House Model Reference Manual
FutureFactory

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1   Introduction

Building energy simulation is a vast field of research that started in the late 50's and that is still highly active nowadays. Building energy simulations are mainly used to help taking design decisions, to analyze current designs and to forecast future building energy use. Building energy modelling methods can mainly be divided into three categories:

- White box models (physics-based)

- Black box models (data-driven)

- Grey box models (hybrid)

White box models are based on the equations related to the fundamental laws of energy and mass balance and heat transfer. White box models can be differentiated in two types, *distributed* parameter models and *lumped* parameter models. Lumped parameter models simplify the description of distributed physical systems into discrete entities that approximate the behavior of a distributed system. The advantage of using lumped models is the decrease in simulation time (**Ramallo-González et al.**[1]). White box models are of special interest for the design phase as they are used to predict and analyse the performance of the building envelope and building systems.

Black box models are based on the statistical relation between input and output system values. The statistical relation between input and output is based on actual data. The relation between the parameters can differ based on the amount of data and the method used to analyze the relation. Currently, there is a large and active field of research about statistical models that are used on black box models (**Coacley et al.**[2]). Black box models are of special interest when there is a large amount of actual input and output data available.

Grey box models are hybrid models that aim to combine the advantages of both approaches. In order to use them it is necessary to implement some equations and it is also required to have actual data of inputs and outputs.

In the FutureFactory project, the modelling research in the HAN-AEA-BES group is extended from a static lumped element white box model into a dynamic model. The extension enables incorporation of building installations for heating and climatization into the model of the building itself. The installations are represented by either their physical parameters or by a grey-box approach. In the latter approach, gas boiler can be modeled as an abstract heat source with a minimum and maximum thermal power, regulated by a (PI(D)) controller with hysteresis which takes the difference between the actual room temperature and the setpoint of the room thermostat as the error signal.

Similarly, a heat pump can be modelled as a heat source which delivers thermal power dependent on outdoor (evaporator) temperature and delivery (condensor) temperature. The efficiency parameter (COP) then depends on the same two basic parameters. Such grey-box models are applied in working standards as he Dutch NTA 8800 (Appendix Q).

This research is aimed at establishing how a dynamic model can be made, depending on lumped elements yet showing the essential control behaviour of basic building HVAC installations. Successful extension of the modelling capacities can be applied to lay a solid foundation under key decisions in the energy transition of the built environment.

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2 White box lumped model for a building: RC networks

The objective of the house model for this project is to serve as test environment for a heating model, which means that the house model is intended as a tool to enable taking building installation design decisions. The house heating demand calculation model implemented for this project is a white box *lumped* model. Specifically, it is a RC network model consisting of thermal resistances (R) and capacities (C). The RC network model is based on the analogy with electrical circuits. The simulation of thermodynamic systems characterizing building elements as resistances or capacities allows to simplify the model while maintaining a high simulation results accuracy (**Bagheri et al.[3], Bacher et al[4].**).

2.1 White box lumped models

There are several types of RC models, the most common being 3R4C models and 3R2C models which are applied on the outer and internal building walls. For the simulation of simple house buildings 3R2C models perform as accurate as more complex 3R4C models (**Fraisse et al.[5]**). Considering that one of the objectives for this project is to obtain a fast but accurate simulation of a simple dwelling the 3R2C network model appeared a good starting point. In the 3R2C model two indoor temperature nodes are present in the dwelling. with capacities (usually an air and a wall temperature) and a well-known outdoor temperature. Between these 3 temperature nodes 3 heat transfer resistances are present. However, the direct heat transfer between the inner walls and the outdoor air is low. Moreover, uncertainties are present about heat transfer coefficients between walls and indoor air, different indoor temperatures in the house rooms and the ground temperature which deviates from the outdoor temperature. In addition, occupancy behaviour varies strongly. For that reason, we have made a further simplification to a 2R2C model. In section 4 it is shown that this dwelling model delivers a reliable annual energy consumption.

2.2 House Model R and C Values

This section presents the basic information for calculating a house model based on an RC network. This category of house models, analogous to electrical impedance networks, may have different numbers of R and C components and may have various component topologies. For the specific model properties, references will be given.

In heat transfer theory the basic thermal circuit contains thermal resistances. Heat transfer occurs via conduction, convection and radiation. In analogy with Ohm's Law for electricity, expressions can be derived for the heat transfer rate (analogous to electrical current) and the thermal resistances (analogous to ohmic resistances) in these three modes of heat transfer. The temperature difference plays a role analogous to the electrical voltage difference. These expressions are shown in Fig.1.

Equations for different heat transfer modes and their thermal resistances.

Transfer Mode	Rate of Heat Transfer	Thermal Resistance
Conduction	$\dot{Q} = \dfrac{T_1 - T_2}{\left(\frac{L}{kA}\right)}$	$\dfrac{L}{kA}$
Convection	$\dot{Q} = \dfrac{T_{\text{surf}} - T_{\text{envr}}}{\left(\frac{1}{h_{\text{conv}} A_{\text{surf}}}\right)}$	$\dfrac{1}{h_{\text{conv}} A_{\text{surf}}}$
Radiation	$\dot{Q} = \dfrac{T_{\text{surf}} - T_{\text{surr}}}{\left(\frac{1}{h_r A_{\text{surf}}}\right)}$	$\dfrac{1}{h_r A}$, where $h_r = \epsilon \sigma (T_{\text{surf}}^2 + T_{\text{surr}}^2)(T_{\text{surf}} + T_{\text{surr}})$

Figure 1: Heat transfer modes [6].

In [7] and [8] the expressions in Fig.1 are derived. For conduction, the expression for absolute thermal resistance is:

$$R = \frac{L}{kA} \qquad \left[\frac{K}{W}\right] \tag{1}$$

- L is the distance over which heat transfer takes place, or the thickness of the material $[m]$.

- k (also denoted with λ) is the thermal conductivity of the material. $[\frac{W}{mK}]$.

- A is the conductive surface area $[m^2]$.

- Thermal resistivity is the reciprocal of thermal conductivity and can be expressed as $r = \frac{1}{k}$ in $[\frac{mK}{W}]$

For convection and radiation the expression for thermal resistance is: $R = \frac{1}{h \cdot A}$ $[\frac{K}{W}]$.

- A is the surface area where the heat transfer takes place $[m^2]$.

- h is the heat transfer coefficient $[\frac{W}{m^2K}]$

The R-value (in Dutch: R-waarde or R_d-waarde) of a building material [9] is the thermal resistance of a square meter surface. It can be calculated by multiplying the thermal *resistivity* with the thickness of the material in m. Alternatively it is calculated by dividing the material thickness by the thermal *conductivity* k or λ.

$$\text{R-value} = r \cdot L \qquad \text{or} \qquad \text{R-value} = \frac{L}{k} \qquad \text{or} \qquad \text{R-value} = \frac{L}{\lambda} \qquad \left[m \cdot \frac{m \cdot K}{W}\right] = \left[\frac{m^2 \cdot K}{W}\right] \tag{2}$$

Some typical heat transfer R-values are: [10]:

- Static layer of air, 40 mm thickness (1.57 in) : R = 0.18 $[\frac{m^2K}{W}]$.

- Inside heat transfer resistance, horizontal current : R = 0.13 $[\frac{m^2K}{W}]$.

- Outside heat transfer resistance, horizontal current : R = 0.04 $[\frac{m^2K}{W}]$.

- Inside heat transfer resistance, heat current from down upwards : R = 0.10 $[\frac{m^2K}{W}]$.

- Outside heat transfer resistance, heat current from above downwards : R = 0.17 $[\frac{m^2K}{W}]$.

Note: in Dutch building physics, R-values with subscripts are used:

- R_d-waarde is used for the R-value of a homogeneous building material. $R = \frac{L}{\lambda}$

- R_c-waarde (compound, construction) is used for the R-value of a surface consisting of several building materials. R_c-waarden are calculated as the surface-area weighted sum of R_d-waarden of the building materials. For the simplest roof surface, R_c is a linear combination of the R-values of the wooden joists and girders (spanten en gordingen) and the areas in between, filled with a certain insulation material sandwich. The R-value of the insulation sandwich, in its turn, is the sum of the R-values of the materials in the sandwich. From inside out, this sandwich may consist of *e.g.* a 9.5 mm plaster board, a PIR/PUR insulation panel, an air gap and a wooden roof deck. All types of R-value have the dimension $[\frac{m^2 \cdot K}{W}]$.
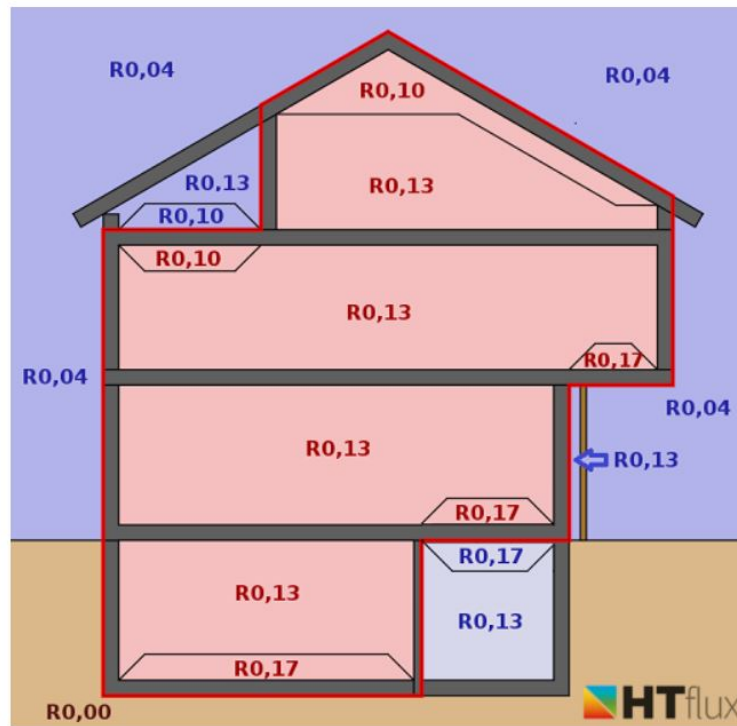
Figure 2: An overview of R-values for heat transfer [11].

The standard R_c-values that have been used for facades, roof and floor until 2020 are summarized in Fig.3:

Construction	New construction	Renovation
Facades [1]	Rc 4.5 m2K / W	Rc 1.3 m2K / W
Roofs [2]	Rc 6.0 m2K / W	Rc 2.0 m2K / W
Floors [3]	Rc 3.5 m2K / W	Rc 2.5 m2K / W

Figure 3: R_c Values [12]

New standard values will be used from 1-1-2021, since the building standard NEN 1068 will be replaced by the NTA 8800 standard. The old and new situation is described in "EnergieVademecum Energiebewust ontwerpen van nieuwbouwwoningen", Hoofdstuk 5: Thermische isolatie, thermische bruggen en luchtdichtheid. [13].

From 2015, the following RC values apply to new construction in the Netherlands:

Location	RC value (NEN 1068, until 1-1-2021) [m2K / W]	Rc value (NTA 8800, from 1-1-2021) [m2K / W]
floor	> = 3.5	> = 3.7
facade	> = 4.5	> = 4.7
roof	> = 6.0	> = 6.3

Figure 4: R_c Values [14]

The values used for different types of houses such as: row houses, detached houses and apartments can be found in the document "Voorbeeldwoningen 2011" [15]. An example with values for a common type of row house, built in the period from 1975 to 1991 is shown in Fig. 5:

Bouwdelen	Huidig			Besparingspakket			Investeringskosten	
	Opp. (m²)	Rc-Waarde (m² K/W)	U-Waarde (W/m²K)	Opp. (m²)	Rc-Waarde (m² K/W)	U-Waarde (W/m²K)	Per m²	Totaal
Begane grondvloer ³	51,0	0,52	1,28	51,0	2,53	0,36	€ 20	€ 1.020
Plat dak ³	-	-	-	-	-	-	-	€ 0
Hellend dak ³	68,6	1,30	0,64	68,6	2,53	0,36	€ 53	€ 3.640
Achter- en voorgevel								
– Gesloten ³	40,6	1,30	0,64	40,6	2,53	0,36	€ 21	€ 850
– Enkelglas ³	3,1		5,20	-		-	€ 139	€ 430
– Dubbelglas ³	16,2		2,90	-		-	€ 142	€ 2.300
– HR⁺⁺ glas	-		-	19,3		1,80		
Zijgevel								
– Gesloten	58,4	1,30	0,64	58,4	2,53	0,36	€ 21	€ 1.230
– Enkelglas	-		-	-		-	-	€ 0
– Dubbelglas	1,8		2,90	-		-	€ 142	€ 260
– HR⁺⁺ glas	-		-	1,8		1,80		

Figure 5: R_c-values for a row house type built between 1975-1991 [15]

2.3 Thermal building (envelope) model analogous to a 2R-2C electrical network

The heat transfer in a building will be modelled in analogy to an electrical circuit where *heat transfer rate* is analogous to by current, *temperature* difference is analogous to potential difference, heat sources are represented by constant current sources, absolute thermal resistances are represented by resistors and thermal capacity ()heat capacity) by capacitors [16]. Figure 6 summarizes the similar term use in different fields.

type	structural analogy[1]	hydraulic analogy	thermal	electrical analogy[2]
quantity	impulse J [N·s]	volume V [m³]	heat Q [J]	charge q [C]
potential	displacement X [m]	pressure P [N/m²]	temperature T [K]	potential V [V = J/C]
flux	load or force F [N]	flow rate Q [m³/s]	heat transfer rate $\dot{Q}$ [W = J/s]	current I [A = C/s]
flux density	stress σ [Pa = N/m²]	velocity $\mathbf{v}$ [m/s]	heat flux $\mathbf{q}$ [W/m²]	current density $\mathbf{j}$ [C/(m²·s) = A/m²]
resistance	flexibility (rheology defined) [1/Pa]	fluid resistance R [...]	**thermal resistance R [K/W]**	electrical resistance R [Ω]
conductance	... ... [Pa]	fluid conductance G [...]	thermal conductance G [W/K]	electrical conductance G [S]
resistivity	flexibility $1/k$ [m/N]	fluid resistivity	thermal resistivity [(m·K)/W]	electrical resistivity ρ [Ω·m]
conductivity	stiffness k [N/m]	fluid conductivity	thermal conductivity k [W/(m·K)]	electrical conductivity σ [S/m]
lumped element linear model	Hooke's law $\Delta X = F/k$	Hagen–Poiseuille equation $\Delta P = QR$	Newton's law of cooling $\Delta T = \dot{Q}R$	Ohm's law $\Delta V = IR$
distributed linear model	... ...	... ...	Fourier's law $\mathbf{q} = -k\boldsymbol{\nabla}T$	Ohm's law $\mathbf{J} = \sigma\mathbf{E} = -\sigma\boldsymbol{\nabla}V$

Figure 6: Table of Analogies [16]

The 2R-2C house model structure is implemented as described below. The schematic of an envelope house model has been shown in figure 7 and the equivalent electrical 2R-2C network with components and topology is given in fig 8.
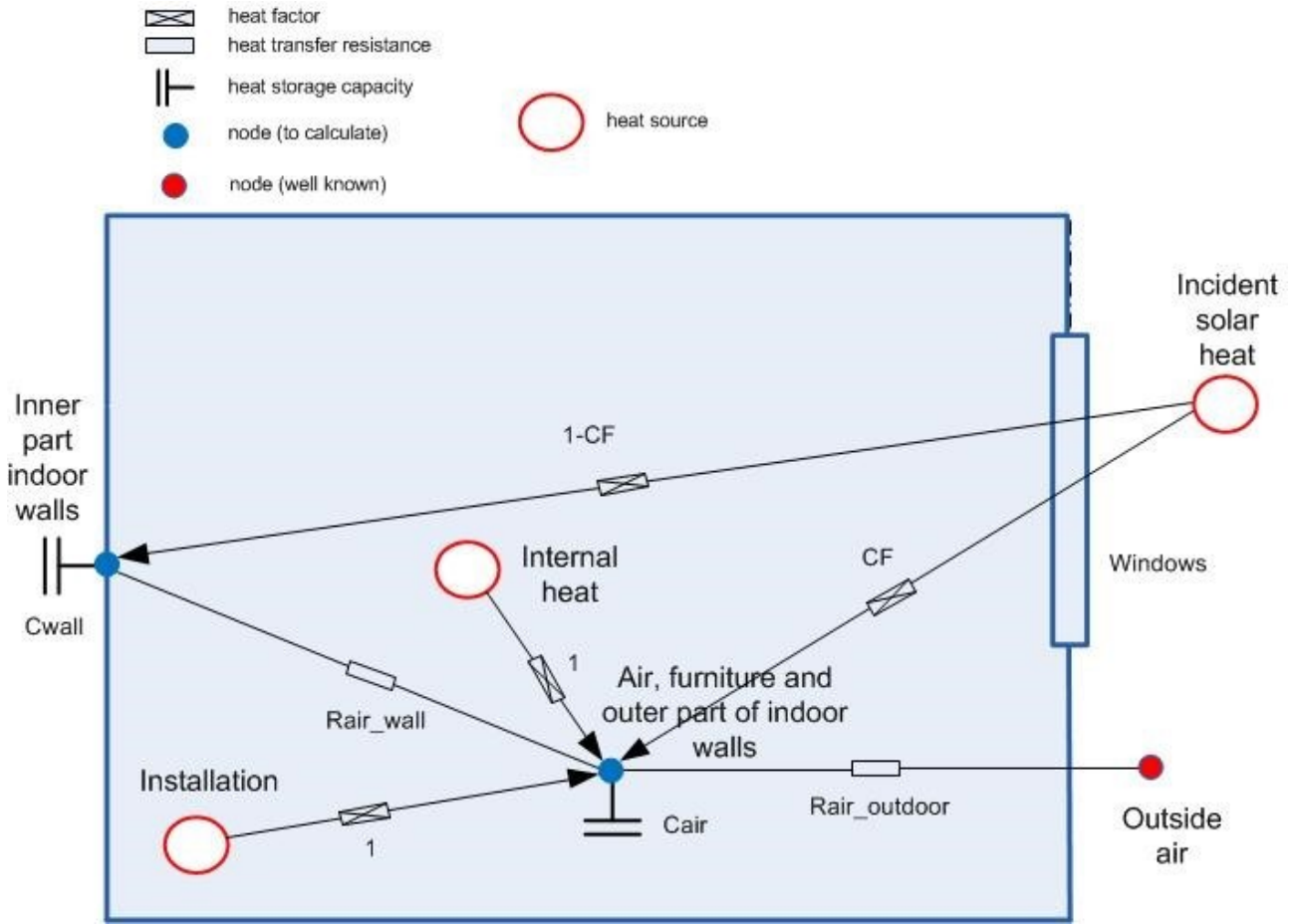
Figure 7: Schematic of envelope model
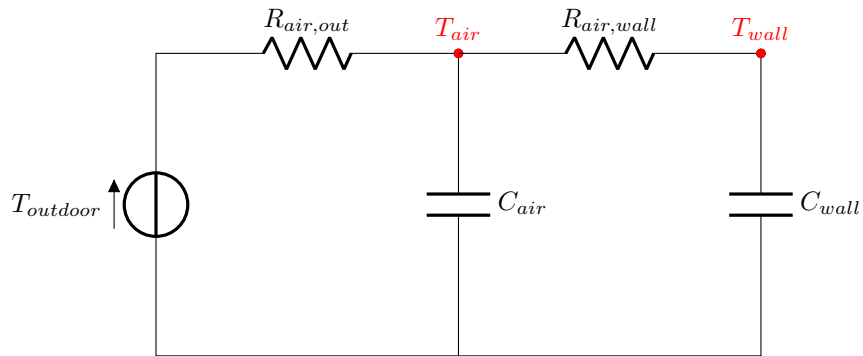
Figure 8: 2R-2C house model.

The model consists of two heat capacities $C_{air,\ indoor}$ and C_{wall} and two resistances R_{wall} and $R_{air,\ outdoor}$. The incident solar energy is divided between C_{wall} and C_{air} through the convection factor CF. It is assumed that both internal heat (lighting, occupancy and electric devices) and supplied heat (installation) initially heat up the indoor air. In Fig. 7, they are fully released at the T_{air} node.

It is also assumed that furniture and the **surface part** of the walls have the same temperature as the air **and the wall mass is divided between the air and wall mass**. Thus, the heat capacity of the air node consists of the air heat capacity, furniture heat capacity and the heat capacity **of a part of the walls**. **Appendix A** presents the coefficients in the dwelling model. In the resistance $R_{air,\ outdoor}$ the influence of heat transmission through the outdoor walls and natural ventilation is considered.

For the air and wall nodes the following power balances can be set up:

$$C_{air} \frac{dT_{air}}{dt} = \frac{T_{outdoor} - T_{air}}{R_{air\_outdoor}} + \frac{T_{wall} - T_{air}}{R_{air\_wall}} + \dot{Q}_{inst} + \dot{Q}_{internal} + CF \cdot \dot{Q}_{solar} \tag{3}$$

$$C_{wall} \frac{dT_{wall}}{dt} = \frac{T_{air} - T_{wall}}{R_{air\_wall}} + (1 - CF) \cdot \dot{Q}_{solar} \tag{4}$$

- CF: convection factor (solar radiation): the convection factor is the part of the solar radiation that enters the room and is released directly convectively into the room.

- $\dot{Q}_{inst}$: delivered heat from heating system (radiator) [W].

- $\dot{Q}_{inernal}$: internal heat [W].

- $\dot{Q}_{solar}$: heat from solar irradiation [W].

- T_{air}: indoor air temperature °C.

- $T_{outdoor}$: outdoor temperature °C.

- T_{wall}: wall temperature °C.

- R_{air_wall}: walls surface resistance $[\frac{K}{W}]$.

- $R_{air\_outdoor}$: outdoor surface resistance $[\frac{K}{W}]$.

- C_{air}: air thermal capacity (heat capacity) $[\frac{J}{K}]$[17].

- C_{wall}: wall thermal capacity (heat capacity) $[\frac{J}{K}]$[17].

Total heat transfer of solar irradiation through the glass windows:

$$\dot{Q}_{solar} = g. \sum (A_{glass}.\dot{q}_{solar}) \tag{5}$$

- $\dot{q}_{solar}$: solar radiation on the outdoor walls $[\frac{W}{m^2}]$.

- g: g value of the glass (ZTA in dutch) [0..1][18]

- A: glass surface $[m^2]$.

3 Lumped-element thermal model of a building

Heat generation and transport inside a building, with heat loss to the surrounding outdoor environment is governed by the same laws of conduction, convection and radiation as elsewhere. A number of approximations is made, however, which will be treated below:

3.1 Heat Conduction: Fourier's Law

Heat transport *within* a solid material is governed by conduction, according to Fourier's Law, illustrated in Figure 9. One side of a rectangular solid is held at temperature T_1, while the opposite side is held at a lower temperature, T_2. The other four sides are insulated so that heat can flow only in the x-direction. For a given material, it is found that the rate, $\dot{Q}_x$, at which heat (thermal energy) is transferred from the hot side to the cold side (the *heat transfer rate*) is proportional to the cross-sectional area, A, across which the heat flows; the temperature difference, $T_1 - T_2$; and inversely proportional to the thickness, Δx, of the material. That is:

$$\dot{Q}_x = -kA\frac{\Delta T}{\Delta x} \tag{6}$$
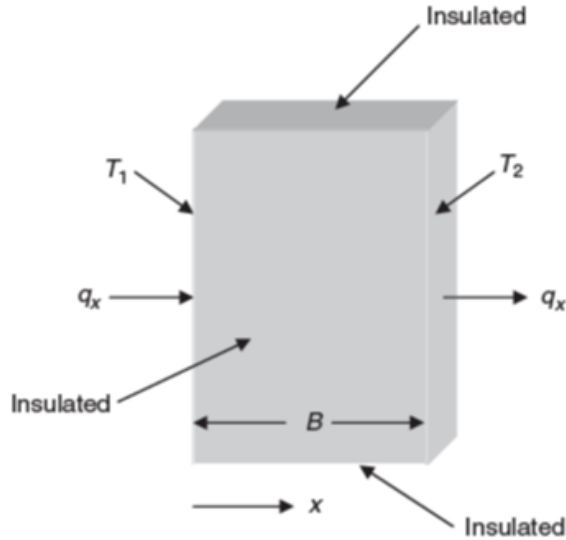
Figure 9: One-dimensional heat conduction in a solid

The constant of proportionality, k, is called the *thermal conductivity*. Equation (6) is also applicable to heat conduction in liquids and gases. However, when temperature differences exist in fluids, convection currents tend to be set up, so that heat is generally not transferred solely by the mechanism of conduction. The thermal conductivity is a property of the material. Values may be found in various handbooks and compendiums of physical property data.

The form of Fourier's law given by Equation (6) is valid only when the thermal conductivity can be assumed constant. A more general result can be obtained by writing the equation for an element of differential thickness. in the limit as Δx approaches zero, $\frac{\Delta T}{\Delta x} \to \frac{dT}{dx}$. Thus, substituting in Equation (6) gives:

$$\dot{Q}_x = -kA\frac{dT}{dx} \tag{7}$$

Equation (7) is not subject to the restriction of constant k. Furthermore, when k is constant, it can be integrated to yield Equation (6). Hence, Equation (7) is the general one-dimensional form of Fourier's law. The negative sign is necessary because heat flows in the positive x-direction when the temperature decreases in the

x-direction. Thus, according to the standard sign convention that $\dot{Q}_x$ is positive when the heat flow is in the positive x-direction, $\dot{Q}_x$ must be positive when dT/dx is negative.

3.1.1 More than one dimension

It is often convenient to formulate Fourier's Law in the original phrasing: the *heat flux* $\dot{\varphi}$ is proportional to the *temperature gradient*. We divide (7) by the area to give:

$$\dot{\varphi_x} \equiv \frac{\dot{Q}_x}{A} - k\frac{dT}{dx} \tag{8}$$

where $\dot{\varphi_x}$ is the heat flux. It has units of $\frac{J}{s \cdot m^2} = \frac{W}{m^2}$. Thus, the units of k are $\frac{W}{m \cdot K}$.

Equation (8) is restricted to the situation in which heat flows in the x-direction only. In the general case in which heat flows in all three coordinate directions, the total heat flux is obtained by vector addition of adding the fluxes in the coordinate directions. Thus,

$$\dot{\boldsymbol{\varphi}} = \dot{\varphi_x}\mathbf{i} + \dot{\varphi_y}\mathbf{j} + \dot{\varphi_z}\mathbf{k} \tag{9}$$

where $\dot{\boldsymbol{\varphi}}$ is the heat flux vector and $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$ are unit vectors in the x-, y-, z-directions, respectively.

Each of the component fluxes is given by a one-dimensional Fourier expression as follows:

$$\dot{\varphi_x} = -k\frac{\partial T}{\partial x} \qquad \dot{\varphi_y} = -k\frac{\partial T}{\partial y} \qquad \dot{\varphi_z} = -k\frac{\partial T}{\partial z} \tag{10}$$

Partial derivatives are used here since the temperature now varies in all three directions. Substituting the above expressions for the fluxes into Equation (9) gives:

$$\dot{\boldsymbol{\varphi}} = -k\left(\frac{\partial T}{\partial x}\mathbf{i} + \frac{\partial T}{\partial y}\mathbf{j} + \frac{\partial T}{\partial z}\mathbf{k}\right) \tag{11}$$

The vector in parenthesis is the temperature gradient vector, and is denoted by ∇T. Hence,

$$\dot{\boldsymbol{\varphi}} = -k\nabla T \tag{12}$$

Equation (12) is the three-dimensional form of Fourier's law. It is valid for homogeneous, isotropic materials for which the thermal conductivity is the same in all directions. Fourier's law states that heat flows in the direction of greatest temperature decrease.

3.1.2 The Heat Conduction Equation

The solution of problems involving heat conduction in solids can, in principle, be reduced to the solution of a single differential equation, the *heat conduction equation*. The equation can be derived by making a thermal power balance on a differential volume element in the solid. For the case of conduction in the x-direction only, such a volume element is illustrated in Figure 10.
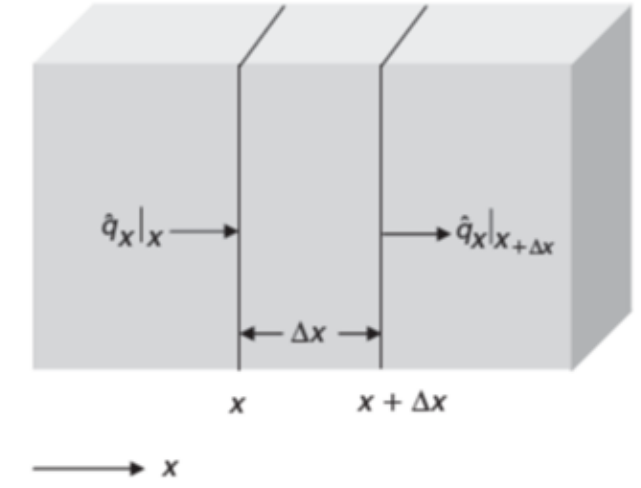
Figure 10: Differential element for 1D heat conduction

The rate at which thermal energy enters the volume element across the face at x is given by the product of the heat flux and the cross-sectional area, $\dot{\varphi}_x|_x \cdot A$. Similarly, the rate at which thermal energy leaves the element across the face at $x + \Delta x$ is $\dot{\varphi}_x|_{x+\Delta x} \cdot A$.

A heat generation term appears in the equation because the balance is made on thermal energy, not total energy. For example, thermal energy may be generated within a solid by an electric current or by decay of a radioactive material.

For a homogeneous heat source of strength $\dot{q}$ *per unit volume*, the net rate of generation is $\dot{q}A\Delta x$. Finally, the rate of accumulation of heat in the material is given by the time derivative of the thermal energy content of the volume element, which is $\rho c(T - T_{ref})A\Delta x$, where T_{ref} is an arbitrary reference temperature. Thus, the balance equation becomes:

$$\left(\dot{\varphi}_x|_x - \dot{\varphi}_x|_{x+\Delta x}\right)A + \dot{q}A\Delta x = \rho c \frac{\partial T}{\partial t} A\Delta x \tag{13}$$

It has been assumed here that the density, ρ, and heat capacity, c, are constant.

Dividing by $A\Delta x$ and taking the limit as $\Delta x \to 0$ yields:

$$\rho c \frac{\partial T}{\partial t} = -\frac{\partial \dot{\varphi}_x}{\partial x} + \dot{q} \tag{14}$$

Using Fourier's law as given by Equation (8), the balance equation becomes:

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\frac{k\partial T}{\partial x}\right) + \dot{q} \tag{15}$$

When conduction occurs in all three coordinate directions, the balance equation contains y- and z-derivatives analogous to the x-derivative. The balance equation then becomes:

$$\rho c \frac{\partial T}{\partial x} = \frac{\partial}{\partial x}\left(\frac{k\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{k\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{k\partial T}{\partial z}\right) + \dot{q} \tag{16}$$

When k is constant, it can be taken outside the derivatives and Equation (16) can be written as:

$$\frac{\rho c}{k} \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} + \frac{\dot{q}}{k} \tag{17}$$

or

$$\frac{1}{\alpha} \frac{\partial T}{\partial t} = \nabla^2 T + \frac{\dot{q}}{k} \tag{18}$$

where $\alpha \equiv k/\rho c$ is the *thermal diffusivity* and ∇^2 is the Laplacian operator. The thermal diffusivity has units of m^2/s.

3.2 Convection: Newton's Law of cooling

When a solid is *immersed* in a fluid or atmospheric gas, heat transfer on the interface occurs by convection. This phenomenon is governed by Newton's Law of cooling:

"The rate of heat lost by a body is directly proportional to the temperature difference of a body and its surroundings"

$$\dot{Q}_x = -hA\Delta T \tag{19}$$

3.3 Radiation

3.4 Approximations: A Simplified Model

In building physics, it is often assumed that Fourier's Law is valid in the form of Eq. (6). This can be done under the condition that

$$\nabla^2 T \equiv 0 \rightarrow \quad \frac{\partial T}{\partial \mathbf{r}} = constant \tag{20}$$

3.5 Lumped-element matrix representation

We take the 2R-2C lumped-element model from Section 2:

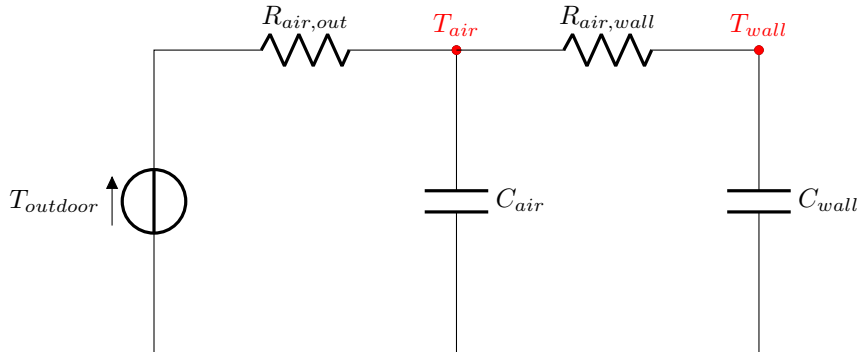**Figure 11:** 2R-2C house model.

The differential equations are:

$$C_{air} \frac{dT_{air}}{dt} = \frac{T_{amb} - T_{air}}{R_{air,amb}} + \frac{T_{wall} - T_{air}}{R_{air,wall}} + \dot{Q}_{heat,air} + \dot{Q}_{int,air} + \dot{Q}_{solar,air}$$

$$\tag{21}$$

$$C_{wall} \frac{dT_{wall}}{dt} = \frac{T_{air} - T_{wall}}{R_{air,wall}} + \dot{Q}_{solar,wall}$$

Writing out the differential equations in the classical notation:

$$C_{air}\frac{dT_{air}}{dt} = \left[\frac{-1}{R_{air,amb}} + \frac{-1}{R_{air,wall}}\right] \cdot T_{air} + \frac{1}{R_{air,wall}} \cdot T_{wall} + \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{heat,air} + \dot{Q}_{int,air} + \dot{Q}_{solar,air}$$

$$C_{wall}\frac{dT_{wall}}{dt} = \frac{1}{R_{air,wall}} \cdot T_{air} + \frac{-1}{R_{air,wall}} \cdot T_{wall} + \dot{Q}_{solar,wall}$$

$$(22)$$

The differential equations can be written in matrix notation as:

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = -\mathbf{K} \cdot \boldsymbol{\theta} + \dot{\mathbf{q}} \tag{23a}$$

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} + \mathbf{K} \cdot \boldsymbol{\theta} = \dot{\mathbf{q}} \tag{23b}$$

with:

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_{air} & 0 \\ 0 & C_{wall} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_{air}}{dt} \\ \frac{dT_{wall}}{dt} \end{bmatrix} \tag{24}$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{air,amb}} + \frac{1}{R_{air,wall}} & \frac{-1}{R_{air,wall}} \\ \frac{-1}{R_{air,wall}} & \frac{1}{R_{air,wall}} \end{bmatrix} \cdot \begin{bmatrix} T_{air} \\ T_{wall} \end{bmatrix} \tag{25}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{heat,air} + \dot{Q}_{int,air} + \dot{Q}_{solar,air} \\ \dot{Q}_{solar,wall} \end{bmatrix} \tag{26}$$

Written out, the differential equation according to (125) becomes:

$$\begin{bmatrix} C_{air} & 0 \\ 0 & C_{wall} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_{air}}{dt} \\ \frac{dT_{wall}}{dt} \end{bmatrix} = \begin{bmatrix} \frac{-1}{R_{air,amb}} + \frac{-1}{R_{air,wall}} & \frac{1}{R_{air,wall}} \\ \frac{1}{R_{air,wall}} & \frac{-1}{R_{air,wall}} \end{bmatrix} \cdot \begin{bmatrix} T_{air} \\ T_{wall} \end{bmatrix} +$$

$$\begin{bmatrix} \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{heat,air} + \dot{Q}_{int,air} + \dot{Q}_{solar,air} \\ \dot{Q}_{solar,wall} \end{bmatrix} \tag{27}$$

In the alternative notation:

$$\begin{bmatrix} C_{air} & 0 \\ 0 & C_{wall} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_{air}}{dt} \\ \frac{dT_{wall}}{dt} \end{bmatrix} + \begin{bmatrix} \frac{1}{R_{air,amb}} + \frac{1}{R_{air,wall}} & \frac{-1}{R_{air,wall}} \\ \frac{-1}{R_{air,wall}} & \frac{1}{R_{air,wall}} \end{bmatrix} \cdot \begin{bmatrix} T_{air} \\ T_{wall} \end{bmatrix} =$$

$$\begin{bmatrix} \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{heat,air} + \dot{Q}_{int,air} + \dot{Q}_{solar,air} \\ \dot{Q}_{solar,wall} \end{bmatrix} \tag{28}$$

The lumped-element equations above are systems of *first-order ordinary differential equations* (ODE). The first order derivative is with respect to *time*. The (silent) assumption that heat conduction within the air and the wall of the previous 2R-2C model is *faster* than the exchange of heat at the *interfaces* between air and wall

and air and ambient surroundings has replaced all spatial information from the *second-order partial differential equations* (PDE) that govern conductive heat transport *within* materials.

Therefore, the lumped-element equations can be solved by:

- the odexxx in Matlab., preferrably ode45.

- the state-space module in Simulink, after conversion to a state-space representation.

- the scipy.integrate.solve_ivp function in Python. In older code, scipy.integrate.odeint is still encountered.

- in C++ several options exist, similar to the options in Python.

The routines in Matlab, Simulink and Python need a *model function* that provides the vector $\dot{\boldsymbol{\theta}}$ for evaluation at any time instance chosen by the algorithm. The equations (125) then should be cast in the following form by left multiplication with $\mathbf{C}^{-1}$.

$$\mathbf{C}^{-1} \cdot \mathbf{C} \cdot \dot{\boldsymbol{\theta}} = -\mathbf{C}^{-1} \cdot \mathbf{K} \cdot \boldsymbol{\theta} + \mathbf{C}^{-1} \cdot \dot{\mathbf{q}} \tag{29a}$$

$$\dot{\boldsymbol{\theta}} = -\mathbf{C}^{-1} \cdot \mathbf{K} \cdot \boldsymbol{\theta} + \mathbf{C}^{-1} \cdot \dot{\mathbf{q}} \tag{29b}$$

Since $\mathbf{C}$ is a *diagonal* matrix with positive elements only, its inverse exists and contains the reciprocal elements on its diagonal:

$$\mathbf{C}^{-1} = \begin{bmatrix} \frac{1}{C_{air}} & 0 \\ 0 & \frac{1}{C_{wall}} \end{bmatrix} \tag{30}$$

This provides the division by the lumped thermal capacitances of the air and wall compartments in the model, necessary for the calculating the derivative vector $\dot{\boldsymbol{\theta}}$ in the model functions.

3.6 Extension of the method to larger lumped-element networks

Take a house model with two stories. Each level in the building is described with a 2R-2C model. Heat transfer occurs between the ground floor and the 1st floor.
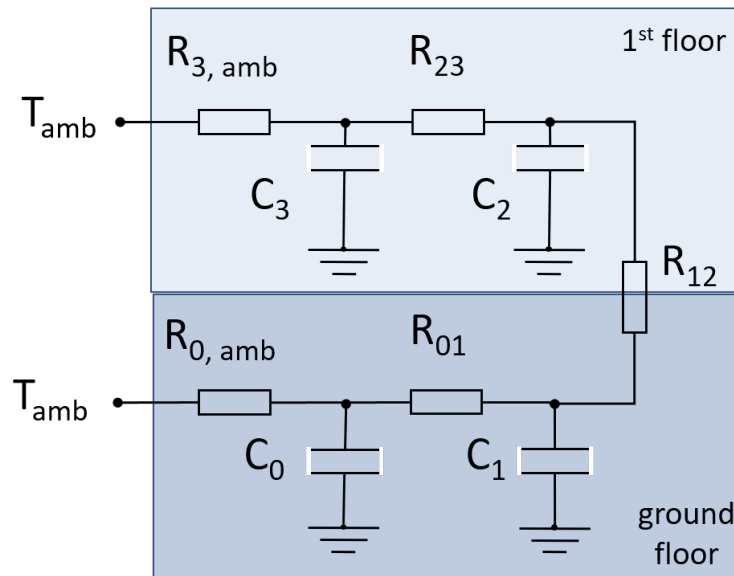

Figure 12: 5R-4C house model

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_0 & 0 & 0 & 0 \\ 0 & C_1 & 0 & 0 \\ 0 & 0 & C_2 & 0 \\ 0 & 0 & 0 & C_3 \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_0}{dt} \\ \frac{dT_1}{dt} \\ \frac{dT_2}{dt} \\ \frac{dT_3}{dt} \end{bmatrix} \tag{31}$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{0,amb}} + \frac{1}{R_{01}} & \frac{-1}{R_{01}} & 0 & 0 \\ \frac{-1}{R_{01}} & \frac{1}{R_{01}} + \frac{1}{R_{12}} & \frac{-1}{R_{12}} & 0 \\ 0 & \frac{-1}{R_{12}} & \frac{1}{R_{12}} + \frac{1}{R_{23}} & \frac{-1}{R_{23}} \\ 0 & 0 & \frac{-1}{R_{23}} & \frac{1}{R_{3,amb}} + \frac{1}{R_{23}} \end{bmatrix} \cdot \begin{bmatrix} T_0 \\ T_1 \\ T_2 \\ T_3 \end{bmatrix} \tag{32}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \frac{1}{R_{0,amb}} \cdot T_{amb} + \dot{Q}_{heat,0} + \dot{Q}_{int,0} + \dot{Q}_{solar,0} \\ \dot{Q}_{solar,1} \\ \dot{Q}_{solar,2} \\ \frac{1}{R_{3,amb}} \cdot T_{amb} + \dot{Q}_{heat,3} + \dot{Q}_{int,3} + \dot{Q}_{solar,3} \end{bmatrix} \tag{33}$$

3.7 Alternative representation of 5R-4C model

The 5R4C model of the previous section can be built from two 2R2C models, one for the ground floor and one for the first floor. The thermal resistance between the construction nodes of the ground and first floor is then added, R_{13} in the figure:
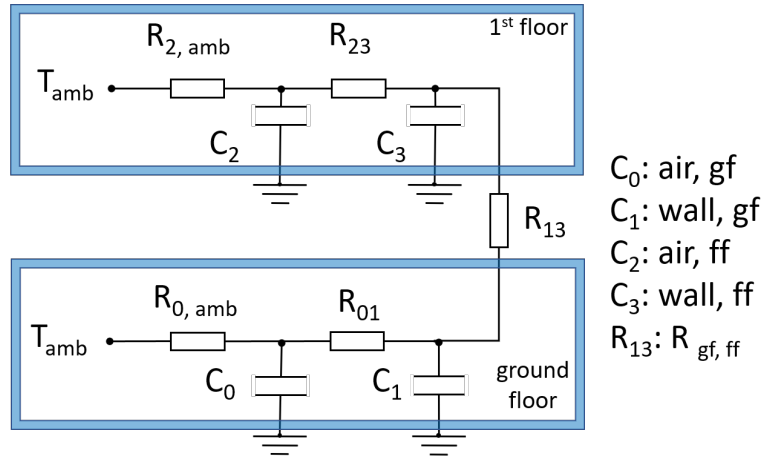
Figure 13: 5R-4C house model, alternative representation

As can be seen in the matrices below, adding R_{13} to the ground floor and first floor "chains" results in a non-symmetric matrix. It has to determined if this disadvantage outweighs the benefit of adding "chains".

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_0 & 0 & 0 & 0 \\ 0 & C_1 & 0 & 0 \\ 0 & 0 & C_2 & 0 \\ 0 & 0 & 0 & C_3 \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_0}{dt} \\ \frac{dT_1}{dt} \\ \frac{dT_2}{dt} \\ \frac{dT_3}{dt} \end{bmatrix} \tag{34}$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{0,amb}} + \frac{1}{R_{01}} & \frac{-1}{R_{01}} & 0 & 0 \\ \frac{-1}{R_{01}} & \frac{1}{R_{01}} + \frac{1}{R_{13}} & 0 & \frac{-1}{R_{13}} \\ 0 & 0 & \frac{1}{R_{2,amb}} + \frac{1}{R_{23}} & \frac{-1}{R_{23}} \\ 0 & \frac{-1}{R_{13}} & \frac{-1}{R_{23}} & \frac{1}{R_{23}} + \frac{1}{R_{13}} \end{bmatrix} \cdot \begin{bmatrix} T_0 \\ T_1 \\ T_2 \\ T_3 \end{bmatrix} \tag{35}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \frac{1}{R_{0,amb}} \cdot T_{amb} + \dot{Q}_{heat,0} + \dot{Q}_{int,0} + \dot{Q}_{solar,0} \\ \dot{Q}_{solar,1} \\ \frac{1}{R_{2,amb}} \cdot T_{amb} + \dot{Q}_{heat,2} + \dot{Q}_{int,2} + \dot{Q}_{solar,2} \\ \dot{Q}_{solar,3} \end{bmatrix} \tag{36}$$

Renumbering restores the matrices to a symmetric representation:
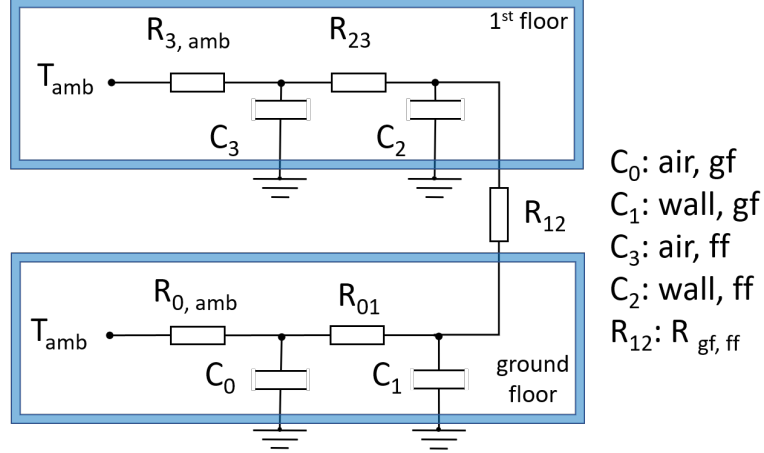
Figure 14: 5R-4C house model, alternative representation, renumbered

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_0 & 0 & 0 & 0 \\ 0 & C_1 & 0 & 0 \\ 0 & 0 & C_2 & 0 \\ 0 & 0 & 0 & C_3 \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_0}{dt} \\ \frac{dT_1}{dt} \\ \frac{dT_2}{dt} \\ \frac{dT_3}{dt} \end{bmatrix} \tag{37}$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{0,amb}} + \frac{1}{R_{01}} & \frac{-1}{R_{01}} & 0 & 0 \\ \frac{-1}{R_{01}} & \frac{1}{R_{01}} + \frac{1}{R_{12}} & \frac{-1}{R_{12}} & 0 \\ 0 & \frac{-1}{R_{12}} & \frac{1}{R_{23}} + \frac{1}{R_{12}} & \frac{-1}{R_{23}} \\ 0 & 0 & \frac{-1}{R_{23}} & \frac{1}{R_{3,amb}} + \frac{1}{R_{23}} \end{bmatrix} \cdot \begin{bmatrix} T_0 \\ T_1 \\ T_2 \\ T_3 \end{bmatrix} \tag{38}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \frac{1}{R_{0,amb}} \cdot T_{amb} + \dot{Q}_{heat,0} + \dot{Q}_{int,0} + \dot{Q}_{solar,0} \\ \dot{Q}_{solar,1} \\ \dot{Q}_{solar,2} \\ \frac{1}{R_{3,amb}} \cdot T_{amb} + \dot{Q}_{heat,3} + \dot{Q}_{int,3} + \dot{Q}_{solar,3} \end{bmatrix} \tag{39}$$

3.8 2R-2C model with buffervessel

The "air" and "wall" nodes of the 2R2C model can be extended with "radiator" node. The radiator has a finite heat capacity of itself. Instead of a thermal resistance, the radiator heat exchange in W/K is entered in the model. The radiator emits heat to the "air" node only. In its turn, the radiator is fed from a "buffervessel" node. The buffervessel loses heat to the radiator and is heated up by a gas boiler or alternatively a heat pump. The gas boiler does not heat the house directly, as was the case in the simplest model. A schematic view is given in Fig. **??**.

18
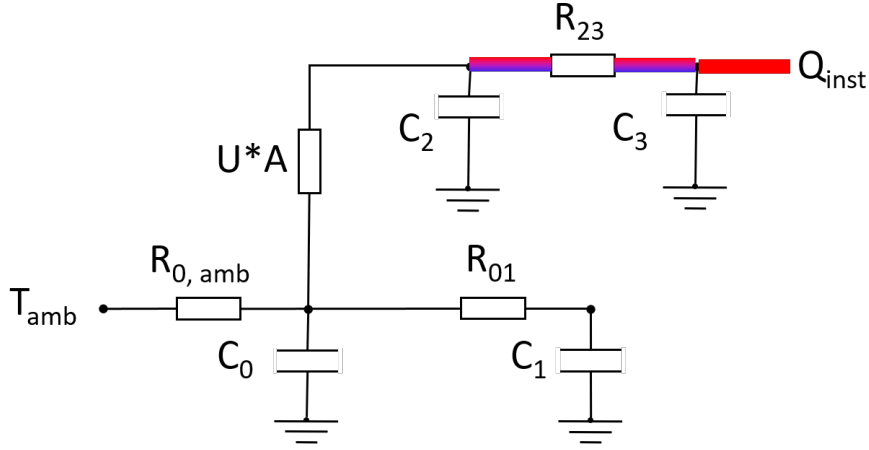
Figure 15: 2R-2C house model with radiator and buffer vessel

The differential equations for heat transport in the model of Fig. **??** are:

$$
\begin{aligned}
C_{air}\frac{dT_{air}}{dt} &= \frac{T_{outdoor} - T_{air}}{R_{air\_outdoor}} + \frac{T_{wall} - T_{air}}{R_{air\_wall}} + U_{rad} \cdot A_{rad} \cdot (T_{return} - T_{air}) + \dot{Q}_{internal} + \dot{Q}_{solar,0} \\
C_{wall}\frac{dT_{wall}}{dt} &= \frac{T_{air} - T_{wall}}{R_{air\_wall}} + \dot{Q}_{solar,1} \\
C_{rad}\frac{dT_{return}}{dt} &= \dot{m} \cdot c_{p,water} \cdot (T_{buffer} - T_{return}) + U_{rad} \cdot A_{rad} \cdot (T_{air} - T_{return}) \\
C_{buffer}\frac{dT_{buffer}}{dt} &= \dot{m} \cdot c_{p,water} \cdot (T_{return} - T_{buffer}) + \dot{Q}_{inst} \\
\frac{dE}{dt} &= \dot{Q}_{inst}
\end{aligned}
\tag{40}
$$

A fifth equation, integrating the heat source energy is sometimes added. Re-arranging the terms in the equation gives:

$$
\begin{aligned}
C_{air}\frac{dT_{air}}{dt} &= \left[\frac{-1}{R_{air\_outdoor}} + \frac{-1}{R_{air\_wall}} + -1 \cdot U_{rad} \cdot A_{rad} \right] \cdot T_{air} + \frac{T_{wall}}{R_{air\_wall}} + U_{rad} \cdot A_{rad} \cdot T_{return} + \\
&\quad \frac{T_{outdoor}}{R_{air\_outdoor}} + \dot{Q}_{internal} + \dot{Q}_{solar,0} \\
C_{wall}\frac{dT_{wall}}{dt} &= \frac{1}{R_{air\_wall}} \cdot T_{air} + \frac{-1}{R_{air\_wall}} \cdot T_{wall} + \dot{Q}_{solar,1} \\
C_{rad}\frac{dT_{return}}{dt} &= U_{rad} \cdot A_{rad} \cdot T_{air} + [-U_{rad} \cdot A_{rad} - \dot{m} \cdot c_{p,water}] \cdot T_{return} + \dot{m} \cdot c_{p,water} \cdot T_{buffer} \\
C_{buffer}\frac{dT_{buffer}}{dt} &= \dot{m} \cdot c_{p,water} \cdot T_{return} - \dot{m} \cdot c_{p,water} \cdot T_{buffer} + \dot{Q}_{heat,3} \\
\frac{dE}{dt} &= \dot{Q}_{inst}
\end{aligned}
\tag{41}
$$

Conversion of the equations to a matrix equation yields:

$$
\mathbf{C} \cdot \dot{\boldsymbol{\theta}} =
\begin{bmatrix}
C_0 & 0 & 0 & 0 \\
0 & C_1 & 0 & 0 \\
0 & 0 & C_2 & 0 \\
0 & 0 & 0 & C_3
\end{bmatrix}
\cdot
\begin{bmatrix}
\frac{dT_0}{dt} \\
\frac{dT_1}{dt} \\
\frac{dT_2}{dt} \\
\frac{dT_3}{dt}
\end{bmatrix}
\tag{42}
$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{0,amb}} + \frac{1}{R_{01}} + U \cdot A & \frac{-1}{R_{01}} & -U \cdot A & 0 \\ \frac{-1}{R_{01}} & \frac{1}{R_{01}} & 0 & 0 \\ -U \cdot A & 0 & U \cdot A + \frac{1}{R_{23}} & \frac{-1}{R_{23}} \\ 0 & 0 & \frac{-1}{R_{23}} & \frac{1}{R_{23}} \end{bmatrix} \cdot \begin{bmatrix} T_0 \\ T_1 \\ T_2 \\ T_3 \end{bmatrix} \tag{43}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \frac{1}{R_{0,amb}} \cdot T_{amb} + \dot{Q}_{int,0} + \dot{Q}_{solar,0} \\ \dot{Q}_{solar,0} \\ 0 \\ \dot{Q}_{heat,3} \end{bmatrix} \tag{44}$$

3.9   2R-2C model with radiator only
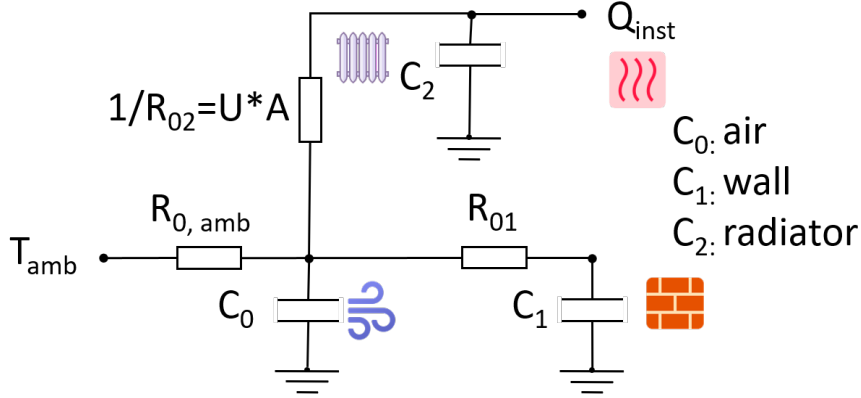
Figure 16: 2R-2C house model with radiator only

The rate of heat transfer from a radiator to the ambient(room) air can be calculated as follows [19]:

$$P = P_{50} \cdot \left[\Delta T_{LMTD} \cdot \frac{1}{49.32} \right]^n$$
$$\Delta T_{LMTD} = \frac{T_{inlet} - T_{return}}{\ln \frac{T_{inlet} - T_{ambient}}{T_{return} - T_{ambient}}} \tag{45}$$
$$n = 1.33$$

This is sometimes simplified to:

$$P = U \cdot A \cdot \Delta T_{LMTD}$$
$$\Delta T_{LMTD} = \frac{T_{inlet} - T_{return}}{\ln \frac{T_{inlet} - T_{ambient}}{T_{return} - T_{ambient}}} \tag{46}$$

or simplified to [20, 21]:

$$P = K_m \cdot \Delta T^n$$
$$\Delta T = \frac{T_{inlet} + T_{return}}{2} - T_{ambient} \tag{47}$$

The differential equations for heat transport in the model of Fig. 16 are:

$$C_{air} \frac{dT_{air}}{dt} = \frac{T_{outdoor} - T_{air}}{R_{air\_outdoor}} + \frac{T_{wall} - T_{air}}{R_{air\_wall}} + U_{rad} \cdot A_{rad} \cdot (T_{rad} - T_{air}) + \dot{Q}_{internal} + \dot{Q}_{solar,0}$$

$$C_{wall} \frac{dT_{wall}}{dt} = \frac{T_{air} - T_{wall}}{R_{air\_wall}} + \dot{Q}_{solar,1} \tag{48}$$

$$C_{rad} \frac{dT_{rad}}{dt} = \dot{Q}_{inst} + U_{rad} \cdot A_{rad} \cdot (T_{air} - T_{rad})$$

Re-arranging the terms in the equation gives:

$$C_{air} \frac{dT_{air}}{dt} = \left[\frac{-1}{R_{air\_outdoor}} + \frac{-1}{R_{air\_wall}} + -1 \cdot U_{rad} \cdot A_{rad} \right] \cdot T_{air} + \frac{T_{wall}}{R_{air\_wall}} + U_{rad} \cdot A_{rad} \cdot T_{rad} +$$

$$\frac{T_{outdoor}}{R_{air\_outdoor}} + \dot{Q}_{internal} + \dot{Q}_{solar,0}$$

$$C_{wall} \frac{dT_{wall}}{dt} = \frac{1}{R_{air\_wall}} \cdot T_{air} + \frac{-1}{R_{air\_wall}} \cdot T_{wall} + \dot{Q}_{solar,1} \tag{49}$$

$$C_{rad} \frac{dT_{rad}}{dt} = U_{rad} \cdot A_{rad} \cdot T_{air} - U_{rad} \cdot A_{rad} \cdot T_{rad} + \dot{Q}_{heat,2}$$

Conversion of the equations to a matrix equation yields:

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_0 & 0 & 0 \\ 0 & C_1 & 0 \\ 0 & 0 & C_2 \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_0}{dt} \\ \frac{dT_1}{dt} \\ \frac{dT_2}{dt} \end{bmatrix} \tag{50}$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{0,amb}} + \frac{1}{R_{01}} + U \cdot A & \frac{-1}{R_{01}} & -U \cdot A \\ \frac{-1}{R_{01}} & \frac{1}{R_{01}} & 0 \\ -U \cdot A & 0 & U \cdot A \end{bmatrix} \cdot \begin{bmatrix} T_0 \\ T_1 \\ T_2 \end{bmatrix} \tag{51}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \frac{1}{R_{0,amb}} \cdot T_{amb} + \dot{Q}_{int,0} + \dot{Q}_{solar,0} \\ \dot{Q}_{solar,1} \\ \dot{Q}_{heat,2} \end{bmatrix} \tag{52}$$
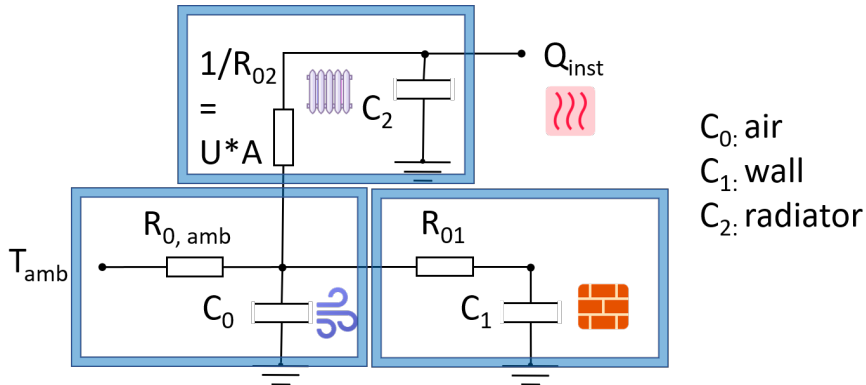
Figure 17: 2R-2C house model with radiator in 3 chains

Starting with the basic 2R2C model we write down the matrices. Note that the heat source for the house is omitted at first. Solar energy entering the house is partitioned between air and wall, Heat generated due to the presence and activities of inhabitants is added to the air node:

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_0 & 0 \\ 0 & C_1 \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_0}{dt} \\ \frac{dT_1}{dt} \end{bmatrix} \tag{53}$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{0,amb}} + \frac{1}{R_{01}} & \frac{-1}{R_{01}} \\ \frac{-1}{R_{01}} & \frac{1}{R_{01}} \end{bmatrix} \cdot \begin{bmatrix} T_0 \\ T_1 \end{bmatrix} \tag{54}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \frac{1}{R_{0,amb}} \cdot T_{amb} + \dot{Q}_{int,0} + \dot{Q}_{solar,0} \\ \dot{Q}_{solar,1} \end{bmatrix} \tag{55}$$

As a third link in the chain, a radiator is added, with a heat capacity C_{rad} and a heat delivery $U \cdot A \cdot (T_{rad} - T_{air})$ to the air node. The heat source $\dot{Q}_{inst}$ is now connected to the radiator.

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_0 & 0 & 0 \\ 0 & C_1 & 0 \\ 0 & 0 & C_2 \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_0}{dt} \\ \frac{dT_1}{dt} \\ \frac{dT_2}{dt} \end{bmatrix} \tag{56}$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{0,amb}} + \frac{1}{R_{01}} + U \cdot A & \frac{-1}{R_{01}} & -U \cdot A \\ \frac{-1}{R_{01}} & \frac{1}{R_{01}} & 0 \\ -U \cdot A & 0 & U \cdot A \end{bmatrix} \cdot \begin{bmatrix} T_0 \\ T_1 \\ T_2 \end{bmatrix} \tag{57}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \frac{1}{R_{0,amb}} \cdot T_{amb} + \dot{Q}_{int,0} + \dot{Q}_{solar,0} \\ \dot{Q}_{solar,1} \\ \dot{Q}_{heat,2} \end{bmatrix} \tag{58}$$

In this example, it becomes visible (in red) that the rank of the C- and K-matrix, and the $\dot{q}$-vector is extended by 1. The heat capacity of the radiator is included as an extra *diagonal* element in the C-matrix. The heat delivery from the radiator to the indoor air is added to or subtracted from the 00, 22, 02 and 20 elements of th K-matrix, so that it remains a *symmetric* matrix. The heater is connected to the radiator, represented by element 2 of the $\dot{q}$-vector.

3.10   2R2C revisited: 2R3C

The 2R2C model as represented in 8 treats the node of the outside temperature (T_{amb}) differently from the other nodes, T_{air} and T_{walls}. This representation is inconsistent, and actually incomplete. Implicitly, the model links a source/sink to the node that controls the outdoor temperature. In literature, one can find models in which this source has been made explicit, such as in [22]. It seems that this representation has been lost over time.

In order to complete the analogy with the other nodes in the model we can connect an additional capacitor (C_{amb}). The capacity will be tending to infinity, as we assume the outside temperature does not change due to heat exchange with the house.

Adding the capacitor and the source also will change the equations. Actually, it results in a more structured set of equations. The equations will be as follows:

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_{amb} & 0 & 0 \\ 0 & C_{air} & 0 \\ 0 & 0 & C_{wall} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_{amb}}{dt} \\ \frac{dT_{air}}{dt} \\ \frac{dT_{wall}}{dt} \end{bmatrix} \tag{59}$$

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$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{amb,air}} & \frac{-1}{R_{amb,air}} & 0 \\ \frac{-1}{R_{amb,air}} & \frac{1}{R_{amb,air}} + \frac{1}{R_{air,wall}} & \frac{-1}{R_{air,wall}} \\ 0 & \frac{-1}{R_{air,wall}} & \frac{1}{R_{air,wall}} \end{bmatrix} \cdot \begin{bmatrix} T_{amb} \\ T_{air} \\ T_{wall} \end{bmatrix} \tag{60}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \dot{Q}_{amb} \\ \dot{Q}_{air} \\ \dot{Q}_{wall} \end{bmatrix} \tag{61}$$

In the equations we now see that the matrix K represents the interaction between the different heat capacities. The off-diagonal elements are equal to (minus) conductance factor $\frac{-1}{R}$ between the respective connected nodes. The structure of K is such that the sum over the rows will always be zero, where the diagonal elements equal the negative sum of the off-diagonal elements.

The vector $\dot{q}$ contains all heat sources (and sinks).

Generalizing the idea above, alternative models can be easily constructed using an underlying graph. In the graph each node is labeled with a heat capacity C_i, and temperature T_i. Nodes i and j can be connected by an edge labeled with $R_{i,j}$, where $\frac{1}{R_{i,j}}$ represents the heat conductance between the two nodes. The K-matrix is the connectivity matrix of the graph, where $K_{i,j} = \frac{-1}{R_{i,j}}$. The diagonal elements, Ki, i are set such that the sums over the rows will be equal to zero.

Additionally, each node can be connected to a source (or sink). Two types of sources are available. A "temperature source" represents a source that will keep the temperature of the connected node constant. This source type can be used to set the ambient temperature.

A heat source represents a source that will provide a continuous constant energy flow into the node. This source type can be used to represent the inflow of energy by for example the sun.

3.10.1 example: 2R-2C house with buffer

3.11 3R2C model

For an apartment building, the simplest model has two nodes with a finite heat capacity, the interior and the building construction. Both nodes have a finite thermal resistance to the ambient environment. Finally there is a thermal resistance between the nodes. Graphically, the model is represented by Figure 18

Figure 18: 3R-2C house model

The differential equations are:

$$C_{air}\frac{dT_{air}}{dt} = \frac{T_{amb} - T_{air}}{R_{air,amb}} + \frac{T_{wall} - T_{air}}{R_{air,wall}} + \dot{Q}_{heat,air} + \dot{Q}_{int,air} + \dot{Q}_{solar,air}$$

(62)

$$C_{wall}\frac{dT_{wall}}{dt} = \frac{T_{air} - T_{wall}}{R_{air,wall}} + \frac{T_{amb} - T_{wall}}{R_{wall,amb}} + \dot{Q}_{solar,wall}$$

Writing out the differential equations in the classical notation:

$$C_{air}\frac{dT_{air}}{dt} = \left[\frac{-1}{R_{air,amb}} + \frac{-1}{R_{air,wall}}\right] \cdot T_{air} + \frac{1}{R_{air,wall}} \cdot T_{wall} + \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{heat,air} + \dot{Q}_{int,air} + \dot{Q}_{solar,air}$$

$$C_{wall}\frac{dT_{wall}}{dt} = \frac{1}{R_{air,wall}} \cdot T_{air} + \left[\frac{-1}{R_{wall,amb}} + \frac{-1}{R_{air,wall}}\right] \cdot T_{wall} + \frac{1}{R_{wall,amb}} \cdot T_{amb} + \dot{Q}_{solar,wall}$$

(63)

The differential equations can be written in matrix notation as:

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = -\mathbf{K} \cdot \boldsymbol{\theta} + \dot{\mathbf{q}} \tag{64a}$$
$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} + \mathbf{K} \cdot \boldsymbol{\theta} = \dot{\mathbf{q}} \tag{64b}$$

with:

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_{air} & 0 \\ 0 & C_{wall} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_{air}}{dt} \\ \frac{dT_{wall}}{dt} \end{bmatrix} \tag{65}$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{air,amb}} + \frac{1}{R_{air,wall}} & \frac{-1}{R_{air,wall}} \\ \frac{-1}{R_{air,wall}} & \frac{1}{R_{wall,amb}} + \frac{1}{R_{air,wall}} \end{bmatrix} \cdot \begin{bmatrix} T_{air} \\ T_{wall} \end{bmatrix} \tag{66}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{heat,air} + \dot{Q}_{int,air} + \dot{Q}_{solar,air} \\ \frac{1}{R_{wall,amb}} \cdot T_{amb} + \dot{Q}_{solar,wall} \end{bmatrix} \tag{67}$$

Written out, the differential equation according to (125) becomes:

$$\begin{bmatrix} C_{air} & 0 \\ 0 & C_{wall} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_{air}}{dt} \\ \frac{dT_{wall}}{dt} \end{bmatrix} = \begin{bmatrix} \frac{-1}{R_{air,amb}} + \frac{-1}{R_{air,wall}} & \frac{1}{R_{air,wall}} \\ \frac{1}{R_{air,wall}} & \frac{-1}{R_{wall,amb}} + \frac{-1}{R_{air,wall}} \end{bmatrix} \cdot \begin{bmatrix} T_{air} \\ T_{wall} \end{bmatrix} +$$

(68)

$$\begin{bmatrix} \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{heat,air} + \dot{Q}_{int,air} + \dot{Q}_{solar,air} \\ \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{solar,wall} \end{bmatrix}$$

In the alternative notation:

$$
\begin{bmatrix} C_{air} & 0 \\ 0 & C_{wall} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_{air}}{dt} \\ \frac{dT_{wall}}{dt} \end{bmatrix} + \begin{bmatrix} \frac{1}{R_{air,amb}} + \frac{1}{R_{air,wall}} & \frac{-1}{R_{air,wall}} \\ \frac{-1}{R_{air,wall}} & \frac{1}{R_{wall,amb}} + \frac{1}{R_{air,wall}} \end{bmatrix} \cdot \begin{bmatrix} T_{air} \\ T_{wall} \end{bmatrix} =
$$

$$
\begin{bmatrix} \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{heat,air} + \dot{Q}_{int,air} + \dot{Q}_{solar,air} \\ \frac{1}{R_{wall,amb}} \cdot T_{amb} + \dot{Q}_{solar,wall} \end{bmatrix}
\tag{69}
$$

it is clear that in this example, where multiple nodes in the thermal network are connected to the ambient surroundings, the approach of Section 3.10 becomes more adventageous:

3.12 3R3C model

The previous 3R2C model representation necessitates an *ad hoc* term in the heat supply vector $\dot{\mathbf{q}}$. Analogous to Section 3.10, we can include the ambient surroundings as a (large) heat capacity into the model. This will change the 3R2C model into a 3R3C model. The equations become:

$$
\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_{amb} & 0 & 0 \\ 0 & C_{air} & 0 \\ 0 & 0 & C_{wall} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_{amb}}{dt} \\ \frac{dT_{air}}{dt} \\ \frac{dT_{wall}}{dt} \end{bmatrix}
\tag{70}
$$

For $\mathbf{K}$ we can start with filling out the non-diagonal symmetic matrix elements:

$$
\mathbf{K} = \begin{bmatrix} 0 & \frac{-1}{R_{amb,air}} & \frac{-1}{R_{amb,wall}} \\ \frac{-1}{R_{amb,air}} & 0 & \frac{-1}{R_{air,wall}} \\ \frac{-1}{R_{amb,wall}} & \frac{-1}{R_{air,wall}} & 0 \end{bmatrix}
\tag{71}
$$

Then we can complete the diagonal elements, so that the sum over each row becomes zero:

$$
\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{amb,air}} + \frac{1}{R_{air,wall}} & \frac{-1}{R_{amb,air}} & \frac{-1}{R_{amb,wall}} \\ \frac{-1}{R_{amb,air}} & \frac{1}{R_{amb,air}} + \frac{1}{R_{air,wall}} & \frac{-1}{R_{air,wall}} \\ \frac{-1}{R_{amb,wall}} & \frac{-1}{R_{air,wall}} & \frac{1}{R_{amb,wall}} + \frac{1}{R_{air,wall}} \end{bmatrix} \cdot \begin{bmatrix} T_{amb} \\ T_{air} \\ T_{wall} \end{bmatrix}
\tag{72}
$$

$$
\dot{\mathbf{q}} = \begin{bmatrix} \dot{Q}_{amb} \\ \dot{Q}_{air} \\ \dot{Q}_{wall} \end{bmatrix}
\tag{73}
$$

3.13 Coupling the housemodel elements

The housemodel is to be extended with modular elements representing the installations that supply the heat demanded by the building. Each subsystem contributes its own set of differential equations to the total system. In Fig. 20, the subsystems are indicated with a color code.
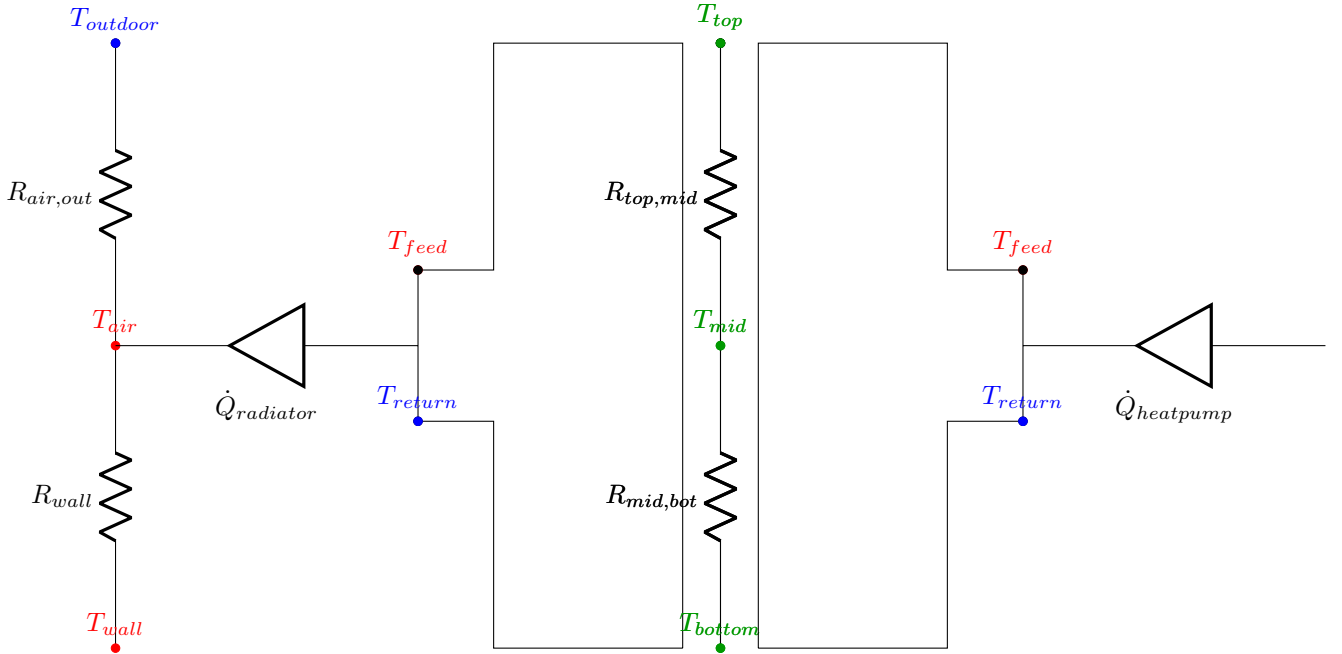
Figure 19: Grand model.
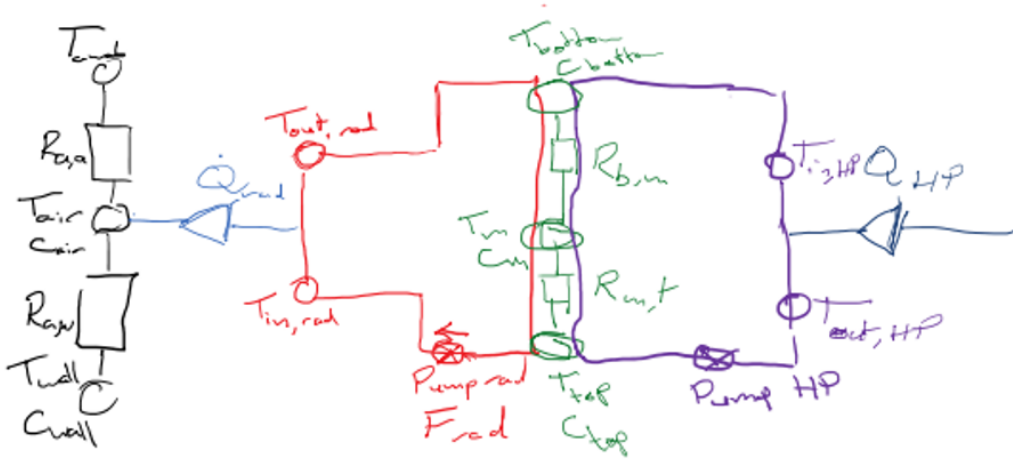
Figure 20: Grand Model

The building itself, in black, generates the differential equations:

$$T_{air}: \quad C_{air}\frac{dT_{air}}{dt} = \frac{T_{amb} - T_{air}}{R_{air,amb}} + \frac{T_{wall} - T_{air}}{R_{air,wall}} + \dot{Q}_{rad,air}$$

$$\tag{74}$$

$$T_{wall}: \quad C_{wall}\frac{dT_{wall}}{dt} = \frac{T_{air} - T_{wall}}{R_{air,wall}}$$

T_{amb}: given as piecewise constant function, in interval $[t_i, t_{i+1}]$, $T_{amb} = T_{amb,i}$

The radiator element, coupled to the node T_{air}, transfers heat to the building at a rate $\dot{Q}_{rad}$. It has a feed temperature T_{feed} and a return temperature T_{return}. The radiator is modeled as a "cross-flow" heat exchanger, obeying the "radiator equation":

26

$$\dot{Q}_{rad}: \quad \dot{Q}_{rad} = C_{rad} \cdot (\Delta T_{LMTD})^n, \text{ with } \Delta T_{LMTD} = \frac{T_{feed} - T_{return}}{\ln\left(\frac{T_{feed} - T_{air}}{T_{return} - T_{air}}\right)}$$

(75)

$$\text{also, :} \quad \dot{Q}_{rad} = F_{rad} \cdot c_w \cdot (T_{feed} - T_{return})$$

when T_{feed}, T_{air} and F_{rad} are known, we have two equations with two unknowns $\dot{Q}_{rad}$ and T_{return}.

Question: when do you solve this system? Do you need to solve this within the time interval $[t_i, t_{i+1}]$?

Further equations:

$$T_{feed} = T_{top}$$

(76)

T_{return} should follow from equations above.

$$T_{top}: \quad C_{top}\frac{dT_{top}}{dt} = \frac{T_{top} - T_{mid}}{-R_{mid,top}} + F_{HP} \cdot c_w \cdot (T_{HP,out} - T_{top}) + \max(F_{rad} - F_{HP}, 0) \cdot c_w \cdot (T_{mid} - T_{top})$$

$$T_{mid}: \quad C_{mid}\frac{dT_{mid}}{dt} = \frac{T_{top} - T_{mid}}{R_{mid,top}} + \frac{T_{mid} - T_{bot}}{-R_{bot,mid}} +$$
$$\max(F_{HP} - F_{rad}, 0) \cdot c_w \cdot (T_{top} - T_{mid}) + \max(F_{rad} - F_{HP}, 0) \cdot c_w \cdot (T_{mid} - T_{bot})$$

$$T_{bot}: \quad C_{bot}\frac{dT_{bot}}{dt} = \frac{T_{mid} - T_{bot}}{R_{bot,mid}} + F_{rad} \cdot c_w \cdot (T_{return} - T_{bot}) +$$
$$\max(F_{HP} - F_{rad}, 0) \cdot c_w \cdot (T_{mid} - T_{bot})$$

(77)

$$T_{HP,in} = T_{bot}$$
$$T_{HP,out}: \quad \dot{Q}_{HP} = F_{HP} \cdot c_w \cdot (T_{HP,out} - T_{HP,in} \dot{Q}_{HP} \quad = f(T_{HP,in}, T_{HP,out}, T_{src,in}, T_{src,out}))$$

(78)

heat pump function? Also here the question is: when to solve this equation?

Writing out the differential equations in the classical notation:

$$C_{air}\frac{dT_{air}}{dt} = \left[\frac{-1}{R_{air,amb}} + \frac{-1}{R_{air,wall}}\right] \cdot T_{air} + \frac{1}{R_{air,wall}} \cdot T_{wall} + \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{heat,air}$$

(79)

$$C_{wall}\frac{dT_{wall}}{dt} = \frac{1}{R_{air,wall}} \cdot T_{air} + \frac{-1}{R_{air,wall}} \cdot T_{wall}$$

The differential equations of the 2R-2C house model (in black) be written in matrix notation as:

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = -\mathbf{K} \cdot \boldsymbol{\theta} + \dot{\mathbf{q}} \tag{80a}$$

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} + \mathbf{K} \cdot \boldsymbol{\theta} = \dot{\mathbf{q}} \tag{80b}$$

with:

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_{air} & 0 \\ 0 & C_{wall} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_{air}}{dt} \\ \frac{dT_{wall}}{dt} \end{bmatrix} \tag{81}$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{air,amb}} + \frac{1}{R_{air,wall}} & \frac{-1}{R_{air,wall}} \\ \frac{-1}{R_{air,wall}} & \frac{1}{R_{air,wall}} \end{bmatrix} \cdot \begin{bmatrix} T_{air} \\ T_{wall} \end{bmatrix} \tag{82}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{heat,air} \\ 0 \end{bmatrix} \tag{83}$$

The routines in Matlab, Simulink and Python need a *model function* that provides the vector $\dot{\boldsymbol{\theta}}$ for evaluation at any time instance chosen by the algorithm. The equations (125) then should be cast in the following form by left multiplication with $\mathbf{C}^{-1}$.

$$\mathbf{C}^{-1} \cdot \mathbf{C} \cdot \dot{\boldsymbol{\theta}} = -\mathbf{C}^{-1} \cdot \mathbf{K} \cdot \boldsymbol{\theta} + \mathbf{C}^{-1} \cdot \dot{\mathbf{q}} \tag{84a}$$

$$\dot{\boldsymbol{\theta}} = -\mathbf{C}^{-1} \cdot \mathbf{K} \cdot \boldsymbol{\theta} + \mathbf{C}^{-1} \cdot \dot{\mathbf{q}} \tag{84b}$$

Since $\mathbf{C}$ is a *diagonal* matrix with positive elements only, its inverse exists and contains the reciprocal elements on its diagonal:

$$\mathbf{C}^{-1} = \begin{bmatrix} \frac{1}{C_{air}} & 0 \\ 0 & \frac{1}{C_{wall}} \end{bmatrix} \tag{85}$$

This provides the division by the lumped thermal capacitances of the air and wall compartments in the model, necessary for the calculating the derivative vector $\dot{\boldsymbol{\theta}}$ in the model functions.

Radiator

$$C_{feed} \frac{dT_{feed}}{dt} = F_{rad} \cdot c_w \cdot (T_{top} - T_{feed}) \tag{86}$$

$$C_{return} \frac{dT_{feed}}{dt} =$$

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_{feed} & 0 \\ 0 & C_{return} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_{feed}}{dt} \\ \frac{dT_{return}}{dt} \end{bmatrix} \tag{87}$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} T_{feed} \\ T_{return} \end{bmatrix} \tag{88}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} 0 \\ \dot{Q}_{rad,air} \end{bmatrix} \tag{89}$$

3.13.1 Buffer vessel

The buffer vessel model is the general model for a "stratified (layered) tank". In order to avoid extensive convection in the tank, the model assumes that addition of hot water from the heat source *and* extraction of hot water to the sink (demand) occurs in the *top* layer. Return flow from the sink is to the *bottom* layer of the vessel.

The differential equations [77] can be rewritten as:

$$C_{top}\frac{dT_{top}}{dt} = \frac{-1}{R_{mid,top}}(T_{top} - T_{mid}) + \max(F_{rad} - F_{HP}, 0) \cdot (T_{mid} - T_{top})$$
$$+ F_{HP} \cdot (T_{HP,out} - T_{top})$$

$$C_{mid}\frac{dT_{mid}}{dt} = \frac{1}{R_{mid,top}}(T_{top} - T_{mid}) + \frac{-1}{R_{bot,mid}}(T_{mid} - T_{bot})$$
$$+ \max(F_{HP} - F_{rad}, 0) \cdot (T_{top} - T_{mid}) + \max(F_{rad} - F_{HP}, 0) \cdot (T_{mid} - T_{bot})$$

$$(90)$$

$$C_{bot}\frac{dT_{bot}}{dt} = \frac{1}{R_{bot,mid}}(T_{mid} - T_{bot}) + \max(F_{HP} - F_{rad}, 0) \cdot (T_{mid} - T_{bot})$$
$$+ F_{rad} \cdot (T_{return} - T_{bot})$$

These differential equations can be written in matrix notation as previously, but a *convection* matrix **F** is added:

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} + \mathbf{K} \cdot \boldsymbol{\theta} + \mathbf{F} \cdot \boldsymbol{\theta} = \dot{\mathbf{q}} \tag{91a}$$

with:

$$\mathbf{C} \cdot \dot{\boldsymbol{\theta}} = \begin{bmatrix} C_{top} & 0 & 0 \\ 0 & C_{mid} & 0 \\ 0 & 0 & C_{bot} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_{top}}{dt} \\ \frac{dT_{mid}}{dt} \\ \frac{dT_{bot}}{dt} \end{bmatrix} \tag{92}$$

$$\mathbf{K} \cdot \boldsymbol{\theta} = \begin{bmatrix} \frac{1}{R_{mid,top}} & \frac{-1}{R_{mid,top}} & 0 \\ \frac{-1}{R_{mid,top}} & \frac{1}{R_{mid,top}} + \frac{1}{R_{bot,mid}} & \frac{-1}{R_{bot,mid}} \\ 0 & \frac{-1}{R_{bot,mid}} & \frac{1}{R_{bot,mid}} \end{bmatrix} \cdot \begin{bmatrix} T_{top} \\ T_{mid} \\ T_{bot} \end{bmatrix} \tag{93}$$

$$\mathbf{F} \cdot \boldsymbol{\theta} = \begin{bmatrix} F_{HP,out} + F_{rad} & F_{rad} & 0 \\ F_{rad} & 0 & F_{rad} \\ 0 & F_{rad} & F_{HP} + F_{rad} \end{bmatrix} \cdot \begin{bmatrix} T_{top} \\ T_{mid} \\ T_{bot} \end{bmatrix} \tag{94}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \frac{1}{R_{air,amb}} \cdot T_{amb} + \dot{Q}_{heat,air} \\ 0 \end{bmatrix} \tag{95}$$

F1: $[0\ 1\ 2\ 0]$

F2: $[2\ 1\ 0\ 2]$

$$\mathbf{DF_{F1}} = \begin{bmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{bmatrix} \tag{96}$$

$$\mathbf{DF_{F2}} = \begin{bmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix} \tag{97}$$

In each time step, when the flow sizes have been determined by the control algorithms, each directed-flow-matrix is multiplied by its respected flow size in $[\frac{m^3}{s}]$. All resulting matrices can then be added together. Assuming a flow of size f_1 and f_2 for the flows $F1$ and $F2$, respectively we now get the matrix $\mathbf{SF}$:

$$\mathbf{SF} = f_1 \cdot \mathbf{DF_{F1}} + f_2 \cdot \mathbf{DF_{F2}} = \begin{bmatrix} 0 & \dot{f}_1 - \dot{f}_2 & \dot{f}_2 - \dot{f}_1 \\ \dot{f}_2 - \dot{f}_1 & 0 & \dot{f}_1 - \dot{f}_2 \\ \dot{f}_1 - \dot{f}_2 & \dot{f}_2 - \dot{f}_1 & 0 \end{bmatrix} \tag{98}$$

The heat transfer induced by the flows is only in the direction of the water flow. The correct elements are obtained by taking the $\min(\mathbf{SF}, 0)$, here we mean for each element in $\mathbf{SF}$ we take the minimum of the respective element and 0. Thus, in the case $f_1 > f_2$ the matrix $\mathbf{SF}$ will become:

$$\min(\mathbf{SF}, 0) = \begin{bmatrix} 0 & \dot{f}_1 - \dot{f}_2 & 0 \\ 0 & 0 & \dot{f}_1 - \dot{f}_2 \\ \dot{f}_1 - \dot{f}_2 & 0 & 0 \end{bmatrix} \tag{99}$$

Now, the diagonal elements can be computed. The diagonal elements are equal to minus the sum of the off-diagonal elements in its respective row. For the matrix given in equation 164 this results in the flow matrix $\mathbf{F}$:

$$\mathbf{F} = \begin{bmatrix} -(\dot{f}_1 - \dot{f}_2) & \dot{f}_1 - \dot{f}_2 & 0 \\ 0 & -(\dot{f}_1 - \dot{f}_2) & \dot{f}_1 - \dot{f}_2 \\ \dot{f}_1 - \dot{f}_2 & 0 & -(\dot{f}_1 - \dot{f}_2) \end{bmatrix} \tag{100}$$

Finally, we need to multiply the resulting flow matrix with the density (ρ_w) and the specific heat (c_w), in order to obtain the heat transferred by the water due to the water flows. The resulting matrix can be added to the K matrix as given in equation 160.

$$\dot{f} = v_{pump} \cdot A_{pipe} \qquad \left[\frac{m}{s} \cdot m^2 = \frac{m^3}{s} \right]$$

$$\dot{f} \cdot \rho_w \cdot c_w \quad \text{has the dimension} \qquad \left[\frac{m^3}{s} \cdot m^2 \cdot \frac{kg}{m^3} \cdot \frac{J}{kg \cdot K} = \frac{J}{K \cdot s} = \frac{W}{K} \right] \tag{101}$$

$$\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$$
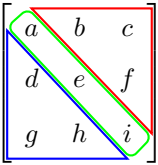
Listing 1: StratifiedBufferNew class

```
class StratifiedBufferNew:
    """parent class for cylindrical stratified buffer vessel

    """
    def __init__(self, name, begin_node=0, volume=0.1, height=1.0, n_layers=5, u=0.12,
        T_ini=20):
        self.name = name
        self.num_nodes = n_layers
        self.nodes = []
        self.begin_node = begin_node                   # anchor point of hot water supply to
            house model
        self.end_node = self.begin_node + n_layers-1   # anchor point of cold water return
            from house model
        self.edges = []
```

```
13          self.volume = volume
            self.height = height
15          self.Uwall = u            # conductivity vessel wall to ambient in [W/K m^2]
            self.T_ini = T_ini
17
            self.boundaries = []
19          self.ambient = None
21          self.tag_list = []
            self.cap_list = []
23          self.edge_list = []
25          self.c_inv_mat = None
            self.k_ext_mat = None
27
            self.rho = 1000           # [kg/m^3]
29          self.cp = 4190            # [J/(K kg)]
            self.conductivity = 0.644  # [W/m K]
31
            self.layer_height = None
33          self.radius = None
            self.A_wall_layer = None
35          self.A_base = None    # contact area between layers (= area of vessel bottom and top
                face)
            self.cap_layer = None
37
            self.temperatures = None
39          self.calculate_buffer_properties()
```

3.13.2 Radiator

In a radiator, the heat transport is in good approximation only due to *convection* of a gas (steam) or liquid (water, glycol, brine) For a liquid, the following points of view may be taken: The equations for the radiator element are:

$$F_{rad} = \dot{f} \cdot \rho \cdot c_w$$
$$F_{rad} = \dot{m} \cdot c_w$$

(102)

where:

ρ is the density of the liquid in $[kg/m^3]$

c_w is the specific heat capacity of water: $4.2 \cdot 10^3 J/(kg \cdot K)$

$\dot{f}$ is the liquid volume flow in $[m^3/s]$

$\dot{m}$ is the liquid mass flow in $[kg/s]$

The equations for the heat transfer of the radiator are:

$$\dot{Q}_{rad} - C_{rad} \cdot (\Delta T_{LMTD})^n \qquad = 0$$
$$\dot{Q}_{rad} - F_{rad} \cdot (T_{feed} - T_{return}) \qquad = 0$$

(103)

$$\text{with } \Delta T_{LMTD} = \frac{T_{feed} - T_{return}}{\ln\left(\frac{T_{feed} - T_{air}}{T_{return} - T_{air}}\right)}$$

This nonlinear system of equations can be solved for the two unknowns $[\dot{Q}_{rad} \quad T_{return}]$, if input data T_{feed},

T_{amb}, C_{rad} and F_{rad} are provided. A solver needs the function template in Eq. 103, with the unknowns vector as input variable. Furthermore, the Jacobian of the function template has to be calculated. Evaluation of an analytical expression of the partial derivatives in the Jacobian always outperforms numerical derivative calculations. Thus, for the upper equation (function) in set 103:

$$\frac{\partial f}{\partial \dot{Q}_{rad}} = 1$$

$$\frac{\partial f}{\partial T_{return}} = -Cn \cdot \frac{\left(\frac{T_1-T_2}{\ln\left(\frac{T_1-T_3}{T_2-T_3}\right)}\right)^{n-1}\left(\frac{T_1-T_2}{T_2-T_3} - \ln\left(\frac{T_1-T_3}{T_2-T_3}\right)\right)}{\ln^2\left(\frac{T_1-T_3}{T_2-T_3}\right)} \tag{104}$$

for the second equation:

$$\frac{\partial f}{\partial \dot{Q}_{rad}} = 1$$
$$\frac{\partial f}{\partial T_{return}} = -F_{rad} \tag{105}$$

See: https://www.derivative-calculator.net/.

The Jacobian matrix

$$\mathbf{J}_{i,j} = \frac{\partial f_i(\mathbf{x})}{\partial x_j}$$

becomes:

$$\begin{bmatrix} \dfrac{\partial f_1}{\partial \dot{Q}_{rad}} & \dfrac{\partial f_1}{\partial T_{return}} \\[2em] \dfrac{\partial f_2}{\partial \dot{Q}_{rad}} & \dfrac{\partial f_2}{\partial T_{return}} \end{bmatrix} \tag{106}$$

with:

$$\mathbf{x} = \begin{bmatrix} \dot{Q}_{rad} \\ T_{return} \end{bmatrix} \tag{107}$$

The properties and the calculation of $\mathbf{x}$ is implemented in Python in the Radiator class. The methods of this class are:

- __init__: initializes the class members. Members starting with __* are private members.

- get_lmtd: returns the value of private member __lmtd.

- func_rad: calculates radiator equations and partial derivatives.

- update: uses scipy.optimize.root() to find the roots $\mathbf{x}$ of the radiator equations.

Listing 2: Radiator class

```
2
class Radiator:
4    """ class for general Radiator object."""
    def __init__(self, exp_rad=1.3):
6        self.T_feed = None
        self.c_rad = None
8        self.exp_rad = exp_rad
        self.c_w = 4.2e3      # [J/kg K]
10       self.rho = 1000       # [kg/m^3]
```

```python
        self.flow = None       # [m^3/s]
        self.F_rad = None       # heat flow in [W/K] = flow * rho * c_w
        self.T_amb = 20.0

        self.q_dot = 0.0
        self.T_ret = None
        self.boundaries = []
        self.return_node = FixedNode

        self.k_mat = None
        self.f_mat = None
        self.q_vec = None

        self.__denominator = None
        self.__lmtd = None

    def boundaries_from_dict(self, lod):
        for n in range(len(lod)):
            node = FixedNode(label=lod[n]["label"],
                             temp=lod[n]["T_ini"],
                             connected_to=lod[n]["connected_to"])
            # append by reference, therefore new node object in each iteration
            self.boundaries.append(node)
        self.return_node = [fn for fn in self.boundaries if fn.label == "return"][0]

    def get_lmtd(self):
        return self.__lmtd

    def func_rad(self, x):
        """model function for scipy.optimize.root().

        Args:
            x: vector with unknowns [self.q_dot, self.T_ret]

        Returns:
            f : vector with model functions evaluated at x
            df : Jacobian (partial derivatives of model functions wrt x
        """
        self.__lmtd = LMTD_radiator(T_feed=self.T_feed, T_return=x[1], T_amb=20.0,
            corrfact=1.0)
        # set of nonlinear functions for root finding
        f = [x[0] - (self.c_rad * self.__lmtd ** self.exp_rad),
             x[0] - self.F_rad * (self.T_feed - x[1])]

        h1 = self.c_rad * self.exp_rad
        h1 *= self.__lmtd ** (self.exp_rad - 1.0)

        h2 = (self.T_feed - x[1]) / (x[1] - self.T_amb)
        denominator = np.log(self.T_feed - self.T_amb) - np.log(x[1] - self.T_amb)
        h2 -= denominator
```

The Radiator class uses a helper function LMTD_radiator to determine the effective temperature drop:

Listing 3: LMTD_radiator function

```python
def LMTD_radiator(T_feed, T_return, T_amb, corrfact=1.0):
    """calculates log mean temperature difference

    representative value in case of varying temperature difference along heat exchanger
    https://checalc.com/solved/LMTD_Chart.html
```

```
8      Args:
            T_feed:      entry  temperature  hot  fluid  or  gas
10          T_return:    exit  temperature  hot  fluid  or  gas
            T_amb:      entry  temperature  cold  fluid  or  gas
12          corrfact:    see:      https://checalc.com/solved/LMTD_Chart.html
                                    https://cheguide.com/lmtd_charts.html
14                                  https://excelcalculations.blogspot.com/2011/06/lmtd-correction-factor.html
                                    http://fchart.com/ees/heat_transfer_library/heat_exchangers/hs2000.htm
16                                  https://yjresources.files.wordpress.com/2009/05/4-3-lmtd-with-tutorial.pdf
                                    https://www.engineeringtoolbox.com/arithmetic-logarithmic-mean-temperature-d
18      Returns:
            LMTD  temperature
20          corr_fact * ( Delta T 1 - Delta T 2 ) / ln (Delta t 1 / Delta T 2)
        """
22      eps = 1e-9
        DeltaT_fr = T_feed - T_return
24      DeltaT_feed = T_feed - T_amb
        DeltaT_ret = T_return - T_amb
26      # assert (DeltaT_fr > 0), "Output temperature difference $\Delta T_1$ is negative"
        # assert DeltaT_in > DeltaT_out, "Input  temperature  difference $\Delta T_1$ is smaller
            than output "
28
        denominator = np.log(DeltaT_feed) - np.log(DeltaT_ret)
30      nominator = DeltaT_fr
        # assert denominator > eps, "Ratio of input/output temperature difference too large"
```

3.14   Model component properties towards an integrated implementation

Here we summarize the properties of the different model components.

3.14.1   Capacity Node

description: A capacity node represents the heat capacity of a part of the system, *for example*, the air in a room, or the water in a layer of the buffer vessel. Within the model, for each capacity node the evolution of the temperature over time will be computed. The capacity nodes are used in the components of the house model and the buffer vessel.

properties

- *label*: unique 'name' for the node. This should be provided in the **input**.

- *tag*: index of the node in the resulting model. Translates to row-index in the matrices and $\dot{\mathbf{q}}$-vector.

- *heat_capacity*: the heat capacity [J/K]. This is constant over time and should be provided in the **input**. Capacity should be greater than zero and finite.

- *temperature*: the temperature [K]. This will be computed by the model. For each node the model should be able to output a temperature profile over the duration of the simulation

In the listing below, from the module `components.py`, the definition of the component as a `dataclass` is shown:

Listing 4: Capacity Node

```
2
  @dataclass
4 class FixedNode:    # external node?
      label: str
6     connected_to: []
```

3.14.2 Fixed temperature Node (external node)

description: This is a node with a predefined temperature. This temperature will not change due to heat exchange with its surrounding nodes. The predefined (external) temperature should be constant within a given time interval. This node represents a part of the system with a very large heat capacity (much larger than other components), *for example*, the ambient air or the ground.

properties

- *label*: unique 'name' for identification. This should be provided in the **input**.

- *connection(s)* to other model nodes: every fixed temperature node is connected to at least one capacity node, via a heat conductance edge. This edge, and its corresponding heat conductance, "belongs" to the fixed temperature node.

- contribution to **K**-matrix: based on the (time-dependent) temperature and the conductances, the diagonal element in the **K**-matrix corresponding to the connected capacity nodes should be updated.

- *temperature* [K] or [°C]: for every given time the temperature of this node should be defined. For this a temperature profile should be provided in the **input**. The temperature profile can be a list of tuples of the form [start_time , temperature]. At every time interval for which the model is evaluated the corresponding temperature of the node should be obtained. For this a function `set_node_temperature` is needed.

- contribution to **q**-vector: based on the (time-dependent) temperature and the conductances, the element in the **q**-vector corresponding capacity nodes should be updated. This is update may be done in the same function as the update for the **K**-matrix. The update value is the same for both terms, except for the sign.

NOTE: The temperature of the node should remain constant over the entire interval of model solving, so moments of switching temperature should coincide with the start and end of these intervals. This may be enforced by limiting the options for 'start_time' (for example only multiples of 10 minutes). An alternative could be that the profile is always defined based on the times as given by the NEN5060. The NEN5060 will, most likely, provide the profile of the ambient air temperature. When we would require all profiles of the same shape and size the reading and processing can be done in the same fashion for all nodes.

In the listing below, from the module `components.py`, the definition of the component as a `dataclass` is shown:

Listing 5: Fixed Node (external node)

```
    def update(self, new_value):
        self.temp = new_value


@dataclass
class CondEdge:
    label: str
    conn_nodes: []   # empty list (tuple, ndarray)
```

The attribute `connected_to` is a list with elements `[tag, conductivity]`. This attribute contains all information for building the **k**-matrix. In most cases the attribute `connected_to` does not change during a simulation. Only the attribute `temp` is updated at regular intervals (see method `update`). The contribution to the $\dot{q}$-vector then has to be updated as well.

3.14.3 Heat conductance Edges

description: A heat conductance edge represents the possibility to exchange heat between the two connected nodes (either capacity node or temperature node). Heat will be transferred from the node with high temperature

to the node with low temperature. For example, an edge between the nodes 'air' and 'walls' indicates that heat can be transferred from the air to the wall, and the other way around.

properties

- *label*: name of the edge. This should be provided in the **input**.

- *connected_nodes*: a pair of connected nodes. Each edge connects two nodes. This should be provided in the **input**.

- *conductance_value* [J/K] or [J/°C]. This should be provided in the **input**.

Listing 6: Conductance Edges

```
    # sink: int
2

4 """ notinuse
  @dataclass
```

3.14.4 Fluid Flow

NOTE: the definition of the fluid flows in this section has its limitations. Only basic closed loops without splits in the 'pipes' can be modeled. This is fine as a starting point. However, when more complex scenarios with complex fluid flows are required a more generic formalism is needed for the modeling of the fluid flows. In this case, a system with flow edges and flow nodes may be a possible solution. The open challenges here are: 1. how to define the flow network (next to / in combination with the heat conductance network), 2. how to compute the flow rates in the more complex system.

description: A fluid flow represents a *closed* loop over a set of nodes (with or without heat capacity). The flow rate is the same for all nodes and edges within the loop. The flow rate may change over time, but is assumed to be constant within a given time interval, and changes are assumed to be instantaneous. Thus, the flow rate can be described by a step-function. This flow rate should be controlled, either in a on/off manner, or in m (???)

properties

- *label*: name of the fluid flow. This should be provided in the **input**.

- *flow_rate*: The flow rate of the fluid in m^3/s (or another unit that fits). This flow rate may change over time, matrices related to the heat transfer induced by the fluid flow need to be updated accordingly, see Section F.6.1.

- *density*: density of the fluid in $[\frac{kg}{m^3}]$. One fixed density will be used (no temperature dependence is taken into account here). This should be provided in the **input**.

- *heat_capacity*: heat capacity of the fluid in $[\frac{J}{kg \cdot K}]$. This should be provided in the **input**.

- *connected_nodes*: An *ordered* list of the nodes through which the fluid flow runs, the order is determined by the direction the fluid will be pumped through the network. Start and end of the list need to be the same node. This ensures the required closed loop. This should be provided in the **input**. From this ordered list a "directed-flow-matrix" can be set-up as indicated in Section F.6.1.

Listing 7: Flow

```
1 class Flow:
      def __init__(self):
3         self.label = None
          self.rate = None
5         self.density = None
          self.cp = None
```

```
7        self.node_list = []  # empty list
         self.edges = []
9        self.f_mat = None
```

3.14.5 flow network

description: multiple fluid flows can be combined in a flow network. The current methodology is limited to two flows (specifically, two flows that both are connected to a buffer vessel).

properties

- *sum_flows*: based on the directed flow matrices and the flow rates, a total matrix can be created (cf. Section F.6.1)

- *heat_transfer_matrix*: from the sum_flow matrix, and the fluid density and heat capacity the corresponding heat transfer matrix can be created.

3.14.6 house module

description: The house module is an abstraction of the main heat capacities of a house, and the heat conductances within. *NOTE*, capacities can be connected to other model modules by means of heat conductance edges or possibly flow edges. There is potentially much freedom in the model design here. Question to be solved here is how do we define the inter-connectivity in the input? Which module is 'leading' in making the connection. My (Marijn) first idea is to let the house module be 'passive' here, that is, connections to the house module are part of the connecting-module.

properties

- list_capacity_nodes. input from (excel) table.

- lis_heat_conductance_edges. input from (excel) table.

- C_matrix: based on capacities a house C-matrix can be composed. (diagonal matrix)

- k_matrix: based on the edges a house k_matrix can be composed. (method based on graph theory functions)

3.14.7 fixed temperatures module

description The fixed temperatures module is a collection of all fixed temperature nodes that are connected to the different other parts of the running model. For each node the temperature profile over time is checked, and the temperature is updated accordingly.

properties

- list_fixed_temperature_nodes

- updating_function: function that loops over all fixed nodes, and makes sure every node is up to date with respect to the temperature at the given time. The updated contributions to **k**-matrix and **q**-vector should be added and passed to the model solver.

3.15 buffer module

description: The buffer module is an abstract representation of a heat buffer vessel. The vessel is build up of a set of n layers. Each layer has a heat conductance edge to the layer directly above and below. Also, a conductance edge to the surrounding air is possible, represented by a fixed temperature node (this works similar as for a house). An alternative is that the surrounding air is a capacity node, which can be part of, or connected

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to the house module. This last scenario is more complex to incorporate in the model, as this connection is not part of either module (buffer or house), but is a 'special' inter-module connection. Next to the heat conductance edges, the buffer also has flow connections. Internally, flow connections exist between adjacent layers, these are bi-directional (the flow can go both directions, but at every moment in time the flow only one direction is active). Also flow connections, coming in and flowing out of both the top and bottom layer are possible.

properties

- nr_layers

- node_list: the buffer consists of multiple flow nodes with capacity. The nodes corresponding to the top and bottom layer will have flow connections.

- internal_conductance_edges: an internal conductance network defines the internal heat-exchange. With this set of internal edges the a **k**-matrix for the buffer can be build. This should be incorporated in the overall model **k**

-

3.16 Heat Pump

A heat pump can be modeled in several ways. A straightforward approach is to reduce the heat pump to two fixed nodes, external to the building system. These nodes represent the evaporator and condensor *exit* temperatures T_{evap} and T_{cond}. In case of a air-water heatpump, T_{evap} can be approched with the instantaneous outdoor (ambient) temperature from the weather conditions. For a heat pump with a liquid heat source this will be the source temperature, in any cases a ground source. T_{cond} can be derived from a heating curve (T_{cond} vs. $T_{outdoor}$) or from a heat pump functional model.

properties

- T_{evap}.

- T_{cond}.

- COP

- Thermal power

The heat pump will deliver its thermal power via an internal heat exchanger from the refrigerant to a liquid heat carrier (water) in a buffer vessel. There are a few options for the connection of the buffer vessel:

- 2-pipe connection

- 4-pipe connection

- 3-pipe connection

3.17 Scripts

Simulations can be run as a Python script or as an IPython (Jupyter) notebook. The structure of a script can be summarized as follows:

- read configuration file. This file is written in *.yaml format. The parameters in the file are converted to a variable (suggested name: `param`) of type `dict`.

- create an instance of the `Building` class. Example: `h = Building("MyHouse")`.

Listing 8: The Building class

```
        self.nodes = []              # np.zeros(self.num_nodes, dtype=object)
2       self.boundaries = []
```

```
          self.ambient = None
 4
          self.c_inv_mat = None    # np.zeros(( self.num_nodes , self.num_nodes ))
 6        self.k_ext_mat = None    # np.zeros_like ( self.c_inv_mat )
          self.q_vec = None        # np.zeros ( self.num_nodes , 1)
 8
          self.tag_list = []
10        self.cap_list = []

12        logging.info(f" Building object {self.name} created")

14    def nodes_from_dict (self , lod: list ):
          """ initializes " nodes " attribute with data from yaml file
16            makes a list from tags belonging to the House object

18        Args :
              lod : list of dicts read from yaml file
20        """
          self.num_nodes = len(lod)
```

- read the nodes of the Building model with the method `nodes_from_dict(param["Building"]["nodes"])`

- fill the inverse of the capacity matrix $\mathbf{C}^{-1}$ using the method `fill_c_inv()`.

- read *all* fixed nodes using the method `boundaries_from_dict(param["boundaries"])`.
  The method copies the "outdoor" external node to the `Building.ambient` node.

- initialize the $\mathbf{K}$-matrix and add the conductivity between the building nodes and ambient to the diagonal elements using the method `make_k_ext_and_add_ambient()`.

- at this point we can read *all* edges in the model using the method `edges_from_dict(param["edges"])` and add the non-diagonal elements to $\mathbf{K}$ with the method `fill_k(param["edges"])`. However, this can only be done for the thermal conductivities *within* the Building subsystem. Thermal conductivities *between* subsystems (*e.g.* between the Building contents and a Radiator) have to be added after assembly of the subsystems (matrices) into a complete model (set of differential equations). Therefore, the $\mathbf{K}$-matrix is completed *after* merging the matrices of the subsystems.

$$
\mathbf{K} \cdot \boldsymbol{\theta} = \left[\underbrace{\begin{bmatrix} \frac{1}{R_{air,wall}} & \frac{-1}{R_{air,wall}} \\ \frac{-1}{R_{air,wall}} & \frac{1}{R_{air,wall}} \end{bmatrix}}_{\mathbf{K}_{int}} + \underbrace{\begin{bmatrix} \frac{1}{R_{air,amb}} & 0 \\ 0 & 0 \end{bmatrix}}_{\mathbf{K}_{ext}} \right] \cdot \begin{bmatrix} T_{air} \\ T_{wall} \end{bmatrix}
\tag{108}
$$

- Similarly, a buffer vessel can be created with `b = StratifiedBuffer("Buffervessel")`.

- run `b.nodes_from_dict(param["Buffer"]["nodes"])` and `b.fill_c_inv()` to create the inverse capacity matrix $\mathbf{C}^{-1}$ for the buffer vessel. The nodes are equivalent to the layers of a stratified buffer tank.

- The buffer vessel has a "ambient" temperature which is an "indoor" temperature for an attic or basement room. This temperature can be taken as a constant for the complete simulation period. Apply the functions `b.boundaries_from_dict(param["boundaries"])` (selects "indoor" as ambient) and `b.add_ambient_to_k()`.

$$\mathbf{K} \cdot \boldsymbol{\theta} = \left[\underbrace{\begin{bmatrix} \frac{1}{R_{top,mid}} & \frac{-1}{R_{top,mid}} & 0 \\ \frac{-1}{R_{top,mid}} & \frac{1}{R_{top,mid}} + \frac{1}{R_{mid,bot}} & \frac{-1}{R_{mid,bot}} \\ 0 & \frac{-1}{R_{mid,bot}} & \frac{1}{R_{mid,bot}} \end{bmatrix}}_{\mathbf{K}_{int}} + \underbrace{\begin{bmatrix} \frac{1}{R_{top,amb}} & 0 & 0 \\ 0 & \frac{1}{R_{mid,amb}} & 0 \\ 0 & 0 & \frac{1}{R_{bot,amb}} \end{bmatrix}}_{\mathbf{K}_{ext}} \right] \cdot \begin{bmatrix} T_{top} \\ T_{mid} \\ T_{bot} \end{bmatrix} \qquad (109)$$

- A very simple radiator model consists of a CapacityNode, coupled to the contents ("air") of the Building subsystem. This can be implemented by calling `r = LinearRadiator("SimpleRadiator")`, `r.nodes_from_dict(param["Radiator"]["nodes"])` and `r.fill_c_inv()`. $\mathbf{C}^{-1}$ is a matrix of rank 1 in this case (numpy.ndarray(1,1)), and not a scalar.

- the LinearRadiator object does not have an "ambient" fixed (external) node contributing to the $\mathbf{K}$-matrix.

$$\mathbf{K} \cdot \boldsymbol{\theta} = \left[\underbrace{\left[\frac{1}{R_{air,rad}} \right]}_{\mathbf{K}_{int}} + \underbrace{\begin{bmatrix} 0 \end{bmatrix}}_{\mathbf{K}_{ext}} \right] \cdot \begin{bmatrix} T_{rad} \end{bmatrix} \qquad (110)$$

- a complete model can be assembled from the partial models. it is created with `total = TotalSystem("HouseWithRadiator", [r, h])`. The list `[r, h]` of partial models is then sorted with `total.sort_parts()` so that the previously assigned tags correspond to the rows of the total system matrices.

- compose the $\mathbf{C}^{-1}$-matrix from the parts with `total.merge_c_inv()`.

- merge the tag_lists with `total.merge_tag_lists()`. TotalSystem.tag_list should be ordered.

- compose the $\mathbf{K}$-matrix from the parts with `total.edges_from_dict(param["edges"])` and `total.fill_k(param["edges"])`.

- compose the $\mathbf{K}_{\mathbf{ext}}$-matrix from the parts with `total.merge_k_ext()`.

- add $\mathbf{K}$ and $\mathbf{K}_{\mathbf{ext}}$ with `total.k_mat += total.k_ext_mat`.

- create an empty $\dot{\mathbf{q}}$-vector with `TotalSystem.make_empty_q_vec()`.

4 Solar irradiation and PV yield

In the house model, energy supply from solar irradition plays an important role. Firstly, solar energy enters the building through windows and poorly insulated surfaces. In winter, this reduces the cost of heating the building. In summer, however, this leads to an extra energy expenditure for cooling the building, which may attain uncomfortable indoor temperature levels in case of large window surfaces or poor insulation.

A second issue is that the yield of PV and PVT panels, which are often installed nowadays, depends on the solar irradiation. Weather conditions, especially the cloud cover density have a strong influence on the electric power and energy yield of these installations.

Therefore, it is important to be able to calculate the solar irradiation quantity, spectral distribution and spatial properties. Only then, a reliable estimation of the energy demand, and of the useful fraction of solar irradiation can be made.

4.1 Solar software

Software for calculation of solar irradiation on the surface of the earth exists in many shapes and implementations. To achieve the final goal, calculation of the solar (power) falling on a surface with a certain orientation, a number of steps have to be carried out.

1. establish the geolocation of the object (building, PV(T) panel) of interest

2. establish the time instant or time range of interest

3. convert the time instant to local, timezone-aware time or UTC

4. find the apparent position of the sun in the sky (azimuth and inclination)

5. determine the attenuation of the earth's atmosphere for the geolocation and time(s) of interest

6. determine the DNI

7. determine the orientation of the surface of interest (azimuth and inclination)

8. determine the direct, diffuse and global irradiation on the surface

9. determine the fraction of the solar irradiation that is effective as an energy source (window transmittance, PV(T) efficiency)

Among the packages available for solar irradiation calculations, we find:

- PV_LIB Toolbox: available for Matlab and Python [23–26].

- solarenergy: available as Python package [27, 28]

- qsun: available as Matlab function or Python function.

4.2 Geolocation

The location of a building or installation needs to be given in *latitude* and *longitude*, in units of degrees with a decimal point. Division in arcminutes and arcseconds is less common nowadays, since the introduction of GPS. Latitude is positive for the northern hemisphere, negative to the south of the equator. The equator itself is zero latitude. Longitude is positive to the east of the Royal Observatory in Greenwich, London, UK, negative to the west of London. The Meridian of Greenwich runs from the North pole to the South Pole through London and has zero longitude. At the poles, latitude is ± 90 degrees and longitude is undefined.

For **Arnhem**, NL, a **latitude of 52.0 degrees** and a **longitude of 6.0 degrees** may be used as an approximation to the geolocation. In reality this geolocation is found in a field between Velp and Rheden, NL.

- PV_LIB Toolbox has a module location.py. In this module, a class Location is defined, with attributes *latitude* and *longitude*. These attributes are in *decimal degrees i.e.* 52.0 and 6.0.

- solarenergy has a module radiation.py with a function sun_position_from_date_and_time. Input parameters to this function are *longitude* and *latitude* in *radians*. The solarenergy has a conversion constant d2r to convert from decimal degrees to radians.

- qsun: longitude and latitude are not input parameters. They are fixed: the chosen location is for De Bilt, NL (52.1 N, 5.1 E).

4.3   Time and timezones

In many programming languages, a datetime object exists. The basic functionality of such an object includes:

- a convention about time "zero".

- a representation of time, stored in an integer or floating-point value.

- a set of conversion routines from various time strings *e.g.* 2021-11-25 17:28:31:321+01:00 to the storage format, and back.

- timezone awareness and daylight savings options.

4.3.1   Time formats and conventions

Many conventions are currently in use. The most "universal" is the UNIX Timestamp. Its *epoch*, the "zero" time is 1 January 1970, 00:00:00 (UTC). The time is represented by an *integer* which counts the *seconds* elapsed since the epoch. Originally, the representation was an int32, which would mean that the computer time is up in the year 2038. Backwards, the beginning of computer time would be in 1901. Fortunately, 64-bit computer registers now also use an int64 for UNIX timestamp representation, which alleviates this shortcoming for all practical situations.

The int64 representation stretches so far into the future and past, that it makes room for improvement. Microsoft Windows maintains a FILETIME structure, built from two DWORD (uint32) entries, which taken together to a 64-bit value represent the number of 100-ns intervals since January 1, 1601 00:00:00.0000000 (UTC).

typedef struct _FILETIME {
DWORD dwLowDateTime;
DWORD dwHighDateTime;
} FILETIME, *PFILETIME, *LPFILETIME;

In Python, the original datetime package contains a datetime class which has its epoch at 1 January 1970, just like the UNIX timestamp. The datetime class has members: year (1-9999), month (1-12), day (1- # of days in month), hour (0-23), minute (0-59), second (0-59) and microsecond (0-999999). Moreover, it has an attribute tzinfo, which handles timezone info and an attribute fold (0, 1) to handle the occurrence of two identical wall times when daylight savings time is reset in autumn.

However, the Python package pandas has an alternative Timestamp class, which uses a int64, representing the number of 1-ns intervals since 1 January 1970. This makes it compatible with UNIX timestamps (divide by 1e9) and with classical Python datetime objects. The type is given as datetime64[ns, Europe/Amsterdam]. This reveals that, apart from the timestamp in UTC, a timezone may be stored. This is done with the helper package pytz, which is installed as a dependency of pandas. It is strongly recommended to always use timezone-aware timestamps, even if UTC is meant. The pytz package also handles daylight savings times smoothly in timezone-aware timestamps.

4.3.2 Examples in Python

The standard Python datetime object is defined in the module datetime.py. On import, it is recommended to also include the timedelta object fom the same module. The use of datetime and timedelta objects without setting timezone information is shown in Listing **??**.

In combination with geolocation, however, it is recommended to use *timezone-aware* datetime objects. This is demonstrated in Listing **??**. Note that the *attribute* of the datetime class is named tzinfo. The input argument for the *method* datetime.now is named tz. The value of this input argument sets datetime.tzinfo from None to a meaningful timezone value.

https://www.alpharithms.com/generating-artificial-time-series-data-with-pandas-in-python-272321/

https://stackoverflow.com/questions/993358/creating-a-range-of-dates-in-python

https://stackoverflow.com/questions/1060279/iterating-through-a-range-of-dates-in-python/1060330#1060330

https://stackoverflow.com/questions/13445174/date-ranges-in-pandas

https://pandas.pydata.org/pandas-docs/stable/user_guide/timeseries.html

https://pandas.pydata.org/pandas-docs/stable/reference/api/pandas.date_range.html

https://www.w3resource.com/pandas/date_range.php

Voorbeeld timestamp and date_range in Pandas.

- PV_LIB Toolbox has a module location.py. In this module, a class Location is defined, with attributes *latitude* and *longitude*. These attributes are in *decimal degrees i.e.* 52.0 and 6.0.

- solarenergy has a module radiation.py with a function sun_position_from_date_and_time. Input parameters to this function are *longitude* and *latitude* in *radians*. The solarenergy has a conversion constant d2r to convert from decimal degrees to radians.

- qsun: longitude and latitude are not input parameters. They are fixed: the chosen location is for De Bilt, NL (52.1 N, 5.1 E).

4.3.3 Conversion of NEN5060 time information

In the spreadsheet *NEN5060-2018.xlsx*, shown in Figure 21a, the first four colums A:D contain the timestamp information. Since the NEN 5060 data is derived from hourly KNMI weather data, it follows the convention of the KNMI records, where the diurnal HOUR data runs from 1-24. The corresponding record of KNMI weather data is given in Figure 21b. KNMI uses UTC timestamps (https://www.knmidata.nl/data-services/knmi-producten-overzicht) pointing to data from the *previous* hour. These UTC timestamps are coded in the columns YYYYMMDD and H, respectively.

In Listing 9 the conversion from the NEN 5060 spreadsheet colums, read into a Pandas Dataframe, is shown. The function pandas.to_datetime correctly handles an offset of $-1\,h$, thereby changing the hour range to 0-23. Thus, the Pandas Timestamps refer to the *following* hour period. The Pandas Timestamps thus obtained are still *naive*. Conversion to *timezone-aware* UTC Timestamps is done by the tz_localize function, which uses a timezone from the pytz package. The *timezone-aware* UTC Timestamps can be converted to the timezone "Europe/Amsterdam" by calling the tz_localize function again. In the local Dutch Timestamps, the Daylight Savings Time (DST) is automatically included. columns with a Pandas UTC and local timestamp are inserted at the beginning of the NEN 5060 DataFrame.

(a) NEN 5060 spreadsheet (detail)

(b) KNMI hourly data in csv format (detail)

Figure 21: NEN 5060 spreadsheet and parent KNMI hourly weather record.

Listing 9: Conversion of NEN5060 timestamp to timezone-aware Pandas Timestamp

```python
def NENdatehour2datetime(nen_df: pd.DataFrame):
    # define timezones
    utz = timezone('UTC')
    nltz = timezone('Europe/Amsterdam')

    # convert columns 'jaar', 'MONTH(datum)', 'DAY(datum)', 'HOUR(uur)' into Pandas timestamps
    # subtracting 1 hour from the 'HOUR(uur)' values (works automatically!)
    pdt_naive = pd.to_datetime(dict(year=nen_df['jaar'],
                                    month=nen_df['MONTH(datum)'],
                                    day=nen_df['DAY(datum)'],
                                    hour=nen_df['HOUR(uur)'] - 1))
    # make NAIVE UTC forward-looking timestamp AWARE
    # Note: this cannot be done inplace because Timestamps are IMMUTABLE
    # Note2: since pdt_naive is a pandas Series object, use Series.dt.tz_localize and
    #     Series.dt.tz_convert
    pdt_utc = pdt_naive.dt.tz_localize(tz=utz)
    # convert AWARE UTC to AWARE local time
    pdt_local = pdt_utc.dt.tz_convert(tz=nltz)

    # insert AWARE UTC and AWARE LOCAL DateTimeIndex as first columns in DataFrame
    nen_df.insert(loc=0, column='utc', value=pdt_utc)
    nen_df.insert(loc=1, column='local_time', value=pdt_local)
    return nen_df
```

4.3.4 Gregorian and Julian time

Today's calendar is the Gregorian calendar, introduced by pope Gregory XIII in 1582. This calendar refines the use of leap years, compared to its predecessor, the Julian calendar, introduced by Julius Caesar in 45 B.C. [29]. In the transition process in October 1582, 10 days had to be skipped. It is clear that this time gap was good for society (finally, Turkey introduced the Gregorian calendar in 1926!), but not for astronomy. That is why astronomers kept using the Julian calendar - between 1582 and 1926 - and ever since. That means they have to define a new epoch every 50 years, to compensate for the imperfections of the Julian calendar. The big advantage is that the planets have kept their undisturbed orbits and that the Harmony of the Spheres is still in sync with ancient times.

4.4 Position of the sun

4.5 Attenuation of the solar radiation

4.6 Direct Normal Incidence (DNI)

4.7 Orientation of the receiving surface

4.8 Direct, diffuse and global irradiation

4.9 Efficiency

5 PV and solar collector modeling

This section presents the (proposed) models that describe the behavior of PV-panels, thermal solar collectors and the combination of the two as PVT panels.

5.1 generic panel properties

PV panels and thermal collectors have a common set of properties. Both are oriented surfaces, which transforms the incoming energy from the solar radiation into useful energy; electrical energy for PV, and heat for thermal collectors. The yield highly depends on the location, orientation with respect to the sun and the total surface area. Below the common properties are listed:

- surface_area: the surface of the panels in m^2.

- longitude: longitude of the location of the panels, given in degrees.

- latitude: latitude of the location of the panels, given in degrees.

- inclination: angle of the panel with the horizontal plane in degrees. The value lies between 0 degrees for horizontal and 90 degrees for vertical.

- azimuth: angle with due south direction in degrees (for the northern hemisphere). The value lies between -180 degrees and 180 degrees, with 90 degrees facing due west and -90 degrees facing due east.

Using these properties one can compute the irradiance level at a given time. Based on the NEN5060 irradiation numbers for the measured global irradiance on the horizontal plane, and the derived diffuse irradiance on the horizontal plane we can find the contributions of the direct and diffuse irradiance.

5.2 splitting global irradiance into direct and diffuse

Most weather data contain only a measurement for the global irradiance on a horizontal plane. In order to make a good estimate for the yield of PV and thermal panels it is important to have an estimate of the direct and diffuse irradiance on the oriented surface of the panels, separately. In literature different experimental models can be found that give a method for making this split. In [30], Dervishi and Mahdavi compare a set of these models that have been published over the years. They conclude that, of the models in their analysis, the model by Erbs et al. [31] gives the best results.

The Erbs model determines a clearness index k_t based on the extraterrestrial solar irradiance (I_o), the sun altitude (α) and the measured global irradiance (I_t):

$$k_t = \frac{I_t}{I_o \cdot \sin(\alpha)}. \tag{111}$$

In the model, I_o is determined with the following equation:

$$I_o = I_{sc} \cdot \left(1 + 0.33 \cdot \cos\frac{360 \cdot n}{365}\right) \cdot \cos(\theta_z), \tag{112}$$

where I_{sc} is the extraterrestrial solar constant irradiance (set to 1367 W/m^2), n is the day number, and θ_z is the zenith angle.

Based on the clearness index k_t the fraction of the diffuse horizontal irradiance (k_d) can be determined:

$$\text{interval:} \quad k_t \leq 0.22 \quad k_d = 1 - 0.09k_t, \tag{113}$$

$$\text{interval:} \quad 0.22 < k_t \leq 0.8 \quad k_d = 0.9511 - 0.1604k_t + 4.39k_t^2 - 16.64k_t^3 + 12.34k_t^4, \tag{114}$$

$$\text{interval:} \quad k_t > 0.8 \quad k_d = 0.165. \tag{115}$$

Now, using k_d we can determine the diffuse contribution of the irradiance on the horizontal plane $I_{dif,h} = k_d \cdot I_t$. The direct irradiance on the horizontal plane is the complementary part, $I_{dir,h} = I_t - I_{diff,h}$.

5.3 irradiation on an inclined surface

In order to be able to compute the output power of the PV-panel we need to compute the contributions of both the diffuse and direct irradiance on the oriented surface of the PV-panel. For the direct irradiance ($I_{dir,p}$) this can be done by using the location and orientation of the panels and the orientation of the sun.

$$I_{dir,p} = \frac{\cos\theta}{\sin h} \tag{116}$$

5.4 PV-panel efficiency

A PV-panel converts the energy of the incoming solar irradiation to electrical energy. The efficiency of the conversion depends on the temperature of the panels according to the relationship [32]:

$$\eta_{\text{cell}}(T_{\text{cell}}) = \eta_{\text{cell,N}} \left(1 + \gamma_{\text{T}} \left(T_{\text{cell}} - T_{\text{cell,N}}\right)\right), \tag{117}$$

where $\eta_{\text{cell,N}}$ is the nominal efficiency according to the panel specifications, γ_{T} is temperature coefficient according to the panel specifications, $T_{\text{cell,N}}$ is the reference temperature at which the nominal efficiency is measured, and T_{cell} is the actual temperature of the panel. The nominal efficiency is measured at a solar irradiance of 1000 W/m^2, and is usually provided in the specs of the PV-panel.

The equation for the efficiency may be extended to accommodate for the effects of the level of irradiation other than the standard conditions. In [33], two variants are provided, both without any further reference:

$$\eta_{\text{cell}}(T_{\text{cell}}) = \eta_{\text{cell,N}} \left(1 + \gamma_{\text{T}} \left(T_{\text{cell}} - T_{\text{cell,N}}\right)\right) \cdot \left(1 - k \cdot (G - G_{stc})\right), \tag{118}$$

and

$$\eta_{\text{cell}}(T_{\text{cell}}) = \eta_{\text{cell,N}} \left(1 + \gamma_{\text{T}} \left(T_{\text{cell}} - T_{\text{cell,N}}\right)\right) \cdot \left(1 - k' \cdot \ln\left[\frac{G}{G_{STC}}\right]\right), \tag{119}$$

where G_{STC} represents the standard solar irradiance level of 1000 W/m^2. Note that the difference between the two equations is that the first considers the difference between the actual irradiance level with the standard level, while the second approach considers the differences of the log of levels. Which of these approximations is the best is unclear at time of writing, and may need some additional investigation. As long as this is unclear, I propose to stick with equation 117, which ignores this effect.

In order to compute the efficiency the temperature of the PV-cells is required. The temperature can be approximated using the formula [32]:

$$T_{\text{cell}} \approx T_a + \left(43.3 \cdot \exp\left[-0.61 \left(\frac{v_w}{\text{m/s}}\right)^{0.63}\right] + 2.1\right) \left(\frac{I_{g,s}}{1000 \text{W/m}^2}\right), \tag{120}$$

where T_a is the ambient temperature, v_w is the wind speed and $I_{g,s}$ is the global irradiance level.

5.5 thermal collector

Schnieders [34] gives a good overview of a set of dynamic collector models, that were available in 1997. Most of these approaches are based on a 3n-node-model, which was proposed by Kamminga in 1985 [35](have not seen the original paper only the summary in Schnieders). This 3n-node-model uses breaks the collector up in n parts of 3 thermal capacities: the glass cover, the absorber plate and the fluid. A basic heat exchange model, similar to the house model, describes the heat exchange in each of the n parts. The heat exchange

between the n parts is only due to the fluid flow through the collector tube. This yield a set of linear partial differential equations. This 3n-node-model is relatively computational intensive. To overcome this issue various approximation approaches have been used over time, which are also mentioned by Schnieders. Although it might be possible to capture this model in our developed modeling formalism of capacities and flows, one can question whether this model fits to the time scales we are considering. Schnieders has made a comparison of the models. For this comparison, measurements were done over some time period, with a sampling interval of 10 seconds. 5 models have been fitted on the data, and the simulation results are shown for a period of 30 minutes. One can observe that the more detailed models match well with the measurements, also on a sub-minute time scale. However this is not the level of detail we will need, since we do not have the input, solar irradiance, on the time-scale. Therefore, a more suited model would possibly be the 1-point model, which only considers the mean temperature, or the stationary model.

(NOTE FOR SELF ended here need to look into the details of the one-point model and stationary model)

5.6 PVT-panel

A PVT-panel combines a PV-panel with a thermal solar collector.

Kramer et al. [33] provide an overview of various models for determining both the thermal and electrical output of PVT-panels. The quality of this overview is varying between sections. Some parts lack the references to the original sources of the models that are discussed. The internal cross-referencing is often 'broken', which makes the relation between the discussed thermal models and electrical models unclear. However, this document can be used as a starting point for setting up a model that captures the both the electrical and thermal output of a PVT-panel.

5.6.1 electrical output

For modeling the electrical yield of a PVT-panel we can refer to the model of the PV-panel. The panel efficiency can be approximated by equation (117). However, the panel temperature is now largely influenced by the solar collector, and Equation (120) does not hold. The most basic approximation for the PV-cell temperature is $T_{\text{cell}} = T_{\text{fl,out}}$, where $T_{\text{fl,out}}$ is the temperature of the collector fluid at the outlet, cf. [33] page 22. The temperature at the outlet should follow from the thermal analysis of the PVT.

5.6.2 thermal output

Section 2.1 of the report Status Quo of PVT Characterization [33] gives an overview of various modelling approaches for obtaining the thermal yield of a thermal solar collector. Here we briefly address the various approaches.

The first approach is based on the **Standard ISO 9806**. Under steady-state test conditions the thermal power $\dot{Q}_{th}$ is given by:

$$\dot{Q}_t h = A_G \cdot G \cdot \left[\eta_{0,hem} - a_1 \cdot \frac{\theta_m - \theta_a}{G} - a_2 \cdot G \cdot \left(\frac{\theta_m - \theta_a}{G} \right)^2 \right], \tag{121}$$

here A_G is the gross area of the collector, G is the hemispherical solar irradiance (Global solar irradiance), θ_m is the mean temperature of the heat transfer fluid and θ_a is the measured ambient temperature. a_1 and a_2 are two coefficients that are specify the collector's temperature dependent heat loss. These coefficients are not directly available, and should be determined by fitting the model to experimental data. (Possibly a manufacturer could provide these parameters?). An additional down side of this model is that it needs the mean temperature of the collector fluid as input. This is largely dependent on the operational conditions. Under the norm's the steady-state test conditions these might be well defined and controlled, in practice these conditions will vary and are not controllable. θ_m will be in general not available as a basic input. This makes the model not directly

practically applicable. The equation 121 is the most basic version of a series. This model has been further extended to add wind speed dependencies and radiation losses. However, the limitation in usability remains.

The second model is a one dimensional energy balance model. The description in [33] is not so clear. It seems that this model provides a steady state solution for the temperature distribution in the direction of the flow of the collector fluid. This yields a function for the outflow temperature dependent on the inflow temperature. According to the description this is a simple linear relationship. However, the exact parameters are obscure. In case we want to use this model the math needs to be worked out in detail. Downside of this model is the lack of time dependence. In a steady state situation, with little fluctuation in the inflow temperature, this model might suffice.

5.6.3 energy balance

6 Manual; how to work with the two zone house model

6.1 Voor wie?

Deze manual is bedoeld om een handreiking te geven aan bedrijven die de impact van hun warmtebron willen doorrekenen.

7 The *housemodel* Python package

7.1 Cloning from Github

The Git repository with the HAN housemodel is located in the cloud, on the GitHub site. The URL is:

https://github.com/hancse/twozone_housemodel

The repository contains a Python package *housemodel*. The Python package is actively updated and upgraded.

Currently, the repository is *public*. This means you do not need a GitHub account for read access permission to download or clone the repository. For contributing, write permission needs to be granted by the administrator(s). In order to obtain a GitHub account, follow the instructions in Appendix A.1.

7.1.1 Option 1

- this option generates a folder with the latest code version for *users*. Contributing is not possible because the .git folder (repository bookkeeping) is not included in the download.

- Follow the link above to the cloud repository.

- Click the button with "**...**" and select "Download repository".

- The downloaded zip archive is named "twozone-housemodel-xxxxxxxxxxxx.zip" Unpack the folder in the zip archive. The xxxxxxxxxxxx code indicates the unique commit (version) number of the downloaded code. Do not change the name of the downloaded and unpacked folder.

7.1.2 Option 2

- this option generates a *local* clone with the complete history of the repository in the .git folder. This is for programmers and contributing *users*. Contributors must be aware of the workflow mentioned in Appendix A.3.

- Follow the instructions in Appendix A.2.

- Read the notes in Appendix A.2.3

- make a new *local* folder on your HDD or SSD disk and name it "housemodel-git".

- go to the (empty) folder and click the right mouse button to open the context menu of Fig. 26.

- choose the menu option "Git clone...".The dialog from Fig. 22 appears.

- fill the entry "URL:" with the internet address (URL) of the repository above.

- fill the entry: "Directory:" with the path to your new local folder. A dummy name with placeholders ⟨*username*⟩ and ⟨*programs*⟩ is given in Fig. 22.

- leave all checkboxes unchecked.

- Press the OK button.

- A dialog with an acrobatic turtle will appear. The dialog will prompt you for your Bitbucket username and password. It will print a "Success" message when cloning has been completed.
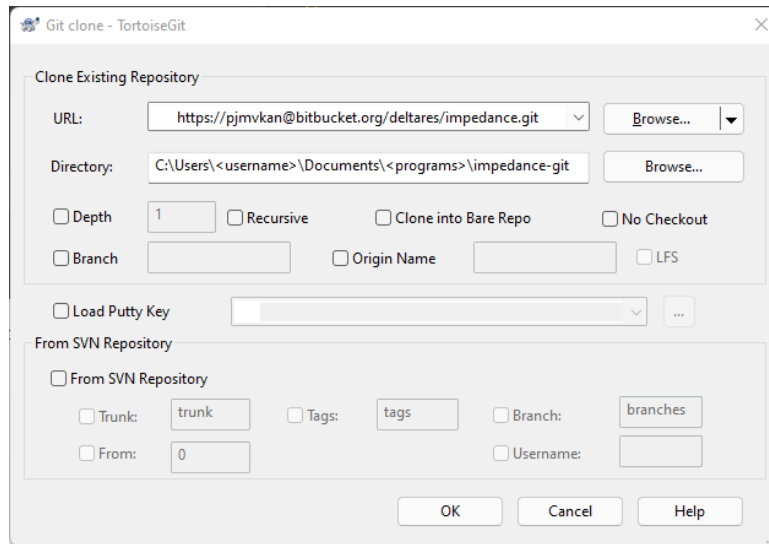
Figure 22: Cloning a repository with TortoiseGit

Note: Running the simulations and tests is best done from the *repository root*. All simulations and tests are designed to find the package, subpackages and configuration files from this directory.

7.2 Working with the Python code

Python scripts and programs can only be run by the Python *interpreter*. Installation of this interpreter and other Python *packages* for mathematical operations, basic plotting and file handling, is done by a *package manager* who bundles the packages in an *environment*.

To get things working, follow the instructions in Appendix B.

- The commands for creating a dedicated *environment* in Appendix B.2 and B.3 are listed in Listing 10.

Listing 10: Example textfile with conda commands for new environment

```
conda config --show

#if not present:
conda config --add channels conda-forge
conda config --set channel_priority strict

conda create -n futurefactory python=3.8

activate futurefactory
conda info -e

conda install -c pvlib pvlib  # downgrades pytorch to 1.4.0, so install pytorch after pvlib

conda install matplotlib
(conda install scipy)
(conda install pandas)
conda install openpyxl
conda install pyyaml
conda install holidays

conda install scikit-learn-intelex
conda install -c pytorch pytorch      # 1.12.1

conda install pytest                  # downgrades pytorch to 1.10.2
conda install colored-traceback
```

```
26
   conda install networkx
28 conda install requests
   conda install tqdm

30
   pip install solarenergy

32
   conda list
```

- after completion of the dedicated *environment* the Python scripts in the folder "twozone_housemodel-xxxxxxxxxxxx" or "housemodel-git" can be run in the Anaconda Prompt console.

- Alternatively, Python scripts can be run and adapted in an "Integrated development Environment (IDE). The recommended choice is the PyCharm IDE. For installation instructions, follow Appendix B.5.

7.3   Package structure

The repository "twozone_housemodel-git" contains the modules for the house model. The customary way to organize the modules is to make a *Python package* with *subpackages*. This opens up the possibility of publishing the package on PyPi, so that it can be imported.

See: https://pypi.org/

From commit e74ce58 the files in the twozone_housemodel-git repository are organized as a package. The proposed structure, implemented in this commit, is:

```
twozone_housemodel-git
├──/Documentation
│  └──LaTeX
│       ├──/Figures
│       ├──/Listings
│       └──/pdf
│            └──this document
├──housemodel
│  ├──__init__.py
│  ├──controls
│  │   └──__init__.py
│  ├──solvers
│  │   └──__init__.py
│  ├──sourcesink
│  │   └──__init__.py
│  └──tools
│      └──__init__.py
├──tests
│  ├──__init__.py
│  ├──context1.py
│  └──test_*.py
├──environment.txt
├──Simulation*.py
├──README
└──setup.py (to be added)
```

- the *repository root* twozone_housemodel-git contains the simulation scripts and configuration files (for now)

- the *package root* housemodel contains the complete package. This can be seen since it contains an (empty) __init__.py module.

- the *subpackage* folders contain the modules with common functions and classes for all simulations. They each contain an (empty) __init__.py module.

- a tests folder is placed carefully as a subfolder of the *repository root*. See: https://docs.python-guide.org/writing/structure/ for the underlying philosophy. Here, testing modules (scripts) can be placed. If the names of the test scripts start with test_, they can be automatically run with the pytest Python package.

Note: Running the simulations and tests is best done from the *repository root*. All simulations and tests have been updated to find the package, subpackages and configuration files from this directory.

7.3.1 Subpackage classes

The subpackage classes contains the following Python modules:

- **constants.py**. This module contains basic physical constants listed in Listing **??**.

- **cells.py**. This module covers Python classes for describing the electrolysis cells used in the experiments and simulations. The (abstract) base class Cell has an attribute cell_constant. Derived classes PlanarCell and CylindricalCell contain specific geometrical parameters used for determining the frequency dependence of electrode polarization. See Listing **??**.

- **electrolytes.py**. This module covers Python classes for describing the basic electrolytes (ionic salt solutions) used in the experiments and simulations. The base class Electrolyte contains the attributes and methods listed in Listing **??**.

- **particles.py**. This module covers Python classes for describing the colloidal particles present in the ionic solutions. The base class Particles contains the attributes and methods listed in Listing **??**.

- **colloids.py**. This module covers Python classes for describing the colloidal systems consisting of a cell, an electrolyte and colloidal particles. The base class Colloids contains the attributes and methods listed in Listing **??**.

7.4 Use Case

- **import classes**
- **instantiate classes**
- **perform calculations**
- **load-short correction**
- **equivalent circuit**

7.5 A Colloid with Particles

The Particle class in the module particles.py has four scalar attributes:

- particle radius in m.
- relative zeta potential in units of eV/kT
- complex permittivity (DC)
- volume fraction of particles in the colloid.

The Particle object represents a collection of monodisperse particles in the colloidal solution. Polydisperse colloids can be modelled by adding a list of Particle objects to the Colloid object. This list is initialized with None for a pure ionic salt solution. The (list of) Particle objects can be added or appended to manually or read from the configuration file in *.yml format.

To be continued...

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A Code Management

Coding in a programming language is a process of trial-and-error, leading to a working control program or modelling code in many incremental steps. When working on this individually, but more so when coding in a team of code contributors, tracking progress is mandatory. Also, keeping track of the coding progress in multiple locations reduces the risk of information or code losses.

A.1 Github or Bitbucket account

For optimal collaboration, programmers communicate their last achievement to their colleagues or key users by *committing* them in a *repository* on their local PC, then *pushing* the changes to a central copy of the repository in the cloud. Before starting their work, colleagues can *pull* the last changes, so that their local copy of the repository is up-to-date. The updated local copy is then used for adding new contributions or trying out the updated features. Changes or improvements can be committed locally and pushed to the cloud repository by each member of the team.

For establishing a team and implementing the workflow above, each contributor must have an account on a Git repository cloud service.

- Github: Go to https://github.com/ and *sign up* with the button in the upper right corner of the web page.
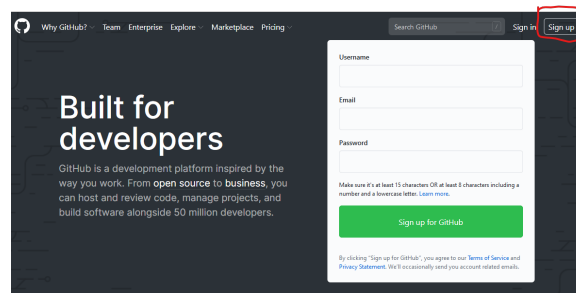
Figure 23: GitHub sign-up

- Bitbucket: Go to https://bitbucket.org/ and sign up with the "Get it free" button in the upper right corner of the web page.
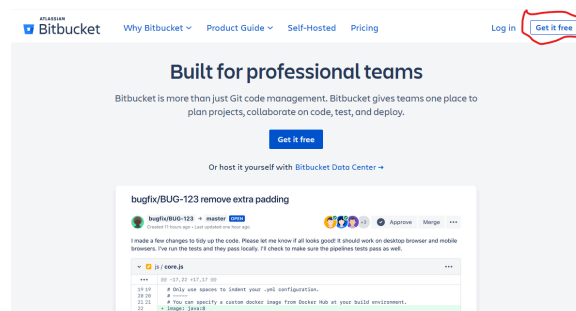
Figure 24: Bitbucket sign-up

Do not forget to store your usernames and passwords. The use of a password *vault* is strongly recommended: https://keepass.info/

Note: Strictly, a GitHub or Bitbucket account is only necessary for all access to *private* repositories or for *contributing* to *public* cloud repositories. Read-only access to *public* repositories is possible without an account.

A.2   Versioning

The starting point for version control is the installation of a version control system on your PC. Historically, a number of systems have been invented. Most of them still exist. Among those, CVS, SVN, Bazaar and Mercurial (hg). In the last few years, however, the Git versioning system seems to gain a major "market share". It has been designed by the inventor of Linux, Linus Torvalds, and has a robust performance. The possibilities of Git are a bit overwhelming for the beginning user, which asks for a careful introduction.

A.2.1   Installation of Git

On Windows, installation of the *Git for Windows* package is the most convenient option. Download the installer at https://gitforwindows.org/.
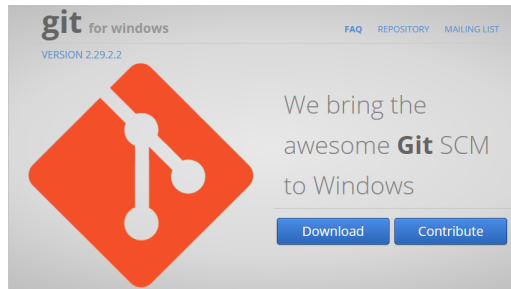

Figure 25: Git for Windows

- Download the latest version for your OS, which is probably 64-bit Git-2.xx.y.z-64-bit.exe

- On execution of the installer, all *default options* can be chosen.

On a computer with a Linux OS, there are several options, e.g.:

- sudo apt install git (Ubuntu, Debian, RPi)

- sudo pacman git (ArchLinux)

For Apple Macintosh installation, consult https://git-scm.com/download/mac.

A.2.2   Installation of a Git client

Using Git can be done from the command line (Windows Command Prompt, Git bash or Linux bash). On Linux, this is the preferred option. On Windows, there are useful Git client programs, which make versioning easier after a while. In the beginning, they may just confront you with the overwhelming capacities of Git. Going through this phase merits the effort, however. A preferred client can be downloaded at https://tortoisegit.org/download/.

- Download and run the installer: TortoiseGit-2.13.0.1-64bit.msi.

- Install with all *default options.*

This client integrates with Windows Explorer as an addition to the context menus under the right-mouse-click button. Installation with the default options is straightforward. Check if the context menus are extended with Git options.

A second client, with extended functionality can be found at https://www.sourcetreeapp.com/. Recommended for regular Git users, who work in teams with more than three collaborators, or with collaborators at external reasearch partners. Sourcetree is also available for Mac, but (unfortunately) not for Linux.
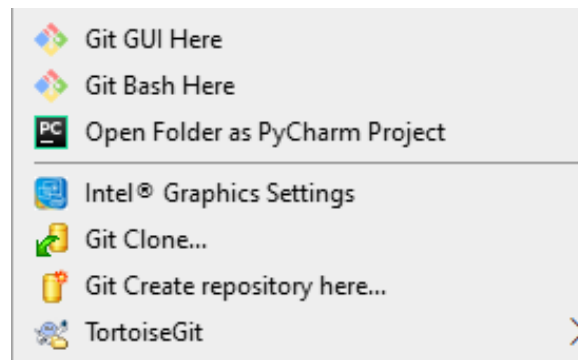
Figure 26: Git options in context menu

A.2.3 Working with Git

After installation of Git and a Git client, you can start working with Git *repositories*. A repository can be *created* locally, on the harddisk of your PC. Alternatively, a repository from the cloud can be *cloned* to your harddisk.

After these initial operations, your contributions to the code can be *staged* and *committed* locally and *pushed* to the cloud. Contributions committed and pushed by colleagues can be *pulled* to your local harddisk.

Regular pulling (before you start coding) and staging-committing-pushing (after you finished coding) cycles will thus assure, that the repositories of all contributors will be synchronized with each other and with the repository in the cloud. The repository in the cloud is often called *origin*.

Note: Each local Git repository should be placed in a separate *local* folder on the physical HDD or SSD. For clarity, it is recommendable to choose a folder name: ⟨*repository_name*⟩-git. (no spaces in the folder name).

Each created or cloned repository folder contains a hidden bookkeeping folder named .**git**. This bookkeeping is not compatible with file sychronization mechanisms. So, please do not create repository folders on Microsoft OneDrive, SharePoint, Teams, Google Drive, OneDrive or SurfDrive shared folders.

Repository folders are possible on WebDAV, NFS or SMB mounted shared folders, **if** only one single user has access to the shared folder (from several personal computers, tablets or phones).

A.3 Git workflow

- Creating a repository locally: https://tortoisegit.org/docs/tortoisegit/tgit-dug-create.html

- Cloning a repository from GitHub or Bitbucket; https://tortoisegit.org/docs/tortoisegit/tgit-dug-clone.html

- Pushing to GitHub or Bitbucket: https://tortoisegit.org/docs/tortoisegit/tgit-dug-push.html

- Pulling the changes from the cloud to your local repository: https://tortoisegit.org/docs/tortoisegit/tgit-dug-pull.html

- Committing and pushing your local changes to the cloud: https://tortoisegit.org/docs/tortoisegit/tgit-dug-commit.html

B Installation of Python and Miniconda

Installation of the software for programming in Python on a computer is easiest with a *package manager*. The recommended package manager for Python is named conda. It can be used as a Windows console (Anaconda Prompt), which is very similar to the implementation in a Linux or MacOS X bash console. The console program is called Miniconda and can be downloaded at:

https://docs.conda.io/en/latest/miniconda.html.

Miniconda is available for Windows, Linux and MacOS. In general, nowadays, one would choose the latest Miniconda Python 3.x version 64-bit installer: Miniconda3-latest-Windows-x86_64.exe on Windows, or the analogous installers for Linux and MacOS X.

- Download and execute your installer

- Install "Just for me" and create C:\Users\⟨*username*⟩\miniconda3. Note: ⟨*username*⟩ should NOT contain spaces. Do not install Miniconda system-wide in the "C:\Program Files" directory.

- Take default options for PATH and REGISTRY update

B.1 Anaconda Prompt

After installation of Anaconda (Miniconda) the Windows Start Menu contains a new group "Anaconda3". A detailed view is shown below:

(a) Anaconda Start Menu
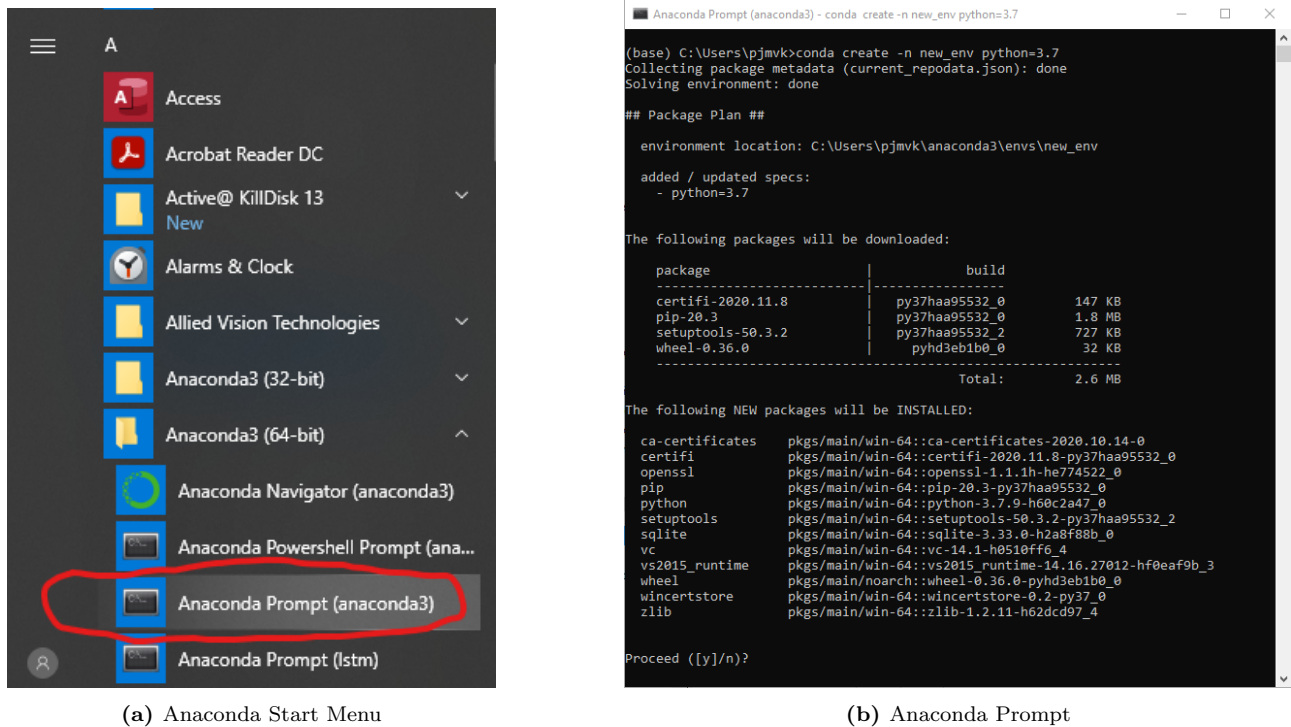
(b) Anaconda Prompt

Figure 27: Anaconda (Miniconda) tools installed on Windows

The Start Menu entry "Anaconda Prompt (miniconda3)" will open a Windows Command Prompt ("MS-DOS window") with special properties. The current directory name (standard prompt) is preceded by (base). This is the name of the default conda *environment*. The (base) environment is *NEVER* used for code development. After installation of the package manager, it contains the latest version of the Python interpreter, which is kept up-to-date with the command:

conda update -n base -c defaults conda

The Python interpreter in the (base) environment may be used by other Windows programs, which will then ask you for the location of the default Python interpreter.

The standard location is: C:\Users\⟨*username*⟩\miniconda3\python.exe.

B.2 Conda configuration

Before creating any dedicated environments, it is recommended to optimize the conda configuration [**stack˙channels**, **stack˙multiple**]. In the previous command, the conda *package* was updated in the base *environment*. The package was read from the defaults *channel*. Other channels exist, that often contain more up-to-date versions of important Python packages. The channel conda-forge is keeping a more recent copy of many packages, including the opencv package, which is a key package used for image analysis. Therefore we add:

- conda config –show   this shows the configuration file. Look for "channels:".

- conda config –add channels conda-forge   this adds the conda-forge channel before the defaults channel (top of the list).

- conda config –set channel˙priority strict   this guarantees that channel priority is maintained according to the list.

The config file now shows:

...

channel˙priority: strict

channels:

- conda-forge

- defaults

...

See also:

https://stackoverflow.com/questions/39857289/should-conda-or-conda-forge-be-used-for-python-environments

https://conda-forge.org/docs/user/tipsandtricks.html#using-multiple-channels

B.3 Conda environments

A dedicated environment can be made with the command:

conda create -n ⟨*env˙name*⟩ python=3.x

The next commands are:

activate ⟨*env˙name*⟩

conda info –envs or conda info -e: note the active environment with asterisk *

conda install ⟨*package˙name*⟩ or pip install ⟨*package˙name*⟩

The result can be seen with: conda list : note the packages are all compatible with your Python version

The commands can be stored in a textfile:

Listing 11: Example textfile with conda commands for new environment

```
1  conda config --show

3  #if not present:
   conda config --add channels conda-forge
5  conda config --set channel_priority strict
```

```
 7  conda create -n futurefactory python=3.8

 9  activate futurefactory
    conda info -e
11
    conda install -c pvlib pvlib   # downgrades pytorch to 1.4.0, so install pytorch after pvlib
13
    conda install matplotlib
15 (conda install scipy)
   (conda install pandas)
17  conda install openpyxl
    conda install pyyaml
19  conda install holidays

21  conda install scikit-learn-intelex
    conda install -c pytorch pytorch      # 1.12.1
23
    conda install pytest                  # downgrades pytorch to 1.10.2
25  conda install colored-traceback

27  conda install networkx
    conda install requests
29  conda install tqdm

31  pip install solarenergy

33  conda list
```

Environments are stored in the private directory of the user. On Windows: C:\Users\⟨*username*⟩\miniconda3\envs

On Linux: /home/⟨*username*⟩/miniconda3/envs

Note: Code development or storage is NEVER done in C:\Users\⟨*username*⟩\miniconda3 NOR in any of its subfolders.

B.4   Python from the console

The Anaconda Prompt program on Windows is a specialized version of the general Windows Command Prompt, formerly known as "MS-DOS window" or "console". The advantage of Anaconda Prompt is that all file paths to the Miniconda installation are automatically set and that the prompt indicates the currently active Python environment. On Linux and MacOS, Anaconda Prompt is integrated in the command-line terminal. Thus Anaconda Prompt looks very similar on all operating systems.

Running a Python script in the console is as simple as:

activate ⟨*env_name*⟩

conda info –envs or conda info -e: note the active environment with asterisk *

cd ⟨*repository_root*⟩

python ⟨*script_name*⟩

For an overview of Python command-line features, see:

https://realpython.com/python-command-line-arguments/#the-command-line-interface
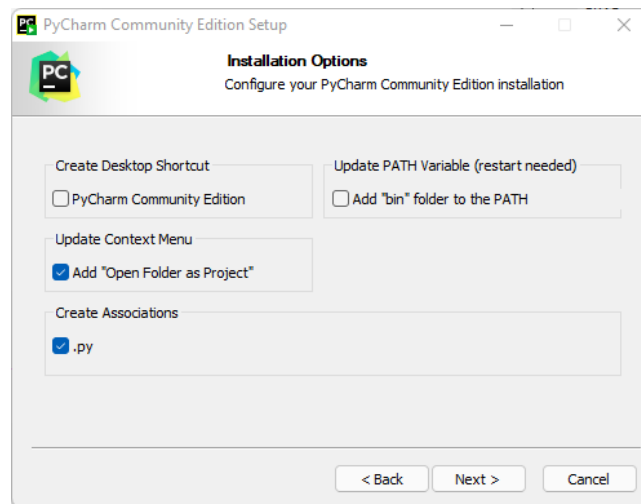
B.5 Python IDE

B.5.1 Installation

Figure 28: PyCharm IDE installation on Windows

After creation of the `conda` environment with the right selection of Python *packages* for the analysis of the impedance measurements, it is recommended to develop the Python software in a dedicated IDE, where Python scripts can be edited, run, and debugged. The recommended program for this purpose is PyCharm, which can be downloaded here:

https://www.jetbrains.com/pycharm/download/#section=windows

https://www.jetbrains.com/community/education/#students

- Download the "Community" installer pycharm-community-2021.3.2.exe and run it.

- Install in default directory.

- Check options according to Figure 28.

- after succesful installation, navigate to the *repository root* folder of your project and right-click on the canvas of the folder window (not on a file or subfolder icon). Choose the "Open Folder as PyCharm Project" item. The PyCharm IDE will start and open the project and subfolders.

- Once a project has been opened in PyCharm, it creates a (hidden) subfolder named .idea in the repository root folder. This folder contains the bookkeeping of the IDE. Do not change anything in this .idea subfolder. If anything goes wrong, delete it entirely, and PyCharm will create a fresh one.

-
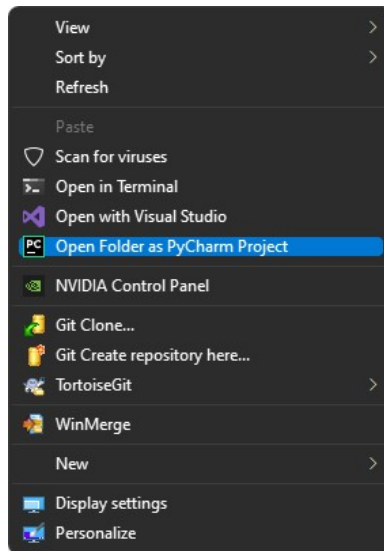
Figure 29: PyCharm context menu after right-click on root folder canvas

B.5.2 Configuration

- To work with your Python code in PyCharm, you need to configure a Python interpreter. Assign the Python interpreter from your (existing!) conda environment created following the guidelines in Appendix B.3 to the open project. See: https://www.jetbrains.com/help/pycharm/configuring-python-interpreter.html.

- After configuring the interpreter, the IDE needs some time to load all the packages from your environment. A progress bar is visible on the bottom of the IDE window.
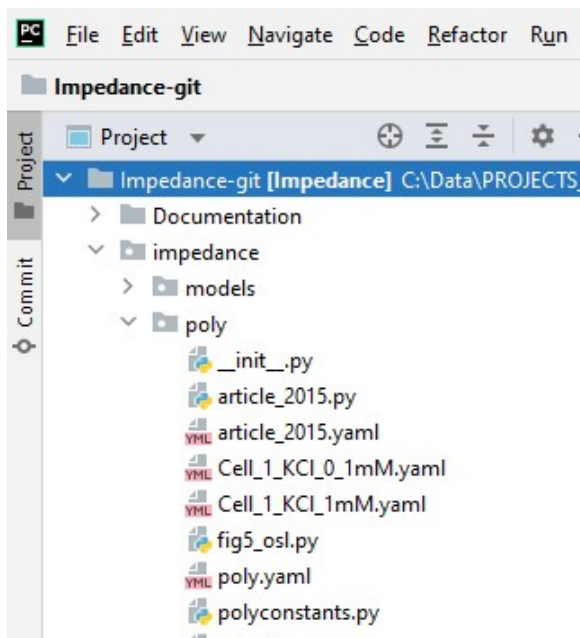
(a) Project tab with root folder and subfolders
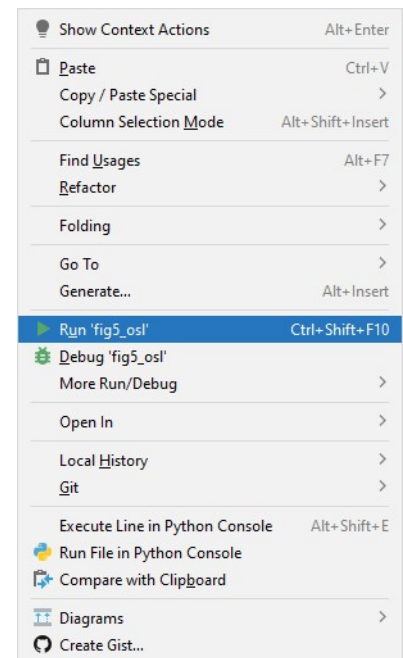
(b) Context menu for right-click

Figure 30: PyCharm project configuration and running

B.5.3 Running and debugging Python scripts

- Selecting a Python script in the Project tab can be done with a left-click. Right-clicking on a Python (*.py) module opens the context menu of Fig. 30b. Clicking the green arrow in the context menu starts

executing the selected script.

- Double-clicking a *.py module in the Project tab opens the module in the editor window of the IDE. Right-clicking on the canvas of the editor window also opens the context menu of Fig. 30b.

C Differential equations for stratified buffervessel MvdB

Python code, for a buffer vessel with 8 layers:

$$
\begin{aligned}
dT1 &= ((F_s * (Tsupply - x[0])) + (F_e * (x[0] - x[1]) * deltaMinus) - (U * As * (x[0] - Tamb)) + ((Aq * lamb)/z) * (x[0] - x[1])) \\
dT2 &= ((F_e * (x[0] - x[1]) * deltaPlus) + (F_e * (x[1] - x[2]) * deltaMinus) - (U * As * (x[1] - Tamb)) + ((Aq * lamb)/z) * (x[0] + x[2] - (2 * x[1]))) \\
dT3 &= ((F_e * (x[1] - x[2]) * deltaPlus) + (F_e * (x[2] - x[3]) * deltaMinus) - (U * As * (x[2] - Tamb)) + ((Aq * lamb)/z) * (x[1] + x[3] - (2 * x[2]))) \\
dT4 &= ((F_e * (x[2] - x[3]) * deltaPlus) + (F_e * (x[3] - x[4]) * deltaMinus) - (U * As * (x[3] - Tamb)) + ((Aq * lamb)/z) * (x[2] + x[4] - (2 * x[3]))) \\
dT5 &= ((F_e * (x[3] - x[4]) * deltaPlus) + (F_e * (x[4] - x[5]) * deltaMinus) - (U * As * (x[4] - Tamb)) + ((Aq * lamb)/z) * (x[3] + x[5] - (2 * x[4]))) \\
dT6 &= ((F_e * (x[4] - x[5]) * deltaPlus) + (F_e * (x[5] - x[6]) * deltaMinus) - (U * As * (x[5] - Tamb)) + ((Aq * lamb)/z) * (x[4] + x[6] - (2 * x[5]))) \\
dT7 &= ((F_e * (x[5] - x[6]) * deltaPlus) + (F_e * (x[6] - x[7]) * deltaMinus) - (U * As * (x[6] - Tamb)) + ((Aq * lamb)/z) * (x[5] + x[7] - (2 * x[6]))) \\
dT8 &= ((F_d * (Treturn - x[7])) + (F_e * (x[6] - x[7]) * deltaPlus) - (U * As * (x[7] - Tamb)) + ((Aq * lamb)/z) * (x[6] - x[7]))
\end{aligned}
\tag{122}
$$

Abbreviations and legend:

$$
\begin{aligned}
C_x &= m_x \cdot c_{p,w} \qquad \text{for} \quad x = 0 \dots \# \text{ of layers} \\
F_{supply} = F_s &= \dot{m}_{supply} \cdot c_{p,w} \\
F_{demand} = F_d &= \dot{m}_{demand} \cdot c_{p,w} \\
\dot{m}_e &= \dot{m}_{supply} - \dot{m}_{demand} \\
F_e &= \dot{m}_e \cdot c_{p,w} \\
\frac{1}{R_{amb}} &= U \cdot A_s \\
\frac{1}{R} = \frac{1}{R_{int}} &= \frac{Aq \cdot \lambda}{z}
\end{aligned}
\tag{123}
$$

The Python code has a "mismatch" between the range of dT_1 (1..8) and the range of x (0 ..7). This is solved by renaming the nodes to T_{top} $T_1 \cdots T_6$ T_{bot}. The set of differential equations the becomes:

$$
\begin{aligned}
C_{top} \cdot \frac{dT_{top}}{dt} &= F_s(T_{sup} - T_{top}) & + F_e(T_{top} - T_1)\Delta_- & \quad -\frac{1}{R_{amb}} \cdot (T_{top} - T_{amb}) + \frac{1}{R}(T_{top} - T_1) \\
C_1 \cdot \frac{dT_1}{dt} &= & F_e(T_{top} - T_1)\Delta_+ + F_e(T_1 - T_2)\Delta_- & \quad -\frac{1}{R_{amb}} \cdot (T_1 - T_{amb}) + \frac{1}{R}(T_0 + T_2 - 2T_1) \\
C_2 \cdot \frac{dT_2}{dt} &= & F_e(T_1 - T_2)\Delta_+ + F_e(T_2 - T_3)\Delta_- & \quad -\frac{1}{R_{amb}} \cdot (T_2 - T_{amb}) + \frac{1}{R}(T_1 + T_3 - 2T_2) \\
C_3 \cdot \frac{dT_3}{dt} &= & F_e(T_2 - T_3)\Delta_+ + F_e(T_3 - T_4)\Delta_- & \quad -\frac{1}{R_{amb}} \cdot (T_3 - T_{amb}) + \frac{1}{R}(T_2 + T_4 - 2T_3) \\
C_4 \cdot \frac{dT_4}{dt} &= & F_e(T_3 - T_4)\Delta_+ + F_e(T_4 - T_5)\Delta_- & \quad -\frac{1}{R_{amb}} \cdot (T_4 - T_{amb}) + \frac{1}{R}(T_3 + T_5 - 2T_4) \\
C_5 \cdot \frac{dT_5}{dt} &= & F_e(T_4 - T_5)\Delta_+ + F_e(T_5 - T_6)\Delta_- & \quad -\frac{1}{R_{amb}} \cdot (T_5 - T_{amb}) + \frac{1}{R}(T_4 + T_6 - 2T_5) \\
C_6 \cdot \frac{dT_6}{dt} &= & F_e(T_5 - T_6)\Delta_+ + F_e(T_6 - T_7)\Delta_- & \quad -\frac{1}{R_{amb}} \cdot (T_6 - T_{amb}) + \frac{1}{R}(T_5 + T_7 - 2T_6) \\
C_{bot} \cdot \frac{dT_{bot}}{dt} &= F_d(T_{ret} - T_{bot}) & + F_e(T_6 - T_{bot})\Delta_+ & \quad -\frac{1}{R_{amb}}(T_{bot} - T_{amb}) + \frac{1}{R}(T_6 - T_{bot})
\end{aligned}
\tag{124}
$$

Note the term in red in the first equation. There is a sign error...

Converting the set of equations to the form

$$
\mathbf{C} \cdot \dot{\boldsymbol{\theta}} + \mathbf{K} \cdot \boldsymbol{\theta} + \mathbf{F} \cdot \boldsymbol{\theta} = \dot{\mathbf{q}}
\tag{125a}
$$

The following set results:

$$
\begin{aligned}
C_{top} \cdot \frac{dT_{top}}{dt} + F_s(T_{top} - T_{sup}) \qquad\qquad\qquad &+ F_e(T_1 - T_{top})\Delta_- &+\frac{1}{R_{amb}}T_{top} + \frac{1}{R}(-T_1 + T_{top}) &\qquad = \frac{1}{R_{amb}}T_{amb} \\
C_1 \cdot \frac{dT_1}{dt} = \qquad\qquad F_e(T_{top} - T_1)\Delta_+ &+ F_e(T_1 - T_2)\Delta_- &-\frac{1}{R_{amb}}T_1 + \frac{1}{R}(-T_0 - T_2 + 2T_1) &\qquad = \frac{1}{R_{amb}}T_{amb} \\
C_2 \cdot \frac{dT_2}{dt} = \qquad\qquad F_e(T_1 - T_2)\Delta_+ &+ F_e(T_2 - T_3)\Delta_- &+\frac{1}{R_{amb}}T_2 + \frac{1}{R}(-T_1 - T_3 + 2T_2) &\qquad = \frac{1}{R_{amb}}T_{amb} \\
C_3 \cdot \frac{dT_3}{dt} = \qquad\qquad F_e(T_2 - T_3)\Delta_+ &+ F_e(T_3 - T_4)\Delta_- &+\frac{1}{R_{amb}}T_3 + \frac{1}{R}(-T_2 - T_4 + 2T_3) &\qquad = \frac{1}{R_{amb}}T_{amb} \\
C_4 \cdot \frac{dT_4}{dt} = \qquad\qquad F_e(T_3 - T_4)\Delta_+ &+ F_e(T_4 - T_5)\Delta_- &+\frac{1}{R_{amb}}T_4 + \frac{1}{R}(-T_3 - T_5 + 2T_4) &\qquad = \frac{1}{R_{amb}}T_{amb} \\
C_5 \cdot \frac{dT_5}{dt} = \qquad\qquad F_e(T_4 - T_5)\Delta_+ &+ F_e(T_5 - T_6)\Delta_- &+\frac{1}{R_{amb}}T_5 + \frac{1}{R}(-T_4 - T_6 + 2T_5) &\qquad = \frac{1}{R_{amb}}T_{amb} \\
C_6 \cdot \frac{dT_6}{dt} = \qquad\qquad F_e(T_5 - T_6)\Delta_+ &+ F_e(T_6 - T_7)\Delta_- &+\frac{1}{R_{amb}}T_6 + \frac{1}{R}(-T_5 - T_7 + 2T_6) &\qquad = \frac{1}{R_{amb}}T_{amb} \\
C_{bot} \cdot \frac{dT_{bot}}{dt} + F_d(T_{bot} - T_{ret}) \quad &+F_e(T_6 - T_{bot})\Delta_+ &+\frac{1}{R_{amb}}T_{bot} + \frac{1}{R}(-T_6 + T_{bot}) &\qquad = \frac{1}{R_{amb}}T_{amb}
\end{aligned}
\tag{126}
$$

Note the correction of the error in the term coloured green. Apparently, the conductive heat loss from the buffervessel to the surroundings is assumed to be equal for *all* layers of the vessel. This translates to a buffer vessel where the top and bottom ends have much better insulation than the side wall.

Writing down the matrix representation of the set we get:

$$
\mathbf{C} \cdot \dot{\boldsymbol{\theta}} =
\begin{bmatrix}
C_{top} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & C_1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & C_2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & C_3 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & C_4 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & C_5 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & C_6 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & C_{bot}
\end{bmatrix}
\cdot
\begin{bmatrix}
\frac{dT_{top}}{dt} \\
\frac{dT_1}{dt} \\
\frac{dT_2}{dt} \\
\frac{dT_3}{dt} \\
\frac{dT_4}{dt} \\
\frac{dT_5}{dt} \\
\frac{dT_6}{dt} \\
\frac{dT_{bot}}{dt}
\end{bmatrix}
\tag{127}
$$

Assuming all thermal conductance values between layers are equal as in the Python code:

$$
\mathbf{K_{int}} \cdot \boldsymbol{\theta} = \frac{1}{R_{int}} \cdot
\begin{bmatrix}
1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 1
\end{bmatrix}
\cdot
\begin{bmatrix}
T_{top} \\
T_1 \\
T_2 \\
T_3 \\
T_4 \\
T_5 \\
T_6 \\
T_{bot}
\end{bmatrix}
\tag{128}
$$

Assuming conductive heat loss from the buffervessel to the surroundings is equal for *all* layers of the vessel, $\mathbf{K_{ext}}$ becomes:

$$
\mathbf{K_{ext}} \cdot \boldsymbol{\theta} = \frac{1}{R_{amb}} \cdot
\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}
\cdot
\begin{bmatrix}
T_{top} \\
T_1 \\
T_2 \\
T_3 \\
T_4 \\
T_5 \\
T_6 \\
T_{bot}
\end{bmatrix}
\tag{129}
$$

The $\dot{q}$-vector becomes:

$$
\dot{\mathbf{q}} =
\begin{bmatrix}
\frac{1}{R_{amb}} \cdot T_{amb} \\
\frac{1}{R_{amb}} \cdot T_{amb} \\
\frac{1}{R_{amb}} \cdot T_{amb} \\
\frac{1}{R_{amb}} \cdot T_{amb} \\
\frac{1}{R_{amb}} \cdot T_{amb} \\
\frac{1}{R_{amb}} \cdot T_{amb} \\
\frac{1}{R_{amb}} \cdot T_{amb} \\
\frac{1}{R_{amb}} \cdot T_{amb}
\end{bmatrix}
\tag{130}
$$

C.0.1 Convective heat transfer in the buffer vessel

The convective part of the heat transfer equations is:

$$
\begin{aligned}
C_{top} \cdot \frac{dT_{top}}{dt} + F_s T_{top} &\quad\quad\quad + F_e(T_1 - T_{top})\Delta_- &&= F_s T_{sup} \\
C_1 \cdot \frac{dT_1}{dt} + &\quad F_e(T_1 - T_{top})\Delta_+ + F_e(T_1 - T_2)\Delta_- &&= 0 \\
C_2 \cdot \frac{dT_2}{dt} + &\quad F_e(T_2 - T_1)\Delta_+ + F_e(T_2 - T_3)\Delta_- &&= 0 \\
C_3 \cdot \frac{dT_3}{dt} + &\quad F_e(T_3 - T_2)\Delta_+ + F_e(T_3 - T_4)\Delta_- &&= 0 \\
C_4 \cdot \frac{dT_4}{dt} + &\quad F_e(T_4 - T_3)\Delta_+ + F_e(T_4 - T_5)\Delta_- &&= 0 \\
C_5 \cdot \frac{dT_5}{dt} + &\quad F_e(T_5 - T_4)\Delta_+ + F_e(T_5 - T_6)\Delta_- &&= 0 \\
C_6 \cdot \frac{dT_6}{dt} + &\quad F_e(T_6 - T_5)\Delta_+ + F_e(T_6 - T_7)\Delta_- &&= 0 \\
C_{bot} \cdot \frac{dT_{bot}}{dt} + F_d T_{bot} &\quad + F_e(T_{bot} - T_6)\Delta_+ &&= F_d T_{ret}
\end{aligned}
\tag{131}
$$

If $\dot{m}_e = \dot{m}_{supply} - \dot{m}_{demand} > 0$, $\Delta_+ = 1$ and $\Delta_- = 0$.

$$
\begin{aligned}
C_{top} \cdot \frac{dT_{top}}{dt} + F_s T_{top} &\quad\quad\quad &&= F_s T_{sup} \\
C_1 \cdot \frac{dT_1}{dt} + &\quad F_e \cdot (T_1 - T_{top}) \cdot \Delta_+ &&= 0 \\
C_2 \cdot \frac{dT_2}{dt} + &\quad F_e \cdot (T_2 - T_1) \cdot \Delta_+ &&= 0 \\
C_3 \cdot \frac{dT_3}{dt} + &\quad F_e \cdot (T_3 - T_2) \cdot \Delta_+ &&= 0 \\
C_4 \cdot \frac{dT_4}{dt} + &\quad F_e \cdot (T_4 - T_3) \cdot \Delta_+ &&= 0 \\
C_5 \cdot \frac{dT_5}{dt} + &\quad F_e \cdot (T_5 - T_4) \cdot \Delta_+ &&= 0 \\
C_6 \cdot \frac{dT_6}{dt} + &\quad F_e \cdot (T_6 - T_5) \cdot \Delta_+ &&= 0 \\
C_{bot} \cdot \frac{dT_{bot}}{dt} + F_d T_{bot} + &\quad F_e(T_{bot} - T_6)\Delta_+ &&= F_d T_{ret}
\end{aligned}
\tag{132}
$$

$$
\mathbf{F} =
\begin{bmatrix}
F_e & 0 & 0 & 0 & 0 & 0 & 0 & -F_e \\
-F_e & F_e & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -F_e & F_e & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -F_e & F_e & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -F_e & F_e & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -F_e & F_e & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -F_e & F_e & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -F_e & F_e
\end{bmatrix}
\tag{133}
$$

If $\dot{m}_e = \dot{m}_{supply} - \dot{m}_{demand} < 0$, $\Delta_+ = 0$ and $\Delta_- = 1$.

$$
\begin{aligned}
C_{top} \cdot \frac{dT_{top}}{dt} + F_s T_{top} &\quad + F_e(T_1 - T_{top})\Delta_- = F_s T_{sup} \\
C_1 \cdot \frac{dT_1}{dt} &\quad + F_e(T_2 - T_1)\Delta_- = 0 \\
C_2 \cdot \frac{dT_2}{dt} &\quad + F_e(T_3 - T_2)\Delta_- = 0 \\
C_3 \cdot \frac{dT_3}{dt} &\quad + F_e(T_4 - T_3)\Delta_- = 0 \\
C_4 \cdot \frac{dT_4}{dt} &\quad + F_e(T_5 - T_4)\Delta_- = 0 \\
C_5 \cdot \frac{dT_5}{dt} &\quad + F_e(T_6 - T_5)\Delta_- = 0 \\
C_6 \cdot \frac{dT_6}{dt} &\quad + F_e(T_7 - T_6)\Delta_- = 0 \\
C_{bot} \cdot \frac{dT_{bot}}{dt} + F_d T_{bot} &\quad = F_d T_{ret}
\end{aligned}
\tag{134}
$$

$$\mathbf{F} = \begin{bmatrix} -F_e & F_e & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -F_e & F_e & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -F_e & F_e & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -F_e & F_e & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -F_e & F_e & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -F_e & F_e & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -F_e & F_e \\ F_e & 0 & 0 & 0 & 0 & 0 & 0 & -F_e \end{bmatrix} \tag{135}$$

Note that since $\dot{m}_e = \dot{m}_{supply} - \dot{m}_{demand} < 0$, the diagonal elements of th $\mathbf{F}$-matrix are positive, like in the case $\dot{m}_e > 0$

Derivation $\mathbf{F}$-matrices:

Directed supply flow: F_{supply} : [top 1 2 3 4 5 6 bottom top]

Directed demand flow: F_{demand} : [bottom 6 5 4 3 2 1 top bottom]

$$\mathbf{DF_{supply}} \cdot \boldsymbol{\theta} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix} \cdot \begin{bmatrix} T_{top} \\ T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_{bot} \end{bmatrix} \tag{136}$$

$$\mathbf{DF_{demand}} \cdot \boldsymbol{\theta} = \begin{bmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} T_{top} \\ T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_{bot} \end{bmatrix} \tag{137}$$

$$\mathbf{SF} = f_s \cdot \mathbf{DF_{supply}} + f_d \cdot \mathbf{DF_{demand}} = \begin{bmatrix} 0 & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s \\ \dot{f}_d - \dot{f}_s & 0 & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 & 0 \\ 0 & \dot{f}_d - \dot{f}_s & 0 & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 \\ 0 & 0 & \dot{f}_d - \dot{f}_s & 0 & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 \\ 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & 0 & \dot{f}_s - \dot{f}_d & 0 & 0 \\ 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & 0 & \dot{f}_s - \dot{f}_d & 0 \\ 0 & 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & 0 & \dot{f}_s - \dot{f}_d \\ \dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & 0 \end{bmatrix} \tag{138}$$

Since we want an $\mathbf{F}$-matrix on the left-hand side of the differential equations, the correct elements are obtained by taking the $\min(\mathbf{SF}, 0)$, here we mean for each element in $\mathbf{SF}$ we take the minimum of the respective element and 0. Thus, in the case $f_s > f_d$ the elements $\dot{f}_s - \dot{f}_d > 0$ are replaced by 0 and the elements $\dot{f}_d - \dot{f}_s < 0$ remain. The matrix $\min(\mathbf{SF}, 0)$ will become:

$$\min(\mathbf{SF}, 0) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s \\ \dot{f}_d - \dot{f}_s & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \dot{f}_d - \dot{f}_s & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \dot{f}_d - \dot{f}_s & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & 0 \end{bmatrix} \tag{139}$$

Now, the diagonal elements can be computed. The diagonal elements are equal to minus the sum of the off-diagonal elements in their respective row. For the matrix given in equation 142 this results in the flow matrix $\mathbf{F}$:

$$\mathbf{F} = \begin{bmatrix} -(\dot{f}_d - \dot{f}_s) & 0 & 0 & 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s \\ \dot{f}_d - \dot{f}_s & -(\dot{f}_d - \dot{f}_s) & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \dot{f}_d - \dot{f}_s & -(\dot{f}_d - \dot{f}_s) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \dot{f}_d - \dot{f}_s & -(\dot{f}_d - \dot{f}_s) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & -(\dot{f}_d - \dot{f}_s) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & -(\dot{f}_d - \dot{f}_s) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & -(\dot{f}_d - \dot{f}_s) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dot{f}_d - \dot{f}_s & -(\dot{f}_d - \dot{f}_s) \end{bmatrix} \tag{140}$$

If the supply and demand flows in the buffervessel are carried by the same liquid medium (water), a differential mass flow $\dot{m}_e = \dot{m}_{supply} - \dot{m}_{demand}$ can be defined, and $F_e = \dot{m}_e \cdot c_{p,w} = \dot{f}_s - \dot{f}_d$. The matrix $\mathbf{F}$ becomes:

$$
\mathbf{F} = \begin{bmatrix}
F_e & 0 & 0 & 0 & 0 & 0 & 0 & -F_e \\
-F_e & F_e & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -F_e & F_e & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -F_e & F_e & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -F_e & F_e & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -F_e & F_e & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -F_e & F_e & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -F_e & F_e
\end{bmatrix}
\tag{141}
$$

In the case $f_s < f_d$ the elements $\dot{f}_d - \dot{f}_s > 0$ are replaced by 0 and the elements $\dot{f}_s - \dot{f}_d < 0$ remain. The matrix $\min(\mathbf{SF}, 0)$ will become:

$$
\min(\mathbf{SF}, 0) = \begin{bmatrix}
0 & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \dot{f}_s - \dot{f}_d & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \dot{f}_s - \dot{f}_d & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \dot{f}_s - \dot{f}_d \\
\dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\tag{142}
$$

Now, the diagonal elements can be computed. The diagonal elements are equal to minus the sum of the off-diagonal elements in their respective row. For the matrix given in equation 142 this results in the flow matrix $\mathbf{F}$:

$$
\mathbf{F} = \begin{bmatrix}
-(\dot{f}_s - \dot{f}_d) & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -(\dot{f}_s - \dot{f}_d) & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -(\dot{f}_s - \dot{f}_d) & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -(\dot{f}_s - \dot{f}_d) & \dot{f}_s - \dot{f}_d & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -(\dot{f}_s - \dot{f}_d) & \dot{f}_s - \dot{f}_d & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -(\dot{f}_s - \dot{f}_d) & \dot{f}_s - \dot{f}_d & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -(\dot{f}_s - \dot{f}_d) & \dot{f}_s - \dot{f}_d \\
\dot{f}_s - \dot{f}_d & 0 & 0 & 0 & 0 & 0 & 0 & -(\dot{f}_s - \dot{f}_d)
\end{bmatrix}
\tag{143}
$$

If the supply and demand flows in the buffervessel are carried by the same liquid medium (water), a differential mass flow $\dot{m}_e = \dot{m}_{supply} - \dot{m}_{demand}$ can be defined, and $F_e = \dot{m}_e \cdot c_{p,w} = \dot{f}_s - \dot{f}_d$. The matrix $\mathbf{F}$ becomes:

$$
\mathbf{F} = \begin{bmatrix}
-F_e & F_e & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -F_e & F_e & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -F_e & F_e & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -F_e & F_e & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -F_e & F_e & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -F_e & F_e & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -F_e & F_e \\
F_e & 0 & 0 & 0 & 0 & 0 & 0 & -F_e
\end{bmatrix}
\tag{144}
$$

D   Documentation buffervessel MvdB

D.1   Introduction

This document describes the buffer vessel model that can be incorporated into the HAN dynamic house model.

List of symbols:

m mass [kg]

$\dot{m}$ mass flow [kg/s]

C_w Specific heat of water [J/kg]

T Temperature [C]

U Thermal transmittance [W/K]

A Area [m^2]

λ Heat conductivity [W/mK]

D.2   Model description

The model for the buffer vessel is derived from the paper of Rakesh Sinha et al. [36]

The model consists of a heating element, located outside of the buffer vessel, which can take water from the vessel and heat the water to a desired temperature.The hot water is then injected to the top of the buffer vessel.

Hot water is is taken from the top of the buffer vessel on the demand side. Cooled water coming from the load is returned tot the bottom of the vessel.

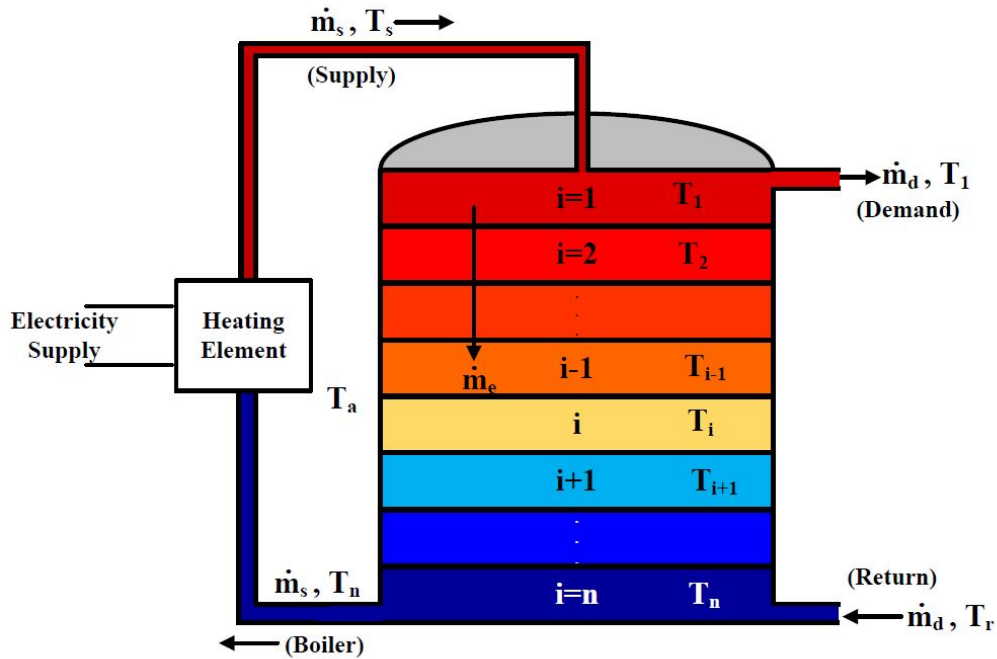A schematic description of the buffer vessel is shown below.

Figure 31: Buffer vessel representation

Due to the fact that the density of water decreases with temperature above 4 °C, different temperature layers are created.

In order to model this, the buffer vessel will be divided into N different sections

D.3 Mathematical description

For the top layer:

$$mC_w \frac{dT_1}{dt} = \dot{m}_s C_w (T_s - T_1) + \dot{m}_e C_w (T_1 - T_2) * sgn(-\dot{m}_e) - UA_s(T_1 - T_a) - \frac{A_q \lambda_w}{z}(T_1 - T_2) \qquad (145)$$

For the middle layers:

$$mC_w \frac{dT_i}{dt} = \dot{m}_e C_w (T_{i-1} - T_i) * sgn(\dot{m}_e) + \dot{m}_e C_w (T_i - T_{i+1}) * sgn(-\dot{m}_e) - UA_s(T_i - T_a) + \frac{A_q \lambda_w}{z}(T_{i-1} + T_{i+1} - 2T_i) \qquad (146)$$

For the bottom layer:

$$mC_w \frac{dT_n}{dt} = \dot{m}_d C_w (T_r - T_n) + \dot{m}_e C_w (T_{n-1} - T_n) * sgn(\dot{m}_e) - UA_s(T_n + T_a) + \frac{A_q \lambda_w}{z}(T_{n-1} - T_n) \qquad (147)$$

D.4 Validation

To check to model from the paper, the following parameters are used:

Parameters	Definition	Value	Units
V	storage volume	200	[m^3]
n	number of stratified layers in storage tank	10	-
λ_w	effective heat conductivity of water	0.644	[W/mK]
U	heat transfer coeff. of the storage walls	0.12	[W/m^{2}K]
x	diameter to height ratio of storage	2.24	-
T_a	ambient Temperature	10	[°C]
x T_s	supply Temperature	80	[°C]
T_r	return Temperature	40	[°C]
P_b	Rated Power of EB	2.4	[MW]
C_w	specific heat capacity of water	4190	[J/kg·K]

Figure 32: Buffer vessel parameters

This results in the following graph:
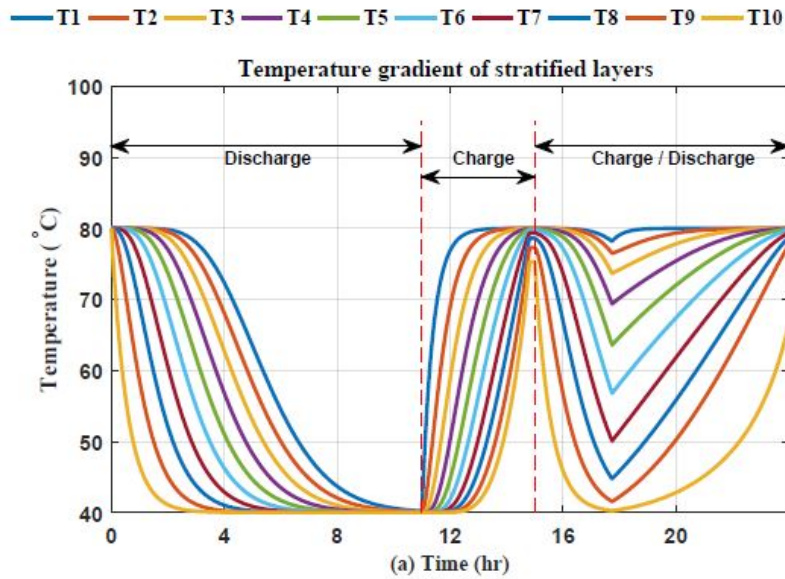
(a) paper results
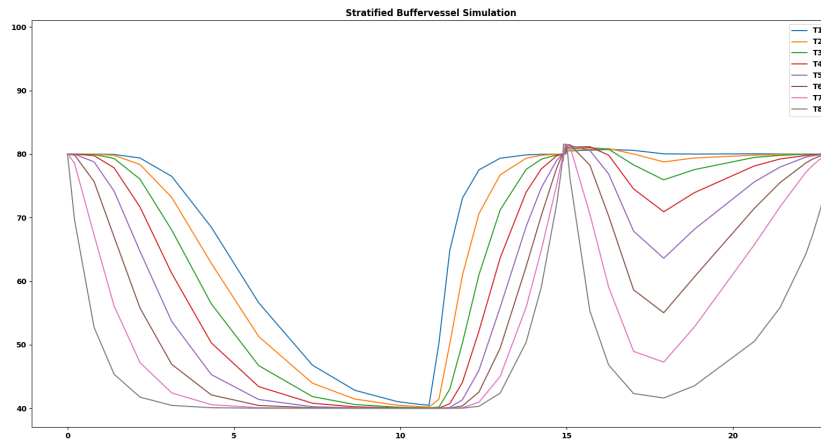
(b) Python results

Figure 33: Comparison between paper and python model

E 2 Zones house model 7R4C network

The 4R-7C house model structure is implemented as described below:
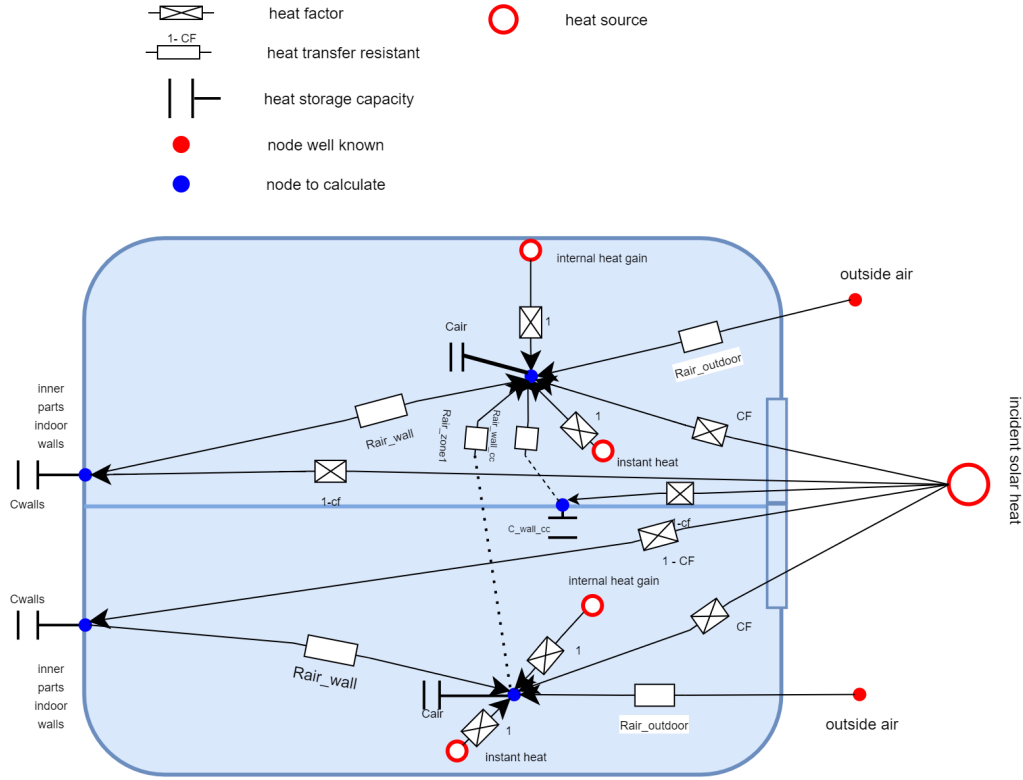

Figure 34: Schematic of a 2 zones house model

The equivalent electrical 7R-4C network with components and topology is given in Fig. 35.
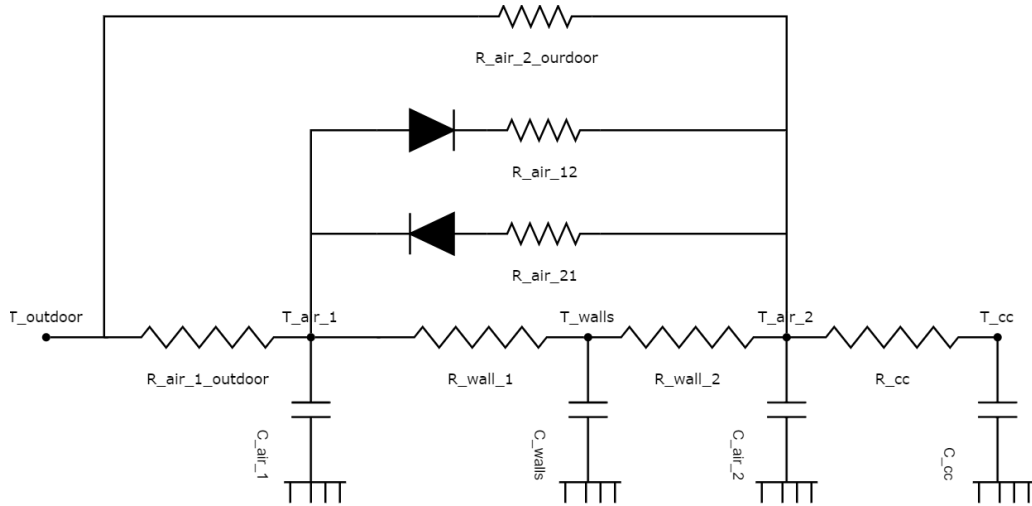

Figure 35: R-C circuits of 2 zones house model

with:

- `T_outdoor` : outdoor temperature $[°C]$

- `T_air_1` : zone 1 air temperature $[°C]$

- `T_walls` : wall temperature $[°C]$

- `T_air_2` : zone 2 air temperature $[°C]$

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- `T_cc` : temperature of the concrete layer between zone 1 and zone 2 $[°C]$

- `R_air_1_outdoor` : outdoor resistance valus.

- `R_wall_1` : walls resistance value.

- `R_wall_2` : walls resistance value.

- `R_cc` : concrete resistance value.

- `R_air_12` : resistance value of air flow from zone 1 to zone 2.

- `R_air_21` : resistance value of air flow from zone 2 to zone 1.

F Finite-element discretization

F.1 Heat pump discretization

Het algemene model van de warmtepomp en airco wordt afgeleid met behulp van het volgende geschematiseerde black box model:

F.2 Buffer vessel discretization

Als voorbeeld van een model met warmtestromen en warmtediffusie wordt het volgende model van een buffervat beschouwd:
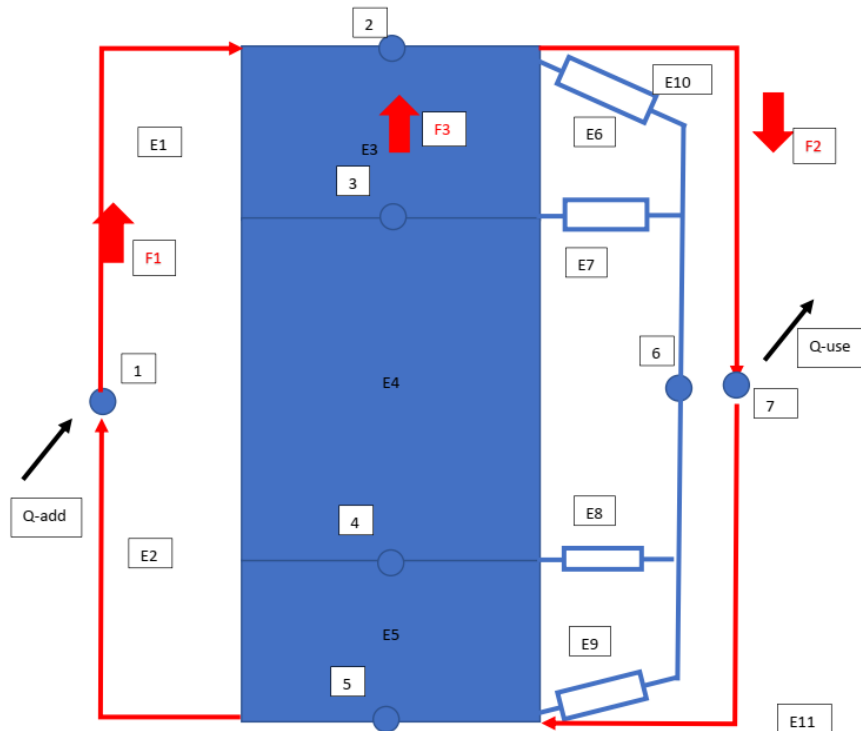

Figure 36: Finite-element buffer vessel

Dit is een buffervat in een verwarmingsinstallatie.

Voor het modelleren hiervan wordt gebruik gemaakt van een tweetal universele elementen:

1. Exchange element. Dit element beschrijft warmtetransportt via een vloeistofstroom F door het element en warmtetransport door geleiding. Het element kan een warmtecapaciteit hebben.

2. Een puntbron. Deze bron beschrijft warmteontwikkeling of warmte-onttrekking in een punt.

Het vat is verdeeld in 3 niveaus over de hoogte:

1. Bovenzijde vat (element 3)

2. Midden vat(element 4)

3. Onderzijde vat (element 5)

In het vat is sprake van:

- Warmteverlies naar andere temperatuurniveau 's en naar de omgeving. De omgevingstemperatuur in dit model is gegeven door de temperatuur in punt 7. De elementen die het volume van het vat beschrijven (E3,E4 en E5) wisselen warmte uit naar elkaar en naar punt 6.

- Warmtetransport door waterstromen. In waterstromen buiten het vat wordt warmte onttrokken of toegevoegd. In het vat is een waterstroom die zorgt voor het kortsluiten van de kringlopen.

Deze beide mechanismen worden meegenomen in het model.

Er wordt verondersteld dat gebruik wordt gemaakt van gelaagdheid. Boven in het vat heerst een hogere temperatuur dan onderin het vat. Daarnaast is er sprake van een tweetal leidingen waarin warmte wordt uitgewisseld met de omgeving:

- Een leiding waarin warmte wordt toegevoegd aan het vat $\dot{Q}_{add}$. Deze leiding neemt vloeistof (water) onder uit het vat (punt 5), verhoogt de temperatuur door warmte-inbreng (punt 1) en brengt het water boven in het vat weer in. Deze leiding bestaat uit de elementen E1 (boven) en E2 (onder). In deze leiding is een vloeistofstroom $F_1(kJ/(Ks))$ aanwezig die de warmte transporteert.

- Een leiding waarin warmte wordt onttrokken aan het vat $\dot{Q}_{use}$. Deze leiding neemt vloeistof (water) boven uit het vat (punt 2), verlaagt de temperatuur door warmteonttrekking (punt 7) en brengt het water boven in het vat weer in. Deze leiding bestaat uit de elementen E10 (boven) en E11 (onder). In deze leiding is een vloeistofstroom $F_2(kJ/(Ks))$ aanwezig die de warmte transporteert.

F.3   Matrixvergelijking

Voor het oplossen van de temperatuurverdeling wordt per knooppunt een energiebalans opgesteld. Deze energiebalans resulteert in een matrixvergelijking.

$$\mathbf{K}\theta + \mathbf{C}\dot{\theta} = \dot{\mathbf{q}} \tag{148}$$

K: de warmtegeleidingsmatrix (W/K) C: de warmtecapaciteitsmatrix (J/K) θ: de temperatuursvector (K) $\dot{\theta}$: de tijdsafgeleide van de temperatuursvector (K/s) $\dot{q}$: de vector met thermische brontermen (W)

F.4   Elementen in de stroming

Om te komen tot het matrixmodel wordt begonnen met één exchange element zoals hierboven geïntroduceerd (E1,E2,E3,E4,E5,E10,E11). Dit element bevat 2 knooppunten. De volgende veronderstellingen worden gedaan:

- Het element bevat 2 knooppunten waarmee deze verbonden is met de omgeving. De nummering bedraagt: n_1 en n_2.

- Binnen het element heerst een lineair verlopende temperatuur, van knooppunt naar knooppunt.

- Binnen het element is een vloeistofstroom F die zorgt voor additioneel warmtetransport. De stroomrichting is van knooppunt 1 naar knooppunt 2.

- De warmtecapaciteit van het element wordt evenredig verdeeld over de knooppunten.

De warmtestroom vanuit het element naar knoopunten 1 en 2 moet in balans zijn met de andere warmtestromen en de warmtegeneratie in de betreffende knooppunten.
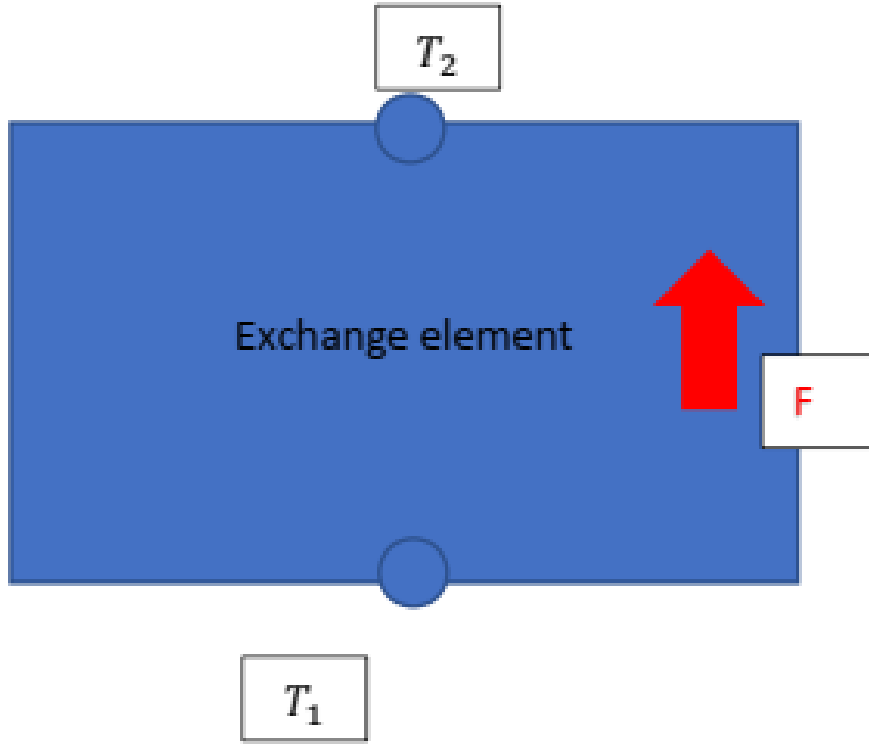
Figure 37: Exchange element buffer vessel

Voor de warmtestromen vanaf knooppunt 1 geldt:

$$(T_1 - T_2) \cdot \frac{1}{R_e} + C_{e1,1} \cdot \frac{dT_1}{dT} = \dot{Q}_{ext,1} \tag{149}$$

T_1: temperatuur in knooppunt 1

T_2: temperatuur in knooppunt 2

R_e: warmteweerstand voor geleiding tussen knooppunt 1 en 2

$C_{e1,1}$: warmtecapaciteit in knooppunt 1 van element 1

$\frac{dT_1}{dT}$: temperatuursverandering in de tijd in knooppunt 1

$\dot{Q}_{ext,1}$: externe warmtetoevoer in knooppunt 1

De vloeistofstroom F vanuit knooppunt T_1 heeft dezelfde temperatuur als T_1 en heeft dus geen invloed op de temperatuur in T_1.

Voor de warmtestromen vanaf punt 2 geldt:

$$(T_2 - T_1) \cdot \frac{1}{R_e} + F \cdot (T_2 - T_1) + C_{e1,2} \cdot \frac{dT_2}{dT} = \dot{Q}_{ext,2} \tag{150}$$

$C_{e1,2}$: warmtecapaciteit in knooppunt 2 van element 1

$\frac{dT_2}{dT}$: temperatuursverandering in de tijd in knooppunt 2

$\dot{Q}_{ext,2}$: externe warmtetoevoer in knooppunt 2

In matrixnotatie:

$$\begin{bmatrix} 1/R_e & -1/R_e \\ -1/R_e - F & 1/R_e + F \end{bmatrix} \cdot \begin{bmatrix} T_1 \\ T_2 \end{bmatrix} + \begin{bmatrix} C_{e1,1} & 0 \\ 0 & C_{e1,2} \end{bmatrix} \cdot \begin{bmatrix} \frac{dT_1}{dt} \\ \frac{dT_2}{dt} \end{bmatrix} = \begin{bmatrix} \dot{Q}_{ext,1} \\ \dot{Q}_{ext,2} \end{bmatrix} \tag{151}$$

Merk op dat door de aanwezigheid van een vloeistofstroom F, de geleidingsmatrix niet langer symmetrisch is.

Daarnaast wordt gebruik gemaakt van elementen die alleen een warmteweerstand weergeven. Deze elementen (E6,E7,E8 en E9) kunnen worden gerepresenteerd met de volgende matrixvergelijking

$$\begin{bmatrix} 1/R_e & -1/R_e \\ -1/R_e & 1/R_e \end{bmatrix} \cdot \begin{bmatrix} T_1 \\ T_2 \end{bmatrix} = \begin{bmatrix} \dot{Q}_{ext,1} \\ \dot{Q}_{ext,2} \end{bmatrix} \tag{152}$$

F.5   Systemmmatrices van het buffervat

Er wordt nu een systeemmatrix opgesteld voor het schematisch weergegeven model. Deze systeemmatrix wordt opgebouwd uit de verschillende elementmatrices. De noodzakelijke rang van deze systeemmatrix is het aantal knooppunten in het warmtestroomschema minus het aantal voorgeschreven knooppunten in dit schema. Er zijn 7 knooppunten in het model. In dit geval wordt in punt 6 de temperatuur voorgeschreven. Er resteren dan 6 onafhankelijke vrijheidsgraden.

F.5.1   Capaciteitsmatrix C

There are 7 nodes in the system. The heat capacities are:

$$\begin{aligned}
\text{node 1} \quad & C_{e1,1} + C_{e2,2} = 0.5 \cdot (C_{e1} + C_{e2}) \\
\text{node 2} \quad & C_{e1,2} + C_{e3,1} + C_{e10,2} + C_{e6,2} = 0.5 \cdot (C_{e1} + C_{e3} + C_{e10} + C_{e6}) \\
\text{node 3} \quad & C_{e3,2} + C_{e4,1} + C_{e7,2} = 0.5 \cdot (C_{e3} + C_{e4} + C_{e7}) \\
\text{node 4} \quad & C_{e4,2} + C_{e5,1} + C_{e8,2} = 0.5 \cdot (C_{e4} + C_{e5} + C_{e8}) \\
\text{node 5} \quad & C_{e5,2} + C_{e2,1} + C_{e9,2} + C_{11,2} = 0.5 \cdot (C_{e5} + C_{e2} + C_{e9} + C_{11}) \\
\text{node 6} \quad & C_{e6,1} + C_{e7,1} + C_{e8,1} + C_{e9,1} = 0.5 \cdot (C_{e6} + C_{e7} + C_{e8} + C_{e9}) \\
\text{node 7} \quad & C_{e10,2} + C_{e11,1} = 0.5 \cdot (C_{e10} + C_{e11})
\end{aligned} \tag{153}$$

$$0.5 \cdot \begin{bmatrix} C_{e1}+C_{e2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & C_{e1}+C_{e3}+C_{e10}+C_{e6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & C_{e3}+C_{e4}+C_{e7} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{e4}+C_{e5}+C_{e8} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{e5}+C_{e2}+C_{e9}+C_{e11} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{e6}+C_{e7}+C_{e8}+C_{e9} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & C_{e10}+C_{e11} \end{bmatrix}$$

The heat capacities of element E1, E2, E10 and E11 (pipelines) are very small and can be approximated to be zero. Also, the elements E6, E7, E8 and E9 are thermal leaks, connected to node 6, which may be a boundary condition.

The capacity matrix thus reduces to:

$$0.5 \cdot \begin{bmatrix} \approx 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & C_{e3} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & C_{e3}+C_{e4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{e4}+C_{e5} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{e5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \approx 0 \end{bmatrix}$$

In the approximation above, the buffer vessel system is not solvable, without adding some heat capacity to nodes N1 and N7. *e.g.* these nodes must be coupled with a house model element with finite heat capacity.

In any case, the node N6 (boundary condition) does not contribute a DOF to the system of equations. Row 6 and column 6 will be removed from the set of equations.

Listing 12: Generation of capacity matrix

```python
    A = nx.adjacency_matrix(G, nodelist=list(range(G.order())))
    B = A.toarray()
    # print(B, "\n")

    row_sums = np.sum(B, axis=1).tolist()
    C_matrix = np.diag(np.array(row_sums), k=0)
    return C_matrix


def K_from_elements(df: pd.DataFrame):
    """assemble K-matrix from Dataframe

    Args:
        df: Dataframe from Excel spreadsheet (float)]

    Returns:
        K_matrix (ndarray):  2D matrix with conductances in network
    """
    # convert Dataframe into list of spreadsheet rows, called "rows"
    # rows becomes a list of lists
    rows = []
    for row in range(len(df.index)):
        rows.append(df.iloc[row].values.tolist())

    # extract element 4: and element 2 of each row into "nodelists"
    nodelists = []
    for row in rows:
        nodelist = [x for x in row[4:] if np.isnan(x) == False]
        nodelist.append(row[3])
        nodelists.append(nodelist)

    # nodelists is a list [node, node, weight], suitable for networkx
    G = nx.Graph()
    G.add_weighted_edges_from(nodelists)
```

F.5.2 q̇-vector

De vector $\dot{\mathbf{q}}$ wordt gegeven door:

$$
\begin{pmatrix}
1 & 1 & \dot{q}_1 = \dot{Q}_{add} \\
2 & 2 & \dot{q}_2 \\
3 & 3 & \dot{q}_3 \\
4 & 4 & \dot{q}_4 \\
5 & 5 & \dot{q}_5 \\
6 & 6 & \dot{q}_6 \\
7 & 7 & \dot{q}_7 = -\dot{Q}_{use}
\end{pmatrix}
$$

$$
\begin{pmatrix}
1 & 2 & 3 \\
4 & 5 & 9
\end{pmatrix}
$$

In nodes N1 and N7 an external een heat source / heat sink is contributing to the power balance.

Het voorgeschreven knooppunt (randvoorwaarde, boundary condition) 6 is verbonden aan knooppunten 2, 3, 4 en 5. Dit zijn de ook de vrijheidsgraden 2, 3, 4 en 5. Vrijheidsgraden worden aangegeven met DOF (degree of freedom). In de overeenkomstige knooppunten wordt de capaciteits? stiffness matrix $\mathbf{K}$ en de bronvector (load vector) $\dot{\mathbf{q}}$ aangepast.De aanpassing van de K-matrix wordt verderop toegelicht. De bronvector wordt als volgt aangepast:

$$
\begin{bmatrix}
1 & 1 & \dot{Q}_{add} \\
2 & 2 & 0 - \frac{1}{R_{2,6}} \\
3 & 3 & 0 - \frac{1}{R_{3,6}} \\
4 & 4 & 0 - \frac{1}{R_{4,6}} \\
5 & 5 & 0 - \frac{1}{R_{5,6}} \\
6 & 7 & -\dot{Q}_{use}
\end{bmatrix}
$$

F.5.3   Geleidingsmatrix K

elements with heat capacity must have two nodes: E3, E4, E5

elements without heat capacity have two nodes as well: E1, E2, E6, E7, E8, E9, E10, E11

elements without heat conduction: E1, E2, E10, E11

elements with heat conduction: E3, E4, E5, E6, E7, E8, E9

elements with heat convection (flow): E1, E2, E3, E4, E5, E10, E11

The "conduction" matrix is equivalent to the stiffness matrix in a mechanical FE analysis. In terms of the thermal system topology this matrix contains the "edges" between the nodes. The matrix is setup as a 7 x 7 square zero matrix with the nodes as DOF.

$$
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\tag{154}
$$

The conductive elements in the system are:

$$
\begin{aligned}
\frac{1}{R_{2,3}} &= \frac{1}{R_{e3}} \\
\frac{1}{R_{3,4}} &= \frac{1}{R_{e4}} \\
\frac{1}{R_{4,5}} &= \frac{1}{R_{e5}} \\
\frac{1}{R_{2,6}} &\quad \frac{1}{R_{3,6}} \quad \frac{1}{R_{4,6}} \quad \frac{1}{R_{5,6}}
\end{aligned}
\tag{155}
$$

The conductive element $\frac{1}{R_{12}} = \frac{1}{R_{e1}} = 0$. This means $R_{12} \to \infty$. We assume, the pipeline is perfectly insulated and creates no heat leak. Thermal energy flowing *through* it is completely delivered to the target node. Likewise, this holds for the elements E2, E10 and E11.

$$
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{-1}{R_{2,3}} & 0 & 0 & \frac{-1}{R_{2,6}} & 0 \\
0 & \frac{-1}{R_{2,3}} & 0 & \frac{-1}{R_{3,4}} & 0 & \frac{-1}{R_{3,6}} & 0 \\
0 & 0 & \frac{-1}{R_{3,4}} & 0 & \frac{-1}{R_{4,5}} & \frac{-1}{R_{4,6}} & 0 \\
0 & 0 & 0 & \frac{-1}{R_{4,5}} & 0 & \frac{-1}{R_{5,6}} & 0 \\
0 & \frac{-1}{R_{2,6}} & \frac{-1}{R_{3,6}} & \frac{-1}{R_{4,6}} & \frac{-1}{R_{5,6}} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\tag{156}
$$

$$
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{R_{2,3}} + \frac{1}{R_{2,6}} & \frac{-1}{R_{2,3}} & 0 & 0 & \frac{-1}{R_{2,6}} & 0 \\
0 & \frac{-1}{R_{2,3}} & \frac{1}{R_{2,3}} + \frac{1}{R_{3,4}} + \frac{1}{R_{3,6}} & \frac{-1}{R_{3,4}} & 0 & \frac{-1}{R_{3,6}} & 0 \\
0 & 0 & \frac{-1}{R_{3,4}} & \frac{1}{R_{3,4}} + \frac{1}{R_{4,5}} + \frac{1}{R_{4,6}} & \frac{-1}{R_{4,5}} & \frac{-1}{R_{4,6}} & 0 \\
0 & 0 & 0 & \frac{-1}{R_{4,5}} & \frac{1}{R_{4,5}} + \frac{1}{R_{5,6}} & \frac{-1}{R_{5,6}} & 0 \\
0 & \frac{-1}{R_{2,6}} & \frac{-1}{R_{3,6}} & \frac{-1}{R_{4,6}} & \frac{-1}{R_{5,6}} & \frac{1}{R_{2,6}} + \frac{1}{R_{3,6}} + \frac{1}{R_{4,6}} + \frac{1}{R_{5,6}} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\tag{157}
$$

If node N6 is a boundary condition *i.e.* T_6 is given as a constant. The corresponding row in the $\mathbf{K}$ and $\mathbf{C}$ matrices can be removed. For the nodes that are connected to node N6 (row 2, 3, 4 and 5) the thermal connection can be moved to the $\dot{\mathbf{q}}$ vector. This can be seen by writing down the differential equation for node N2:

$$
0.5\,C_{e3} \cdot \frac{dT_2}{dt} = \frac{1}{R_{2,3}}(T_3 - T_2) + \frac{1}{R_{2,6}}(T_6 - T_2) = (-\frac{1}{R_{2,3}} - \frac{1}{R_{2,6}}) \cdot T_2 + \frac{1}{R_{2,3}} \cdot T_3 + \frac{1}{R_{2,6}} \cdot T_6
\tag{158}
$$

$$
\begin{array}{ccccc}
\mathbf{K}\theta & + & \mathbf{C}\dot{\theta} = & & \dot{\mathbf{q}} \\[6pt]
(\frac{1}{R_{2,3}} + \frac{1}{R_{2,6}}) \cdot T_2 - \frac{1}{R_{2,3}} \cdot T_3 + & & 0.5\,C_{e3} \cdot \frac{dT_2}{dt} = & & \frac{1}{R_{2,6}} \cdot T_6
\end{array}
\tag{159}
$$

Note: the sum of each row in $\mathbf{K}$ is not *zero* anymore, but equals the corresponding vector element in $\dot{\mathbf{q}}$.

This reduces the matrices to:

$$\mathbf{C} = 0.5 \cdot \begin{bmatrix} \approx 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & C_{e3} & 0 & 0 & 0 & 0 \\ 0 & 0 & C_{e3} + C_{e4} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{e4} + C_{e5} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{e5} & 0 \\ 0 & 0 & 0 & 0 & 0 & \approx 0 \end{bmatrix}$$

$$\mathbf{K} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{R_{2,3}} + \frac{1}{R_{2,6}} & \frac{-1}{R_{2,3}} & 0 & 0 & 0 \\ 0 & \frac{-1}{R_{2,3}} & \frac{1}{R_{2,3}} + \frac{1}{R_{3,4}} + \frac{1}{R_{3,6}} & \frac{-1}{R_{3,4}} & 0 & 0 \\ 0 & 0 & \frac{-1}{R_{3,4}} & \frac{1}{R_{3,4}} + \frac{1}{R_{4,5}} + \frac{1}{R_{4,6}} & \frac{-1}{R_{4,5}} & 0 \\ 0 & 0 & 0 & \frac{-1}{R_{4,5}} & \frac{1}{R_{4,5}} + \frac{1}{R_{5,6}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{160}$$

$$\dot{\mathbf{q}} = \begin{bmatrix} \dot{Q}_{add} \\ \frac{1}{R_{2,6}} \cdot T_6 \\ \frac{1}{R_{3,6}} \cdot T_6 \\ \frac{1}{R_{4,6}} \cdot T_6 \\ \frac{1}{R_{5,6}} \cdot T_6 \\ -\dot{Q}_{use} \end{bmatrix}$$

Listing 13: Generation of stiffness matrix

```python
    A = nx.adjacency_matrix(G, nodelist=list(range(G.order())))
    B = A.toarray()
    # print(B, "\n")

    row_sums = np.sum(B, axis=1).tolist()
    K_matrix = B - np.diag(np.array(row_sums), k=0)
    return K_matrix


def flowlist_to_edges(fl: list):
    # fl = list(range(10))
    # el = [[fl[i], fl[i+1]] for i in range(len(fl)-1)]
    # el2 = [[i, j] for i, j in zip(fl[:-1], fl[1:])]
    el3 = [[i, j] for i, j in zip(fl, fl[1:])]
    # print(el3)
    return el3


def flow_to_F_matrix(flowlist: list, rank: int):
    """

    Args:
        flowlist: list of lists! hence flatten  why?
        rank:
```

nodes: E1 has 1 and 2

E2 has 1 and 5

E3 has 2 and 3

E4 has 3 and 4

E5 has 4 and 5

E6 has 2 and 6

E7 has 3 and 6
E8 has 4 and 6
E9 has 5 and 6
E10 has 2 and 7
E11 has 5 and 7

edges conductivity R and convection F:

1 and 2
1 and 5
2 and 3
3 and 4
4 and 5
2 and 6
3 and 6
4 and 6
5 and 6
2 and 7
5 and 7

F.6 Water flow heat transfer

In the buffer vessel model, cf. Figure 36, two water flows run through the system. The first, labeled with $F1$, draws cold water from the bottom layer of the tank. This water is heated up in node 1. In the figure this is done using the external heat flow Q_{add}, but in a full system model another model component, for example a heat pump, can be connected here. (*Note*: In order to be able to add heat in a sensible way to the system node 1 has to have some heat capacity. The approximation done above making the capacity of the pipes zero is then not valid.) The heated water flows back into the vessel in the top level. The water flow $F1$ outside the vessel, induces an equal sized flow of water in side the vessel from the top layer towards the bottom, through the elements $E3$, $E4$ and $E5$.

The second water flow $F2$ draws water from the hot top layer. In node 7 a heat flow Q_{use} is extracted. Here, similar to node 1, another model component (for example a radiator) may be connected. (*Note*: the note made for node 1 is valid here is well). The cooled water will flow back into the vessel in the bottom layer. F2 induces a flow in the buffer vessel opposite to $F1$, running though $E5$, $E4$ and $E3$, consecutively.

The water flows will be controlled by pumps, either by a on/off manner (switching between a fixed water volume per second and 0) or a more advanced varying flow rate. Since $F1$ and $F2$ can be controlled separately, the flow in the vessel, labeled with $F3$ can run either direction, from bottom to top, or from top to bottom. The size of the flow $F3$ is given by: $F3 = F1 - F2$. When $F3$ is positive it flows from top to bottom in the vessel. A negative value, implies a water flow from bottom to top.

F.6.1 Setting up the flow matrix

As indicated earlier, the flow rates can be controlled, and thus may change over time. This means that the terms for the heat exchange due to the water flows need to be generated at each time step, or at least after each change in the flow rates. A matrix that represents the flows may be generated in the following process.

- First of all, the flows in the system need to be defined in the input file. For each flow we need to know the order it traverses the elements in the system, and more specifically the nodes it passes. This can be done by considering each flow separately, and listing the nodes you pass in the direction of the flow. For $F1$

this gives Nodes_{F1} $[0, 1, 2, 3, 4, 0]$, and for $F2$ this gives Nodes_{F2} $[6, 4, 3, 2, 1, 6]$. (note the labeling of the nodes used here is the number in Figure 36 minus one.) In the list the first element is equal to the last element, which shows that the flow is a closed loop. The depicted flow $F3$ is only the difference between $F1$ and $F2$, and does not need to be defined by itself.

- From the ordered list of nodes, we can create a "'directed-flow-matrix"' ($\mathbf{DF}$) for each flow. This matrix should be of the same size as the conductance-matrix ($\mathbf{K}$) and the capacity-matrix ($\mathbf{C}$). The directed-flow-matrix contains a 1 for each matrix-element that corresponds to a connection between nodes in the direction of the flow, and -1 for a connection between nodes in the opposite direction. Thus for flows $F1$ and $F2$ the matrix will be:

$$\mathbf{DF_{F1}} = \begin{bmatrix} 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{161}$$

$$\mathbf{DF_{F2}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \tag{162}$$

These matrices can be build up from the list as defined in the previous step, by looping through the list and taking the elements $\text{Nodes}(i, i+1)$, and filling in a one at the matrix element $(\text{Node}(i), \text{Node}(i+1))$. After looping through all these pairs we have filled in all connections in the direction of the flow, $\mathbf{DF^{+1}}$. The connections against the flow, $\mathbf{DF^{-1}}$, are given by: $\mathbf{DF^{-1}} = -1 \cdot (\mathbf{DF^{+1}})^T$. Finally, $\mathbf{DF} = \mathbf{DF^{+1}} + \mathbf{DF^{-1}}$.

- In each time step, when the flow sizes have been determined by the control algorithms, each directed-flow-matrix is multiplied by its respected flow size in $[\frac{m^3}{s}]$. All resulting matrices can then be added together. Assuming a flow of size f_1 and f_2 for the flows $F1$ and $F2$, respectively we now get the matrix $\mathbf{SF}$:

$$\mathbf{SF} = f_1 \cdot \mathbf{DF_{F1}} + f_2 \cdot \mathbf{DF_{F2}} = \begin{bmatrix} 0 & f_1 & 0 & 0 & -f_1 & 0 & 0 \\ -f_1 & 0 & f_1 - f_2 & 0 & 0 & 0 & f_2 \\ 0 & f_2 - f_1 & 0 & f_1 - f_2 & 0 & 0 & 0 \\ 0 & 0 & f_2 - f_1 & 0 & f_1 - f_2 & 0 & 0 \\ f_1 & 0 & 0 & f_2 - f_1 & 0 & 0 & -f_2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -f_2 & 0 & 0 & f_2 & 0 & 0 \end{bmatrix} \tag{163}$$

- The heat transfer induced by the flows is only in the direction of the water flow. The correct elements are obtained by taking the $\min(\mathbf{SF}, 0)$, here we mean for each element in $\mathbf{SF}$ we take the minimum of the

respective element and 0. Thus, in the case $f_1 > f_2$ the matrix $\mathbf{SF}$ will become:

$$
\min(\mathbf{SF}, 0) = \begin{bmatrix}
0 & 0 & 0 & 0 & -f_1 & 0 & 0 \\
-f_1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & f_2 - f_1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & f_2 - f_1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & f_2 - f_1 & 0 & 0 & -f_2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -f_2 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\tag{164}
$$

- Now, the diagonal elements can be computed. The diagonal elements are equal to minus the sum of the of diagonal elements in its respective row. For the matrix given in equation 164 this results in the flow matrix $\mathbf{F}$:

$$
\mathbf{F} = \begin{bmatrix}
f_1 & 0 & 0 & 0 & -f_1 & 0 & 0 \\
-f_1 & f_1 & 0 & 0 & 0 & 0 & 0 \\
0 & f_2 - f_1 & -(f_2 - f_1) & 0 & 0 & 0 & 0 \\
0 & 0 & f_2 - f_1 & -(f_2 - f_1) & 0 & 0 & 0 \\
0 & 0 & 0 & f_2 - f_1 & f_1 & 0 & -f_2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -f_2 & 0 & 0 & 0 & 0 & f_2
\end{bmatrix}
\tag{165}
$$

- Finally, we need to multiply the resulting flow matrix with the density (ρ_{water}) and the specific heat ($c_{p,water}$), in order to obtain the heat transferred by the water due to the water flows. The resulting matrix can be added to the K matrix as given in equation 160.

$$
v_{pump} \cdot A_{pipe} \cdot \rho_{water} \cdot c_{p,water} = \qquad \left[\frac{m}{s} \cdot m^2 \cdot \frac{kg}{m^3} \cdot \frac{J}{kg \cdot K} = \frac{J}{K \cdot s} = \frac{W}{K} \right]
\tag{166}
$$

Note 1, when the system contains flows of different fluids, the described steps need to be followed for each fluid type separately. Each fluid will have its own matrix which will contribute to the overall system. This also implies the need to define the density and specific heat for each flow.

Note 2, at this moment the process does not deal with splitting and merging of the water flows. Therefore, a system that may control valves to distribute the water over different radiators using one supply pipe, and one pump, is not feasible in this concept, yet.

F.7 House model (2R2C-model) in finite element structure

Although the equations of the house model as presented in Section ?? have a very similar structure, one should not mix the lumped-element approach presented in Section ?? with the finite-element approach of this chapter. Therefore, we revisit the 2R2C-model in order to incorporate the house model in the finite-element approach.

Recall that, in the lumped-element model, the 2R2C model contained two connected elements with a heat capacity, one for the air in the house and one for the building structure. In the lumped element model these heat capacities cold be directly modeled with one capacitor for the air and one for the walls. The heat transfer between the two capacities was modeled with a single heat conductor (resistor). Finally, the air could exchange heat with the node fro the ambient temperature, which has a fixed temperature. This resulted in the model as presented in Figure 38.
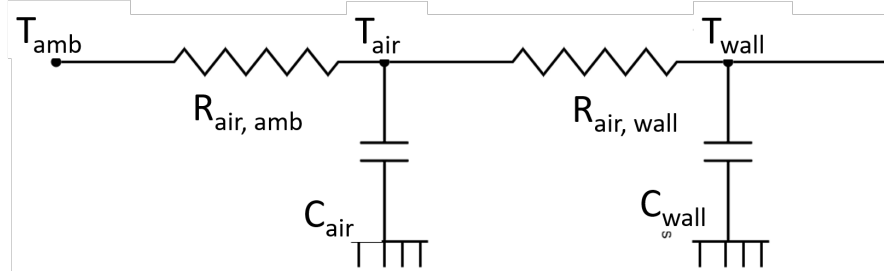
Figure 38: 2R-2C house model revisited

When we want to model this same concept in the finite-element structure, we need four elements: one element that represents the air, one that represents the walls, one element for the interaction between the air and the wall, and one element for the interaction between the air and the ambient surroundings. The model is sketched in Figure **??**.
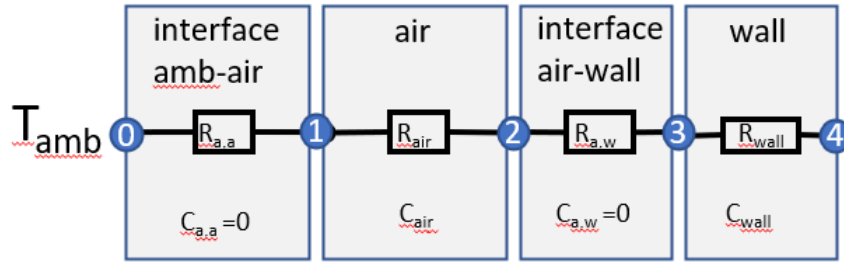

Figure 39: Finite element representation of the 2R2C house model

In this model the heat capacity of the air will be divided over the nodes 1 and 2, with $0.5 \cdot C_{air}$ for each node. In the same manner, the heat capacity of the wall will be divided over the nodes 3 and 4. The elements that are needed for the heat exchange between air and wall, and air and ambient surroundings do not have any heat capacity.

In the lumped-element model the air and wall were considered to have a homogeneous temperature. This is no longer the case in the finite element model. Theoretically, one could make the heat resistance within the air and wall elements zero, which would lead to an instantaneous heat transfer between the nodes 1 and 2, and 3 and 4, respectively. Thus resulting in an equal temperature for nodes 1 and 2, and 3 and 4. However, computationally this will lead to problems, since the corresponding **K** matrix will have $\frac{1}{R} = \infty$ entries in the representative positions. Therefore, in practice, an internal heat resistance has to be applied in the air and wall elements. Thus, resulting in a gradient within the elements.

The **C** and **K** matrices of the system will be:

$$
\mathbf{C} = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0.5 \cdot C_{air} & 0 & 0 & 0 \\
0 & 0 & 0.5 \cdot C_{air} & 0 & 0 \\
0 & 0 & 0 & 0.5 \cdot C_{wall} & 0 \\
0 & 0 & 0 & 0 & 0.5 \cdot C_{wall}
\end{bmatrix}
$$

$$
\mathbf{K} = \begin{bmatrix}
\frac{1}{R_{a,a}} & -\frac{1}{R_{a,a}} & 0 & 0 & 0 \\
-\frac{1}{R_{a,a}} & \frac{1}{R_{a,a}} + \frac{1}{R_{air}} & -\frac{1}{R_{air}} & 0 & 0 \\
0 & -\frac{1}{R_{air}} & \frac{1}{R_{air}} + \frac{1}{R_{a,w}} & -\frac{1}{R_{a,w}} & 0 \\
0 & 0 & -\frac{1}{R_{a,w}} & \frac{1}{R_{a,w}} + \frac{1}{R_{wall}} & -\frac{1}{R_{wall}} \\
0 & 0 & 0 & -\frac{1}{R_{wall}} & \frac{1}{R_{wall}}
\end{bmatrix}
$$

(167)

G   NEN and ISO

The list of NEN and ISO standard used in the calculation:

- NTA 8800
- NEN 1068
- ISO 6946
- ISO 10077-2
- NEN 7120