Heat and mass transfers in the context of energy geostructures

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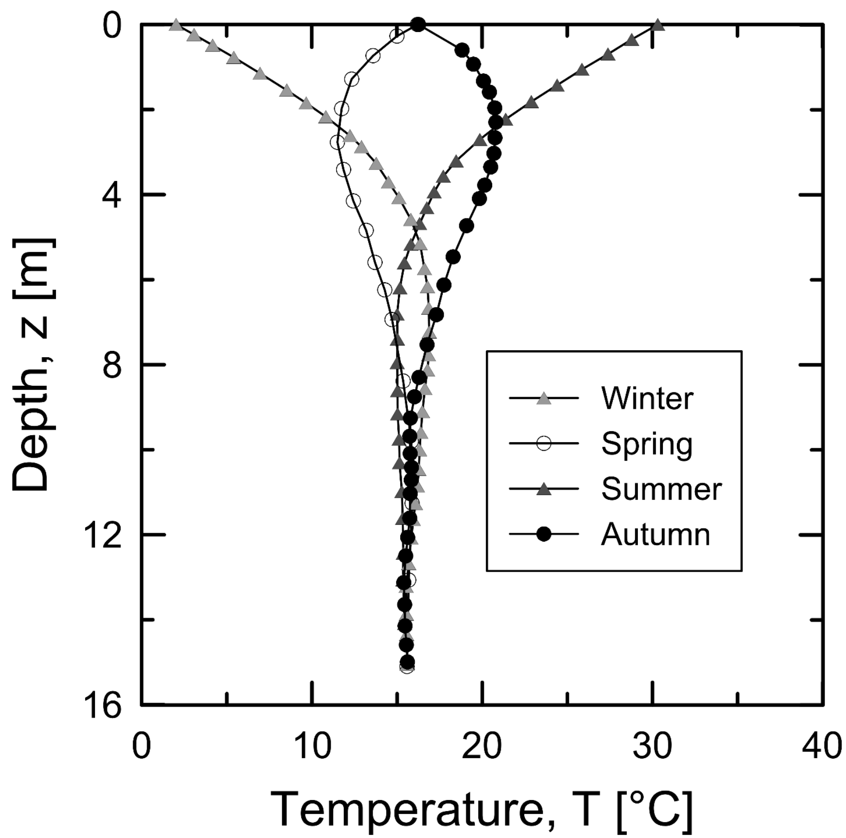
Outline

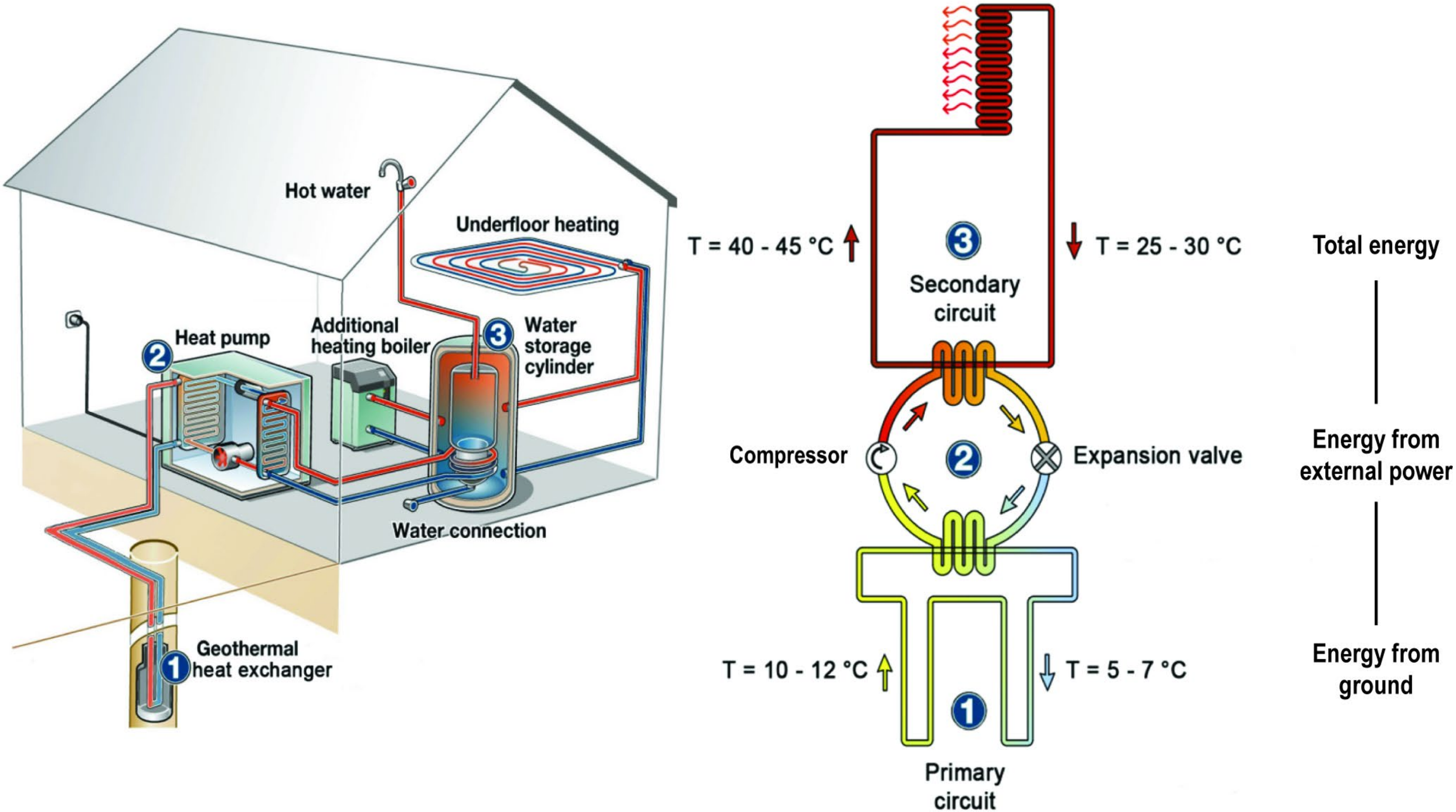
- Principles and modes of heat transfer
- Energy conservation equation
- Initial and boundary conditions for energy conservation
- Principles and modes of mass transfer
- Mass conservation equation
- Initial and boundary conditions for mass conservation

Temperature field in the subsurface

- The temperature field in the subsurface is typically sensitive to atmospheric conditions within the first 10-15 m

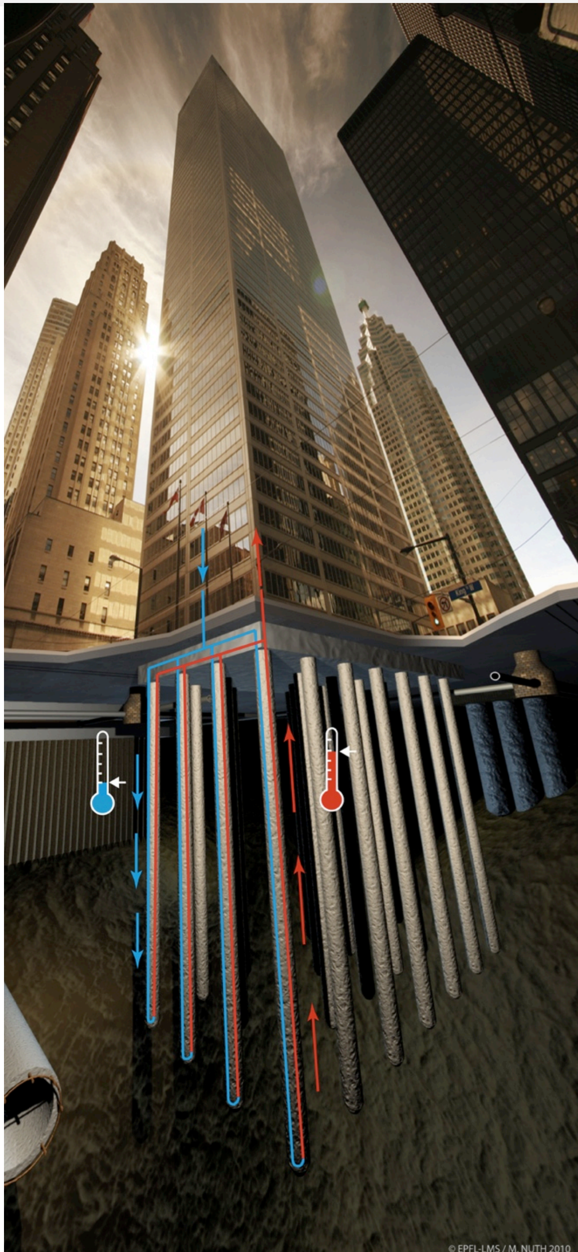


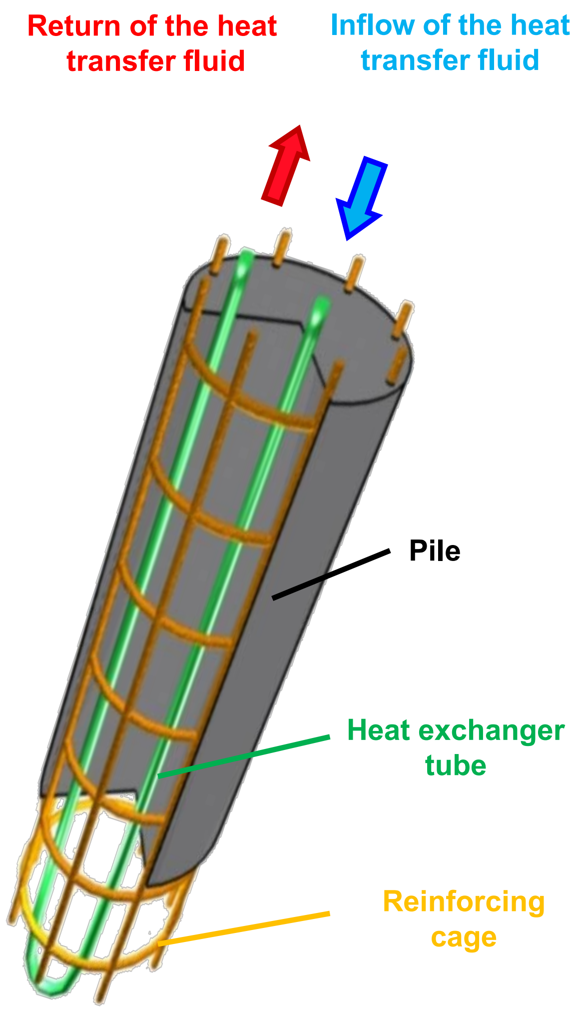
The Ground Source Heat Pump System



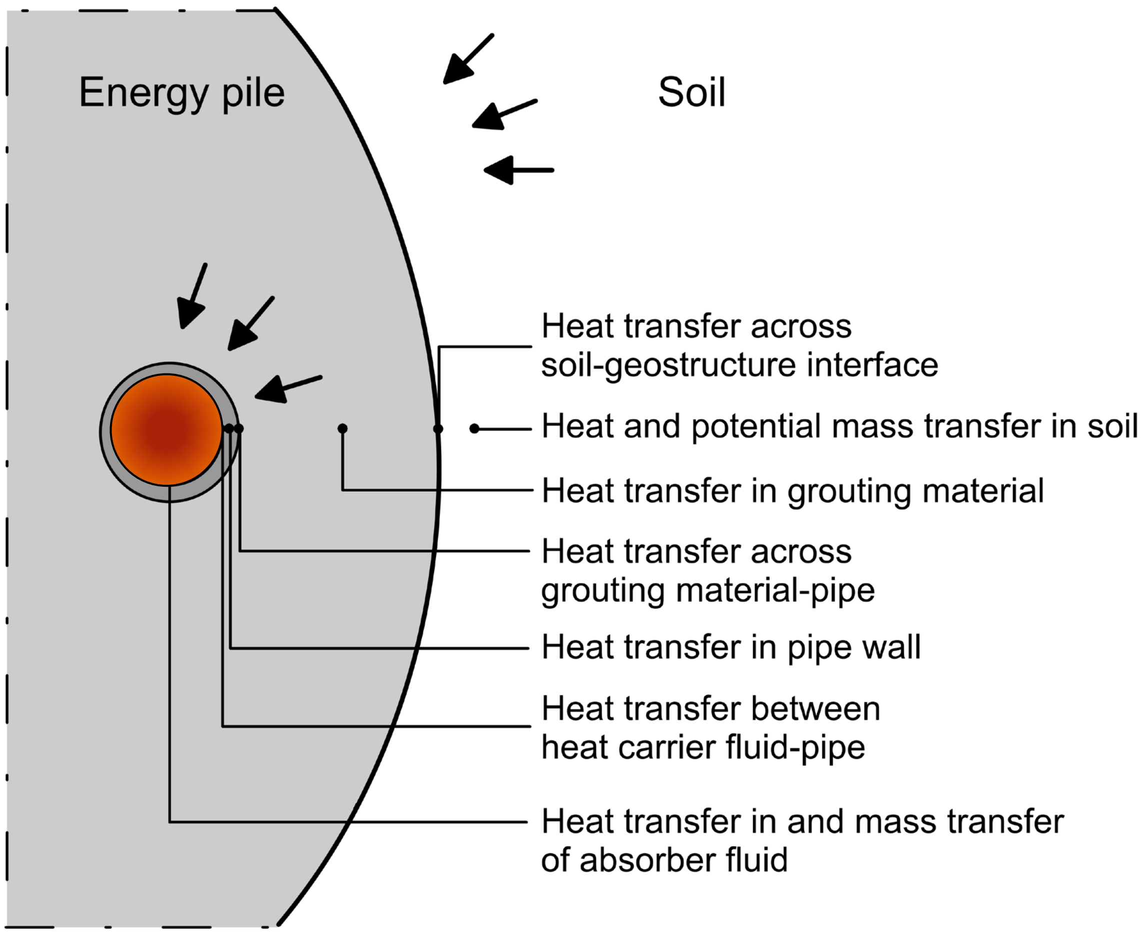
Modified after Agentur für Erneuerbare Energien (reproduced with permission)

The technology





The typical problem



- Four typical materials:
  - Heat carrier fluid
  - Pipes
  - Reinforced concrete
  - Soil/rock
- Two phenomena:
  - Heat transfer
  - Mass transfer
- Two master equations:
  - Energy cons. eq.
  - Mass cons. eq.

Principles and modes of heat transfer

Fundamentals of heat transfer

- (Thermal) Energy in the form of heat is transferred between any two particles of matter that are at different temperatures

- These particles can be, for example, part of
  - the same solid body
  - two different solids
  - a fluid mass
  - a solid and a fluid

- Heat transfer cannot be measured directly, but its occurrence can be related to a scalar quantity, i.e., temperature, T

- Heat (as mass) transfer can be described via *rate equations*

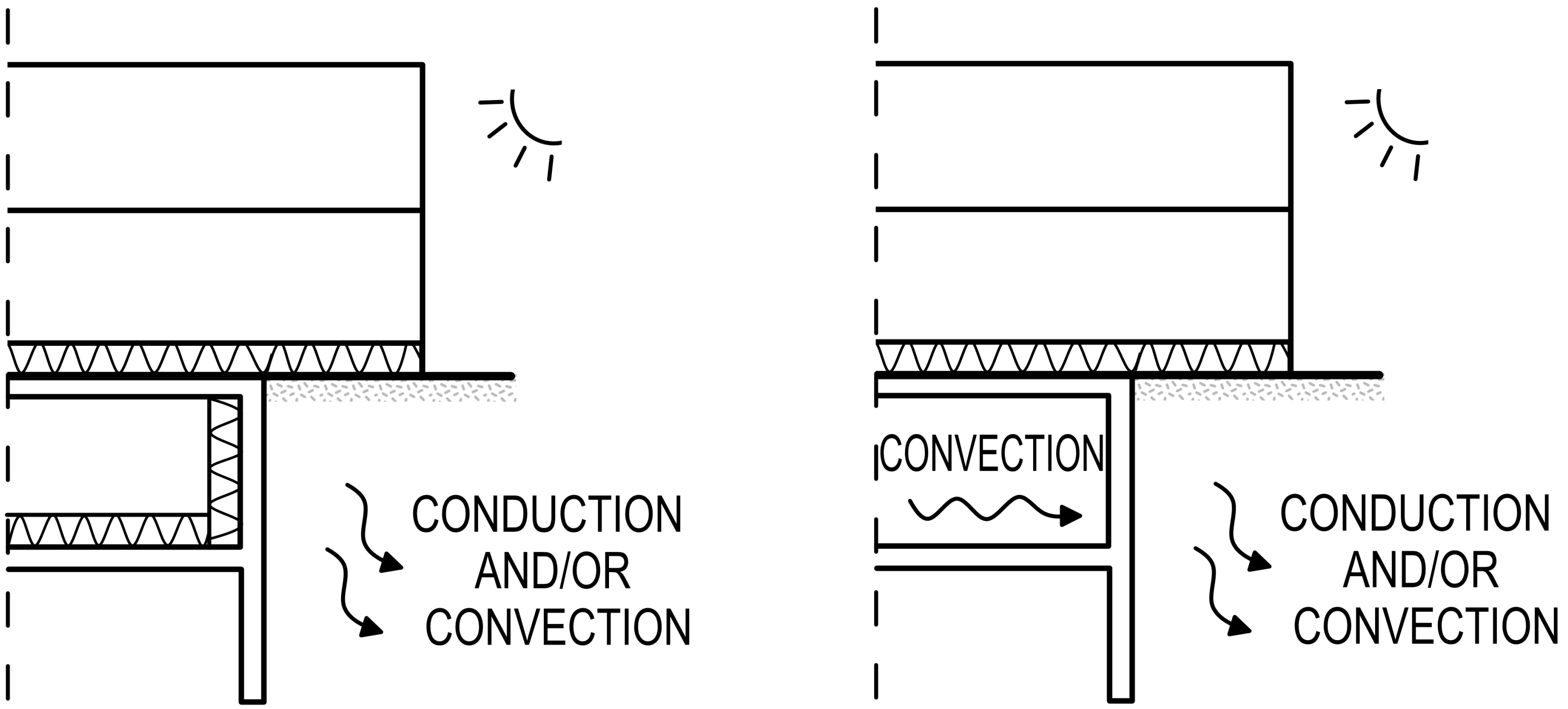
Modes of heat transfer

- There are 2 fundamental modes of heat transfer:
  - Conduction
  - Convection

- *Radiation phenomena* may also characterise heat transfer, however they generally play a negligible role in energy geostructure applications

- *Latent processes* caused by phase changes of the constituents of the medium may characterise heat transfer, but are generally negligible in energy geostructure applications

Examples of heat transfer phenomena

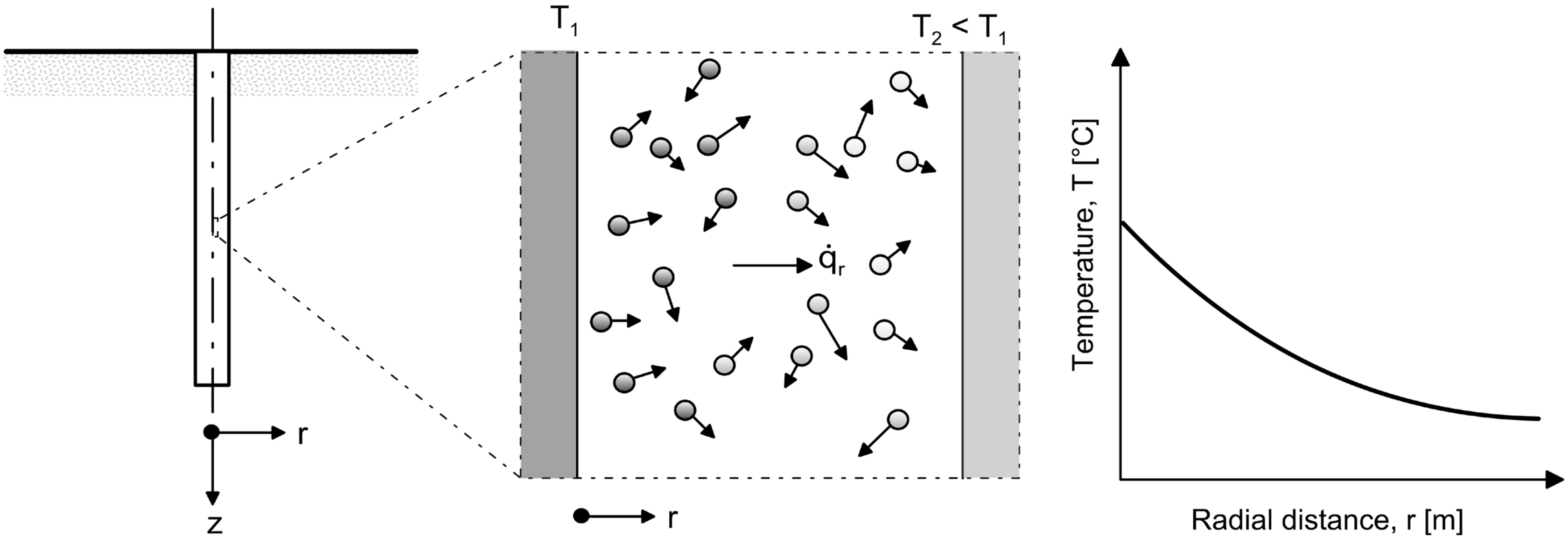


(Laloui and Rotta Loria, 2019)

Conduction

- Heat transfer mode that occurs at the molecular and atomic levels between particles of a solid or a fluid at different temperatures

- Conduction is generally associated to an invisible motion of the particles that constitute the medium



(Laloui and Rotta Loria, 2019)

Fourier's law

- The rate equation describing conduction is Fourier's law

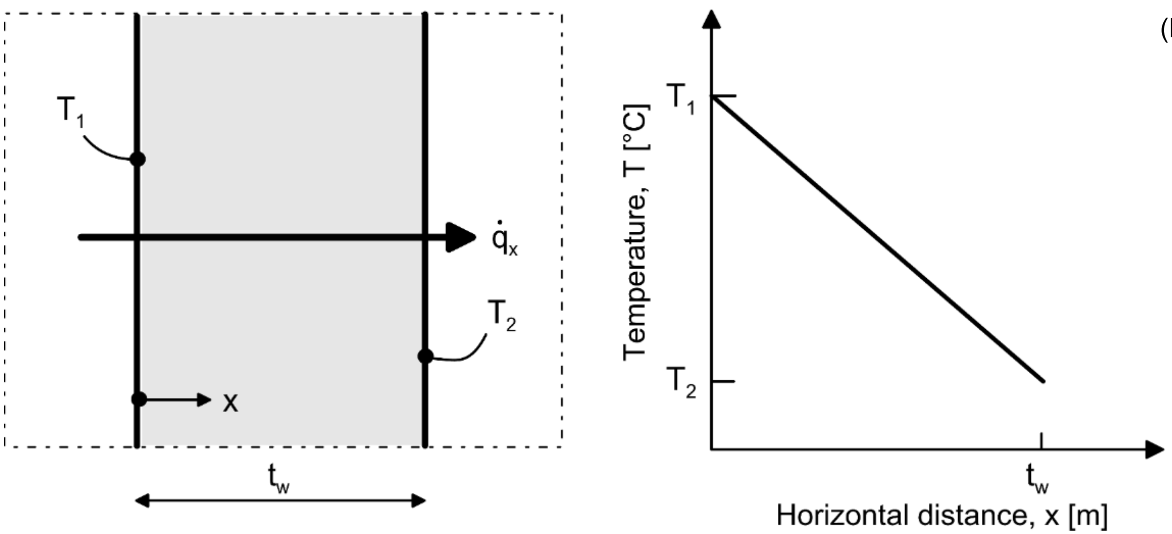
$$\dot{q}_{cond,i} = \frac{Q}{At} = \frac{\dot{Q}}{A} = -\lambda \frac{\partial T}{\partial n_i} = -\lambda \nabla T = -\lambda\left(\frac{\partial T}{\partial x}\hat{e}_x + \frac{\partial T}{\partial y}\hat{e}_y + \frac{\partial T}{\partial z}\hat{e}_z\right)$$

- $\dot{q}_{cond,i}$ = energy density by conduction
- Q = heat energy
- $\dot{Q}$ = heat power
- A = Area
- t = time
- λ = thermal conductivity

Fourier's law: simplified formulation

- Fourier's law can be markedly simplified for problems involving plane geometries under steady state conditions
- These situations characterise, e.g., the operation of energy walls

$$\dot{q}_x = -\lambda \frac{dT}{dx} = -\lambda \frac{(T_2 - T_1)}{t_w} = \frac{\lambda (T_1 - T_2)}{t_w}$$



(Laloui and Rotta Loria, 2019)

Thermal conductivity

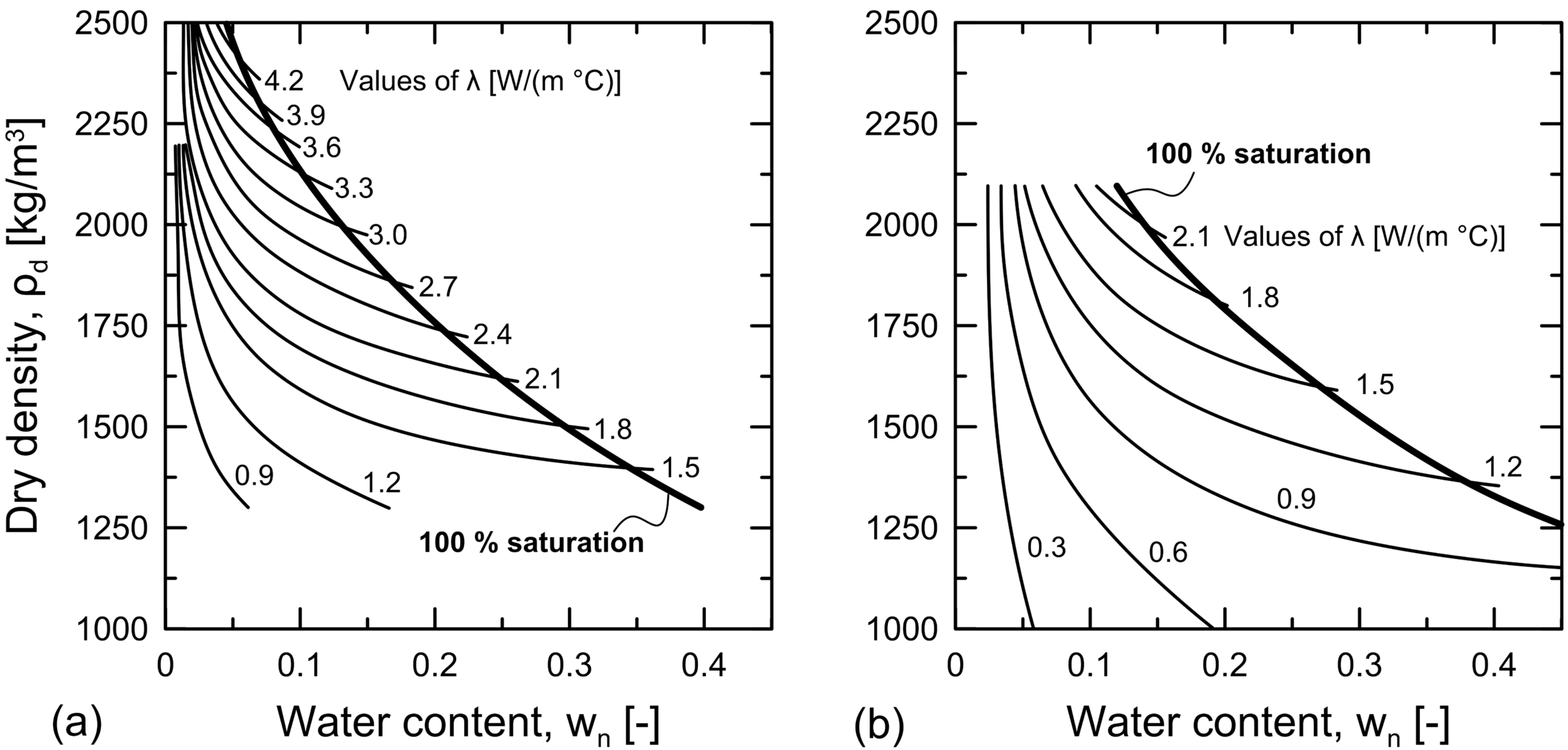
- The thermal conductivity of soils markedly depends on (see, e.g., Brandon and Mitchell, 1989; Alrtimi et al., 2016; Vulliet et al., 2016)
  - Mineralogy
  - Dry density
  - Water content
  - Gradation
- In a similar way, the thermal conductivity of concrete markedly depends on (see, e.g., Morabito, 1989; Lanciani et al., 1989; Neville, 1995; Kim et al., 2003)
  - Aggregate types and sources
  - Dry density
  - Water content
  - Mix proportioning

Thermal conductivity of constituents

Material	Thermal conductivity, λ_i [W/(m °C)]
Air	0.024
Water	0.6
Feldspar	1.4 – 2.5
Plagioclase	1.5 – 2.0
Mica	1.6 – 3.5
Amphibole	2.8 – 4.8
Garnet	3.1 – 5.5
Olivine	3.2 – 5.0
Pyroxene	3.5 – 5.7
Calcite	3.6
Chlorite	5.2
Quartz	7.7

(Laloui and Rotta Loria, 2019;
data from Banks (2012), Côté and Konrad (2005) and Midttømme et al. (2008), after Loveridge (2012))

Typical soil thermal conductivity



Typical relationship for an unfrozen (a) coarse-grained soil and (b) fine-grained soil (redrawn after Brandl (2006))

Typical calculation approach for λ

- The effective thermal conductivity of porous materials, such as soils, rocks and concrete, assumed to be isotropic and with pores fully filled with a fluid, can be evaluated as

$$\lambda = \lambda_f n + \lambda_s (1 - n)$$

- λ_f = thermal conductivity of the general fluid filling the pores
- λ_s = thermal conductivity of the solid particles
- n = material porosity

- For materials with pores fully saturated with water, λ_f is replaced by the thermal conductivity of the water λ_w.

Convection

- Heat transfer mode that characterises fluids in motion with a temperature gradient

- Convection is associated with the superposition of two mechanisms:
  - Energy transport by a diffusion motion of the fluid
  - Energy transport by a bulk motion of the fluid (mass transfer)

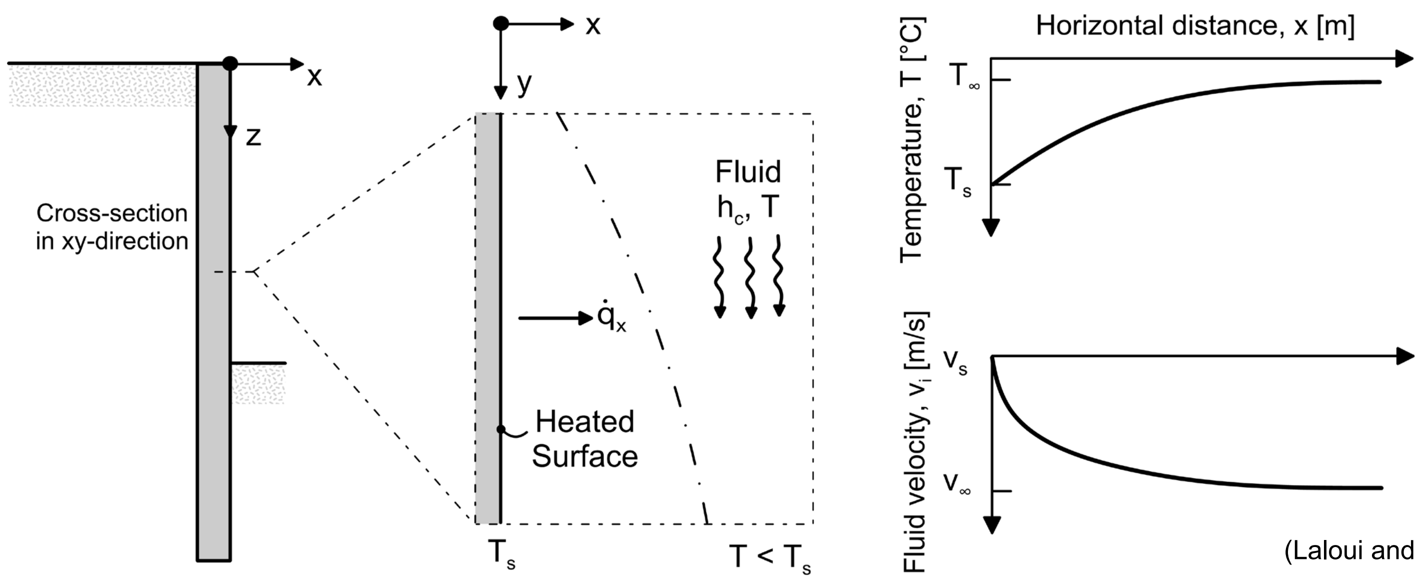
- Convection heat (and mass) transfer can be associated to:
  - Internal flow problems: the fluid in motion is completely bounded by a surface
  - External flow problems: the fluid in motion is not completely bounded by a surface
  - Seepage flow problems: the fluid is in motion across a permeable material medium

Newton's law of cooling

- The rate equation governing convection is Newton's law of cooling

$$\dot{q}_{conv,i} = h_c(T_s - T_\infty)$$

- $\dot{q}_{cond,i}$ = energy density by convection
- h_c = convection heat transfer coefficient
- T_s = surface temperature
- T_∞ = fluid temperature



(Laloui and Rotta Loria, 2019)

Natural and forced convection

- The motion of fluids is the result of a force
  - Free or natural convection: when the force that causes the motion of the fluid is due entirely to density variations caused by a non-uniform temperature distribution
  - Forced convection: the force that causes the motion of the fluid is due to any other cause
- In soils, the moving particles that typically transport heat are water molecules

Convection heat transfer coefficient

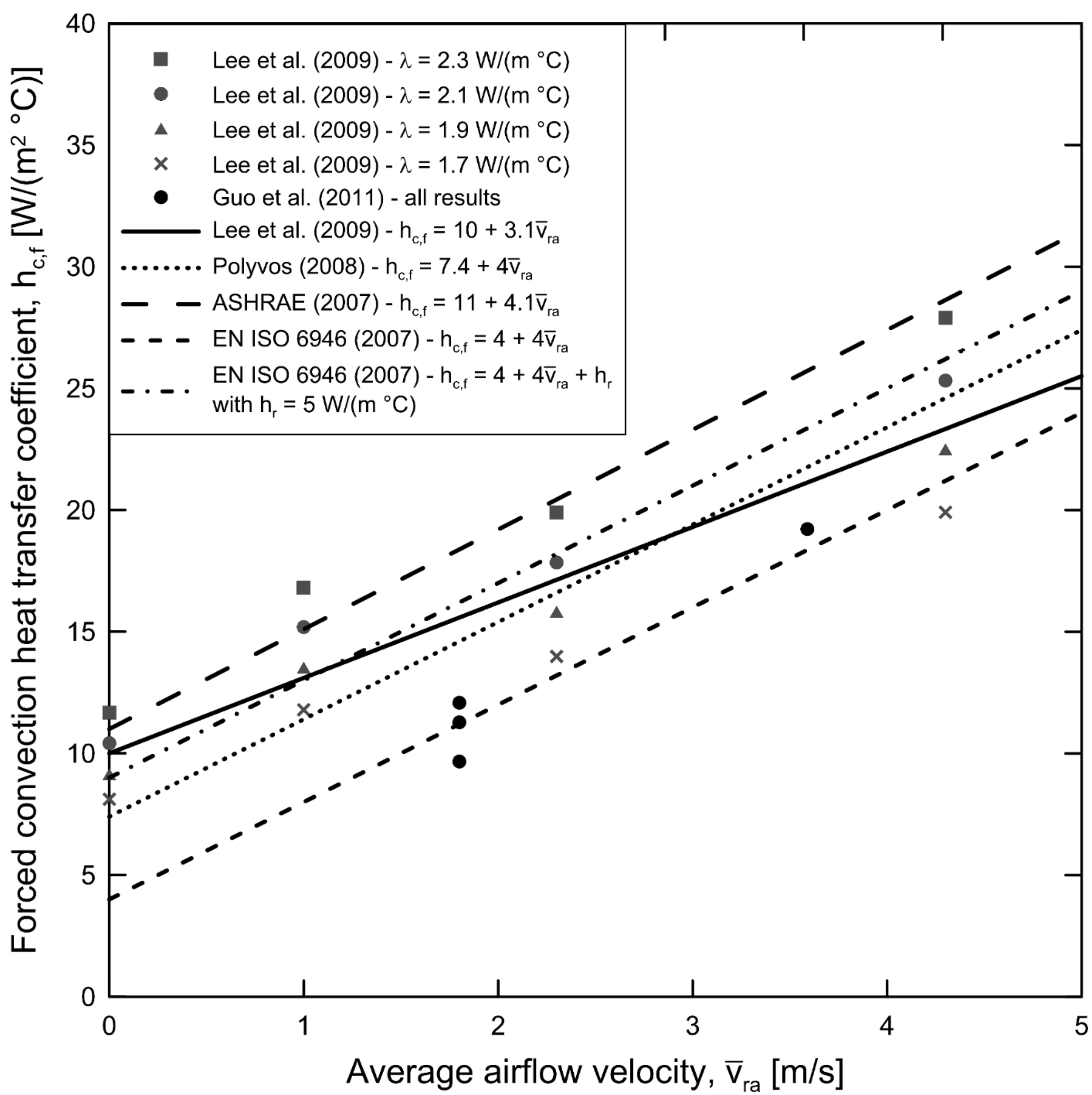
- The convection heat transfer coefficient h_c and the separate terms $\rho_f c_{pf} \bar{v}_{rf,i}$ depend on:
  - The nature of the fluid in motion
  - An assortment of fluid thermodynamic and transport (mass) properties

- In the analysis of internal and external flows related to airflows, the convection heat transfer coefficient is often expressed as

$$h_c = h_{c,n} + h_{c,f}$$

Convection heat transfer coefficient

(Laloui and Rotta Loria, 2019;
redrawn after Bourne-Webb et al., 2016)



Newton's law of cooling

- In the context of the analysis of convection heat transfer associated with seepage problems, Newton's law of cooling reads

$$\dot{q}_{conv,i} = \rho_f c_{p,f} \bar{v}_{rf,i} (T_s - T_\infty)$$

- $c_{p,f}$ = specific heat of fluid
- ρ_f = density of fluid
- $\bar{v}_{rf,i}$= relative velocity of water with respect to the solid skeleton

- Convection is significant only if consistent fluid flow is present

- In soils, this is often the case in sandy or gravelly materials (highly permeable materials), while it is not for clays (low permeable materials)

Typical calculation approach for ρc_p

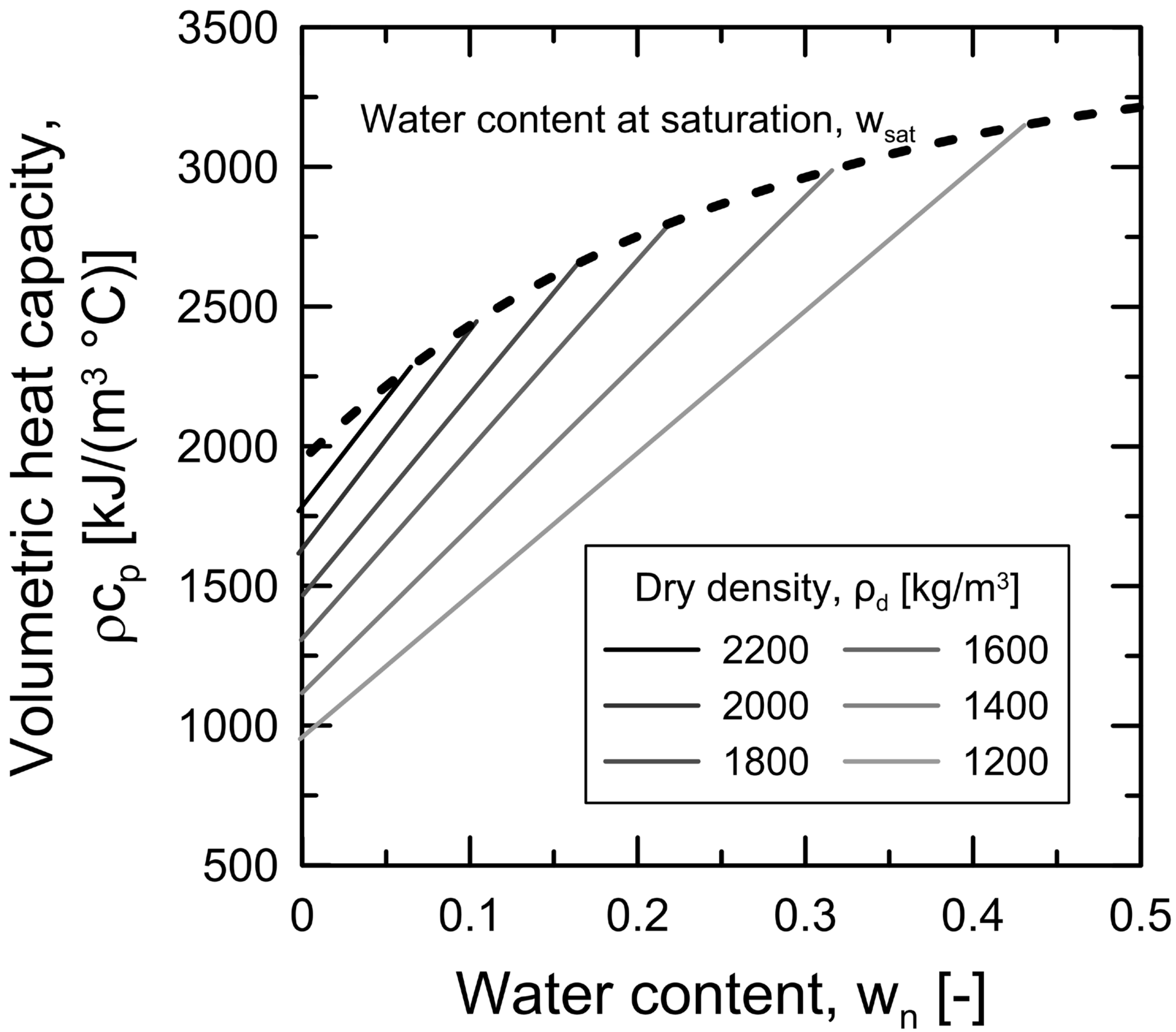
- The effective volumetric heat capacity of porous materials fully saturated with a fluid can be calculated as

$$\rho c_p = \rho_f c_{p,f} n + \rho_s c_{p,s} (1 - n)$$

- $\rho_f c_{p,f}$= volumetric heat capacity of the general fluid filling the pores
- $\rho_s c_{p,s}$= volumetric heat capacity of the solid particles

- For soils fully saturated with water, $\rho_f c_{p,f}$ is replaced by the volumetric heat capacity of the water $\rho_w c_{p,w}$

Typical soil volumetric heat capacity



(Laloui and Rotta Loria, 2019;
redrawn after Dysli, 1991)

Energy conservation equation

Rationale

- The energy conservation equation is the master equation that governs heat transfer phenomena in physical systems

- For any isolated domain, the considered equation expresses that the amount of energy remains constant, i.e., energy is neither created nor destroyed but can only be converted

- Usually derived in an elementary manner based on an energy balance for an elementary volume

$$\begin{bmatrix} \text{Rate of heat entering through} \\ \text{the bounding surfaces of a volume} \end{bmatrix} + \begin{bmatrix} \text{Rate of heat} \\ \text{generation in a volume} \end{bmatrix} = \begin{bmatrix} \text{Rate of energy} \\ \text{storage in a volume} \end{bmatrix}$$

Energy conservation equation

- The Fourier heat conduction equation is obtained in this way, *neglecting any conversion of mechanical energy into heat* and considering an isotropic body subjected to:
  - arbitrary thermal conditions on its surfaces
  - internal volumetric heat generation $\dot{q}_v$ per unit time

$$\lambda \nabla^2 T + \dot{q}_v = \rho c_p \frac{\partial T}{\partial t}$$

The quantity $\nabla^2 T$ is as follows in Cartesian coordinates x, y, z:

$$\nabla^2 T = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}$$

Simplified Fourier heat conduction equation

- If no heat is generated in the medium, the Fourier equation reads

$$\alpha_d \nabla^2 T = \frac{\partial T}{\partial t}$$

- $\alpha_d = \frac{\lambda}{\rho c_p} =$ thermal diffusivity

- α_d measures the ability of a material to conduct thermal energy relative to its ability to store thermal energy (Hermansson et al. 2009)

- Soils of large α_d will respond quickly to changes in their thermal environment and vice versa

- The higher the value of α_d the faster the heat propagation in the medium

Other formulations of the Fourier heat conduction equation

- The case in which the temperature distribution is independent of time and no heat sources are present can be of interest

- The above involves the Laplace's equation

$$\nabla^2 T = 0$$

- When convection is aimed to be included in the heat transfer analysis, the energy conservation equation

$$\lambda \nabla^2 T + \dot{q}_v = \rho c_p \frac{\partial T}{\partial t} + \rho_f c_{p,f} \bar{v}_{rf,i} \nabla T$$

Initial and boundary conditions

- The full mathematical description of heat transfer needs initial and boundary conditions to be solved

- The unique case in which no initial conditions are needed is in the steady state problem governed by $\nabla^2 T = 0$

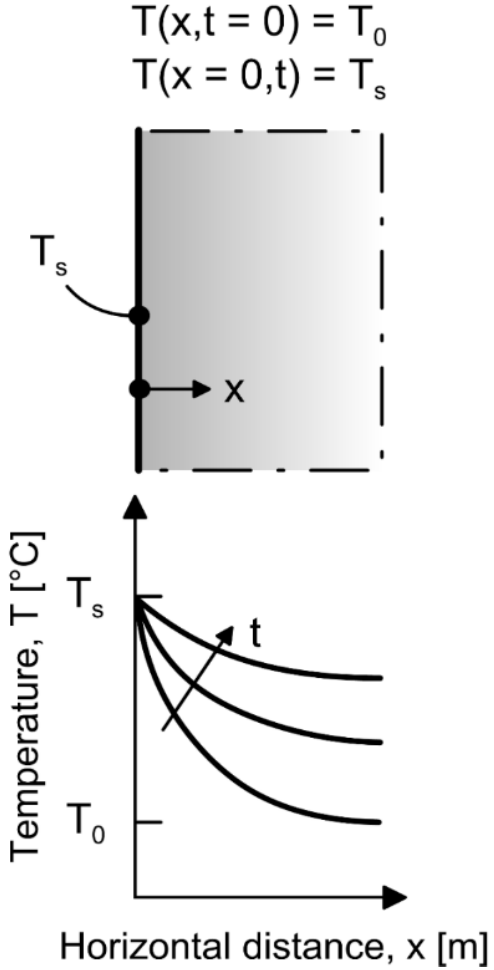
- In almost all problems, the typical initial condition employed is to assume a constant initial temperature, i.e., $T_0 = \text{const}$

Prescribed surface temperature

- Also known as Dirichlet's boundary condition or boundary condition of the first kind

$$T(\mathcal{H}, t) = f(\mathcal{H}, t)$$

- $\mathcal{H}$ = point on the considered surface
- $f(M, t)$ = prescribed function



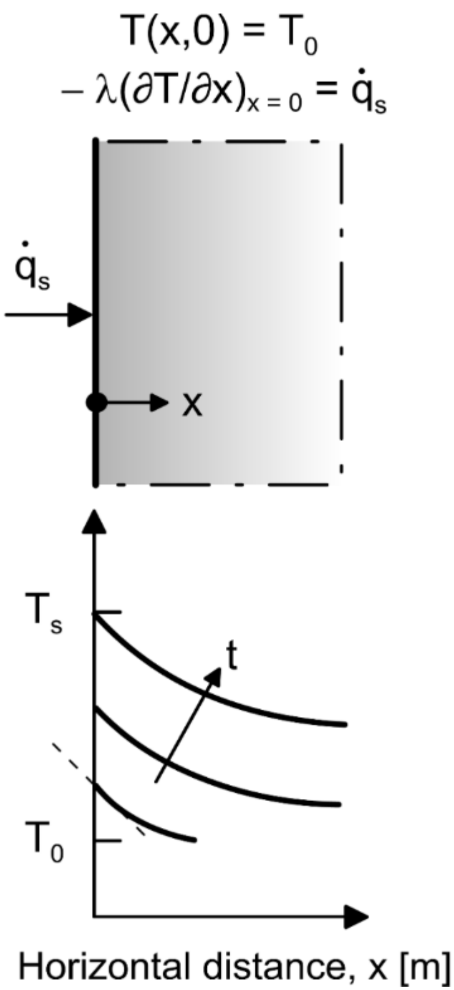
(Laloui and Rotta Loria, 2019)

Prescribed heat input

- Also known as Neumann's boundary condition or boundary condition of the second kind

$$-\lambda \frac{\partial T}{\partial n_i}(\mathcal{H}, t) = \dot{q}(\mathcal{H}, t)$$

- n_i = outward normal to the surface at point $\mathcal{H}$

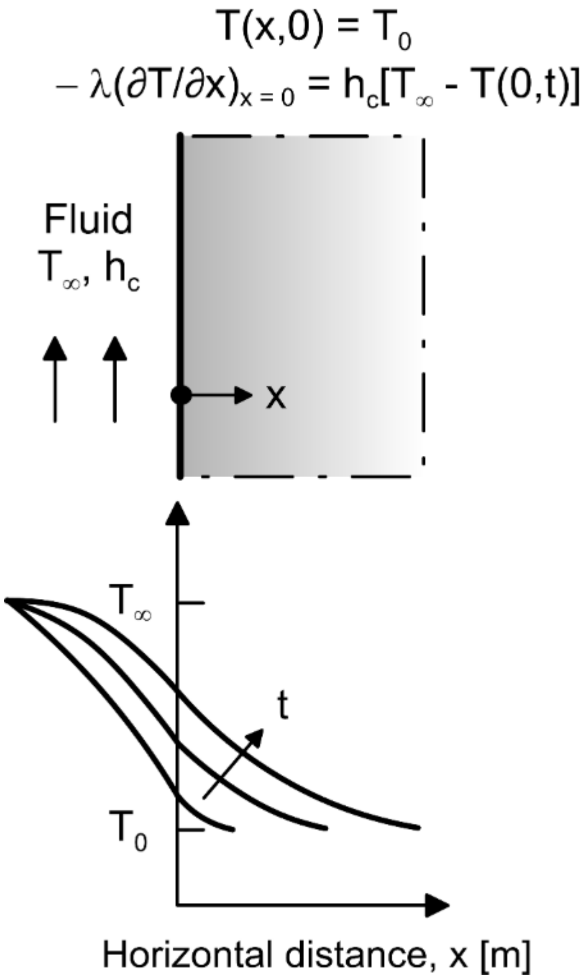


(Laloui and Rotta Loria, 2019)

Convection boundary condition

- Also known as Cauchy's or mixed Neumann's boundary condition or boundary condition of the third kind

$$-\lambda \frac{\partial T}{\partial n_i}(\mathcal{H}, t) = h_c[T_\infty - T(\mathcal{H}, t)]$$



(Laloui and Rotta Loria, 2019)

Interface boundary condition (perfect thermal contact)

- If two bodies are in *perfect thermal contact*
  - their temperature at the surface contact must be the same
  - the heat flux leaving one body through the contact surface must be equal to that entering the other body

$$T_1(\mathcal{H}, t) = T_2(\mathcal{H}, t)$$

$$\lambda_1 \frac{\partial T_1}{\partial n_i}(\mathcal{H}, t) = \lambda_2 \frac{\partial T_2}{\partial n_i}(\mathcal{H}, t)$$

- 1 and 2 = labels for the two bodies
- n_i = common normal to the contact surface at $\mathcal{H}$

Principles and modes of mass transfer

Fundamentals of mass transfer

- Mass, in the form of generic particles constituting a fluid volume, is transferred by convection between any two regions of a continuous system that are characterised by different hydraulic heads

- Hydraulic heads are the potential variable that governs mass transfer

- The gradient of these variables govern mass transfer in much as the same way a temperature gradient characterises heat transfer

Fundamentals of mass transfer

- The global hydraulic potential that describes mass transfer is the total head, H

- This potential is made of three contributions that characterise fluids at each point:

  - the elevation head, h_z, due to the weight of the fluid
  - the pressure head, h_p, due to the static pressure
  - the velocity head, h_v, due to the bulk motion of the fluid

- The expression of the total head, e.g., considering water, reads

$$H = h_z + h_p + h_v = z + \frac{p_w}{\gamma_w} + \frac{v_w^2}{2g}$$

Modes of mass transfer

- There are 2 fundamental modes of mass transfer:
  - Laminar flow
  - Turbulent flow

- *Laminar flow - the trajectories of the single particles constituting the fluid in motion coincide with the effective trajectories of the average fluid motion*

- *Turbulent flow - the trajectories of the single particles constituting the fluid in motion are random and no more coincident with the effective trajectories of the average fluid motion*

Reynolds number

- The distinction between laminar and turbulent flows is based on the knowledge of the Reynolds number

$$Re_x = \frac{\rho_f v_\infty x}{\mu_f}$$

- v_∞ = characteristic velocity of the fluid (i.e., mean relative velocity)
- x = characteristic length of the considered problem (i.e., hydraulic diameter for a flow within a circular pipe)
- μ_f = the dynamic viscosity of the fluid

- Reynolds number represents the ratio of inertia to viscous forces

Critical values of Reynolds number

- For flows over plane surfaces: $10^5 \leq Re_c \leq 3 \cdot 10^6$ (Bergman et al., 2011)
- For seepage flows within soils: $2000 \leq Re_c \leq 3000$
- The previous markedly different values are a result of the different characteristic length that is considered to describe the problem
- Under laminar conditions

$$H = h_z + h_p = z + \frac{p_w}{\gamma_w} = h$$

Darcy's law

- Darcy's law allows expressing a relation between the hydraulic gradient and the mean flow velocity under steady conditions

$$\bar{v}_{rw,i} = -k\nabla h = -k\nabla\left(z + \frac{p_w}{\gamma_w}\right)$$

- k = hydraulic conductivity
- h = piezometric head
- p_w = pore water pressure
- g = gravity
- z = vertical coordinate

- If a relationship between the mass flux density $\dot{q}_{D,i}$ and ∇h is considered, the *rate equation* describing mass transfer is found

$$\dot{q}_{D,i} = -k\nabla h$$

Hydraulic conductivity

- The hydraulic conductivity of geomaterials depends on the characteristics of the medium across which the fluid flows as well as on the physical properties of the fluid (Vulliet et al., 2016), i.e.:
  - Granulometry
  - Soil fabric
  - Dry density
  - Temperature

- In rock masses, hydraulic conductivity depends on the characteristics of the fractures network

Mass conservation equation

Rationale

- The mass conservation equation is the master equation that governs mass transfer phenomena in physical systems
- This equation expresses a relation between the kinematic characteristics of a fluid motion and the density of the fluid
- This master equation is also often termed continuity equation
- Usually derived in an elementary manner based on a mass balance for an elementary volume, similar to what presented for the energy conservation equation

Mass conservation equation

- The mass conservation equation is obtained for a volume in which mass flows in and out, subjected to arbitrary hydraulic conditions on its surfaces with internal volumetric mass generation $\dot{q}_v$ per unit time

$$-\nabla \cdot \left(\rho_f \bar{v}_{rf,i}\right) + \dot{q}_v = \frac{\partial \rho_f}{\partial t}$$

- In many practical cases, no volumetric mass generation is considered and the fluid is assumed incompressible. Hence

$$\nabla \cdot \bar{v}_{rf,i} = 0$$

Mass conservation equation

- For analyses of seepage flows within geomaterials fully saturated with water, it is common to assume that the solid grains are incompressible and the volume fraction of the fluid is characterised by a bulk density of $\rho \equiv n\rho_w$. Hence

$$-\nabla \cdot \left(\rho_w \bar{v}_{rw,i}\right) + \dot{q}_v = \frac{\partial n\rho_w}{\partial t}$$

- If the porous medium is also assumed to be incompressible and no volumetric mass generation occurs, the above can be rewritten as

$$\nabla \cdot \bar{v}_{rw,i} = 0$$

Initial and boundary conditions

- Analogous considerations to those presented for characterising heat transfer problems hold for fully describing mass transfer problems with reference to the initial and boundary conditions

- In this case, the boundary conditions are generally expressed either as a function of a hydraulic head, $\bar{H}$ (Dirichlet's condition) or a flux, $\partial H/\partial n_i$ (Neumann's condition)

Summary of typical thermal and hydraulic parameters

Material	Hydraulic conductivity, k [m/s]	Thermal conductivity, λ [W/(m °C)]		Volumetric heat capacity, ρc_p [MJ/(m^3°C)]	
		Dry	Saturated	Dry	Saturated
Clay	10^{-8}–10^{-10}	0.4 – 1.0	0.9 – 2.3	0.3 – 0.6	2.1 – 3.2
Silt	10^{-5}–10^{-8}	0.4 – 1.0	0.9 – 2.3	0.6 – 1.0	2.1 – 2.4
Sand	10^{-3}–10^{-4}	0.3 – 0.8	1.7 – 5.0	1.0 – 1.3	2.2 – 2.4
Gravel	10^{-1}–10^{-3}	0.4 – 0.5	1.8	1.2 – 1.6	2.2 – 2.4
Concrete	10^{-9}–10^{-12}	0.9 – 2.0		1.8 – 2.0	
Steel	-	14 – 60		3.12	
Water	-	0.57		4.186	
Air	-	0.025		0.0012	

(data from Phaud, 2002; Vulliet et al., 2016)