraction of energy leaving a surface that arrives at a second surface. For surfaces with finite areas, the view factors are defined by

$$F_{k-j} = \frac{1}{A_k} \int_{A_k} \int_{A_k} \int_{A_j} \frac{\cos \theta_k \cos \theta_j}{\pi S^2} dA_k dA_j$$
(2.76)

where S is the distance from a point on surface A_j to a point on surface A_k . The angles θ_j and θ_k are measured between the line S and the normal to the surface as shown in Figure 11.



Figure 11. Nomenclature for enclosure radiation

From equation(2.76), following equation is obtained:

$$A_k F_{k-j} = A_j F_{j-k}$$
(2.77)

There are several ways to calculate view factors. One of them is the "cross-string" rule which is illustrated in Figure 12.


Figure 12. Cross-string rule

and given by following equation:

$$F_{ij} = \frac{r_{12} + r_{21} - (r_{11} + r_{22})}{2L_i}$$
(2.78)

When partial, or third shadowing exists, the two radiating surfaces are subdivided into n finite subsurfaces and contribute to the summation in equation

$$F_{ij} = \sum_{k=1}^{n} \sum_{l=1}^{n} F_{kl}$$
(2.79)

of those subsurfaces in which ray r_{kl} intersects a shadowing surface is excluded (Figure 13).



Figure 13. Third Surface Shadowing

2.1.6 Moisture Transfer in Air Cavities

Moisture transport in air cavities follows the approach for heat transfer in air cavities (Chapter 2.1.5) and treats the frame cavity as though it contains an opaque solid, which is assigned an effective water vapor diffusion coefficient. The water vapor transfer coefficient depends on the convective heat transfer coefficient according to the Lewis Formula (2.87). The convective heat transfer coefficient, h_c , depends on the Nusselt number, Nu, which depends on several geometric and environmental parameters (Chapter 2.1.5). The effective mass transfer shall be determined as follows.

$$\delta_{eff} = Nu \cdot \beta_{conv} \cdot d = Nu \cdot \frac{\mathbb{Z}_c}{\rho_a c_{pa}} \cdot d$$
(2.80)

Where

 $\delta_{\rm eff}$ is the effective water vapor permeability (m²/s);

Nu is the Nusselt number;

 β_{conv} is the water vapor transfer coefficient (m/s);

 h_c is the convective heat transfer coefficient (W/m²K);

 ρ_a is the density of air (kg/m³);

 c_{pa} is the heat capacity of air (J/(kgK));

d is the thickness or width of the air cavity in the direction of heat flow.

2.1.7 Boundary Conditions

There are two different options for defining the boundary conditions. The simple option is to provide temperature and relative humidity boundary conditions right at the surface nodes. In this

case, equation (2.81) applies:

$$T_{surf} = T_{boundary}$$

$$RH_{surf} = RH_{boundary}$$

$$P_{surf} = P_{boundary}$$
(2.81)

The second option is to provide surrounding air properties and calculate the resulting heat/mass flux on the surfaces depending on the surface heat and moisture transfer coefficients. For pressure boundary conditions, Equation (2.81) always applies.

The difference in absolute air pressure on the inside and outside of the component is a function of three primary mechanisms: Wind, stack effect and mechanical air handling equipment. Various methods to calculate wind and stack effect pressures exist, which are always applicable under certain conditions. They can be utilized to calculate dynamic pressure differences ΔP between inside and outside. The resulting pressure boundary conditions are found in Equation (2.82):

$$P_{surf,in} = P_{atm}$$

$$P_{surf,ex} = P_{atm} - \Delta P$$
(2.82)

With

$$P_{surf,in}$$
 = Absolute pressure on interior surface (Pa)
 $P_{surf,ex}$ = Absolute pressure on exterior surface (Pa)
 ΔP = Pressure difference between inside and outside surface (Pa)

The total heat flux on a surface boundary consists of advection heat flux, shortwave solar heat flux and long-wave radiation heat flux. The shortwave heat flux does not depend on the conditions of the element; advection and long-wave radiation heat exchange do depend on the temperature conditions of the surface.

The total heat flux on a component surface follows Equation (2.83):

$$\dot{q}_{tot} = \dot{q}_{conv} + \dot{q}_{sw} + \dot{q}_{lw} + \dot{q}_{vapor}$$
(2.83)

With

 \dot{q}_{tot} = total heat flux density (W/m²)

 q_{sw} = shortwave radiation heat flux density (W/m²)

 q_{lw} = long-wave radiation heat flux density (W/m²)

 \dot{q}_{vapor} = heat flux density from vapor (W/m²)

The convective heat flux can be calculated according to (2.84):

$$\dot{q}_{conv} = \alpha_{conv} \cdot (T_{surf} - T_{air})$$
(2.84)

With

$$\alpha_{conv}$$
 = convective heat transfer coefficient (W/(m²K))

 T_{surf} = surface temperature (C)

 T_{air} = air temperature (C)

The vapor heat flux density can be calculated as:

$$\dot{q}_{vapor} = \beta_{conv} \cdot h_{lg} \cdot \left(\varphi_{air} \cdot \gamma_{v,sat,air} - \varphi \cdot \gamma_{v,sat,surf} \right)$$
(2.85)

Where,

 φ_{air} = humidity of ambient air,

$$\gamma_{v,sat,air}$$
 = saturation concentration at air temperature (see (2.49)),

 φ = humidity at the surface,

 $\gamma_{v.sat.surf}$ = saturation concentration at surface temperature (see (2.49)),

 h_{lg} = heat of evaporation

 β_{conv} = Lewis formula coefficient (see (2.87))

Similarly, the water vapor flux density can be calculated according to (2.86):

$$\dot{g}_{conv} = \beta_{conv} \cdot (\gamma_{surf} - \gamma_{air})$$
(2.86)

 \dot{g}_{conv} = water vapor flux density (kg/(m²s))

 β_{conv} = water vapor transfer coefficient (m/s)

 γ_{surf} = water vapor content on the surface (kg/m³)

 γ_{air} = water vapor content in the air (kg/m³)

The water vapor transfer coefficient depends on the convective heat transfer coefficient according to Lewis Formula (2.87):

$$\beta_{conv} = \frac{\alpha_{conv}}{\rho_a c_{pa}}$$
(2.87)

With

 ρ_a = density of air (kg/m³)

$$c_{pa}$$
 = heat capacity of air (J/(kgK))

The following sections will provide information on how to calculate the convective heat transfer

coefficient. In case the required input information is missing, it should also be possible to provide a user defined h_{comp} .

2.1.7.1 Exterior surface – Heat transfer

2.1.7.1.1 Short-wave radiative flux

The total solar gain on any exterior surface it a combination of the absorption of direct and diffuse solar radiation and is calculated according to equation (362) in the *Engineering Reference Manual for Energy Plus* (Plus).

2.1.7.1.2 Long-wave radiative flux

The long-wave radiative flux describes the radiation exchange between the surface and its surroundings. The heat flux is calculated from the surface absorptivity, the temperature of the surface, and of all surfaces in sight of this surface with the corresponding view factors. For simplification, the area in view is usually divided into ground, air and sky. The ground surface temperature is assumed to be the same as the air temperature. Therefore the total long-wave heat flux is the sum of all those components:

$$q_{lw,ex} = q_{gnd} + q_{sky} + q_{air}$$

$$(2.88)$$

With

 $\dot{q}_{lw,ex}$ = exterior long wave radiation heat flux density (W/m²)

$$\dot{q}_{gnd}$$
 = heat flux density to the ground (W/m²)

 \dot{q}_{sky} = heat flux density to the sky (W/m²)

 \dot{q}_{air} = heat flux density to the exterior air (W/m²)

With the application of the Stefan-Boltzmann Law to each component we get:

$$q_{lw,ex} = \varepsilon \sigma W_{gnd} \left(T_{gnd}^4 - T_{surf,ex}^4 \right) + \varepsilon \sigma W_{sky} \left(T_{sky}^4 - T_{surf,ex}^4 \right)$$
(2.89)

With

$$\begin{split} & \mathcal{E} = \text{long-wave emissivity of the surface (-)} \\ & \sigma = \text{Stefan-Boltzmann constant} = 5.6704 (W/(m^2\text{K}^4)) \\ & T_{surf,ex} = \text{temperature of the external surface (C)} \\ & W_{gnd} = \text{view factor to the ground (C)} \\ & T_{gnd} = \text{temperature of the ground (C)} \\ & W_{sky} = \text{view factor to the sky (C)} \\ & T_{sky} = \text{temperature of the sky (C)} \end{split}$$

The view factors to ground and sky can be calculated according to Walton (Walton 1983):

$$W_{gnd} = 0.5 \cdot (1 - \cos \kappa)$$

$$W_{sky} = 0.5 \cdot (1 + \cos \kappa)$$
(2.90)

With

 $_{\kappa}$ = tilt angle of the surface (-)

2.1.7.1.3 Convective heat flux

The convective heat flux is calculated according to equation (2.84). There are numerous models to estimate the exterior convection coefficient. As the moisture transfer coefficient depends on the convective heat transfer coefficient, an accurate model is desirable. The total convective heat transfer on an external surface is a result of combined natural and forced convection. The total convective heat transfer coefficient is therefore:

$$\alpha_{conv,ex,tot} = \alpha_{conv,ex,f} + \alpha_{conv,ex,n}$$
(2.91)

With

 $\alpha_{conv,ex,tot}$ = convective heat transfer coefficient, external, total (W/(m²K))

 $\alpha_{conv,ex,f}$ = convective heat transfer coefficient, external, forced (W/(m²K))

$$\alpha_{conv.ex.n}$$
 = convective heat transfer coefficient, external, natural (W/(m²K))

A new and comprehensive model to calculate the forced convective heat transfer coefficient for very smooth surfaces is presented in (Montazeri, Blocken 2017). It computes the convective heat transfer coefficient based on building dimensions and reference wind speed for windward, leeward and side facades as well as roofs. However, this model is only applicable for very smooth surfaces. The TARP algorithm (as described in (Plus 2008) referencing (Walton 1983)) uses surface roughness multipliers to adjust the coefficients. A combination of both approaches yields:

$$\alpha_{conv,ex,f} = R_i \cdot v_{w10}^{a_{exp}} \cdot (a_0 + a_1 \cdot W + a_2 \cdot W^2 + a_3 \cdot W^3 + a_4 \cdot W^4 + a_5 \cdot H + a_6 \cdot H^2 + a_7 \cdot H^3 + a_8 \cdot H^4 + a_9 \cdot W \cdot H + a_{10} \cdot W \cdot H^2 + a_{11} \cdot W \cdot H^3 + a_{12} \cdot W^2 \cdot H + a_{13} \cdot W^2 \cdot H^2$$

$$+ a_{14} \cdot W^2 \cdot H^3 + a_{15} \cdot W^3 \cdot H + a_{16} \cdot W^3 \cdot H^2 + a_{17} \cdot W^3 \cdot H^3)$$
(2.92)

With

 R_i = Roughness index (-) (see Table 3)

 V_{w10} = reference wind speed in 10 m height (m/s)

 a_{exp} = windspeed exponent coefficient (-)

 $a_0 - a_{17}$ = equation coefficients (-) (see Table 2)

W =Building Width (m)

H =Building Height (m)

With the coefficients in Table 2:

Coefficient	Windward	Leeward	Side facade	Roof
a _{exp}	0.84	0.89	0.88	0.90
a ₀	7.559	3.691E-1	3.217	5.383
a ₁	-2.277E-1	5.848E-2	-4.235E-3	-1.320E-1
a ₂	6.0337E-3	-3.662E-3	1.118E-3	2.211E-3
a ₃	-7.801E-5	6.995E-5	-2.301E-5	-6.099E-6
a ₄	3.810E-7	-4.174E-7	1.382E-7	-6.369E-8
a ₅	4.485E-2	5.621E-2	6.551E-3	2.320E-1
a ₆	-8.190E-4	-2.847E-3	1.843E-3	-4.653E-3
a ₇	1.080E-5	5.155E-5	-4.576E-5	4.830E-5
a ₈	-6.020E-8	-3.011E-7	3.014E-7	-2.004E-7
a 9	1.047E-3	7.582E-3	-6.985E-3	5.224E-3
a ₁₀	-2.430E-5	-1.455E-4	1.402E-4	-1.244E-4
a ₁₁	1.793E-7	8.924E-7	-8.728E-7	9.642E-7
a ₁₂	-3.591E-6	-1.488E-4	1.043E-4	-1.643E-4
a ₁₃	1.385E-7	2.751E-6	-2.052E-6	3.810E-6
a ₁₄	-1.353E-9	-1.646E-8	1.268E-8	-2.892E-8
a ₁₅	-9.369E-8	8.907E-7	-5.537E-7	1.115E-6
a ₁₆	1.757E-9	-1.569E-8	1.070E-8	-2.541E-8
a ₁₇	-9.134E-12	9.019E-11	-6.574E-11	1.921E-10

 Table 2. Coefficients for the calculation of external forced convective heat transfer coefficient for windward, leeward and side facades and for roofs

And with the surface roughness indexes in Table 3:

Roughness Index	R _i	Example Material
1 (Very Rough)	2.17	Stucco
2 (Rough)	1.67	Brick
3 (Medium Rough)	1.52	Concrete
4 (Medium Smooth)	1.13	Clear Pine
5 (Smooth)	1.11	Smooth Plaster
6 (Very Smooth)	1	Glass

 Table 3. Roughness index values for the calculation of the exterior forced surface transfer coefficients

The heat transfer coefficient due to natural convection is also calculated with the TARP algorithm. The part of the convective heat transfer coefficient due to natural ventilation for a vertical surface computes to:

$$\alpha_{conv,ex,n} = 1.31 \cdot \left| (T_{surf,ex} - T_{air,ex}) \right|^{\frac{1}{3}}$$
(2.93)

With

 $T_{suf,ex}$ = Temperature of the exterior surface (C) $T_{oir,ex}$ = Temperature of the exterior air (C)

For an inclined surface, upward facing and lower air temperature than surface temperature, or downward facing and higher air temperature than surface temperature:

$$\alpha_{conv,ex,n} = \frac{9.482 \cdot \left| (T_{surf,ex} - T_{air,ex}) \right|^{\frac{1}{3}}}{7.283 - \left| \cos \phi \right|}$$
(2.94)

With

 ϕ = tilt angle of the surface (-)

And for an inclined surface, upward facing and higher air temperature than surface temperature or downward facing and lower air temperature than surface temperature:

$$\alpha_{conv,ex,n} = \frac{1.810 \cdot \left| (T_{surf,ex} - T_{air,ex}) \right|^{\frac{1}{3}}}{1.382 - \left| \cos \phi \right|}$$
(2.95)

2.1.7.2 Exterior surface – Moisture transfer

2.1.7.2.1 Convective moisture flux

The exterior convective moisture flux is calculated with equation (2.97):

$$\dot{g}_{conv,ex} = \beta_{conv,ex} \cdot (\gamma_{v,surf,ex} - \gamma_{v,air,ex})$$
(2.96)

With

 $\dot{g}_{conv,ex}$ = water vapor flux density, exterior (kg/(m²s)) $\beta_{conv,ex}$ = water vapor transfer coefficient, exterior (kg/(m²sPa)) $\gamma_{v,surf,ex}$ = partial water vapor concentration on the exterior surface (kg/m³)

 $\gamma_{v,air,ex}$ = partial water vapor concentration of the exterior air (kg/m³) Utilizing (2.48) and (2.49) the equation can be rewritten to

$$\dot{g}_{conv,ex} = \beta_{conv,ex} \cdot \left(\frac{e^{\left(77.345+0.0057 \cdot T_{surf,ex} - \frac{7235}{T_{surf,ex}}\right)}}{461.4 \cdot T_{surf,ex}^{9.2}} \cdot \varphi - \frac{e^{\left(77.345+0.0057 \cdot T_{air,ex} - \frac{7235}{T_{air,ex}}\right)}}{461.4 \cdot T_{air,ex}^{9.2}} \cdot \varphi_{ext}\right)$$
(2.97)

With

 $\dot{g}_{conv,ex}$ = water vapor flux density, exterior (kg/(m²s))

 $\beta_{conv,ex}$ = water vapor transfer coefficient, exterior (kg/(m²sPa))

 $\gamma_{v,surf,ex}$ = partial water vapor concentration on the exterior surface (kg/m³)

 $\gamma_{v,air,ex}$ = partial water vapor concentration of the exterior air (kg/m³)

The exterior vapor transfer coefficient $\beta_{conv,e}$ is calculated according to (2.87) with:

$$\beta_{conv,ex} = \frac{\alpha_{conv,ex,tot}}{\rho_a C_{air,ex}}$$
(2.98)

With

 $\beta_{conv,ex}$ = water vapor transfer coefficient, exterior (kg/(m²sPa))

 $\alpha_{conv.ex.tot}$ = convective heat transfer coefficient, exterior, total (W/(m²K))

2.1.7.2.2 Source - Rain Load

For rain, the amount of water sitting on a vertical surface can be estimated using ASHRAE 160 (Standard), Section 4.6. In this standard, the rain deposit is referred to as:

$$r_{bv} = F_E \cdot F_D \cdot F_L \cdot U \cdot \cos\theta \cdot r_h \tag{2.99}$$

where

 r_{bv} = Rain deposition on vertical wall [kg/(m²s)]

 F_E = Rain exposure factor [-]

 F_D = Rain deposition factor [-]

 F_L = Empirical constant, 0.2 kg·s/(m³·mm)

U = Hourly average wind speed at 10 m (33 ft) height [m/s]

 θ = Angle between wind direction and normal to the wall [-]

 r_h = Rainfall intensity, horizontal surface [mm/h]

The rain deposition, r_{bv} , will be accounted for through capillary suction of water liquid at the material surface. The presence of water liquid typically increases the material liquid uptake significantly, which results in an altered liquid transfer coefficient, D. Whether D changes or not depends on the amount of deposited water at the surface. This "coating" of water can be defined

through a water film thickness, d_f , and if the thickness is less than critical, $d_{f,crit}$ (value tbd),

significant capillary suction will not occur; thus the liquid transfer coefficient will remain indifferent. Other tools (Künzel 1995) alter the liquid transfer coefficient of all the materials in the simulation model, once the critical thickness criterium is met.

The maximum amount of water that can deposit at a material surface, before rolling off or evaporating, depends of many factors. The surface inclination, contact angle (hydrophobic tendency) and contact area, droplet size and weight, and surface smoothness ((Yilbas et al. 2017) and (Künzel 2007)) all have an impact on maximum d_f . Subsequently, since surface materials can

only be coated with a certain amount of water, the rainwater uptake is cut off when maximum d_f is obtained.

At present, no good models exist to include the remaining water on surfaces. A promising approach seems to be to add a layer of an artificial material on the surface that can store and release the water according to a model that considers the surface properties, e.g. surface roughness and inclination, among others.

2.1.7.3 Interior surface – heat transfer

For the total heat flux on an internal surface, Equation (2.83) applies as well. The radiant parts $\dot{q}_{_{SW}}$

and \dot{q}_{bv} cannot be calculated for a building component simulation. The location of the 2D element in

a real building is not known and therefore the potential impacts of solar radiation from nearby windows or long-wave radiation exchange with other interior components, occupants and equipment need to be approximated.

As the vapor transfer coefficient depends on the convective part of the heat transfer coefficient, the latter needs to be calculated in more detail. The heat transfer coefficient due to natural convection is calculated with the TARP algorithm the same way the natural convection proportion is calculated for the exterior surface. However, there is no forced air flow on the inside, so the interior convective heat transfer coefficient due to natural convection is the total heat transfer coefficient.

The convective heat transfer coefficient due to natural ventilation for a vertical surface computes to:

$$\alpha_{conv,in,n} = 1.31 \cdot \left| (T_{surf,in} - T_{air,in}) \right|^{\frac{1}{3}}$$

(2.100)

With

$$T_{surf,in}$$
 = Temperature of the interior surface (C)

$$T_{air,in}$$
 = Temperature of the interior air (C)

For an inclined surface, upward facing and lower air temperature than surface temperature, or downward facing and higher air temperature than surface temperature:

$$\alpha_{conv,i,n} = \frac{9.482 \cdot \left| (T_{surf,in} - T_{air,in}) \right|^{\frac{1}{3}}}{7.283 - \left| \cos \phi \right|}$$
(2.101)

With

 ϕ = tilt angle of the surface (-)

And for an inclined surface, upward facing and higher air temperature than surface temperature, or downward facing and lower air temperature than surface temperature:

$$\alpha_{conv,i,n} = \frac{1.810 \cdot \left| (T_{surf,in} - T_{air,in}) \right|^{\frac{1}{3}}}{1.382 - \left| \cos \phi \right|}$$
(2.102)

2.1.7.4 Interior surface – Moisture transfer

2.1.7.4.1 Convective moisture flux

The interior convective moisture flux is calculated with equation (2.103):

1

$$\dot{g}_{conv,in} = \beta_{conv,in} \cdot (\gamma_{air,in} - \gamma_{surf,in})$$
(2.103)

With

 $\dot{g}_{conv,in}$ = water vapor flux density, interior (kg/(m²s))

 $b_{conv.in}$ = water vapor transfer coefficient, interior (kg/(m²sPa))

 $\gamma_{surf.in}$ = water vapor content on the interior surface (Pa)

 $\gamma_{air,in}$ = water vapor content of the interior air (Pa)

Utilizing (2.48) and (2.49) the equation can be rewritten to

$$\dot{g}_{conv,\text{int}} = \beta_{conv,\text{int}} \cdot \left(\frac{e^{\left(77.345+0.0057 \cdot T_{surf,in} - \frac{7235}{T_{surf,in}}\right)}}{461.4 \cdot T_{surf,in}^{9.2}} \cdot \varphi - \frac{e^{\left(77.345+0.0057 \cdot T_{air,in} - \frac{7235}{T_{air,in}}\right)}}{461.4 \cdot T_{air,in}^{9.2}} \cdot \varphi_{\text{int}}\right)$$
(2.104)

The exterior vapor transfer coefficient $eta_{{\it conv},e}$ is calculated according to (2.87) with:

$$\beta_{conv,in} = \frac{\alpha_{conv,in,n}}{\rho_a C_{air,in}}$$
(2.105)

With

 $\beta_{conv,in}$ = water vapor transfer coefficient, interior(kg/(m²sPa))

 $\alpha_{conv,in,n}$ = convective heat transfer coefficient, interior, natural (W/(m²K))

2.1.7.4.2 Interior surface – Moisture sources

Rain does not apply to interior surfaces. Currently no other moisture sources are available for the interior surface.

3 Numerical Model:

3.1 Nomenclature

Variable	Description	Units	
u	General state variable that finite element model is	Units depend on state variable	
	set up for.	used.	
k	Thermal conductivity coefficient	W/(m·K) or J/(m·K·s)	
$ ilde{\psi}$	Shape function in master coordinate system	-	
ع ج	Horizontal axis in master coordinate system (corresponds to x-axis)	-	
η	Vertical axis in master coordinate system (corresponds to y-axis)	-	
[A]	Matrix	-	
{B}	Vector	-	
$m{J}_{ij}$	Element of Jacobian matrix (at i-th row and j-th column)	-	
$m{J}_{ij}^{*}$	Element of inverse Jacobian matrix (at i-th row and j-th column)	-	
det[A]	Determinant of matrix [A]	-	
Е	Diffusion coefficient for stagnant air m ² /s		
μ	Water vapor transfer resistance factor -		
D	Liquid transport coefficient	m ² /s for liquid and kg/(m ² ·s) for humidity	
γ	Material mass over given domain	kg/m ³	
Т	Temperature	K	

Subscripts and superscripts

Subscript/Superscript	Description
[i]	Timestep number
(a)	Iteration number
Х	Value in x-axis direction
у	Value in y-axis direction
i	Index of node
j	Index of node
W	Water total

3.2 Discretization of Governing Equations

This chapter provides concrete discretization of heat and mass transfer equations.

3.2.1 Notation

Some common notation will be used in this document:

 $\{V\}$ - vector of variables or constants

[M] - matrix

 $\psi \equiv \psi(x, y)$ - shape function in global coordinate system

 $\tilde{\psi} \equiv \psi(\xi, \eta)$ - shape function in local coordinate system

 $V^{(a)}$ - variable from iteration "a".

 V_{ii1} - variable from timestep "i".

 $[M]_{ii}$ - matrix element at position (i, j)

 $\{V\}_i$ - vector element at position i

3.2.2 Pressure

The pressure equation is given in following form:

$$\frac{\partial \gamma_{air}}{\partial P_{air}} \frac{\partial P_{air}}{\partial t} = \frac{\partial}{\partial x} \left(\frac{k_{air} \cdot \rho_{air}}{\eta_{air}} \cdot \frac{\partial P_{air}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{k_{air} \cdot \rho_{air}}{\eta_{air}} \cdot \frac{\partial P_{air}}{\partial y} \right)$$
(3.1)

When discretizing (3.1) it will be considered that $\frac{k_{air} \cdot \rho_{air}}{\eta_{air}}$ and $\frac{\partial \gamma_{air}}{\partial P_{air}}$ are constant. Because that is

not true, it is important to note that equation (3.1) will be considered non-linear where solution will be found through iterations. Meaning that program will solve (3.1) for set of ΔP_{air} and then will

recalculate $\frac{k_{air} \cdot \rho_{air}}{\eta_{air}}$ and $\frac{\partial \gamma_{air}}{\partial P_{air}}$ for new solution. Iterations will be repeated till tolerance is

achieved.

3.2.2.1 Domain Equation

Discretization of the entire equation will follow the procedure described in Chapter 7.2.4. The pressure equation will always have non-linear form because of ρ_{air} and $\frac{\partial \gamma_{air}}{\partial P_{air}}$ being dependent on

$$P_{air}$$
.

The final matrix equation will have the following form:

$$\frac{\left[M_{air}^{P}\right]}{\Delta t}\left\{\Delta P_{air,[i]}\right\} - \left[K_{air}^{P}\right]\left\{\Delta P_{air,[i]}\right\} = \frac{\left[M_{air}^{P}\right]}{\Delta t}\left\{P_{air,[i-1]} - P_{air,[i]}\right\} + \left[K_{air}^{P}\right]\left\{P_{air,[i]}\right\}$$

where the coefficients of the matrices are calculated as:

$$\begin{bmatrix} M_{air}^{P} \end{bmatrix}_{ij} = \sum_{\xi,\eta=-\frac{1}{\sqrt{3}}}^{\xi,\eta=-\frac{1}{\sqrt{3}}} \left(\frac{\partial \gamma_{air}}{\partial P_{air}} \tilde{\psi}_{i} \tilde{\psi}_{j} \det[J] \right)$$

$$\begin{bmatrix} K_{air}^{P} \end{bmatrix}_{ij} = \sum_{\xi,\eta=-\frac{1}{\sqrt{3}}}^{\xi,\eta=-\frac{1}{\sqrt{3}}} \begin{bmatrix} \frac{k_{air} \cdot \rho_{air}}{\eta_{air}} \left(\left(J_{11}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \eta} \right) \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \eta} \right) \\ + \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \eta} \right) \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \eta} \right) \end{bmatrix} \det[J]$$

COMPLETE DOMAIN EQUATION

$$\left(\frac{\left[M_{air}^{P}\right]}{\Delta t} - \left[K_{air}^{P}\right]\right) \left\{\Delta P_{air,[i]}^{(a)}\right\} = \frac{\left[M_{air}^{P}\right]}{\Delta t} \left\{P_{air,[i-1]}\right\} + \left(\left[K_{air}^{P}\right] - \frac{\left[M_{air}^{P}\right]}{\Delta t}\right) \left\{P_{air,[i]}^{(a-1)}\right\}$$
(3.2)

3.2.3 Mass Transfer

3.2.3.1 Domain Equation

The mass transfer equation is given in following form:

$$\frac{\partial \gamma_{w}}{\partial \varphi} \frac{\partial \varphi}{\partial t} = \frac{\partial}{\partial x} \left(\frac{E}{\mu_{x}} \frac{\partial \left(\varphi \gamma_{v_{sat}} \right)}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{E}{\mu_{y}} \frac{\partial \left(\varphi \gamma_{v_{sat}} \right)}{\partial y} \right) + \frac{\partial}{\partial y} \left(\frac{k_{air,x} \cdot \varphi \gamma_{v_{sat}}}{\eta_{air}} \cdot \frac{\partial P_{air}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{k_{air,y} \cdot \varphi \gamma_{v_{sat}}}{\eta_{air}} \cdot \frac{\partial P_{air}}{\partial y} \right) + \frac{\partial}{\partial y} \left(\frac{k_{air,y} \cdot \varphi \gamma_{v_{sat}}}{\eta_{air}} \cdot \frac{\partial P_{air}}{\partial y} \right) + S_{l} + S_{v}$$

$$(3.3)$$

3.2.3.1.1 Diffusion Equation

The first term on the right side of (3.3) represents the diffusion equation: $2\left(\frac{1}{2} \partial \left(\frac{1}{2} \partial \left(\frac{1}{2}$

$$0 = \frac{\partial}{\partial x} \left(\frac{E}{\mu_x} \frac{\partial \left(\varphi \gamma_{v_{sat}}\right)}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{E}{\mu_y} \frac{\partial \left(\varphi \gamma_{v_{sat}}\right)}{\partial y} \right)$$

It can be written as

$$0 = \frac{\partial}{\partial x} \left(\delta_x \frac{\partial \left(\varphi \gamma_{v_{sat}} \right)}{\partial x} \right) + \frac{\partial}{\partial y} \left(\delta_y \frac{\partial \left(\varphi \gamma_{v_{sat}} \right)}{\partial y} \right); \qquad \delta_x = \frac{E}{\mu_x}; \delta_y = \frac{E}{\mu_y}$$

The saturation vapor content, $\gamma_{v_{sat}}$ is a function of humidity that will be calculated from the sorption curve. To obtain the correct humidity solution from the diffusion equation, successive iterations need to be applied. Before discretization is applied, the diffusion part of the mass transfer equation needs to be written in the form of a partial derivative of separate terms:

$$0 = \frac{\partial}{\partial x} \left(\delta_x \gamma_{v_{sat}} \frac{\partial \varphi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\delta_y \gamma_{v_{sat}} \frac{\partial \varphi}{\partial y} \right) + \frac{\partial}{\partial x} \left(\delta_x \varphi \frac{\partial \gamma_{v_{sat}}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\delta_y \varphi \frac{\partial \gamma_{v_{sat}}}{\partial y} \right)$$
(3.4)

Applying discretization to this equation will give:

$$-\left(\left[\delta^{\gamma}\right]+\left[\delta^{\varphi}\right]\right)\left\{\Delta\varphi\right\}=\left(\left[\delta^{\gamma}\right]+\left[\delta^{\varphi}\right]\right)\left\{\varphi\right\}$$

where

$$\begin{split} \left[\delta^{\gamma}\right]_{ij} &= \sum_{\xi,\eta=-\frac{1}{\sqrt{3}}}^{\xi,\eta=\frac{1}{\sqrt{3}}} \left[\delta\gamma_{v_{sat}} \left(\left(J_{11}^{*}\frac{\partial\tilde{\psi}_{i}}{\partial\xi} + J_{12}^{*}\frac{\partial\tilde{\psi}_{i}}{\partial\eta}\right) \left(J_{11}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{12}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right) \left(J_{21}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right) \right] \det[J] \right] \\ &+ \left(J_{21}^{*}\frac{\partial\tilde{\psi}_{i}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right) \left(J_{21}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right) \right) \det[J] \\ &\left[\delta^{\varphi}\right]_{ij} = \sum_{\xi,\eta=-\frac{1}{\sqrt{3}}}^{\xi,\eta=\frac{1}{\sqrt{3}}} \left[\delta \left(\frac{\tilde{\psi}_{i}\left(J_{11}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{12}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right)\sum_{k=1}^{n} \left(\gamma_{v_{sat},k}\left(J_{11}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\xi} + J_{12}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\eta}\right)\right) \\ &+ \tilde{\psi}_{i}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right)\sum_{k=1}^{n} \left(\gamma_{v_{sat},k}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\eta}\right)\right) \\ &+ \tilde{\psi}_{i}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right)\sum_{k=1}^{n} \left(\gamma_{v_{sat},k}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\eta}\right)\right)\right) \\ &+ \tilde{\psi}_{i}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right)\sum_{k=1}^{n} \left(\gamma_{v_{sat},k}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\eta}\right)\right)\right) \\ &+ \tilde{\psi}_{i}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right)\sum_{k=1}^{n} \left(\gamma_{v_{sat},k}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\eta}\right)\right)\right) \\ &+ \tilde{\psi}_{i}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right)\sum_{k=1}^{n} \left(\gamma_{v_{sat},k}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\eta}\right)\right) \\ &+ \tilde{\psi}_{i}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right)\sum_{k=1}^{n} \left(\gamma_{v_{sat},k}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\eta}\right)\right) \\ &+ \tilde{\psi}_{i}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right)\sum_{k=1}^{n} \left(J_{21}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\eta}\right)\right) \\ &+ \tilde{\psi}_{i}\left(J_{21}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{j}}{\partial\eta}\right)\sum_{k=1}^{n} \left(J_{21}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\xi} + J_{22}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\eta}\right)\sum_{k=1}^{n} \left(J_{2}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\xi} + J_{2}^{*}\frac{\partial\tilde{\psi}_{k}}{\partial\eta}\right)$$

Note that for equation (3.4) the state variable is humidity and because of that, discretization of the first and second part are different, and thus coefficients for δ^{γ} and δ^{φ} .

3.2.3.1.2 Water Liquid Transportation Liquid Transportation is given as:

$$0 = \frac{\partial}{\partial x} \left(D_{\varphi} \left(\frac{\partial \varphi}{\partial x} \right) \right) + \frac{\partial}{\partial y} \left(D_{\varphi} \left(\frac{\partial \varphi}{\partial y} \right) \right)$$

which will lead to the following matrix form after discretization:

$$-\left[D_{\varphi}\right]\left\{\Delta\varphi\right\}=\left[D_{\varphi}\right]\left\{\varphi\right\}$$

where

$$\begin{bmatrix} D_{\varphi} \end{bmatrix}_{ij} = \sum_{\xi,\eta = -\frac{1}{\sqrt{3}}}^{\xi,\eta = -\frac{1}{\sqrt{3}}} \begin{bmatrix} D_{\varphi} \left(\left(J_{11}^* \frac{\partial \tilde{\psi}_i}{\partial \xi} + J_{12}^* \frac{\partial \tilde{\psi}_i}{\partial \eta} \right) \left(J_{11}^* \frac{\partial \tilde{\psi}_j}{\partial \xi} + J_{12}^* \frac{\partial \tilde{\psi}_j}{\partial \eta} \right) \\ + \left(J_{21}^* \frac{\partial \tilde{\psi}_i}{\partial \xi} + J_{22}^* \frac{\partial \tilde{\psi}_i}{\partial \eta} \right) \left(J_{21}^* \frac{\partial \tilde{\psi}_j}{\partial \xi} + J_{22}^* \frac{\partial \tilde{\psi}_j}{\partial \eta} \right) \end{bmatrix} \det[J]$$

3.2.3.1.3 Pressure Transport

Pressure transportation is given as:

$$0 = \frac{\partial}{\partial x} \left(\frac{k_{air,x} \cdot \varphi \gamma_{v_{sat}}}{\eta_{air}} \cdot \frac{\partial P_{air}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{k_{air,y} \cdot \varphi \gamma_{v_{sat}}}{\eta_{air}} \cdot \frac{\partial P_{air}}{\partial y} \right)$$

which will lead to the following matrix equation:

$$-[P]{\Delta\varphi} = [P]{\varphi}$$

where:

$$\left[P\right]_{ij} = \sum_{\xi,\eta=-\frac{1}{\sqrt{3}}}^{\xi,\eta=-\frac{1}{\sqrt{3}}} \left[\frac{k_{air}\gamma_{v_{sat}}}{\eta_{air}} \left(\frac{\tilde{\psi}_i \left(J_{11}^* \frac{\partial \tilde{\psi}_j}{\partial \xi} + J_{12}^* \frac{\partial \tilde{\psi}_j}{\partial \eta}\right) \sum_{k=1}^n \left(P_{air,k} \left(J_{11}^* \frac{\partial \tilde{\psi}_k}{\partial \xi} + J_{12}^* \frac{\partial \tilde{\psi}_k}{\partial \eta}\right)\right) + \tilde{\psi}_i \left(J_{21}^* \frac{\partial \tilde{\psi}_j}{\partial \xi} + J_{22}^* \frac{\partial \tilde{\psi}_j}{\partial \eta}\right) \sum_{k=1}^n \left(P_{air,k} \left(J_{21}^* \frac{\partial \tilde{\psi}_k}{\partial \xi} + J_{22}^* \frac{\partial \tilde{\psi}_k}{\partial \eta}\right)\right) \right) \right] det[J]$$

3.2.3.1.4 Internal Mass Generation

Internal mass generation is defined by a simple equation:

$$0 = S_l + S_v$$

which converts to a simple vector equation:

$$0 = \{Q_l\} + \{Q_v\}$$

where,

$$\begin{split} \left\{ Q_{l} \right\}_{i} &= \sum_{\xi,\eta=-\frac{1}{\sqrt{3}}}^{\xi,\eta=\frac{1}{\sqrt{3}}} \left(\tilde{\psi}_{i} \cdot S_{l,i} \cdot \det[J] \right) \\ \left\{ Q_{v} \right\}_{i} &= \sum_{\xi,\eta=-\frac{1}{\sqrt{3}}}^{\xi,\eta=\frac{1}{\sqrt{3}}} \left(\tilde{\psi}_{i} \cdot S_{v,i} \cdot \det[J] \right) \end{split}$$

3.2.3.1.5 Mass Transfer Capacitance

Mass transfer capacitance is defined by:

$$\frac{\partial \gamma_{w}}{\partial \varphi} \frac{\partial \varphi}{\partial t} = 0$$

Which then transfers to the following matrix equation:

$$\frac{\left[\gamma_{w}^{\varphi}\right]}{\Delta t}\left\{\Delta\varphi_{\left[i\right]}^{\left(a\right)}\right\} = \frac{\left[\gamma_{w}^{\varphi}\right]}{\Delta t}\left\{\varphi_{\left[i-1\right]}\right\} - \frac{\left[\gamma_{w}^{\varphi}\right]}{\Delta t}\left\{\varphi_{\left[i\right]}^{\left(a-1\right)}\right\}$$

where,

$$\left[\gamma_{w}^{\varphi}\right]_{ij} = \sum_{\xi,\eta=-\frac{1}{\sqrt{3}}}^{\xi,\eta=\frac{1}{\sqrt{3}}} \left(\frac{\partial\gamma_{w}}{\partial\varphi} \cdot \tilde{\psi}_{i} \cdot \tilde{\psi}_{j} \cdot \det[J]\right)$$

COMPLETE DOMAIN EQUATION

$$\begin{pmatrix} \left[\frac{\gamma_{w}^{\varphi}}{\Delta t} - \left[\delta^{\gamma} \right] - \left[\delta^{\varphi} \right] - \left[D_{\varphi} \right] - \left[P \right] \end{pmatrix} \left\{ \Delta \varphi_{[i]}^{(a)} \right\} = \frac{\left[\gamma_{w}^{\varphi} \right]}{\Delta t} \left\{ \varphi_{[i-1]} \right\} + \left\{ \left[\delta^{\gamma} \right] + \left[\delta^{\varphi} \right] + \left[D_{\varphi} \right] + \left[P \right] - \frac{\left[\gamma_{w}^{\varphi} \right]}{\Delta t} \right] \left\{ \varphi_{[i]}^{(a-1)} \right\} + \left\{ Q_{l} \right\} + \left\{ Q_{v} \right\}$$
(3.5)

3.2.3.2 Boundary Conditions

There are two different boundary conditions that can be used together with domain equation (3.5):

- Boundary Conditions with fixed convective film coefficient
- Boundary Condition with variable film coefficient

Regardless of whether the film coefficient is fixed or calculated, the same boundary condition equation will be applied. And because the mass transfer calculations are already solved through iterations, the same solution approach will be used in both cases. The moisture boundary condition is defined by equation:

$$\dot{g}_{conv,ex} = \beta_{conv} \cdot \left(\frac{e^{\left(77.345 + 0.0057 \cdot T_{surf} - \frac{7235}{T_{surf}}\right)}}{461.4 \cdot T_{surf}^{9.2}} \cdot \varphi - \frac{e^{\left(77.345 + 0.0057 \cdot T_{air} - \frac{7235}{T_{air}}\right)}}{461.4 \cdot T_{air}^{9.2}} \cdot \varphi_{ext} \right)$$

which will give discretization: -[G] $\left\{\Delta \varphi_{[i]}^{(a)}\right\} = [G]\left\{\varphi_{[i]}^{(a-1)}\right\} - \left\{Q_{air}\right\}$

Where,

$$\begin{bmatrix} G \end{bmatrix}_{ij} = \sum_{\xi} \left(\beta_{conv} \cdot \frac{e^{\left(77.345 + 0.0057 \cdot T_{surf} - \frac{7235}{T_{surf}} \right)}}{461.4 \cdot T_{surf}^{9.2}} \cdot \tilde{\psi}_i \cdot \tilde{\psi}_j \cdot \det[J] \right)$$

$$\{ Q_{air} \}_i = \sum_{\xi} \left(\frac{e^{\left(77.345 + 0.0057 \cdot T_{air} - \frac{7235}{T_{air}} \right)}}{461.4 \cdot T_{air}^{9.2}} \cdot \varphi_{ext} \cdot \tilde{\psi}_i \cdot \det[J] \right)$$

3.2.4 Heat Transfer Equation

3.2.4.1 Domain Equation

Heat transfer equation defined in the following form:

$$\begin{aligned} \rho_{eq} \cdot C_{eq} &\frac{\partial T}{\partial t} + S \cdot h_{il} \cdot I_{il} = \\ &= \frac{\partial}{\partial x} \left(k \cdot \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \cdot \frac{\partial T}{\partial y} \right) - h_{lg} \left(\frac{\partial \vec{g}_v}{\partial x} + \frac{\partial \vec{g}_v}{\partial y} \right) \\ &- C_l \left(\vec{g}_{l,x} \cdot \frac{\partial T}{\partial x} + \vec{g}_{l,y} \cdot \frac{\partial T}{\partial y} \right) - C_v \left(\vec{g}_{v,x} \cdot \frac{\partial T}{\partial x} + \vec{g}_{v,y} \cdot \frac{\partial T}{\partial y} \right) - C_{air,d} \left(\vec{g}_{air,x} \cdot \frac{\partial T}{\partial x} + \vec{g}_{air,y} \cdot \frac{\partial T}{\partial y} \right) + Q \end{aligned}$$

This equation needs to be developed before discretization is applied:

$$\begin{split} \rho_{eq} C_{eq} &\frac{\partial T}{\partial t} + Sh_{il} I_{il} = \\ &= \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) \\ &+ h_{lg} \left(\delta_x \frac{\partial}{\partial x} \left(\frac{\partial \gamma_v}{\partial x} \right) + \delta_y \frac{\partial}{\partial y} \left(\frac{\partial \gamma_v}{\partial y} \right) \right) + h_{lg} \rho_{air} \frac{k_{air}}{\eta_{air}} x \left(\frac{\partial}{\partial x} \left(\frac{\partial P_{air}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\partial P_{air}}{\partial y} \right) \right) \\ &+ C_l D_{\varphi} \left(\frac{\partial \varphi}{\partial x} \frac{\partial T}{\partial x} + \frac{\partial \varphi}{\partial y} \frac{\partial T}{\partial y} \right) + C_v \frac{E}{\mu} \left(\frac{\partial \gamma_v}{\partial x} \frac{\partial T}{\partial x} + \frac{\partial \gamma_v}{\partial y} \frac{\partial T}{\partial y} \right) \\ &+ C_v \rho_{air} x \frac{k_{air}}{\eta_{air}} \left(\frac{\partial P_{air}}{\partial x} \frac{\partial T}{\partial x} + \frac{\partial P_{air}}{\partial y} \frac{\partial T}{\partial y} \right) + C_{air,d} \frac{k_{air,x}}{\eta_{air}} \left(\frac{\partial P_{air}}{\partial x} \frac{\partial T}{\partial x} + \frac{\partial P_{air}}{\partial y} \frac{\partial T}{\partial y} \right) + Q \end{split}$$

3.2.4.1.1 Conduction Equation

The conduction equation is given in the following form:

$$0 = \frac{\partial}{\partial x} \left(k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T}{\partial y} \right)$$
(3.6)

The discretization of this equation is simple:

$$-[K]{\Delta T} = [K]{T}$$

where the elements of matrix $\begin{bmatrix} K \end{bmatrix}$ can be calculated as:

$$\begin{bmatrix} K \end{bmatrix}_{ij} = \sum_{\xi,\eta} \begin{bmatrix} k \left(\int_{11}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \eta} \right) \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \eta} \right) \\ + \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \eta} \right) \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \eta} \right) \end{bmatrix} \det[J]$$

3.2.4.1.2 Conversion from Liquid to Gas (Vapor Part)

Conduction in the domain from liquid to gas is defined with the following equation:

$$0 = h_{lg} \left(\delta_x \frac{\partial}{\partial x} \left(\frac{\partial \gamma_v}{\partial x} \right) + \delta_y \frac{\partial}{\partial y} \left(\frac{\partial \gamma_v}{\partial y} \right) \right)$$

which is defined in matrix form (Note that this equation is given in linear form because vector $\{\gamma_{\nu}\}$ is considered to be constant in the heat balance equation.):

$$0 = \left[H_{lg}^{\nu} \right] \left\{ \gamma_{\nu} \right\}$$

where,

$$\begin{bmatrix} H_{1g}^{\nu} \end{bmatrix}_{ij} = \sum_{\xi,\eta} \begin{bmatrix} h_{1g} \delta \left(\int_{11}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \eta} \right) \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \eta} \right) \\ + \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{i}}{\partial \eta} \right) \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \eta} \right) \end{bmatrix} \det[J]$$

3.2.4.1.3 Conversion from Liquid to Gas (Air Part) The conduction equation from air is:

$$0 = h_{lg} \rho_{air} \frac{k_{air}}{\eta_{air}} x \left(\frac{\partial}{\partial x} \left(\frac{\partial P_{air}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\partial P_{air}}{\partial y} \right) \right)$$

and in matrix form:

$$0 = \left[H_{\rm lg}^{air} \right] \left\{ P_{air} \right\}$$

where

$$\begin{bmatrix} H_{1g}^{air} \end{bmatrix}_{ij} = \sum_{\xi,\eta} \begin{bmatrix} h_{lg} \rho_{air} \frac{k_{air}}{\eta_{air}} x \begin{pmatrix} \left(J_{11}^* \frac{\partial \tilde{\psi}_i}{\partial \xi} + J_{12}^* \frac{\partial \tilde{\psi}_i}{\partial \eta} \right) \begin{pmatrix} J_{11}^* \frac{\partial \tilde{\psi}_j}{\partial \xi} + J_{12}^* \frac{\partial \tilde{\psi}_j}{\partial \eta} \end{pmatrix} \\ + \left(J_{21}^* \frac{\partial \tilde{\psi}_i}{\partial \xi} + J_{22}^* \frac{\partial \tilde{\psi}_i}{\partial \eta} \right) \begin{pmatrix} J_{21}^* \frac{\partial \tilde{\psi}_j}{\partial \xi} + J_{22}^* \frac{\partial \tilde{\psi}_j}{\partial \eta} \end{pmatrix} \end{bmatrix} \det[J]$$

3.2.4.1.4 Conduction from Liquid

Conduction from liquid is given in the form of:

$$0 = C_l D_{\varphi} \left(\frac{\partial \varphi}{\partial x} \frac{\partial T}{\partial x} + \frac{\partial \varphi}{\partial y} \frac{\partial T}{\partial y} \right)$$

which needs to contain a non-linear part, because equation is solved by temperature:

$$-[K_{l}]{\Delta T} = [K_{l}]{T}$$

where,

$$\begin{bmatrix} K_{l} \end{bmatrix}_{ij} = \sum_{\xi,\eta} \begin{bmatrix} C_{l} D_{\varphi} \begin{pmatrix} \tilde{\psi}_{i} \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \eta} \right) \sum_{k=1}^{n} \left(\varphi_{k} \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{k}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{k}}{\partial \eta} \right) \right) \\ + \tilde{\psi}_{i} \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \eta} \right) \sum_{k=1}^{n} \left(\varphi_{k} \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{k}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{k}}{\partial \eta} \right) \right) \end{bmatrix} \det[J]$$

3.2.4.1.5 Conduction from Vapor

Conduction from vapor is given as:

$$0 = C_{\nu} \frac{E}{\mu} \left(\frac{\partial \gamma_{\nu}}{\partial x} \frac{\partial T}{\partial x} + \frac{\partial \gamma_{\nu}}{\partial y} \frac{\partial T}{\partial y} \right)$$

which in matrix form is equal to:

$$-[K_{\nu}]{\Delta T} = [K_{\nu}]{T}$$

where,

$$\begin{bmatrix} K_{\nu} \end{bmatrix}_{ij} = \sum_{\xi,\eta} \begin{bmatrix} \mathcal{W}_{i} \left(J_{11}^{*} \frac{\partial \tilde{\mathcal{W}}_{j}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\mathcal{W}}_{j}}{\partial \eta} \right) \sum_{k=1}^{n} \left(\gamma_{\nu,k} \left(J_{11}^{*} \frac{\partial \tilde{\mathcal{W}}_{k}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\mathcal{W}}_{k}}{\partial \eta} \right) \right) \\ + \tilde{\mathcal{W}}_{i} \left(J_{21}^{*} \frac{\partial \tilde{\mathcal{W}}_{j}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\mathcal{W}}_{j}}{\partial \eta} \right) \sum_{k=1}^{n} \left(\gamma_{\nu,k} \left(J_{21}^{*} \frac{\partial \tilde{\mathcal{W}}_{k}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\mathcal{W}}_{k}}{\partial \eta} \right) \right) \end{bmatrix} \det[J]$$

3.2.4.1.6 Conduction from Airflow

Conduction from airflow is combined from two equations:

$$0 = \left(\left(C_{v} \cdot \rho_{air} \cdot x + C_{air,d} \right) \frac{k_{air}}{\eta_{air}} \right) \left(\frac{\partial P_{air}}{\partial x} \frac{\partial T}{\partial x} + \frac{\partial P_{air}}{\partial y} \frac{\partial T}{\partial y} \right)$$

which in matrix form is:

$$-\left[K_{air}\right]\left\{\Delta T\right\}=\left[K_{air}\right]\left\{T\right\}$$

where

$$\begin{bmatrix} K_{air} \end{bmatrix}_{ij} = \sum_{\xi,\eta} \left[\left(\left(C_{\nu} \rho_{air} x + C_{air,d} \right) \frac{k_{air}}{\eta_{air}} \right) \left(\begin{array}{c} \tilde{\psi}_{i} \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \eta} \right) \sum_{k=1}^{n} \left(P_{air,k} \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{k}}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{k}}{\partial \eta} \right) \right) \\ + \tilde{\psi}_{i} \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{j}}{\partial \eta} \right) \sum_{k=1}^{n} \left(P_{air,k} \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{k}}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{k}}{\partial \eta} \right) \right) \right) det[J]$$

3.2.4.1.7 Internal Heat Generation

Internal heat generation is defined with a simple equation:

$$0 = Q$$

which in matrix form is a simple vector:

$$0 = \{Q\}$$

Where,

$$\left\{ Q \right\}_i = \sum_{\xi,\eta} \left(\tilde{\psi}_i \cdot Q_i \cdot \det[J] \right)$$

3.2.4.1.8 Thermal Capacitance

Thermal capacitance is given by following equation:

$$\rho_{eq}C_{eq}\frac{\partial T}{\partial t}=0$$

Discretization of this equation is:

$$\frac{\left[RC_{p}\right]}{\Delta t}\left\{\Delta T_{\left[i\right]}^{\left(a\right)}\right\} = \frac{\left[RC_{p}\right]}{\Delta t}\left\{T_{\left[i-1\right]}\right\} - \frac{\left[RC_{p}\right]}{\Delta t}\left\{T_{\left[i\right]}^{\left(a-1\right)}\right\}$$

where

$$\left[RC_{p}\right]_{ij} = \sum_{\xi,\eta} \left(\rho \cdot C_{p} \cdot \tilde{\psi}_{i} \cdot \tilde{\psi}_{j} \cdot \det[J]\right)$$

3.2.4.1.9 Ice to Liquid Energy Conversion Ice to liquid conversion is given with:

$$Sh_{il}I_{il} = 0$$

or in vector form:

$$\left\{hI_{il}\right\}=0$$

where

$$\left\{hI_{l}\right\}_{i} = \sum_{\xi,\eta} \left(\tilde{\psi}_{i} \cdot h_{il} \cdot I_{il} \cdot \det[J]\right)$$

COMPLETE DOMAIN EQUATION

$$\begin{pmatrix} \begin{bmatrix} RC_p \end{bmatrix} \\ \Delta t \end{bmatrix} - \begin{bmatrix} K \end{bmatrix} - \begin{bmatrix} K_l \end{bmatrix} - \begin{bmatrix} K_v \end{bmatrix} - \begin{bmatrix} K_{air} \end{bmatrix} \end{pmatrix} \left\{ \Delta T_{[i]}^{(a)} \right\} + \left\{ hI_{il} \right\} = \\ \frac{\begin{bmatrix} RC_p \end{bmatrix}}{\Delta t} \left\{ T_{[i-1]} \right\} + \left[\begin{bmatrix} K \end{bmatrix} + \begin{bmatrix} K_l \end{bmatrix} + \begin{bmatrix} K_v \end{bmatrix} + \begin{bmatrix} K_{air} \end{bmatrix} - \frac{\begin{bmatrix} RC_p \end{bmatrix}}{\Delta t} \right\} \left\{ T_{[i]}^{(a-1)} \right\} + \left[H_{lg}^v \end{bmatrix} \left\{ \gamma_v \right\} + \left[H_{lg}^{air} \right] \left\{ P_{air} \right\} + \left\{ Q \right\}$$

3.2.4.2 Boundary Conditions

The following boundary condition types are considered:

- Convection with moisture transfer (with fixed and variable film coefficient),
- Temperature and
- Black body radiation

3.2.4.3 Convection

The convection boundary condition is defined with following equation:

$$q = h_c \cdot (T - T_{air}) + \beta_{conv} \cdot h_{lg} \cdot (\varphi \cdot \gamma_{v,sat,surf} - \varphi_{air} \cdot \gamma_{v,sat,air})$$
(3.7)

which will give discretization:

$$-[H_{c}]\left\{\Delta T_{[i]}^{(a)}\right\} = [H_{c}]\left\{T_{[i]}^{(a-1)}\right\} - \left\{Q_{c,air}\right\} - \left\{Q_{v,surf}\right\} - \left\{Q_{v,air}\right\}$$

Where,

$$\begin{split} \left[H_{c}\right]_{ij} &= \sum_{\xi} \left(h_{c} \cdot \tilde{\psi}_{i} \cdot \tilde{\psi}_{j} \cdot \det[J]\right) \\ \left\{Q_{c,air}\right\}_{i} &= \sum_{\xi} \left(h_{c} \cdot T_{air} \cdot \tilde{\psi}_{i} \cdot \det[J]\right) \\ \left\{Q_{v,surf}\right\}_{i} &= -\sum_{\xi} \left(\beta_{conv} \cdot h_{lg} \cdot \gamma_{v,sat,surf} \cdot \varphi \cdot \tilde{\psi}_{i} \cdot \det[J]\right) \\ \left\{Q_{v,air}\right\}_{i} &= \sum_{\xi} \left(\beta_{conv} \cdot h_{lg} \cdot \gamma_{v,sat,air} \cdot \varphi_{air} \cdot \tilde{\psi}_{i} \cdot \det[J]\right) \end{split}$$

3.2.4.4 Temperature

Temperature boundary condition is a special case of the convection boundary condition where the heat transfer coefficient is infinitely large. It will come down to equation (3.7) where the film convection coefficient will be set to a large number and the moisture component can be taken away since air temperature is equal to surface temperature.

$$q = h_c \cdot \left(T - T_{air}\right)$$

Discretization is performed as shown in chapter 3.2.4.3.

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5 Appendix A: Mathematics and Thermodynamic Preliminaries

5.1 Nabla symbol (∇)

The differential operator given in Cartesian coordinates (x, y) on a two-dimensional Euclidean space is defined by:

$$\nabla = \vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y}$$

where \vec{i} and \vec{j} are unit vectors in x and y axes respectively.

5.2 Material derivative or Eulerian derivative operator

The material derivative describes the time rate of change of some physical quantity for a material element subjected to a space-and-time-dependent macroscopic velocity field.

The material derivative is defined for any tensor field φ that is macroscopic, with the sense that is depends only on position and time coordinates, $\varphi = \varphi(x, y, t)$:

$$\frac{D\varphi}{Dt} \equiv \frac{\partial\varphi}{\partial t} + \vec{v} \cdot \nabla\varphi = \frac{\partial\varphi}{\partial t} + v_x \cdot \frac{\partial\varphi}{\partial x} + v_y \cdot \frac{\partial\varphi}{\partial y}$$
(5.1)

Where $\vec{v}(x, y, t)$ is the fluid velocity.

5.3 Enthalpy

Enthalpy is a measurement of energy in a thermodynamic system. It is the thermodynamic quantity equivalent to the total heat content of a system. It is equal to the internal energy of the system plus the product of pressure and volume.

$$H = U + pV$$

H = Enthalpy of the system [Energy]

U = Internal energy of the system [Energy]

p = pressure of the system [Force/Area]

V = volume of the system [Volume]

5.3.1 Specific Enthalpy

The specific enthalpy of a uniform system is defined as:

$$h = \frac{H}{m}$$

m = mass of the system [mass]

It can be expressed in other specific quantities by:

h = u + pv

ll = Specific internal energy [Energy/Mass]

p = pressure of the system [Force/Area]

v = specific volume [Volume/Mass]

Specific volume is equal to:

$$v = \frac{1}{\rho}$$

 ρ = is the density [Mass/Volume]

Enthalpy can also be expressed per unit volume, ${\cal H}$ [Energy/Volume].

$$\mathcal{H} = \frac{H}{V}$$

5.3.2 Specific Heat at Constant Pressure (C_p)

Specific heat at constant pressure is the change of specific enthalpy with respect to temperature changes when the pressure is held constant (isobaric process).

$$C_p = \left(\frac{\partial h}{\partial T}\right)_p$$

For constant pressure process:

$$\left(\Delta h\right)_{P}=\int_{T_{1}}^{T_{2}}C_{P}dT$$

6 Appendix B: Theoretical Background

6.1 Conservation of Momentum

While we don't expect to model fluid flow, which is governed by the conservation of momentum equations, we will briefly describe them here for completeness. The principle of conservation of linear momentum (or Newton's second law of motion) states that the time rate of change of linear momentum of a given set of particles is equal to the vector sum of all the external forces acting on the particles of the set, provided Newton's Third Law of action and reaction governs the internal forces. Newton's second law can be written as:

$$\frac{\partial(\rho\vec{u})}{\partial t} + \nabla(\rho\vec{u}\otimes\vec{u}) = \nabla\cdot\sigma + \rho\vec{f}$$
(6.1)

where

 \otimes = Tensor product of two vectors

 σ = Cauchy stress tensor [N/m²]

 \vec{f} = The body force vector, measured per unit mass and normally taken to be the gravity vector

Equation (6.1) is actually set of 3 equations (in 3-D) and they describe the motion of a continuous medium, and in fluid mechanics they are also known as the Navier-Stokes equations.

The form of the momentum equations shown in (6.1) is the conservation (divergence) form that is most often utilized for compressible flows. This equation may be simplified to a form more commonly used with incompressible flows. Expanding the first two derivatives and collecting terms:

$$\rho\left(\frac{\partial \vec{u}}{\partial t} + \vec{u}\nabla\cdot\vec{u}\right) + \vec{u}\left(\frac{\partial\rho}{\partial t} + \nabla\cdot\rho\vec{u}\right) = \nabla\sigma + \rho\vec{f}$$
(6.2)

The second term in parentheses in the continuity equation (6.19) and neglecting this term allows (6.2) to reduce to the non-conservation (advective) form:

$$\rho \frac{D\vec{u}}{Dt} = \nabla \sigma + \rho \vec{f}$$

where the material derivative has been employed.

6.2 Conservation of Energy

The law of conservation of energy (or the First Law of Thermodynamics) states that the time rate of change of the total energy is equal to the sum of the rate of work done by applied forces and the change of heat content per unit time. In general case, the First Law of Thermodynamics cab be expressed in conservation form as:

$$\frac{\partial \left(\rho e^{t}\right)}{\partial t} + \nabla \cdot \left(\rho \vec{v} e^{t}\right) = -\nabla \cdot \vec{q} + \nabla \cdot \left(\sigma \vec{v}\right) + Q + \rho \vec{f} \cdot \vec{v}$$
(6.3)

 $e^{t} = e + \frac{1}{2}\vec{v}\cdot\vec{v}$ = The total energy [Energy/Volume]

- σ = The Cauchy stress tensor [N/m²]
- \vec{f} = The body force vector, measured per unit mass and normally taken to be the gravity vector
- ℓ = The internal energy [Energy/Volume]

 \vec{q} = The heat flux vector [Energy/(Time·Area)]

Q = The internal heat generation [Energy/(Time·Volume)]

6.2.1 Incompressible Fluids

For incompressible flows, an internal energy equation is more appropriate. Taking the dot product of the velocity vector with the momentum equation produces an equation for the kinetic energy. This equation is subtracted from the internal energy equation:

$$\frac{\partial(\rho e)}{\partial t} + \nabla \cdot (\rho \vec{v} e) = -\nabla \cdot \vec{q} + Q + \mu \Phi$$
(6.4)

 Φ = Dissipation function

μ = Dynamic viscosity [Mass/(Length*Time)]

The thermal energy equation (6.4) can be simplified further by expanding the derivatives on the left-hand side of the equation and using the continuity equation. The resulting equation is the non-conservative (advective) form of the energy equation

$$\rho \frac{De}{Dt} = -\nabla \cdot \vec{q} + Q + \mu \Phi \tag{6.5}$$

Which is the standard form used for incompressible flows.

6.2.2 Equation of State

In addition to the conservation laws described above, two thermodynamic relations or equations of state are required. A caloric equation of state relates the internal energy of the materials to two (intensive) thermodynamic variables. Of many possible forms for this equation, one of the most common for fluid dynamics is the functional relation:

$$e = e(T, v)$$

 $v = \frac{1}{\rho}$ = The specific volume [Volume/Mass]

The change in internal energy is then:

$$de = \frac{\partial e}{\partial T} \Big|_{v} dT + \frac{\partial e}{\partial v} \Big|_{T} dv$$
$$de = C_{v} dT + \left(T \frac{\partial P}{\partial T} \Big|_{v} - P \right) dv$$

where standard Maxwell relations from thermodynamics have been used. When converted to material derivative the change in internal energy becomes:

$$\rho \frac{De}{Dt} = \rho C_{\nu} \frac{DT}{Dt} = \rho C_{p} \frac{DT}{Dt} = \rho C \frac{DT}{Dt}$$
(6.6)

C = Specific heat [Energy/(Mass·Temperature)]

The specific heat at constant volume C_ν is the same as the specific heat at constant pressure C_p for constant density processes.

The equation of state provides a relation among three (intensive) thermodynamic variables. The perfect gas law:

$$P = \rho RT$$

is one common equation of state with R being the universal gas constant. For most of the applications considered here, the incompressible flow assumption leads to the equation of state:

$$\rho = \rho_0$$

which implies that the pressure is no longer a thermodynamic variable.

6.2.3 Continuity Equation and Equation of State

Combining equations (6.5) and (6.6), continuity equation can be expressed in terms of the primitive variables (u, P, T):

$$\rho C_{p} \frac{DT}{Dt} = -\nabla \cdot \vec{q} + Q_{s} + \Phi$$

$$\rho C_{p} \left(\frac{\partial T}{\partial t} + v_{x} \frac{\partial T}{\partial x} + v_{y} \frac{\partial T}{\partial y} \right) = -\left(\frac{\partial q}{\partial x} + \frac{\partial q}{\partial y} \right) + Q_{s} + \Phi$$
(6.7)

T = Temperature [Temperature]

C_p = Specific heat at constant pressure [Energy/(Mass·Temperature)]

For flow velocities and velocity gradients that are sufficiently small (applicable to building science), viscous dissipation term, Φ , can be ignored. Conservation of energy equation then becomes:

$$\rho C_{p} \left(\frac{\partial T}{\partial t} + v_{x} \frac{\partial T}{\partial x} + v_{y} \frac{\partial T}{\partial y} \right) = - \left(\frac{\partial q}{\partial x} + \frac{\partial q}{\partial y} \right) + Q_{s}$$
(6.8)

6.2.3.1 Fourier Heat Conduction

The <u>Fourier heat conduction</u> law states that:

$$\vec{q}_{c} = -k \cdot \nabla T = -\left(k_{x} \frac{\partial T}{\partial x} + k_{y} \frac{\partial T}{\partial y}\right)$$
(6.9)

Replacing equation (6.9) into (6.8) we finally get:

$$\rho C_p \left(\frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} \right) = \frac{\partial}{\partial x} \left(k_x \cdot \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \cdot \frac{\partial T}{\partial y} \right) + Q_s$$
(6.10)

For *isotropic* materials, conservation of energy equation becomes:

$$\rho C_p \left(\frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} \right) = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + Q_s$$

6.2.3.2 Steady-State

For steady-state problems, time derivative is equal to zero

$$\rho C_p \left(v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} \right) = \frac{\partial}{\partial x} \left(k_x \cdot \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \cdot \frac{\partial T}{\partial y} \right) + Q_s$$

For *isotropic* materials, steady-state conservation of energy equation is:

$$\rho C_p \left(v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} \right) = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + Q_s$$

6.2.3.3 Solid stationary region

In the solid region Ω_s where velocities are equal to zero, (the advective transport of energy), the energy equation reduces to:

$$\rho C_{p} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k_{x} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_{y} \frac{\partial T}{\partial y} \right) + Q_{s}$$
(6.11)

Or for *isotropic* materials:

$$\rho C_p \frac{\partial T}{\partial t} = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + Q_s$$

6.2.3.4 Steady-State in Stationary Region

For steady-state problems, conservation of energy equation for solid regions becomes:

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T}{\partial y} \right) + Q_s = 0$$
(6.12)

Or for *isotropic* materials:

$$k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + Q_s = 0$$

6.3 Conservation of Energy in Porous Media

Energy transfer through solid non-deformable material is described with equation (6.11).

6.3.1 Conservation of Energy in Dry Porous Media

Introducing porosity (ϕ) to such material (see chapter 6.4 for more details), energy equation through such material becomes:

$$(1-\phi)\rho_d C_p \frac{\partial T}{\partial t} = (1-\phi) \left(\frac{\partial}{\partial x} \left(k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T}{\partial y} \right) \right)$$
(6.13)

where:

 $C_{p,d}$ = Specific heat of dry material [Energy/(Mass·Temperature)]

 ρ_d = Dry material density [Mass/Volume]

k_d = Dry material conductivity [Energy/(Time·Length·Temperature)]

Equation (6.13) considers energy only through porous dry material where all coefficients were scaled down for material porosity. This means that energy contained in solid dry small domain of volume "V" is scaled down by $(1-\phi)$ because that is amount of material contained within that domain. Equation (6.13) describes part of energy flow through porous material. Second part must include gas or fluid flow that happens in pores.

6.3.2 Conservation of Energy in Moist Media

Energy conservation of moving media given by (6.10) can be simplified. If the heat transfer through radiation and convection within porous structure can be neglected, equation becomes:

$$\phi_k \rho_k C_{p,k} \frac{\partial T}{\partial t} = \phi_k \left(\frac{\partial}{\partial x} \left(k_{x,k} \cdot \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_{y,k} \cdot \frac{\partial T}{\partial y} \right) \right) + I_k h_{ph,k} + Q$$
(6.14)

where:

 $C_{p,k}$ = Specific heat of fluid/liquid/vapor [Energy/(Mass·Temperature)]

 ϕ_k = fraction of the domain filled with fluid/liquid/vapor [-]

 ρ_k = Fluid/liquid/vapor density [Mass/Volume]

 k_k = Fluid/liquid/vapor conductivity [Energy/(Time·Length·Temperature)]

 $v_{\phi,x}$ and $v_{\phi,y}$ = Speed of fluid/liquid/vapor through porous media [Length/Time]

 I_k = Mass of fluid/liquid/vapor from phase change [Mass/(Volume Time)]

 $h_{ph,k}$ = Specific enthalpy of fluid/liquid/vapor (phase change from state to state) [Energy/(Mass·Temperature)]

Term $I_k h_{ph,k}$ has been added to account from phase change between different media states. Considering that medium (water) can have different states. Equation (6.14) should be written to include all mediums:

$$\sum_{k=1}^{k=numOfMediums} \left(\phi_k \rho_k C_{p,k} \frac{\partial T}{\partial t} \right) = \sum_{k=1}^{k=numOfMediums} \left[\phi_k \left(\frac{\partial}{\partial x} \left(k_{x,k} \cdot \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_{y,k} \cdot \frac{\partial T}{\partial y} \right) \right) \right] + \sum_{k=1}^{k=numOfMediums} \left(I_k h_{ph,k} \right) + Q_k \left(\frac{\partial}{\partial x} \left(k_{x,k} \cdot \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_{y,k} \cdot \frac{\partial T}{\partial y} \right) \right) \right]$$

6.3.3 Combined

By interposing equations (6.13) and (6.14) we finally get energy equation for porous media:

$$\left((1-\phi)\rho_d C_p + \phi \rho_k C_{p,k} \right) \frac{\partial T}{\partial t} =$$

$$\frac{\partial}{\partial x} \left(\left((1-\phi)k_x + \phi k_{x,k} \right) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\left((1-\phi)k_y + \phi k_{y,k} \right) \frac{\partial T}{\partial y} \right) + m_{ph,k} h_{ph,k}$$

$$(6.15)$$

by introducing equivalent coefficients:

$$\rho_e C_{p,e} = (1-\phi) \rho_d C_p + \sum_{k=1}^{numOfMedulims} \phi \rho_k C_{p,k}$$
$$k_{x,e} = (1-\phi) k_x + \sum_{k=1}^{numOfMedulims} \phi k_{x,k}$$
$$k_{y,e} = (1-\phi) k_y + \sum_{k=1}^{numOfMedulims} \phi k_{y,k}$$

equation (6.15) can be written as:

$$\rho_e C_{p,e} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k_{x,e} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_{y,e} \frac{\partial T}{\partial y} \right) + \sum_{k=1}^{numOfMediums} I_k h_{ph,k}$$
(6.16)

6.4 Definition of Material Porosity

Porosity or void fraction is a measure of the void spaces in a material and is a fraction of the volume of voids over the total volume, between 0 and 1, or as percentage between 0 and 100%. It is defined by the ratio:

$$\phi = \frac{V_p}{V_t} \tag{6.17}$$

Where,

 V_p = is the volume of void-space

 V_t = is the total bulk volume of material, including the solid and void components.

6.5 Pores Filled with Air and Water

Volume of entire domain contains of solid material, humid air, liquid water and ice:

$$V = V_d + V_{air} + V_l + V_i$$

Defining that as partial volumes:

$$1 = \frac{V_d}{V} + \frac{V_{air}}{V} + \frac{V_l}{V} + \frac{V_i}{V}$$
$$1 = (1 - \phi) + \phi_{air} + \phi_l + \phi_i$$

Which then finally leads to:

$$\phi = \phi_{air} + \phi_l + \phi_i \tag{6.18}$$

Relations between material content and partial porosities can be established as:

$$\gamma_{air} = \frac{m_{air}}{V} = \frac{\rho_{air} \cdot V_{air}}{V} = \rho_{air} \cdot \phi_{air}$$

and same for liquid and ice.

6.6 Conservation of Mass

The law of conservation of mass states that the total time rate of change of a matter in a fixed region is equal to the net rate of flow of matter across the surface or effectively, no matter can be created or destroyed. The mathematical statement of the principle results in the following equation, known as the conservation of mass, or also as continuity equation:

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \vec{v} = 0$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$$
(6.19)

 ρ = density of the fluid [Mass/Volume]

 \vec{v} = velocity vector [Length/Time]

Or, in its developed form for 2-D geometry:

$$\frac{\partial \rho}{\partial t} + v_x \frac{\partial \rho}{\partial x} + v_y \frac{\partial \rho}{\partial y} + \rho \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} \right) = 0$$
(6.20)

Assuming that <u>material density</u> is <u>constant over the region</u>, equation (6.19) becomes:

$$\frac{\partial \rho}{\partial t} + \rho \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} \right) = 0$$

For <u>incompressible fluids</u>, or fluids where compressibility is negligible, material derivative of the density is zero:

$$\frac{\partial \rho}{\partial t} = 0$$

The continuity equation (6.19) then becomes:

$$\nabla \cdot \vec{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0$$

For solids, this equation is satisfied automatically, since $v_x = v_y = 0$.

Mass conservation equation (6.19) can also be written in terms of mass flow rate:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{g} = 0 \tag{6.21}$$

where,

 \vec{g} = Flux of the material [Mass/(Area·Time)]

6.7 Mass Transport

Mass transfer is net movement of mass from one location to another. The phrase is commonly used in engineering for physical processes that involve diffusive and convective transport within physical systems.

6.7.1 Diffusion

Diffusion is the net movement of molecules or atoms from a region of high concentration to a region of low concentration. This is also referred to as movement of a substance down a concentration gradient. Diffusion is described by Fick's Laws of diffusion.

6.7.1.1 Fick's First Law

Fick's first law relates the diffusive flux to the concentration under the assumption of steady state. It postulates that the flux goes from regions of high concentration to regions of low concentration.

$$\vec{g}_{k} = -D_{f,k} \nabla \rho_{k} = -D_{f,k} \left(\frac{\partial \rho_{k}}{\partial x} \vec{i} + \frac{\partial \rho_{k}}{\partial y} \vec{j} \right)$$
(6.22)

 \vec{g}_{k} = Diffusion flux vector [Mass/(Area·Time)]

*D*_{*f,k*} = Diffusion coefficient or diffusivity [Area/Time]

 ρ_k = Specific Mass of substance [Mass/Volume]

6.7.1.2 Fick's Second Law

Fick's second law predicts how diffusion causes the concentration to change with time.

$$\frac{\partial \rho_k}{\partial t} = D_{f,k} \nabla^2 \rho_k = D_{f,k} \left(\frac{\partial^2 \rho_k}{\partial x^2} + \frac{\partial^2 \rho_k}{\partial y^2} \right)$$
(6.23)

6.7.1.3 Temperature Dependence of the Diffusion Coefficient in Solids

The diffusion coefficient in solids at different temperatures is generally found to be well predicted by the Arrhenius equation.

 $D_f = D_0 \cdot e^{-E_A/(\sigma T)}$

 D_0 = maximal diffusion coefficient (at infinite temperature) [Area/Time]

*E*_A = Activation energy for diffusion [Energy/atom]

T = Absolute temperature [Temperature]

 σ = Boltzmann constant [Units?]

6.7.2 Capillary Transport (Darcy's Law)

Equation that describes the flow of fluid through a porous medium is called Darcy's law. Darcy's law is a simple proportional relationship between the instantaneous discharge rate through a porous medium, the viscosity of the fluid and the pressure drop over a given distance. Equation for single phase (fluid) flow in vertical pipe is:

$$\begin{aligned} \boldsymbol{\mathcal{G}} &= -\frac{\boldsymbol{\pounds}A\left(P_{b}-P_{a}\right)}{\mu L} + \frac{\boldsymbol{\pounds}A}{\mu L}\left(\rho GL\right) \\ \boldsymbol{\mathcal{G}} &= \text{Total liquid discharge [Volume/Time]} \\ \boldsymbol{\pounds} &= \text{Intrinsic permeability of the medium [Area]} \\ \boldsymbol{A} &= \text{Cross-sectional area to flow [Area]} \\ \boldsymbol{P}_{b} - \boldsymbol{P}_{a} &= \text{Total pressure drop [Pressure]} \\ \boldsymbol{\mu} &= \text{Dynamic viscosity of the fluid [Pressure Time, or Mass/(Length Time)]} \\ \boldsymbol{L} &= \text{Length over which pressure drop is taking place [Length]} \\ \boldsymbol{G} &= \text{Gravity acceleration (9.81 m/s^{2}) [Length/Time^{2}]} \\ \text{The negative sign is because fluid flows from high to low pressure.} \\ \text{Dividing both sides of equation by the area:} \\ \boldsymbol{v} &= -\frac{\boldsymbol{\pounds}}{\mu}\frac{P_{b}-P_{a}}{L} + \frac{\boldsymbol{\pounds}}{\mu}\rho \boldsymbol{G} \end{aligned}$$
(6.24)

and applying it to infinitesimal distance (
$$L - > dy$$
):

$$v_{y} = -\frac{\mathbf{k}_{y}}{\mu_{y}} \frac{\partial P_{y}}{\partial y} + \frac{\mathbf{k}_{y}}{\mu_{y}} \rho G$$

and finally, equation in general (vector) form:

$$\vec{v} = -\frac{\mathbf{k}}{\mu} \Big(\nabla P - \rho \vec{G} \Big) \tag{6.25}$$

 \vec{v} = Darcy's velocity [Length/Time]

P = Pressure gradient vector [Pressure]

$$\vec{v} = -\left(\frac{\boldsymbol{k}_x}{\mu_x}\frac{\partial P_x}{\partial x}\vec{i} + \frac{\boldsymbol{k}_y}{\mu_y}\frac{\partial P_y}{\partial y}\vec{j}\right) + \frac{\boldsymbol{k}_y}{\mu_y}\rho G\vec{j}$$
(6.26)

Multiplying both sides of equation (6.26) with density of the fluid:

$$\vec{g} = \vec{v}\rho = -\rho \left(\frac{\boldsymbol{k}_x}{\mu_x} \frac{\partial P_x}{\partial x} \vec{i} + \frac{\boldsymbol{k}_y}{\mu_y} \frac{\partial P_y}{\partial y} \vec{j} \right) + \frac{\boldsymbol{k}_y}{\mu_y} \rho^2 G \vec{j}$$
(6.27)

6.7.3 Fluid/Liquid Flow Through Porous Media

As commonly observed, some fluid/liquid flows through the media while some mass of the fluid is stored in the pores present in the media. Mass conservation of fluid across the porous medium can be derived with (6.19). Furthermore, we have that $m = \rho V_p$, where V_p is the pore volume of the medium in the domain volume V. This can be expressed as:

$$m = \rho \phi V$$

where

 ϕ = is the porosity of the material (V_p / V) [-]

Mass conservation equation in this case will be:

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot \left(\rho\phi\vec{v}\right) = 0$$

$$\frac{\partial(\rho_k\phi)}{\partial t} + \nabla \cdot \vec{g}_k = 0$$
(6.28)

where

 \vec{g}_k = fluid mass flow rate [Mass/(Area·Time)]

 ρ_k = density of the fluid [Mass/Volume].

k = subscript used to designate liquid, vapor or solid

Introducing γ_k as fluid content in the medium ($\gamma_k = \phi \rho_k$), we can write continuity equation for fluid in porous media:

$$\frac{\partial \gamma_k}{\partial t} + \nabla \cdot \vec{g}_k = 0 \tag{6.29}$$

Mass flow rate of a fluid, *k*, through porous media can be calculated by applying Darcy's law (6.24):

$$v_k = -\frac{\mathbf{k}_k}{\mu_k} \frac{P_{k,b} - P_{k,a}}{L} + \frac{\mathbf{k}_k}{\mu_k} \gamma_k G \tag{6.30}$$

where pressure of the fluid from the gravity field is reduced by porosity of the material. This will lead to slightly modified equation (6.27) that will be valid for fluid in porous materials:

$$\vec{g}_{k} = -\frac{\boldsymbol{k}_{k}\rho_{k}}{\mu} \left[\frac{\partial P_{k,x}}{\partial x} \vec{i} + \left(\frac{\partial P_{k,y}}{\partial y} + \gamma_{k}G \right) \vec{j} \right]$$
(6.31)

Applying (6.31) into mass continuity equation for porous media in (6.29):

$$\frac{\partial \gamma_{k}}{\partial t} = \frac{\partial}{\partial x} \left(\frac{\mathbf{k}_{k,x} \cdot \rho_{k}}{\mu_{k}} \frac{\partial P_{k,x}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\mathbf{k}_{k,y} \cdot \rho_{k}}{\mu_{k}} \frac{\partial P_{k,y}}{\partial y} \right) - \frac{\partial}{\partial y} \left(\frac{\mathbf{k}_{k} \cdot \rho_{k}}{\mu_{k}} \gamma_{k} G \right)$$
(6.32)
6.8 Summary of Equations for Heat and Mass Transfer

Basic equations for heat and moisture transport are given in separate document and will be inserted here just for reference purpose.

6.8.1 Air flow through porous media

Governing Equation

$$\begin{split} \phi_{air} K_{1} \frac{\partial P_{air}}{\partial t} &= \frac{\partial}{\partial x} \left(\frac{\mathbf{f}_{air}}{\mu_{air}} P_{air} \cdot K_{1} \cdot \frac{\partial P_{air}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\mathbf{f}_{air}}{\mu_{air}} P_{air} \cdot K_{1} \cdot \frac{\partial P_{air}}{\partial y} \right) - \frac{\partial}{\partial y} \left(\frac{\mathbf{f}_{air} \cdot K_{1} \cdot P_{air}}{\mu_{air}} K_{1} \cdot \phi_{air} P_{air} G \right) \\ \rho_{air} &= \frac{P_{air} \left(1 + x \right)}{287.042 \left(T + 273.15 \right) \left(1 + 1.607858x \right)} = P_{air} \cdot K_{1} \\ x &= 0.621945 \cdot \frac{P_{v}}{P_{aam} - P_{v}} \\ P_{v} &= \varphi \cdot P_{v_{sat}} \\ p_{v} &= \varphi \cdot P_{v_{sat}} \end{split}$$

$$P_{v_{sat}} = \frac{e}{T^{8.2}}$$

6.8.2 Water mass transfer

Governing Equation

$$\frac{\partial \gamma_{w}}{\partial \varphi} \frac{\partial \varphi}{\partial t} = \frac{\partial}{\partial x} \left(\delta_{x} \frac{\partial \left(\varphi \gamma_{v_{sat}} \right)}{\partial x} \right) + \frac{\partial}{\partial y} \left(\delta_{y} \frac{\partial \left(\varphi \gamma_{v_{sat}} \right)}{\partial y} \right) + \frac{\partial}{\partial y} \left(\frac{\kappa_{air,x} \cdot \varphi \gamma_{v_{sat}}}{\mu_{air}} \cdot \frac{\partial P_{air}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\kappa_{air,y} \cdot \varphi \gamma_{v_{sat}}}{\mu_{air}} \cdot \frac{\partial P_{air}}{\partial y} \right) - \frac{\partial}{\partial y} \left(\frac{\kappa_{air,y} \cdot \varphi \gamma_{v_{sat}}}{\mu_{air}} \gamma_{air} G \right) + \frac{\partial}{\partial x} \left(D_{\varphi} \left(\frac{\partial \varphi}{\partial x} \right) \right) + \frac{\partial}{\partial y} \left(D_{\varphi} \left(\frac{\partial \varphi}{\partial y} - \frac{\kappa_{l} \rho_{l}}{\mu_{l} D_{\varphi}} \gamma_{l} \cdot G \right) \right) + S_{l} + S_{v}$$

Boundary Conditions

$$g_n = \beta (\gamma_a - \gamma)$$
$$\beta = \frac{h_c}{\rho_{air} C_{p,air}}$$

6.8.3 Heat transfer

Governing Equation

$$\rho_e \cdot C_{p,e} \cdot \frac{\partial T}{\partial t} = -\left[\frac{\partial}{\partial x}\left(k_{x,e}\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_{y,e}\frac{\partial T}{\partial y}\right)\right] - I_{il} \cdot h_{il} - I_{lg} \cdot h_{lg} + Q_s$$

$$\begin{aligned} \rho_e \cdot C_{p,e} &= (1 - \phi) \cdot \rho_d \cdot C_d + \phi_{air} \cdot \rho_{air} \cdot C_{p,air} + \phi_l \cdot \rho_l \cdot C_{p,l} + \phi_{ice} \cdot \rho_{ice} \cdot C_{p,ice} \\ k_{x,e} &= (1 - \phi) \cdot k_{x,d} + \phi_{air} \cdot k_{x,air} + \phi_l \cdot k_{x,l} + \phi_{ice} \cdot k_{x,ice} \\ k_{y,e} &= (1 - \phi) \cdot k_{y,d} + \phi_{air} \cdot k_{y,air} + \phi_l \cdot k_{y,l} + \phi_{ice} \cdot k_{y,ice} \end{aligned}$$

Boundary Conditions

With defined temperature:

$$T = f(x, y, t) \quad on \ \Gamma_T$$
$$T = T_{const} \qquad on \ \Gamma_T$$

With defined flux:

$$q_f = f(x, y, t) \text{ on } \Gamma_Q$$
$$q_f = q_{const} \text{ on } \Gamma_Q$$

Convection boundary condition:

$$q_c = h_c \left(T - T_c \right)$$

Radiation boundary condition:

$$q_r = h_r (x, y, t, T) (T - T_r)$$
$$h_r (x, y, t, T) = \varepsilon \sigma (T + T_r) (T^2 + T_r^2)$$

6.8.4 Combining Equations

In general, heat and mass transfer are divided in three separate models that will be solved through iterations. Pressure distribution will be solved first followed by mass transfer and finally temperature distribution. After solving each of these systems, results with previous state need to be examined. This is necessary because while solving for one unknown, it is considered that other two variables are constant. However, new solution will require that other two variables are recalculated again. All this needs to be repeated until all variables are within given tolerance.

6.9 Boundary Conditions

To complete the description of the general problem described in the previous section, suitable boundary and initial conditions are required. Boundary conditions are most easily understood and described by considering the fluid mechanics separate from other transport processes. In the following sections, boundary conditions associated with the viscous flow, porous flow, and thermal transport are discussed, followed by a discussion of the initial conditions.





6.10 Porous Flow Boundary Conditions

The flow conditions that can be applied to the boundary of a fluid-saturated porous medium depend on the specific model used to describe the problem. A Forchheimer or simple Darcy model allows the following type of boundary conditions:

Dirichlet or essential boundary conditions

$$\vec{v}_i \vec{n}_i = f^u(s,t)$$
 on Γ_i

Neumann or natural boundary conditions

$$T_i \vec{n}_i = -\hat{P}(s,t)\delta_{ij}n_j(s)\vec{n}_i = -\hat{P}(s,t) = f^{\tau}(s,t) \qquad on \quad \Gamma_{\tau}$$

Where,

s = coordinate along the boundary []

t = time [Time]

 \vec{n}_i = the outward unit normal to the boundary [-]

 \vec{v}_i = velocity vector [Length/Time]

The specified functions f^{u} and f^{τ} are generally simple expressions for standard situations where the fluid is contained by fixed boundaries ($f^{u} = 0$) or planes/lines of symmetry ($f^{\tau} = 0$), or

enters/leaves the domain (f^{τ} = constant) Ω_{f} . In essence these conditions state that the fluid velocity normal to the boundary may be specified (outflow/inflow) or the normal force (pressure) on the boundary may be imposed. Also, note that only one type of boundary condition can be specified at any point on the boundary.

For many applications a saturated porous layer will adjoin a clear fluid region and certain continuity conditions will be required at the open interface. The applicable conditions vary with the type of porous media model and in cases have not been rigorously verified. The major difficulty stems from the heterogeneous nature of the porous medium and the fact that a continuum

description is derived by and averaging process. Clearly, averaging within a distance $\approx \sqrt{k}$ of a boundary or interface is not valid and some loss of information will occur. The standard assumptions are that the pressure is continuous and the shear stress in the bulk fluid is related to the tangential velocity in the porous layer.

$$\frac{\partial v_f}{\partial n} = \frac{\alpha}{\sqrt{k}} \left(v_f - v_p \right)$$

Where,

 v_f = clear fluid velocity [Length/Time]

 V_p = velocity in porous media [Length/Time]

 α = material parameter [-]

6.11 Thermal and Transport Boundary Conditions

The thermal part of the boundary value problem for the fluid or solid requires the temperature (Dirichlet or essential condition) or the heat flux (Neumann or natural condition) to be specified on all parts of the boundary enclosing the heat transfer region:

$$T = \hat{T}(s,t) \quad on \quad \Gamma_T$$

$$k_x \frac{\partial T}{\partial x} \vec{n}_x + k_y \frac{\partial T}{\partial y} \vec{n}_y + q_f + q_c + q_r = q(s,t) \quad on \quad \Gamma_q$$

Where $\Gamma_{hT} = \Gamma_T \bigcup \Gamma_q$ is the total boundary enclosing the heat transfer region. Also, q_f , q_c and q_r refer to the flux, convective and radiative components given by:

$$q_{f} = cons$$

$$q_{c} = h_{c}(s,T,t)(T - T_{c})$$

$$q_{r} = h_{r}(s,T,t)(T - T_{r})$$
(6.33)

Where,

 h_c = the convective heat transfer coefficient

 T_c = the reference (or sink) temperature for convective transfer

 h_r = the effective radiation heat transfer coefficient

 T_r = the reference temperature for radiative transfer

Effective radiation heat transfer coefficient can be calculated as:

$$h_r = F\sigma(T+T_r)(T^2+T_r^2)$$

Where,

F = form factor σ = the Stefan-Boltzmann constant

The form factor given in the previous equation is dependent on geometry and is called view factor. View factor is the proportion of the radiation which leaves surface one that strikes surface two.

6.11.1 View Factors

The view factor is defined as the fraction of energy leaving a surface that arrives at a second surface. For surfaces with finite areas, the view factors are defined by:

$$F_{k \to j} = \frac{1}{A_k} \int_{A_k} \int_{A_j} \frac{\cos \theta_k \cos \theta_j}{\pi S^2} dA_k dA_j$$
(6.34)

Where S is the distance from a point on surface A_j to a point on surface A_k .

The angles θ_j and θ_k are measured between the line S and the normal to the surface (see Figure 15).



Figure 15. Nomenclature for Enclosure Radiation

From equation (6.34) it is clear that:

$$A_k F_{k \to j} = A_j F_{j \to k}$$

There are several ways to calculate view factors and one of them is "cross-string" rule illustrated in Figure 16.



and given by following equation:

$$F_{ij} = \frac{r_{12} + r_{21} - (r_{11} + r_{22})}{2L_i}$$

In the case when partial or third surface shadowing exist, the two radiating surfaces are subdivided into n finite sub-surfaces. Each subsurface will have its view factor calculated and finally, summation will give the view factor between two surfaces that do not fully see each other:

$$F_{ij} = \sum_{k=1}^{n} \sum_{l=1}^{n} F_{kl}$$

7 Appendix D: Finite Element Method Background

7.1 Preliminaries

7.1.1 Weighted Residual Method

In applied mathematics, the method of mean weighted residuals are methods for solving differential equations. The solutions of these differential equations are assumed to be well

approximated by a finite sum of test functions ϕ_i .

7.1.1.1 Exact solution

Boundary value problem: differential equation + boundary conditions. Displacement in a uniaxial bar subject to a distributed force p(x).

$$\frac{d^2u}{dx^2} + p(x) = 0, \qquad 0 \le x \le 1$$
(7.1)

and boundary conditions

$$u(0) = 0$$

$$\frac{du}{dx}(1) = 1$$
(7.2)

The exact solution is a twice differential function. In general, it is difficult to find the exact solution when the domain and/or boundary conditions are complicated. Sometimes the solution might not exist even if the problem is well defined.

7.1.1.2 Approximate Solution

The solution above satisfies the essential boundary conditions, but not natural boundary conditions (essential boundary conditions are conditions that are imposed explicitly on the solution and natural boundary conditions are those that automatically will be satisfied after solution of the problem).

The residual form of differential equation (7.1):

$$\frac{d^2u}{dx^2} + p(x) = R(x)$$

Minimize the residual by multiplying with a weight W and integrate over the domain:

$$\int_{0}^{1} R(x)W(x)dx = 0$$

If it satisfies for any W(x), then R(x) will approach zero and the approximate solution will approach the exact solution.

The approximate solution is a linear combination of trial functions.

$$u(x) = \sum_{i=1}^{N} c_i \phi_i(x)$$
(7.3)

Accuracy depends on the choice of trial functions. The approximate solution must satisfy the

essential BC.

7.1.1.2.1 Galerkin Method

Use N trial functions for weighting functions.

$$\int_{0}^{1} R(x)\phi_{i}(x)dx = 0, \qquad i = 1,...,N$$

$$\int_{0}^{1} (\frac{d^{2}u}{dx^{2}} + p(x))\phi_{i}(x)dx = 0, \qquad i = 1,...,N$$

$$\int_{0}^{1} \frac{d^{2}u}{dx^{2}}\phi_{i}(x)dx = -\int_{0}^{1} p(x)\phi_{i}(x)dx, \quad i = 1,...,N$$

Integration by parts reduces the order of differentiation in u(x).

$$\frac{du}{dx}\phi_{i}\Big|_{0}^{1}-\int_{0}^{1}\frac{du}{dx}\frac{d\phi_{i}}{dx}dx=-\int_{0}^{1}p(x)\phi_{i}(x)dx, \quad i=1,...,N$$

applying natural boundary conditions and rearranging:

$$\int_{0}^{1} \frac{d\phi_{i}}{dx} \frac{du}{dx} dx = \int_{0}^{1} p(x)\phi_{i}(x)dx + \frac{du}{dx}(1)\phi_{i}(1) - \frac{du}{dx}(0)\phi_{i}(0), \qquad i = 1, \dots, N$$

Substituting the approximate solution (7.3):

$$\int_{0}^{1} \frac{d\phi_{i}}{dx} \sum_{j=1}^{N} c_{j} \frac{d\phi_{j}}{dx} dx = \int_{0}^{1} p(x)\phi_{i}(x) dx + \frac{du}{dx}(1)\phi_{i}(1) - \frac{du}{dx}(0)\phi_{i}(0), \ i = 1, ..., N$$
(7.4)

Equation (7.4) can be rewritten in matrix form:

$$\sum_{j=1}^{N} K_{ij} c_j = F_i, \quad i = 1, ..., N$$

or

$$[K]_{(N\times N)} \{c\} = \{F\}_{(N\times 1)}$$

where

$$K_{ij} = \int_{0}^{1} \frac{d\phi_{i}}{dx} \frac{d\phi_{j}}{dx} dx$$

$$F_{i} = \int_{0}^{1} p(x)\phi_{i}(x)dx + \frac{du}{dx}(1)\phi_{i}(1) - \frac{du}{dx}(0)\phi_{i}(0)$$

The coefficient matrix is symmetric; $K_{ij} = K_{ji}$ and we get N equations with N unknown coefficients.

7.1.1.2.2 Example 1

We will consider the differential equation

$$\frac{d^2u}{dx^2} + 1 = 0, \qquad 0 \le x \le 1$$

with the following boundary conditions:

$$u(0) = 0$$
$$\frac{du}{dx}(1) = 1$$

Using the following trial functions:

$$\phi_1(x) = x$$

 $\phi_2(x) = x^2$
 $\phi_1(x) = 1$
 $\phi_1(x) = 2x$

The approximate solution (which satisfies essential boundary conditions):

$$u(x) = \sum_{i=1}^{2} c_i \phi_i(x) = c_1 x + c_2 x^2$$

The coefficient matrix and right-hand side vector:

$$K_{11} = \int_{0}^{1} (\phi_{1}(x))^{2} dx = 1$$

$$K_{12} = K_{21} = \int_{0}^{1} (\phi_{1}(x))^{2} dx = 1$$

$$K_{22} = \int_{0}^{1} (\phi_{2}(x))^{2} dx = \frac{4}{3}$$

$$F_{1} = \int_{0}^{1} \phi_{1}(x) dx + \phi_{1}(1) - \frac{du}{dx}(0) \phi_{1}(0) = \frac{3}{2}$$

$$F_{2} = \int_{0}^{1} \phi_{2}(x) dx + \phi_{2}(1) - \frac{du}{dx}(0) \phi_{2}(0) = \frac{4}{3}$$

The matrix equation:

$$[K] = \frac{1}{3} \begin{bmatrix} 3 & 3 \\ 3 & 4 \end{bmatrix}; \qquad F = \frac{1}{6} \begin{cases} 9 \\ 8 \end{cases}; \qquad \{c\} = [K]^{-1} \{F\} = \begin{cases} 2 \\ -\frac{1}{2} \end{cases}$$

Therefore, the approximate solution is:

$$u(x) = 2x - \frac{x^2}{2}$$

The approximate solution is also the exact solution because the linear combination of the trial functions can represent the exact solution.

7.1.1.2.3 Example 2

In this example, the differential equation is slightly changed:

$$\frac{d^2u}{dx^2} + x = 0, \quad 0 \le x \le 1$$

and the boundary conditions are:

$$u(0) = 0$$
$$\frac{du}{dx}(1) = 1$$

Using the same trial functions as in example 1:

$$\phi_1(x) = x$$

 $\phi_1(x) = 1$
 $\phi_2(x) = x^2$
 $\phi_1(x) = 1$
 $\phi_1(x) = 2x$

Because the trial functions are identical as in example 1, the coefficient matrix is the same. However, the force vector is different this time:

$$[K] = \frac{1}{3} \begin{bmatrix} 3 & 3 \\ 3 & 4 \end{bmatrix}; \qquad F = \frac{1}{12} \begin{bmatrix} 16 \\ 15 \end{bmatrix}; \quad \{c\} = [K]^{-1} \{F\} = \begin{cases} \frac{19}{12} \\ -\frac{1}{4} \end{cases}$$

which would lead to following approximate solution:

$$u(x) = \frac{19}{12}x - \frac{x^2}{4}$$

In this case, trial functions could not express the exact solution. Thus, the approximate solution is different from the exact one. The exact solution is:

$$u(x) = \frac{3}{2}x - \frac{x^3}{6}$$

7.2 Description of Method

The finite element method is a numerical method for determining approximate solutions to a large class of engineering problems. Regardless of the physical nature of the problem, a standard finite-element method primarily involves the following steps:

- 1. Definition of the problem and its domain
- 2. Discretization of the domain
- 3. Identification of state variables
- 4. Formulation of the problem
- 5. Establishing coordinate systems
- 6. Constructing approximate functions for the elements
- 7. Obtain element matrices and equations
- 8. Numerical integration
- 9. Assembly of element equations
- 10. Introduction of boundary conditions
- 11. Solution of the final set of simultaneous equations
- 12. Interpretation of the results

7.2.1 Definition of the Problem and its Domain

In finite element methods, there are primarily three sources of approximation. The first one is the definition of the domain (physically and geometrically); the other two are the discretization and solution algorithms. The approximation used in defining the physical characteristics of different regions.

7.2.2 Discretization of the Domain

Since the problem is usually defined over a continuous domain, the governing equations, with the exception of essential boundary conditions, are valid for the entirety of, as well as for any portion of, that domain. This allows idealization of the domain in the form of interconnected finite-sized domains (elements) of different sizes and shapes.

In finite-element idealization of the domain, we shall, in general, make reference to the following elements: finite element $\Omega_{_{\rho}}$ and master element $\tilde{\Omega}_{_{m}}$.

Finite elements are those which, when put together, result in a discrete version of the actual continuous domain. Their geometric approximations are controlled by the number of nodes utilized at the exterior of the elements to define their shape. The physical approximations are controlled by the total number of nodes utilized in defining the trial functions (shape functions) for state variable.

For a moment, let us assume that it is possible to systematically generate the approximation field function for the element Ω_{e} :

$$u(x, y, t) \approx u^{e}(x, y, t) = \sum_{j=1}^{n} u_{j}^{e}(t) \psi_{j}^{e}(x, y)$$
(7.5)

where, $u^{e}(x, y, t)$ represents an approximation of u(x, y, t) over the element Ω_{e} , u_{j}^{e} denote the values of function $u^{e}(x, y, t)$ at selected number of points, called *element nodes*, in the element Ω_{e} and $\psi_{i}^{e}(x, y, t)$ are the approximation functions associated with the element. The n parameters (or

nodal values) u_j^e in equation (7.5) must be determined such that the approximate solution $u^e(x, y, t)$ satisfies the boundary conditions of the problem. This process leads to n algebraic equations among the nodal values ($u_1^e, u_2^e, ..., u_n^e$). The set of algebraic equations is termed a *finite element model* of the original equation.

Master elements are those which are used in place of finite elements in order to facilitate computations in the element domain. Figure 17 illustrates and actual finite element Ω_e and corresponding master element $\tilde{\Omega}_w$.



Figure 17. Demonstration of Coordinate Transformation for a Rectangular Element

In general, the master elements are straight lines, right triangle or prisms, squares, and cubes. They are defined in reference to normalized coordinate axes (ξ , η , ς). The actual elements can be any shape and size.

7.2.3 Identification of State Variables

Until this step, no reference has been made to the physical nature of the problem. Whether it is a heat-transfer problem, fluid or solid-mechanics problem, etc., comes into the picture at this stage. The mathematical description of steady-state physical phenomena, for instance, leads to an elliptic boundary-value problem in which the formula contains the state variable and the flux. These variables are related to each other by a constitutive equation representing a mathematical expression of a physical law.

In our case, where we are trying to solve heat and mass transfer, there are three different equations and therefore, three different state variables.

According to given equations, the three state variables are air pressure, relative humidity (water content) and temperature. Therefore, approximation functions for our state variables are:

$$T(x, y, t) \approx T^{e}(x, y, t) = \sum_{j=1}^{n} T_{j}^{e}(t) \psi_{j}^{e}(x, y)$$
$$\varphi(x, y, t) \approx \varphi^{e}(x, y, t) = \sum_{j=1}^{n} \varphi_{j}^{e}(t) \psi_{j}^{e}(x, y)$$

$$P_{air}(x, y, t) \approx P_{air}^{e}(x, y, t) = \sum_{j=1}^{n} P_{air, j}^{e}(t) \psi_{j}^{e}(x, y)$$

7.2.4 Formulation of the Problem

Very often a physical problem is formulated via set of differential equations:

$$\overline{L}\overline{u} = \overline{f}$$

with boundary conditions or by an integral equation:

$$\pi = \int_{\Omega} G(x, y, z, u) d\Omega + \int_{\Gamma} g(x, y, z, u) d\Gamma$$

where "*u*" represents the state variable(s).

7.2.4.1 The Model Equation

Consider the problem of finding the solution *u* of the second-order partial differential equation:

$$-\frac{\partial}{\partial x}\left(a_{11}\frac{\partial u}{\partial x} + a_{12}\frac{\partial u}{\partial y}\right) - \frac{\partial}{\partial y}\left(a_{21}\frac{\partial u}{\partial x} + a_{22}\frac{\partial u}{\partial y}\right) + b\frac{\partial u}{\partial t} + a_{00}u - f = 0$$
(7.6)

for given data a_{ij} (i, j = 1, 2), *b*, a_{00} and f, and specified boundary conditions.

7.2.4.2 Weak Form

The weak form of a differential equation is a weighted-integral statement that is equivalent to both the governing differential equation as well as the associated natural boundary conditions. We shall develop the weak form of equation (7.6) over the typical element Ω_{e} .

$$0 = \int_{\Omega_e} \omega \left[-\frac{\partial}{\partial x} \left(a_{11} \frac{\partial u}{\partial x} + a_{12} \frac{\partial u}{\partial y} \right) - \frac{\partial}{\partial y} \left(a_{21} \frac{\partial u}{\partial x} + a_{22} \frac{\partial u}{\partial y} \right) + b \frac{\partial u}{\partial t} + a_{00} u - f \right] dxdy$$
(7.7)

In the second step, we distribute the differentiation among u and ω equally, so that both u and ω are required to be differentiable only once with respect to x and y. To achieve this we use integrationby-parts on the first two terms in equation (7.7). First we note the following identities for any differentiable functions $\omega(x,y)$, $F_1(x,y)$ and $F_2(x,y)$:

$$\frac{\partial}{\partial x}(\omega F_1) = \frac{\partial\omega}{\partial x}F_1 + \omega\frac{\partial F_1}{\partial x} \quad or \quad -\omega\frac{\partial F_1}{\partial x} = \frac{\partial\omega}{\partial x}F_1 - \frac{\partial}{\partial x}(\omega F_1)$$

$$\frac{\partial}{\partial y}(\omega F_2) = \frac{\partial\omega}{\partial y}F_2 + \omega\frac{\partial F_2}{\partial y} \quad or \quad -\omega\frac{\partial F_2}{\partial y} = \frac{\partial\omega}{\partial y}F_2 - \frac{\partial}{\partial y}(\omega F_2)$$
(7.8)

Next, we recall the component form of the gradient (or divergence) theorem:

$$\int_{\Omega_{e}} \frac{\partial}{\partial x} (\omega F_{1}) dx dy = \prod_{\Gamma_{e}} (\omega F_{1}) n_{x} ds$$

$$\int_{\Omega_{e}} \frac{\partial}{\partial y} (\omega F_{2}) dx dy = \prod_{\Gamma_{e}} (\omega F_{2}) n_{y} ds$$
(7.9)

where n_x and n_y are the components of the unit normal vector:

 $\vec{n} = n_x \vec{i} + n_y \vec{j} = \cos \alpha \cdot \vec{i} + \sin \alpha \cdot \vec{j}$

on the boundary Γ_e , and ds is the arclength of an infinitesimal line element along the boundary (see Figure 18).



Figure 18. Typical triangular element

Using (7.8) and (7.9) in (7.7), we obtain:

$$0 = \int_{\Omega_{e}} \left[\frac{\partial \omega}{\partial x} \left(a_{11} \frac{\partial u}{\partial x} + a_{12} \frac{\partial u}{\partial y} \right) + \frac{\partial \omega}{\partial y} \left(a_{21} \frac{\partial u}{\partial x} + a_{22} \frac{\partial u}{\partial y} \right) + \omega b \frac{\partial u}{\partial t} \right] dx dy$$

+
$$\iint_{\Gamma_{e}} \omega \left[n_{x} \left(a_{11} \frac{\partial u}{\partial x} + a_{12} \frac{\partial u}{\partial y} \right) + n_{y} \left(a_{21} \frac{\partial u}{\partial x} + a_{22} \frac{\partial u}{\partial y} \right) \right] ds$$
(7.10)

From an inspection of the boundary term in this equation, we note that the specification of u constitutes the essential boundary condition, and hence u is the primary variable. The specification of the coefficient of the weight function in the boundary expression:

$$q_{n} \equiv n_{x} \left(a_{11} \frac{\partial u}{\partial x} + a_{12} \frac{\partial u}{\partial y} \right) + n_{y} \left(a_{21} \frac{\partial u}{\partial x} + a_{22} \frac{\partial u}{\partial y} \right)$$
(7.11)

constitutes the natural boundary condition; thus q_n is the secondary variable of the formulation. The function $q_n = q_n(s)$ denotes the projection of the vector ∇u along the unit normal \vec{n} . By definition, q_n is positive outward from the surface as we move counter-clockwise along the boundary Γ_e .

The last step is to use definition (7.11) in (7.10) and write the weak form of equation (7.6):

$$0 = \int_{\Omega_{e}} \left[\frac{\partial \omega}{\partial x} \left(a_{11} \frac{\partial u}{\partial x} + a_{12} \frac{\partial u}{\partial y} \right) + \frac{\partial \omega}{\partial y} \left(a_{21} \frac{\partial u}{\partial x} + a_{22} \frac{\partial u}{\partial y} \right) + \omega b \frac{\partial u}{\partial t} + a_{00} \omega u - \omega f \right] dxdy$$

$$- \iint_{\Gamma_{e}} \omega q_{n} ds$$
(7.12)

7.2.5 Establishing a Coordinate System

There are primarily two reasons for choosing special coordinate axes for elements in addition to the global axes for the entire system. The first case is construction of the trial functions for the elements, and the second is ease of integration over the elements.

Once the coordinate axes are established, the element equations are ordinarily computed first in master element $\tilde{\Omega}_m$. Then are they transformed into Ω_e and finally into the global system for assembly.

7.2.6 Constructing Approximate Functions for the Elements

The finite element method involves the discretization of both the domain and the governing equations. By dividing the solution into a number of small regions, called finite elements, and approximating the solution over these regions by a suitable known function, a relation between the differential equations and the elements is established. The functions employed to represent the nature of the solution within each element are called shape functions, or interpolating functions, or basis functions. They are called interpolating functions as they are used to determine the value of the field variable within an element by interpolating the nodal values. Polynomial type functions have been most widely used as they can be integrated or differentiated easily and the accuracy of the results can be improved by increasing the order of the polynomial.

7.2.7 Obtain Element Matrices and Equations

The weak form described in above in the Weak Form section (see equation (7.12)) requires that the approximation chosen for u should be at least linear in both x and y so that there are no terms in (7.12) that are identically zero. Suppose that variable u is approximated over a typical finite element Ω_e as given by (7.5). Substituting the finite element approximation given by (7.5) for *u* into weak form (7.12), we obtain:

$$0 = \int_{\Omega_{e}} \left[\frac{\partial \omega}{\partial x} \left(a_{11} \sum_{j=1}^{n} u_{j} \frac{\partial \psi_{j}}{\partial x} + a_{12} \sum_{j=1}^{n} u_{j} \frac{\partial \psi_{j}}{\partial y} \right) + \frac{\partial \omega}{\partial y} \left(a_{21} \sum_{j=1}^{n} u_{j} \frac{\partial \psi_{j}}{\partial x} + a_{22} \sum_{j=1}^{n} u_{j} \frac{\partial \psi_{j}}{\partial y} \right) \right] dx dy - \iint_{\Gamma_{e}} \omega q_{n} ds$$

$$+ \omega b \sum_{j=1}^{n} \psi_{j} \frac{\partial u_{j}}{\partial t} + a_{00} \omega \sum_{j=1}^{n} u_{j} \psi_{j} - \omega f$$

$$(7.13)$$

This equation must hold for any weight function ω . Since we need n independent algebraic equations to solve for n unknowns $u_1, u_2, ..., u_n$, we choose n independent functions for $\omega = \Psi_1, \Psi_2$,

..., Ψ_n . This choice is a natural one when the weight function is viewed as a virtual variation of the dependent unknown. For each choice of ω , we obtain an algebraic relation among (u₁, u₂, ..., u_n). We label the algebraic equation result from substitution of Ψ_1 for ω into (7.13) as the first algebraic equation. The ith algebraic equation is obtained by substituting $\omega = \Psi_i$ into (7.13):

$$0 = \sum_{j=1}^{n} \left\{ \int_{\Omega_{e}} \left[\frac{\partial \psi_{i}}{\partial x} \left(a_{11} \frac{\partial \psi_{j}}{\partial x} + a_{12} \frac{\partial \psi_{j}}{\partial y} \right) + \frac{\partial \psi_{i}}{\partial y} \left(a_{21} \frac{\partial \psi_{j}}{\partial x} + a_{22} \frac{\partial \psi_{j}}{\partial y} \right) + a_{00} \psi_{i} \psi_{j} \right] dxdy \right\} u_{j}$$

$$0 = \sum_{j=1}^{n} \left\{ \int_{\Omega_{e}} b \psi_{i} \psi_{j} \frac{\partial u_{j}}{\partial t} - \int_{\Omega_{e}} f \psi_{i} dxdy - \prod_{\Gamma_{e}} \psi_{i} q_{n} ds \quad (i = 1, 2, ..., n) \right\}$$

or in matrix form:

$$\sum_{j=1}^{n} M_{ij} \frac{\partial u_{j}^{e}}{\partial t} + \sum_{j=1}^{n} K_{ij}^{e} u_{j}^{e} + \sum_{j=1}^{n} A_{ij} u_{j}^{e} = f_{i}^{e} + Q_{i}^{e}$$
(7.14)

where:

$$M_{ij}^{e} = \int_{\Omega_{e}} b\psi_{i}\psi_{j}dxdy$$

$$K_{ij}^{e} = \int_{\Omega_{e}} \left[\frac{\partial\psi_{i}}{\partial x} \left(a_{11} \frac{\partial\psi_{j}}{\partial x} + a_{12} \frac{\partial\psi_{j}}{\partial y} \right) + \frac{\partial\psi_{i}}{\partial y} \left(a_{21} \frac{\partial\psi_{j}}{\partial x} + a_{22} \frac{\partial\psi_{j}}{\partial y} \right) \right] dxdy$$

$$A_{ij}^{e} = \int_{\Omega_{e}} a_{00}\psi_{i}\psi_{j}dxdy$$

$$f_{i}^{e} = \int_{\Omega_{e}} f\psi_{i}^{e}dxdy, \qquad Q_{i}^{e} = \prod_{\Gamma_{e}} q_{n}\psi_{i}^{e}ds$$

$$(7.15)$$

In matrix notation, equation (7.14) takes the form:

$$\begin{bmatrix} M^e \end{bmatrix} \left\{ \dot{u}^e \right\} + \begin{bmatrix} K^e \end{bmatrix} \left\{ u^e \right\} + \begin{bmatrix} A^e \end{bmatrix} \left\{ u^e \right\} = \left\{ f^e \right\} + \left\{ Q^e \right\}$$
(7.16)

For given timestep value, the previous equation can be written as:

$$\frac{\left[M^{e}\right]}{\Delta t}\left\{u_{i}^{e}-u_{i-1}^{e}\right\}+\left[K^{e}\right]\left\{u_{i}^{e}\right\}+\left[A^{e}\right]\left\{u_{i}^{e}\right\}=\left\{f^{e}\right\}+\left\{Q^{e}\right\}$$
(7.17)

where u_{i-1}^{e} is a state variable from the previous timestep or the initial state in case i=1, and u_{i}^{e} is the unknown value of the state variable for the current timestep. This equation finally can be solved as:

$$u_i^e = \left(\frac{\left[M^e\right]}{\Delta t} + \left[K^e\right] + \left[A^e\right]\right)^{-1} \cdot \left(\frac{\left[M^e\right]}{\Delta t} \left\{u_{i-1}^e\right\} + \left\{f^e\right\} + \left\{Q^e\right\}\right)$$
(7.18)

7.2.8 Numerical Integration

Since the interpolation functions are easily derivable for a rectangular element and it is easier to evaluate integrals over rectangular geometries, we transform the finite element integral statement defined over quadrilaterals to a rectangle (see Figure 17). The transformation results in complicated expressions in terms of the coordinates used for the rectangular element. Therefore, numerical integration is used to evaluate such expressions. Numerical integration schemes, such as the Gauss-Legendre scheme, require that the integral be evaluated on a specific domain or with respect to a specific coordinate system. Gauss quadrature, for example, require that the integral be

expressed over a square region $\tilde{\Omega}_m$ of dimensions 2 by 2 and that the coordinate system (ξ, η) be such that $-1 \leq (\xi, \eta) \leq 1$. The transformation of a given integral expression, defined over the element Ω_e , to the domain $\tilde{\Omega}_m$ must be such as to facilitate numerical integration. Each element of the finite element mesh is transformed to $\tilde{\Omega}_m$, only for the purpose of numerically evaluating the integrals.

7.2.8.1 Coordinate Transformation

Coordinate transformations of physical entities such as vectors and matrices follow well-defined rules. They are often done in the form of a Jacobian matrix.

7.2.8.1.1 Rectangular Element

For instance, let us assume that there are two different coordinate systems, for example x, y located in the element domain, and ξ , η , located in the master element:

$$T: \frac{x = x(\xi, \eta)}{y = y(\xi, \eta)}$$

The transformation between actual element Ω_e and the master element $\tilde{\Omega}_m$ [or equivalently between (x,y) and (ξ , η)] is accomplished by a coordinate transformation of the form:

$$x = \sum_{j=1}^{m} x_{j}^{e} \tilde{\psi}_{j}^{e}(\xi, \eta)$$

$$y = \sum_{j=1}^{m} y_{j}^{e} \tilde{\psi}_{j}^{e}(\xi, \eta)$$
(7.19)

where $\tilde{\psi}_{i}^{e}$ denotes the finite element interpolation functions of the master element $\tilde{\Omega}_{m}$.

An infinitesimal line segment (or area and volume) in one coordinate system can be transformed into another by following the usual rules of differentiation:

$$\begin{bmatrix} \frac{\partial \tilde{\psi}_{i}^{e}}{\partial \xi} \\ \frac{\partial \tilde{\psi}_{i}^{e}}{\partial \eta} \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial \psi_{i}^{e}}{\partial x} \\ \frac{\partial \psi_{i}^{e}}{\partial y} \end{bmatrix}$$
(7.20)

The matrix on right-hand side of this equation is known as *Jacobian*. The inverse transformation which defines mapping of element Ω_e back into the master element $\tilde{\Omega}_m$ follows a similar rule. This is referred to as the *inverse transformation*:

$$\begin{bmatrix} \frac{\partial \psi_i^e}{\partial x} \\ \frac{\partial \psi_i^e}{\partial y} \end{bmatrix} = J^{-1} \cdot \begin{bmatrix} \frac{\partial \tilde{\psi}_i^e}{\partial \xi} \\ \frac{\partial \tilde{\psi}_i^e}{\partial \eta} \end{bmatrix}$$
(7.21)

where J^{-1} is the inverse matrix of the Jacobian:

$$J^{-1} = \begin{bmatrix} J_{11}^* & J_{12}^* \\ J_{21}^* & J_{22}^* \end{bmatrix} = \frac{1}{\det[J]} \cdot \begin{bmatrix} \frac{\partial y}{\partial \eta} & -\frac{\partial y}{\partial \xi} \\ -\frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \xi} \end{bmatrix}$$

This implies that the condition of |J| > 0 must be satisfied for every point in both domains.

The elemental area dA = dxdy in the element Ω_e is transformed to:

$$dA \equiv dxdy = \det[J]d\xi d\eta$$

When a typical element of the finite element mesh is transformed to its master element for the purpose of numerically evaluating integrals, the integrand must also be expressed in terms of the coordinates (ξ , η) of the master element. For example, consider the element coefficients:

$$K_{ij}^{e} = \int_{\Omega_{e}} \left(k_{11}(x, y) \frac{\partial \psi_{i}^{e}(x, y)}{\partial x} \frac{\partial \psi_{j}^{e}(x, y)}{\partial x} + k_{22}(x, y) \frac{\partial \psi_{i}^{e}(x, y)}{\partial y} \frac{\partial \psi_{j}^{e}(x, y)}{\partial y} \right) dxdy$$
$$C_{ij}^{e} = \int_{\Omega_{e}} c(x, y) \psi_{i}^{e}(x, y) \psi_{j}^{e}(x, y) dxdy$$

The integrand (i.e., expression in square brackets under the integral) is a function of global coordinates x and y. We must rewrite it in terms of ξ and η using the transformation (7.21):

$$K_{ij}^{e} = \int_{\tilde{\Omega}_{m}} \left(\hat{k}_{11}(\xi,\eta) \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{i}(\xi,\eta)}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{i}(\xi,\eta)}{\partial \eta} \right) \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \eta} \right) \right) \right) \det[J] d\xi d\eta$$
$$+ k_{22} \left(\xi, \eta \right) \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{i}(\xi,\eta)}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{i}(\xi,\eta)}{\partial \eta} \right) \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \eta} \right) \right) \det[J] d\xi d\eta$$
$$C_{ij}^{e} = \int_{\Omega} \hat{c}(\xi,\eta) \cdot \tilde{\psi}_{i}^{e}(\xi,\eta) \cdot \tilde{\psi}_{j}^{e}(\xi,\eta) \cdot \det[J] \cdot d\xi d\eta$$

Note that conversion of k_{11} , k_{22} and c coefficients can be simply achieved by applying coordinate transformation shown in (7.19).

7.2.8.1.2 Line Element

For line element coordinate transformation is:

$$T: s = s(x, y) = \sum_{j=1}^{m} s_j^e \tilde{\psi}_j^e(\xi)$$

An infinitesimal line segment in one coordinate system can be transformed into another by following the usual rules of differentiation:

$$ds = \det d\xi$$

7.2.8.1.2.1 Linear Line Element

The determinant for the linear line element can simply be calculated as the distance between two points:

$$\det = \frac{ds}{d\xi} = \frac{1}{2} (s_2 - s_1) = \frac{1}{2} \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$
(7.22)

7.2.9 Numerical Integration Over Master Element

Integrals defined over a rectangular master element $\tilde{\Omega}_m$ can be numerically evaluated using the Gauss-Legendre quadrature formulas:

$$\int_{\tilde{\Omega}_m} F(\xi,\eta) d\xi d\eta = \int_{-1-1}^{1} F(\xi,\eta) d\xi d\eta \approx \sum_{I=1}^{M} \sum_{J=1}^{N} F(\xi_I,\eta_J) W_I W_J$$

where M and N denote the number of Gauss quadrature points, (ξ_I, η_J) denote the Gauss point coordinates, and W_I and W_J denote the corresponding Gauss weights.

Similarly, integration over line elements can be done in the same way:

$$\int_{\tilde{\Gamma}_m} F(\xi) d\xi = \int_{-1}^{1} F(\xi) d\xi \approx \sum_{I=1}^{M} F(\xi_I) W_I$$

Quadrature weights and points for different number of integration points are given in Table 4.

Points ξ _ι	r	Weights W ₁	
0.0000000	One-point formula	2.000000	
$\pm \frac{1}{\sqrt{3}}$	Two-point formula	1.0000000	
0.0000000	Three-point formula	0.8888889	
$\pm\sqrt{\frac{3}{5}}$		0.5555556	

Table 4. Quadrature weights and points

7.2.10 Assembly of Element Equations

The assembly of element matrix equations ($p_e = k_e u_e$) is done according to the topological configuration of the elements after this equation is transformed into the global system. The assembly is done through the nodes as the interfaces which are common to the adjacent elements. At these nodes, the continuities are established with respect to the state variable and possibly with respect to its derivatives. Sometimes this assembly is done through certain nodes only, referred to as the *primary nodes* (e.g. corner nodes), instead of to all the nodes at the interfaces. This reduces the overall size of the assembled matrix. The nodes that are not used in the assembly, the so-called *secondary nodes*, are used together with the primary nodes to increase the degree of approximation at the element level. Assume that the complete element matrix is partitioned as follows:

$$\begin{bmatrix} P_I \\ P_{II} \end{bmatrix} = \begin{bmatrix} K_{I,I} & K_{I,II} \\ K_{II,I} & K_{II,II} \end{bmatrix} \begin{bmatrix} U_I \\ U_{II} \end{bmatrix}$$

in which subscripts I and II identify the portions of the equations corresponding to primary and secondary nodes, respectively. The equation can be brought to the following form:

$$P_{I} - K_{I,II} K_{II,II}^{-1} P_{II} = \left[K_{I,I} - K_{I,II} K_{II,II}^{-1} K_{II,I} \right] U_{I}$$

which, in short, can be written as:

$$P_e = K_e U_e$$

this is the final equation assembled. It contains the unknown value of the function at the primary nodes only. To illustrate the assembly, let assume that domain Ω in 2D space consist of three elements (rectangular, triangular and line), as shown in Figure 19.



Figure 19. Assembly of Three Elements

The element submatrices are identified as the dyadic product of element designations using primary nodes (i, j, q and r are the numbers assigned to nodes).

$$\begin{bmatrix} i\\ j\\ q\\ r \end{bmatrix} \begin{bmatrix} i & j & q & r \end{bmatrix} = \begin{bmatrix} ii & ij & iq & ir\\ ji & jj & jq & jr\\ qi & qj & qq & qr\\ ri & rj & rq & rr \end{bmatrix}$$

Which, for the example shown in Figure 19, leads to the following element submatrices:

$$\begin{bmatrix} P_{1} \\ P_{5} \\ P_{4} \\ P_{3} \end{bmatrix} = \begin{bmatrix} K_{ii}^{I} & K_{ij}^{I} & K_{iq}^{I} & K_{ir}^{I} \\ K_{ji}^{I} & K_{jj}^{I} & K_{jq}^{I} & K_{jr}^{I} \\ K_{qi}^{I} & K_{qj}^{I} & K_{qq}^{I} & K_{qr}^{I} \\ K_{ri}^{I} & K_{rj}^{I} & K_{rq}^{I} & K_{rr}^{I} \end{bmatrix} \cdot \begin{bmatrix} U_{1} \\ U_{5} \\ U_{4} \\ U_{3} \end{bmatrix}$$

$$\begin{bmatrix} P_{3} \\ P_{2} \\ P_{3} \end{bmatrix} = \begin{bmatrix} K_{ii}^{II} & K_{ij}^{II} & K_{iq}^{II} \\ K_{ji}^{II} & K_{jj}^{II} & K_{jq}^{II} \\ K_{qi}^{II} & K_{qj}^{II} & K_{qq}^{II} \end{bmatrix} \cdot \begin{bmatrix} U_{3} \\ U_{2} \\ U_{1} \end{bmatrix}$$
$$\begin{bmatrix} P_{2} \\ P_{4} \end{bmatrix} = \begin{bmatrix} K_{ii}^{III} & K_{ij}^{III} \\ K_{ji}^{III} & K_{jj}^{III} \end{bmatrix} \cdot \begin{bmatrix} U_{2} \\ U_{4} \end{bmatrix}$$

With this designation, the assembled version of the complete matrix of the configuration shown in Figure 19 will be:

$$\begin{bmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \\ P_5 \end{bmatrix} = \begin{bmatrix} K_{ii}^{I} + K_{qq}^{II} & K_{qj}^{II} & K_{ir}^{I} + K_{qi}^{II} & K_{iq}^{I} & K_{ij}^{I} \\ & K_{jj}^{II} + K_{ii}^{III} & K_{ji}^{II} & K_{ij}^{II} & 0 \\ & K_{rr}^{I} + K_{ii}^{II} & K_{rq}^{I} & K_{rj}^{I} \\ & & K_{qq}^{I} + K_{jj}^{III} & K_{qj}^{I} \\ & & & K_{qq}^{I} + K_{jj}^{III} & K_{qj}^{I} \\ & & & & & K_{qq}^{I} + K_{jj}^{III} & K_{qj}^{I} \\ \end{bmatrix} \cdot \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \\ U_5 \end{bmatrix}$$

The final results of assembling all these elements is the system of linear equations which is solved by unknown nodal values (state variable).

 $||K|| \cdot \{U\} = \{P\}$

7.2.11 Introduction of Boundary Conditions

In most problems of interest, one encounters situations where the portion of the boundary on which natural boundary conditions are specified has points in common with the portion of the boundary on which the essential boundary conditions are specified. In other words, at a few nodal points of the mesh, both the primary and secondary degrees of freedom may be specified. Such points are called singular points. Obviously, one cannot impose boundary conditions on both the primary and secondary variables at the same point.

At this stage, the essential boundary conditions are introduced. The most common forms of boundary conditions are:

$$\int_{\Gamma_h} h(u-u_\infty) d\Gamma_h + \int_{\Gamma_q} q_f d\Gamma_q = 0$$

where h is a given "film" coefficient, q_f is the flux through the boundary, u_{∞} is the value of the state variable at the boundary condition.

Using the weak form:

$$\int_{\Gamma_h} \omega h(u-u_\infty) d\Gamma_h + \int_{\Gamma_q} \omega q_f d\Gamma_q = 0$$

Creating ith algebraic equation ($\omega = \psi_i^e$) from above:

$$\int_{\Gamma_h} \psi_i^e(s) \cdot h \cdot \left(\sum_{j=1}^n u_j^e \psi_j^e(s) - u_\infty \right) d\Gamma_h + \int_{\Gamma_q} \psi_i^e(s) \cdot q_f d\Gamma_q = 0$$

and transforming it to local coordinate system:

$$\sum_{i=1}^{n} h \cdot \tilde{\psi}_{i}^{e}(\xi) \cdot \sum_{j=1}^{n} u_{j}^{e} \tilde{\psi}_{j}^{e}(\xi) \cdot \det - \sum_{i=1}^{n} h \cdot \tilde{\psi}_{i}^{e}(\xi) \cdot u_{\infty} \cdot \det + \sum_{i=1}^{n} q_{f} \cdot \tilde{\psi}_{i}^{e}(\xi) \cdot \det = 0$$

Where det is calculated by using equation (7.22) and $\tilde{\psi}_{j}^{e}$ are local shape functions. Finally, this will lead to matrix equations:

$$\begin{bmatrix} H_{ij} \end{bmatrix} \{ u_j \} = \{ HU_i \} - \{ Q_{fi} \}$$

where:

$$H_{ij} = h \cdot \tilde{\psi}_i^e(\xi) \cdot \tilde{\psi}_j^e(\xi) \cdot \det$$

 $HU_i = h \cdot \tilde{\psi}_i^e(\xi) \cdot u_\infty \cdot \det$

$$Q_{fi} = q_f \cdot \tilde{\psi}_i^e(\xi) \cdot \det$$

7.2.12 Solution of the Final Set of Simultaneous Equations

Until this step, there was no reference to whether the problem is linear or nonlinear. Regardless of the nature of the problem, the finite element method will eventually yield to the solution of a set of simultaneous differential equations. The solution procedure for simultaneous equations in general is categorized into the three parts: (1) direct, (2) iterative and (3) stochastic.

In the case of thermal and mass transfer, the solution will be achieved in a direct way or in cases when a direct solution is impossible, an iterative approach will be applied.

7.2.13 Interpretation of Results

The previous step resulted in the approximate values of the state variable at discrete points (nodes) of the domain. Normally these values are interpreted and used for calculations of other physical entities, such as flux, either throughout the domain or in certain regions of it.

This is the decision-making step and is probably the most important step in the entire process. Two important questions must be answered at this point: *How good are the results?* and *What should be done with them?* The first requires the estimation of error bounds, and the second involves the physical nature of the problem.

7.2.14 Nonlinear Problem

A nonlinear problem will be introduced in certain cases of heat and mass transfer. A good example is a radiation boundary condition in heat transfer where the radiation heat transfer coefficient is dependent on an unknown temperature. While the governing equation for heat transfer is linear and can be solved directly, that is not the case with pressure and water transfer, and therefore a non-linear approach must be applied. The problem also becomes non-linear if any of the coefficients are dependent on the state variable (see chapter 7.2.15).

Considering that the nonlinear equation f(u) = 0 cannot be directly solved by variable u, one approach that can be applied is to replace u with $u + \Delta u$, so that equation $f(u + \Delta u) = 0$ will be solved by Δu . Finally, the solution of the state variable u will be achieved through the following equation:

$$u^{(a)} = u^{(a-1)} + \alpha \cdot \Delta u^{(a)}$$
(7.23)

where α is the relaxation parameter ($0 < \alpha \le 1$), "(a)" denotes the current iteration step, $u^{(a)}$ is the evaluated value of the state variable at current iteration "(a)", $u^{(a-1)}$ is the evaluated value at the previous iteration and $\Delta u^{(a)}$ is the evaluated change of state variable in the current iteration. Note that setting the relaxation parameter to zero will not converge since the next solution is going to be estimated to be equal to the previous.

To achieve convergence of the state variable (*u*), the following equation has been used:

$$enorm = \sqrt{u_1^2 + u_2^2 + u_3^2 + \dots + u_n^2}$$

Convergence Criteria

If $enorm^{a-1}$ is from the previous iteration, then the solution is achieved when:

$$dif = \frac{\left|enorm^{a} - enorm^{a-1}\right|}{enorm^{a}} < tolerance$$

Where dif is the achieved tolerance.

7.2.15 Coefficients Dependence on State Variables

It is often the case that coefficients are expressed as a function of a state variable when they need to be evaluated when solving a system of nonlinear equations. Even if the coefficient dependence of the state variable is linear, the solution method that needs to be applied in this case must be for the nonlinear case.

A coefficient that is dependent on the value of the state variable c(u) will have a different value when a small change in the state variable happens $c(u + \Delta u)$. Since the value of Δu will be unknown at the moment, it is important to provide an approximation of $c(u + \Delta u)$:

$$\frac{\partial c}{\partial t} = \frac{c(u + \Delta u) - c(u)}{\Delta u} \implies \qquad c(u + \Delta u) = c(u) + \Delta u \frac{\partial c}{\partial t}$$
(7.24)

The above equation can be used in the iterative process since the value of c(u) will be able to be calculated by applying the state value from the previous iteration, while Δu is a vector of

unknowns by which the matrix equations will be solved.

This approach can be used to estimate conduction coefficients over the entire domain as well as on coefficients at boundary conditions. The state variable and change of state variable can be approximated as:

$$u(x, y) + \Delta u(x, y) \approx u^{e}(x, y) + \Delta u^{e}(x, y) = \sum_{j=1}^{n} u_{j}^{e} \psi_{j}^{e}(x, y) + \sum_{j=1}^{n} \Delta u_{j}^{e} \psi_{j}^{e}(x, y)$$
(7.25)

Further on, we will consider more general cases of element equations along with boundary conditions when coefficients are some function of state variable.

7.2.16 Equations and Matrices for Common Structures

In this section, we will consider common equation structures that can be found in the governing equations. By common structure we consider a type of differential equation. For example, we can consider capacitance part of the governing equations:

$$\phi_{air}K_1 \frac{\partial P_{air}}{\partial t}$$
, $\frac{\partial \gamma_w}{\partial \varphi} \frac{\partial \varphi}{\partial t}$ and $\rho_e \cdot C_{p,e} \cdot \frac{\partial T}{\partial t}$

It is important to notice that all three differential equations have the same structure related to the state variable (pressure, relative humidity and temperature), which will make the conversion to finite element matrices identical.

7.2.16.1 Capacitance Coefficients and Matrix

The capacitance part of the differential equation is written as:

$$r \cdot \frac{\partial u}{\partial t}$$

Where r is any coefficient that can be constant or state dependent, and u is a state variable. Related to timesteps, this equation can be written as:

$$r\frac{\partial u}{\partial t} \Longrightarrow r\frac{u_{[t]} - u_{[t-1]}}{\Delta t}$$

Converting it to the weak form:

$$\int_{\Omega_m} \omega \frac{r}{\Delta t} \left(\sum_{j=1}^n \psi_j^e(x, y) u_{[t]}^e - \sum_{j=1}^n \psi_j^e(x, y) u_{[t-1]}^e \right) = 0$$

Where $u_{[t-1]}^{e}$ is the state solution from the previous timestep or the initial state, $u_{[t]}^{e}$ is an unknown value of state at timestep t by which the matrix needs to be solved.

Further discretization will lead to:

$$\sum_{i=1}^{n} \int_{\Omega_{m}} \psi_{i}^{e}(x, y) \frac{r}{\Delta t} \left(\sum_{j=1}^{n} \psi_{j}^{e}(x, y) u_{[t]} - \sum_{j=1}^{n} \psi_{j}^{e}(x, y) u_{[t-1]} \right) = 0$$

Which finally in matrix form is:

$$M_{ij}^{e} u_{[t]} - M_{ij}^{e} u_{[t-1]} = 0$$

Where,

$$M_{ij}^{e} = \frac{r}{\Delta t} \tilde{\psi}_{i}^{e} (\xi, \eta) \tilde{\psi}_{j}^{e} (\xi, \eta) \det[J]$$
(7.26)

7.2.16.2 Conduction Coefficient and Matrix

The conduction equation is given in the following form:

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial u}{\partial y} \right) = 0$$

Where conductivity k represents either thermal conductivity, a suction curve or a diffusion coefficient. Introducing the weak form over the master element:

$$\int_{\Omega_m} \left(\frac{\partial \omega}{\partial x} \left(k_x \sum_{j=1}^n \frac{\partial \psi_j^e(x, y) u_j^e}{\partial x} \right) + \frac{\partial \omega}{\partial y} \left(k_y \sum_{j=1}^n \frac{\partial \psi_j^e(x, y) u_j^e}{\partial y} \right) \right) dx dy = 0$$

Where the system of equations will look like:

$$\int_{\Omega_m} \sum_{i=1}^n \left(\frac{\partial \psi_i^j(x, y)}{\partial x} \left(k_x \sum_{j=1}^n \frac{\partial \psi_j^e(x, y) u_j^e}{\partial x} \right) + \frac{\partial \psi_i^j(x, y)}{\partial y} \left(k_y \sum_{j=1}^n \frac{\partial \psi_j^e(x, y) u_j^e}{\partial y} \right) \right) dx dy = 0$$

Which will finally give following matrix equation:

$$\left[K_{ij}^{e}\right]\left\{u_{j}^{e}\right\}=0$$

Where:

$$\left[K_{ij}^{e}\right] = \int_{\Omega_{m}} \left(k_{11}(x, y) \frac{\partial \psi_{i}^{e}(x, y)}{\partial x} \frac{\partial \psi_{j}^{e}(x, y)}{\partial x} + k_{22}(x, y) \frac{\partial \psi_{i}^{e}(x, y)}{\partial y} \frac{\partial \psi_{j}^{e}(x, y)}{\partial y}\right) dx dy$$

Or in the local coordinate system:

$$\begin{bmatrix} K_{ij}^{e} \end{bmatrix} = \int_{\tilde{\Omega}_{m}} \begin{pmatrix} \hat{k}_{11}(\xi,\eta) \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{i}(\xi,\eta)}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{i}(\xi,\eta)}{\partial \eta} \right) \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \eta} \right) \\ + k_{22}(\xi,\eta) \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{i}(\xi,\eta)}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{i}(\xi,\eta)}{\partial \eta} \right) \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \eta} \right) \end{pmatrix} \det[J] d\xi d\eta$$

7.2.16.3 Conduction Coefficient with Derivative and Matrix

Sometimes the conduction coefficient will have a derivative over a known variable, which is the case in the moisture equation. In general terms, the equation can be written as:

$$\frac{\partial \gamma}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial \gamma}{\partial y}\frac{\partial u}{\partial y} = 0$$

Introducing the weak form over the master element:

$$\int_{\Omega_m} \left(\omega \cdot \sum_{j=1}^n \frac{\partial \psi_j^e(x, y)}{\partial x} u_j^e \cdot \sum_{k=1}^n \left(\frac{\partial \psi_k^e(x, y)}{\partial x} \cdot \gamma_k^e \right) + \\ \omega \cdot \sum_{j=1}^n \frac{\partial \psi_j^e(x, y)}{\partial y} u_j^e \cdot \sum_{k=1}^n \left(\frac{\partial \psi_k^e(x, y)}{\partial y} \cdot \gamma_k^e \right) + \right) dx dy = 0$$

Then forming a system of equations:

$$\int_{\Omega_m} \sum_{i=1}^n \left(\psi_i^e(x,y) \cdot \sum_{j=1}^n \left(\frac{\partial \psi_j^e(x,y)}{\partial x} u_j^e \right) \cdot \sum_{k=1}^n \left(\frac{\partial \psi_k^e(x,y)}{\partial x} \cdot \gamma_k^e \right) + \right) \\ \psi_i^e(x,y) \cdot \sum_{j=1}^n \left(\frac{\partial \psi_j^e(x,y)}{\partial y} u_j^e \right) \cdot \sum_{k=1}^n \left(\frac{\partial \psi_k^e(x,y)}{\partial y} \cdot \gamma_k^e \right) + \right) \\ dxdy = 0$$

This will then lead to the matrix equation:

$$\left[\gamma_{ij}^{e}\right]\left\{u_{j}^{e}\right\}=0$$

Where:

$$\begin{bmatrix} \gamma_{ij}^{e} \end{bmatrix} = \int_{\Omega_{m}} \begin{pmatrix} \psi_{i}^{e}(x, y) \cdot \frac{\partial \psi_{j}^{e}(x, y)}{\partial x} \cdot \sum_{k=1}^{n} \begin{pmatrix} \frac{\partial \psi_{k}^{e}(x, y)}{\partial x} \cdot \gamma_{k}^{e} \end{pmatrix} + \\ \psi_{i}^{e}(x, y) \cdot \frac{\partial \psi_{j}^{e}(x, y)}{\partial y} \cdot \sum_{k=1}^{n} \begin{pmatrix} \frac{\partial \psi_{k}^{e}(x, y)}{\partial y} \cdot \gamma_{k}^{e} \end{pmatrix} + \end{pmatrix} dxdy$$

And then in the local coordinate system:

$$\begin{bmatrix} \gamma_{ij}^{e} \end{bmatrix} = \int_{\tilde{\Omega}_{m}} \begin{pmatrix} \psi_{i}^{e}(\xi,\eta) \cdot \left(J_{11}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \eta}\right) \cdot \sum_{k=1}^{n} \left(\int_{11}^{*} \frac{\partial \tilde{\psi}_{k}(\xi,\eta)}{\partial \xi} + J_{12}^{*} \frac{\partial \tilde{\psi}_{k}(\xi,\eta)}{\partial \eta} \right) \cdot \gamma_{k}^{e} \end{pmatrix} + \\ \psi_{i}^{e}(\xi,\eta) \cdot \left(J_{21}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{j}(\xi,\eta)}{\partial \eta} \right) \cdot \sum_{k=1}^{n} \left(\int_{21}^{*} \frac{\partial \tilde{\psi}_{k}(\xi,\eta)}{\partial \xi} + J_{22}^{*} \frac{\partial \tilde{\psi}_{k}(\xi,\eta)}{\partial \eta} \right) \cdot \gamma_{k}^{e} \end{pmatrix} + det[J]d\xi d\eta$$

7.2.16.3.1 Boundary Conditions

When considering boundary conditions, there are two forms of interest: Natural and Neumann.

Natural Boundary Condition

Boundary conditions with a state variable dependent "film" coefficient "h" can be written as:

$$\int_{\Gamma_{h}} \omega \cdot h(u + \Delta u) \cdot \left[\left(u + \Delta u \right) - u_{\infty} \right] \cdot d\Gamma_{h}$$
(7.27)

Equation (7.27) has to be discretized and solved by state variable difference. Combining (7.24) into (7.27):

$$\int_{\Gamma_{h}} \omega \cdot \left(h(u) + \Delta u \frac{\partial h}{\partial t} \right) \cdot \left[(u + \Delta u) - u_{\infty} \right] \cdot d\Gamma_{h} = 0$$
(7.28)

Using a state function approximation (7.25) will end up creating a system of "n" equations:

$$\int_{\Gamma_c} \sum_{i=1}^{n} \psi_i^e(x, y) \cdot \left(h(u) + \frac{\partial h}{\partial t} \sum_{j=1}^{n} \Delta u_j^e \psi_j^e(x, y) \right) \cdot \left[\left(\sum_{j=1}^{n} u_j^e \psi_j^e(x, y) + \sum_{j=1}^{n} \Delta u_j^e \psi_j^e(x, y) \right) - u_{\infty} \right] d\Gamma_c = 0$$
(7.29)

Which leads to:

$$\int_{\Gamma_{c}} \sum_{i=1}^{n} \psi_{i}^{e}(x, y) \cdot h(u) \cdot u + \int_{\Gamma_{c}} \sum_{i=1}^{n} \psi_{i}^{e}(x, y) \cdot h(u) \cdot \Delta u - \int_{\Gamma_{c}} \sum_{i=1}^{n} \psi_{i}^{e}(x, y) \cdot h(u) \cdot u_{\infty} + \int_{\Gamma_{c}} \sum_{i=1}^{n} \psi_{i}^{e}(x, y) \cdot \Delta u \cdot \frac{\partial h}{\partial t} \cdot u + \int_{\Gamma_{c}} \sum_{i=1}^{n} \psi_{i}^{e}(x, y) \cdot \Delta u \cdot \frac{\partial h}{\partial t} \cdot \Delta u - \int_{\Gamma_{c}} \sum_{i=1}^{n} \psi_{i}^{e}(x, y) \cdot \Delta u \cdot \frac{\partial h}{\partial t} \cdot u_{\infty} = 0$$

The above equation will be solved through iterations by calculating the change in state variable Δu_j^e and simply using it to calculate the state variable by applying the iterative equation (7.23). If we consider that the current iteration is "(a)", then the values of the state variables from previous iterations are $u_j^{(a-1)}$ and its change $\Delta u_j^{(a-1)}$. The above equation can be written in matrix form:

$$\left\{ \left[A_{ij}^{e} \right] + \left[C_{ij}^{e} \right] + \left[D_{ij}^{e} \right] + \left[E_{ij}^{e} \right] \right\} \left\{ \Delta u_{j}^{(a)} \right\} = \left\{ B_{i}^{e} \right\} - \left[A_{ij}^{e} \right] \left\{ u_{j}^{(a-1)} \right\}$$

Where matrices are calculated as:

$$\begin{bmatrix} A_{ij}^{e} \end{bmatrix} = \tilde{\psi}_{i}^{e} \left(\xi \right) \cdot \tilde{\psi}_{j}^{e} \left(\xi \right) \cdot h \cdot \det$$

$$\left\{ B_{i}^{e} \right\} = \tilde{\psi}_{i}^{e} \left(\xi \right) \cdot h \cdot u_{\infty} \cdot \det$$

$$\begin{bmatrix} C_{ij}^{e} \end{bmatrix} = \tilde{\psi}_{i}^{e} \left(\xi \right) \cdot \tilde{\psi}_{j}^{e} \left(\xi \right) \cdot \frac{\partial h}{\partial t} \cdot \det \cdot \left(\sum_{k=1}^{n} \tilde{\psi}_{k}^{e} \left(\xi \right) \cdot u_{k}^{(a-1)} \right)$$

$$\begin{bmatrix} D_{ij}^{e} \end{bmatrix} = \tilde{\psi}_{i}^{e} \left(\xi \right) \cdot \tilde{\psi}_{j}^{e} \left(\xi \right) \cdot \frac{\partial h}{\partial t} \cdot \det \cdot \left(\sum_{k=1}^{n} \tilde{\psi}_{k}^{e} \left(\xi \right) \cdot \Delta u_{k}^{(a-1)} \right)$$

$$\begin{bmatrix} E_{ij}^{e} \end{bmatrix} = \tilde{\psi}_{i}^{e} \left(\xi \right) \cdot \tilde{\psi}_{j}^{e} \left(\xi \right) \cdot \frac{\partial h}{\partial t} \cdot \det \cdot u_{\infty}$$

Note that equation (7.29) is linearized for some matrix coefficients, because the equation is nonlinear by itself. Instead of applying the state variable from the current iteration, the equation will simply take the solution from the previous iteration (a-1). The iterative process will eventually lead to a solution within the given tolerance. Also, since the solution for Δu is converging towards zero, the matrix $\left[D_{ij}^{e}\right]$ can be removed from the above equation.

Neumann

A boundary condition with a state variable dependent flux can be written as:

$$\int_{\Gamma_q} \omega q_f \left(u + \Delta u \right) d\Gamma_q = 0 \tag{7.30}$$

As already explained in a previous section, the variable $q_f(u + \Delta u)$ can be written as:

$$q_{f}\left(u+\Delta u\right) = q_{f}\left(u\right) + \Delta u \frac{\partial q_{f}}{\partial u}$$

Applying this to (7.30):

$$\int_{\Gamma_q} \omega \cdot \left[q_f(u) + \frac{\partial q_f}{\partial u} \sum_{j=1}^n \Delta u_j^e \cdot \psi_j^e(x, y) \right] d\Gamma_q = 0$$

Which then in developed form and the local coordinate system leads to:

$$\int_{\Gamma_q} \psi_i^e(x, y) \cdot \left[q_f(u) + \frac{\partial q_f}{\partial t} \sum_{j=1}^n \Delta u_j^e \cdot \psi_j^e(x, y) \right] \cdot d\Gamma_q = 0$$

And finally, in matrix form:

$$\left[F_{ij}^{e}\right]\left\{\Delta u_{j}^{(a)}\right\}-\left\{Q_{i}\right\}=0$$

Where:

$$F_{ij}^{e} = \int_{\tilde{\Gamma}_{q}} \tilde{\psi}_{i}^{e}(\xi) \cdot \tilde{\psi}_{j}^{e}(\xi) \cdot \frac{\partial q_{f}}{\partial t} \cdot \det d\tilde{\Gamma}_{q}$$
$$Q_{i} = \int_{\tilde{\Gamma}_{q}} \tilde{\psi}_{i}^{e}(\xi) \cdot q_{f} \cdot \det d\tilde{\Gamma}_{q}$$

7.3 Shape Functions

7.3.1 One-dimensional linear elements

Let us consider a typical linear element with end nodes "i" and "j" with the corresponding temperature being denoted by T_i and T_j respectively.



Figure 20. One-dimensional finite linear element

The linear temperature variation in the element is represented by:

$$T(x) = \alpha_1 + \alpha_2 \cdot x \tag{7.31}$$

Where T is the temperature at any location x, and the parameters α_1 and α_2 are constants. Since there are two arbitrary constants in the linear representation, it requires only two nodes to determine the values α_1 and α_2 namely.

$$T_i = \alpha_1 + \alpha_2 x_i$$
$$T_j = \alpha_1 + \alpha_2 x_j$$

From the above set we get:

$$\alpha_1 = \frac{T_i x_j - T_j x_i}{x_j - x_i}$$
$$\alpha_2 = \frac{T_j - T_i}{x_j - x_i}$$

Substituting the values of α_1 and α_2 into equation (7.31) we get:

$$T = T_i \left[\frac{x_j - x}{x_j - x_i} \right] + T_j \left[\frac{x - x_i}{x_j - x_i} \right]$$

or

$$T = N_i T_i + N_j T_j = \begin{bmatrix} N_i & N_j \end{bmatrix} \left\{ \frac{T_i}{T_j} \right\}$$
(7.32)

Where N_i and N_j are called *Shape functions* or *Interpolation functions* or *Basis functions*.

$$N_{i} = \begin{bmatrix} \frac{x_{j} - x_{i}}{x_{j} - x_{i}} \end{bmatrix}$$

$$N_{j} = \begin{bmatrix} \frac{x - x_{i}}{x_{j} - x_{i}} \end{bmatrix}$$
(7.33)

The derivatives of the shape functions are constant within an element. From equation (7.32), the temperature gradient is calculated as:

$$\frac{dT}{dx} = \frac{dN_i}{dx}T_i + \frac{dN_j}{dx}T_j = -\frac{1}{x_j - x_i}T_i + \frac{1}{x_j - x_i}T_j$$

or

 $\frac{dT}{dx} = \begin{bmatrix} -\frac{1}{l} & \frac{1}{l} \end{bmatrix} \begin{cases} T_i \\ T_j \end{cases}$

1

Where l is the length of an element equal to $(x_j - x_i)$.



Figure 21. Non-dimensional coordinates of one-dimensional linear element

Transforming one-dimensional linear element coordinates to a system where $x_i = -1$ and $x_j = 1$ (non-dimensional coordinates), the shape functions will become (from equations (7.33)):

$$\psi_1^e = \frac{1}{2}(1-\xi)$$

$$\psi_2^e = \frac{1}{2}(1+\xi)$$
(7.34)

7.3.2 Two-dimensional quadrilateral linear elements

The quadrilateral element has four nodes located at the vertices as shown in Figure 22.



Figure 22. Two-dimensional quadrilateral element

The temperature within the quadrilateral is represented by:

$$T = \alpha_1 + \alpha_2 x + \alpha_3 y + \alpha_4 x y \tag{7.35}$$

thus, the temperature gradients may be written as:

$$\frac{\partial T}{\partial x} = \alpha_2 + \alpha_4 y$$
$$\frac{\partial T}{\partial y} = \alpha_3 + \alpha_4 x$$

Therefore, the gradient varies within the element in a linear way. On substituting the values for T_1 , T_2 , T_3 and T_4 into equation (7.35) for the nodes 1, 2, 3 and 4 and solving, we obtain the values of α_1 ,

 α_2 , α_3 and α_4 . Substituting these relationships back into equation (7.35) and collating the coefficients of T₁, T₂, T₃ and T₄ we get:

$$T = N_1 T_1 + N_2 T_2 + N_3 T_3 + N_4 T_4$$

In the simplest form, the quadrilateral element becomes a rectangular element with the boundaries of the element parallel to a coordinate system.



Figure 23. A simple rectangular element

For the rectangular element shown in Figure 23, the shape functions are:

$$N_{1} = \frac{1}{4ab}(b-x)(a-y)$$

$$N_{2} = \frac{1}{4ab}(b+x)(a-y)$$

$$N_{3} = \frac{1}{4ab}(b+x)(a+y)$$

$$N_{4} = \frac{1}{4ab}(b-x)(a+y)$$



Figure 24. Non-dimensional coordinates of a rectangular system

We can express these shape functions in terms of length ratios x/b and y/a as:

$$N_1 = \frac{1}{4ab}(b-x)(a-y) = \frac{1}{4}(1-\frac{x}{b})(1-\frac{y}{a}) = \frac{1}{4}(1-\xi)(1-\eta)$$

All shape functions for rectangular element shown in Figure 24 are:

$$\begin{split} \psi_{1}^{e} &= \frac{1}{4} (1 - \xi) (1 - \eta) \\ \psi_{2}^{e} &= \frac{1}{4} (1 + \xi) (1 - \eta) \\ \psi_{3}^{e} &= \frac{1}{4} (1 + \xi) (1 + \eta) \\ \psi_{4}^{e} &= \frac{1}{4} (1 - \xi) (1 + \eta) \end{split}$$
(7.36)

7.4 Nonlinear Method Solution

Section 7.2.14 describes the approach in the case of nonlinear problems. This appendix gives simple example of iterations and how the entire process works.

Example 1

In this first example, the idea is to present the iterative process on a simple equation:

 $3u^2 + 5u = 8$

If we linearize this equation around $u + \Delta u$:

 $3u(u + \Delta u) + 5(u + \Delta u) = 8$

Solving this by Δu will give:

$$\Delta u = \frac{8 - 5u - 3u^2}{3u + 5}$$

Applying starting condition to be u = 0 and relaxation parameter to be equal to one:

u	∆u
0	
1.6	1.6
0.81632653	-0.7836735
1.0739726	0.25764607
0.973009	-0.1009636
1.01022512	0.03721612
0.99618023	-0.0140449
1.00143447	0.00525424
0.99946236	-0.0019721
1.00020165	0.00073929
0.99992439	-0.0002773
1.00002836	0.00010397
0.99998937	-3.899E-05
1.00000399	1.4621E-05
0.9999985	-5.483E-06
1.00000056	2.0561E-06

A solution within a tolerance of 1e-5 is obtained in 14 iterations. However, applying the same starting value (u = 0) and a relaxation parameter of 0.75 will give following iterations:

Х	$\Delta \mathbf{x}$
0	
1.2	1.6
0.99767442	-0.2697674
1.00007325	0.00319844

0.99999771	
1.0000007	3.1465E-06

Now we can see that solution is achieved with just five iterations.