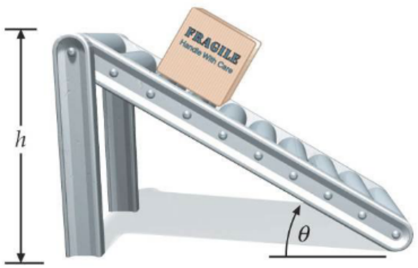
SW 1: Introduction

Model's three properties

- **Mapping**: models act as a representation of natural or artificial originals and can be models in turn;
- **Reduction**: models function as abstraction. They do not capture every attribute of the original; instead, they isolate and retain only those attributes relevant to the specific objective, intentionally omitting detail to manage complexity and focus on the problem at hand;
- **Pragmatic**: models function as utilitarian substitutes. They do not replace the original universally but serve as a representative for a specific user (subject), within a defined time frame, and for a particular purpose or operation.

Example



- **Generaliz.**: point mass sliding down an inclined plane;
- **Mapping**: box as mass, conveyor slope as an angle θ, vertical drop as height h, gravity;
- **Reduction**: no structure flexibility, no air movement, no friction, no rollers $\to$ flat plane;
- **Pragmatic**: it allows a, v_f, t of the box to be calculated, it enables the prediction of how to build a belt mockup.

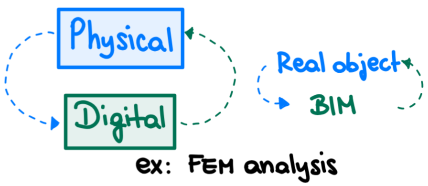
Digital representation

- - - - - - - → Manual Data Flow (Offline)

——————→ Automatic Data Flow (Real-time)

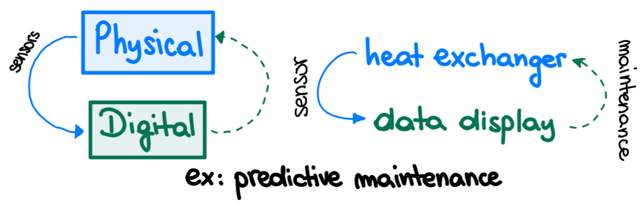
Digital model (simulation)

No direct connection between digital and physical object:



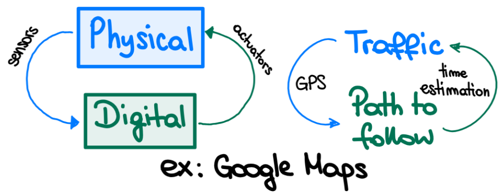
Digital shadow

Unidirectional, automated data flow from physical object to digital model:



Digital twin

Automated data exchange between physical object and model:



Role of time

Stationary behavior

Steady-state operation: $\dot{m}_\alpha = \dot{m}_\omega$

Dynamic behavior

Non stationary/transient/unsteady: $\dfrac{dm}{dt} = \dot{m}_\alpha - \dot{m}_\omega$

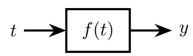
Governing dynamics

Empirical (black box)

Data based, without direct physics link. (ex: machine learning, fitting of functions)

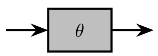
Physics-based (white box)

Based on physical laws.
(ex: conservation of mass)



Grey-box (hybrid)

Combining physics and data parameters.



Role of space

Point model (0D)

Assumes the whole system is perfectly mixed. (ex: ideal mixer with isotropic distribution). Software: Excel, MATLAB

Linked point

Connects several simple models together to create a basic network or layout. (ex: space shown via linking of 0D-models). Software: Simulink, Modelica

Spatial model (1-3D)

Considers real position of state variables or entities; spatial relationships affect the dynamics. (ex: real mixer with anisotropic, heterogeneous distribution). Software: COMSOL, ANSYS, AutoCAD, REVIT

Example with a heat pump

- **Purpose**: digital shadow $\to$ automated data;
- **Governing dynamics**: physics-based $\to$ based on thermodyn. laws;
- **Time**: time dependent, dynamic behavior $\to$ heating load, power of the hp, on/off cycles;
- **Space**: linked point $\to$ el. inputs, thermal energy exchange, 4 components to monitor.

Solvability of models

Analytical

Closed formula as solution. Only for simple problems.

$$A = \frac{x^3}{3}\Big|_0^2 = \frac{8}{3}$$

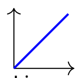
Numerical

Numerical approximation. For complex problems.

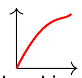
$$A \approx \sum_{i=1}^{n} f(x_i)dx \approx 2.6667$$

Further modelling properties

Linear vs Non-linear

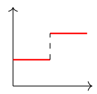


Linear

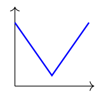


Non-Linear

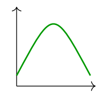
Continuity vs Differentiability



Non-Cont

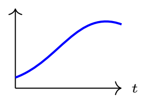


Cont/Non-Diff

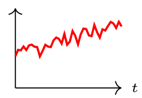


Differentiable

Deterministic vs Stochastic



Deterministic



Stochastic

Modelling approaches

Top-down

Largest components broken down into smaller. ex: marble block sculpture, railway network.
⊕ Efficient model, ⊖ Misses details

Bottom-up

Individual components combined into larger. ex: LEGO model, human body.
⊕ Detailed model, ⊖ Complex

SW2: How to model a system

1. Problem formulation
2. Mathematical representation
3. Mathematical analysis
4. Interpretation and evaluation of results

Problem formulation

Task 1 - Defining goals

What do we want to achieve?
How well/closely does our model need to represent reality?
What could be the goals for this specific system?

Task 2 - Characterize the system

What are the relevant parameters and variables of the system?
What are the system boundaries?
What are the inputs and outputs of the system?

Task 3 - Simplify and idealize the system

Still reproduce the significant behaviors of the system, while reducing complexity.
Reduce model to the main parameters and variables (ex. for hp: COP? Max. power? Avg power? Yearly values? Temperature levels?).

Mathematical formulation

Task 1 - Identify fundamental theories and laws

If no laws are available, use ad-hoc or empirical data to derive relationships:
Thermodynamic laws, material properties, ad-hoc
$P_{out} = COP(T_{amb}) \cdot P_{in}$

Task 2 - Derivation of relationships

Transfer system into a mathematical formulation.
Top-down (black/grey box): Use generic relationship, data from measurement to determine parameters. For more complex systems, add more parameters. Use techniques such as machine learning.
Bottom-up: Detailed physical modelling of the device. Physical laws to describe each component. Exact geometry, material properties, boundary conditions.

Task 3 - Reduce to standard mathematical problem

Simple algebra, linear programming, differential equation, diffusion problem, wave propagation, FEM problem, using suitable methods and software/programming tools.

Interpretation and evaluation of the results

Task 1 - Calibration of results

Use existing data to calibrate the model.

Task 2 - Validation

Check underlying physics law, such as energy or mass conservation, compare to known solutions, look at extreme cases, compare to measured data.
→ What is it and why do we have to do it?

Before the modelling:
What do we model how?:

a) Aims: does the model describe the process under test?
b) Output: does the model provide the required output to describe the process?
c) Type: is the type of the model suitable to describe the process?

During modelling:
Can we reproduce the measurements?
Does the model behave like to system under study?

d) Fitting data: does the model reproduce the fitting data? How to measure accuracy?
e) Reproducing novel data: does the model also predict novel measurement data correctly?
f) Sensitivity analysis: does the model predict the behavior of the system correctly when system parameters are changed?

After modelling:
Does the model also work with new data?

g) System potentially changed.
h) Differences in system behavior is only manifest in new experiments.

SW 3: Data-based modelling

Linear regression

Used to find a linear function $y = f(x) = a + bx$ that best fits a dataset (x_i, y_i).

Least squares method

Minimize the sum of squared errors (SSE):

$$S = \sum_{i=1} (y_i - (a + bx_i))^2$$

If measurement uncertainties Δy_i exist, weight the error:

$$S_i = \frac{y_i - y(x)}{\Delta y_i}$$

Optimal parameter formulas

Finding a and b when S is minimal:

$$\frac{\partial S}{\partial a} = 0 \quad ; \quad \frac{\partial S}{\partial b} = 0$$

Slope b:

$$b = \frac{\sum_i x_i y_i - \frac{1}{n}\left(\sum_i x_i\right)\left(\sum_i y_i\right)}{\sum_i x_i^2 - \frac{1}{n}\left(\sum_i x_i\right)^2}$$

Intercept a:

$$a = \bar{y} - b\bar{x}$$

where:

$$\bar{x} = \frac{\sum_i x_i}{n} \quad ; \quad \bar{y} = \frac{\sum_i y_i}{n}$$

Quality of fit ($\mathbf{R^2}$)

The coefficient of determination R^2 indicates the percentage of variation explained by the model:

$$R^2 = \frac{\sum_i (y(x) - \bar{y})^2}{\sum_i (y_i - \bar{y})^2}$$

- $R^2 = 1$ (100%): the model explains all data;
- $R^2 = 0$ (0%): the model doesn't (random).

Multilinear regression

Used when the target depends on multiple variables:

$$y(x_1, \dots, x_n) = a + b_1 x_1 + \dots + b_n x_n = a + \sum_{j=1}^{n} b_j x_j$$

Non-linear regression

The goal is to fit data using non-linear functions when the underlying process is not linear.

Linearization techniques

Function	Equation	Trasformation	Variables
Exp	$y = ae^{bx}$	$\ln y = \ln a + bx$	x vs $\ln y$
Power	$y = ab^x$	$\ln y = \ln a + x \ln b$	x vs $\ln y$
Inverse	$y = \frac{a}{x}$	$\frac{1}{y} = \frac{x}{a}$	x vs $\frac{1}{y}$
Square offset	$y = ax^2 + b$	$y = a(x^2) + b$	x^2 vs y
Root / Cubic	$y = \sqrt{ax^3 + b}$	$y^2 = ax^3 + b$	x^3 vs y^2

Maximum likelihood method (MLE)

Determines the parameters of a probability distribution that best describes a dataset, independent of histogram binning.

Likelihood function

Defines as the product of probability densities for all data points:

$$L(\sigma, \mu) = \prod_i f(x_i, \sigma, \mu)$$

Log-likelihood

To simplify calculation and avoid small numbers, minimize the negative logarithm:

$$-\log L = -\sum_i \log(f(x_i, \sigma, \mu))$$

Common distribution

Normal distribution:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)$$

Weibull distribution (Reliability):

$$f(x) = \begin{cases} \lambda k(\lambda x)^{k-1} e^{-(\lambda x)^k}, & x > 0 \\ 0 & \text{else} \end{cases}$$

Weibull cumulative distribution function

$$F(x) = \int_{-\infty}^{x} f(u)\, du = \begin{cases} 1 - e^{-(\lambda x)^k} & for x > 0 \\ 0 & \text{else} \end{cases}$$

SW4: Modelling with ODEs

Fundamentals of ODEs

An ODE contains functions of one independent variable and their derivatives.

Ordinary (ODE)

Involves one independent variable:

$$\frac{d^2x}{dt^2} = -g$$

Partial (PDE)

Involves multiple independent variables:

$$\frac{d^2u}{dt^2} = c^2 \frac{d^2u}{dx^2}$$

Analytical solution method

Separation of variables

Used when terms involving y and x can be moved to opposite sides.

Variation of parameters

Used for inhomogeneous linear ODEs. General solution is the sum of the homogeneous solution and a particular solution.

Numerical solution methods

Euler method

A simple iterative method to approximate ODEs defined as $\frac{df}{dx} = g(x)$.

The approximation uses the finite difference slope:

$$\frac{df}{dx} \approx \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$$

Iterative steps:

$$f(x_0 + \Delta x) = f(x_0) + g(x_0)\Delta x$$

Modelling principles

Balance equations

Based on the conservation principle:

$$\frac{d}{dt} f(t) = f(t_\alpha) - f(t_\omega)$$

Example in a capacitor

$$U_0 = U_R + U_C \Rightarrow U_0 = RI + \frac{Q}{C} = R\frac{dQ}{dt} + \frac{Q}{C}$$

Mechanics and forces

Equation of motion is derived from Newton's second law $F_{net} = ma$.

Example of a falling drop with drag

$$m\dot{v} = mg - bv \Rightarrow v(t) = \frac{mg}{b}\left(1 - e^{-bt/m}\right)$$

Growth and decay

Describes processes where a quantity increases or decreases over time.

$$\frac{dN}{dt} = kN \Rightarrow N(t) = N_0 e^{kt}$$

with half-time / doubling factor τ:

$$\tau = \left|\frac{\ln 2}{k}\right|$$

Example of logistic growth

$$\frac{dN}{dt} = KN(t) - \frac{K}{K}N^2 \Rightarrow N(t) = \frac{L}{1 + \left(\frac{L}{N_0} - 1\right)e^{-kt}}$$

Recipe to derive the equation of motion

1. Make a sketch of the situation;
2. Define the coordinate system and select variables of interest;
3. Identify all forces and momenta;
4. Formulate the equation of motion;
5. Solve it.

Linear algebra and systems of ODEs

Matrix representation

System of equations:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

Matrix form ($Ax = b$):

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

If $x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$, then $\dot{x} = \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix}$

Inversion and diagonalization

Inverse matrix R^{-1}: $R \cdot R^{-1} = I$ (Identity matrix).

$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Diagonalization: Special matrices can be rewritten as:

$$A = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$$

This transforms the matrix into a diagonal matrix containing eigenvalues λ.

Why is it called linear algebra

Linearization:
Complex, non-linear functions can be approximated by linear functions in a small neighborhood of a point a:

$$f(x) \approx f(a) + f'(a)(x - a)$$

Benefit of solving ODEs

If A were a number, $\dot{x} = Ax$ would solve to $x(t) = ke^{At}$.
Since A is a matrix, if we diagonalize it using eigenvalues λ, the solution becomes a mixture of exponentials:

$$x(t) = R^{-1} \begin{pmatrix} k_1 e^{\lambda_1 t} & 0 & 0 \\ 0 & k_2 e^{\lambda_2 t} & 0 \\ 0 & 0 & k_3 e^{\lambda_3 t} \end{pmatrix} R$$

Solvability of linear systems

Geometric interpretation:
Solving $Ax = b$ is finding the intersenction of lines/planes.

- **Case 1**, consistent: lines intersect at exactly one point;
- **Case 2**, inconsistent: lines are parallel and distinct, there is no solution;
- **Case 3**, infinite solutions: lines are identical and overlap completely.

Determinant

A scalar value derived from a square matrix that tells us if it is invertible. If det $\boldsymbol{A} = 0$, the matrix is not invertible.

2x2 formula: For $\boldsymbol{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$, det $\boldsymbol{A} = ad - bc$.

3x3 formula: For $\boldsymbol{A} = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$,

$$\det \boldsymbol{A} = a_{11} \det \begin{bmatrix} e & f \\ h & i \end{bmatrix} - a_{12} \det \begin{bmatrix} d & f \\ g & i \end{bmatrix} + a_{13} \det \begin{bmatrix} d & e \\ g & h \end{bmatrix}$$

$$\det \boldsymbol{A} = \sum_{j}^{n} a_{1j} C1j, \quad \underbrace{C1j = (-1)^{1+j} \det \boldsymbol{A}_{ij}}_{\text{Cofactors}}$$

The Eigenvalue problem

For a square n×n matrix $\boldsymbol{A}$, we look for a Eigenvector x and a Eigenvalues a such that:

$$\boldsymbol{A}x = \lambda x$$

Calculation method:

1. Solve the characteristic equation det$(\boldsymbol{A} - \lambda I) = 0$
2. This result in an n-th order polynomial $(a_1 \lambda^n + \cdots = 0)$
3. The roots of this polynomial are the Eigenvalues.

SW5-10: Modelica

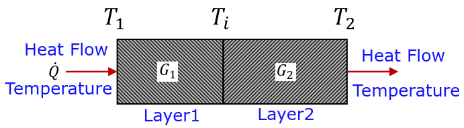
Equation-based modelling

Problem definition - Double layer wall

A wall consists of two layers with different thermal conductance values G_1 and G_2.

We consider two steady-state cases:

1. A heat flow $\dot{Q}_1$ passes througs the wall and the right temperature is T_2. The interface temperature T_i and the left temperature T_1 are unknown.
2. Both boundary temperatures T_1 and T_2 are given and the interface temperature T_i and the heat flow $\dot{Q}$ are unknown.



Formulas

Heat conduction equation [W]:

$$\dot{Q} = G\Delta T = G\,(T_\alpha - T_\omega) = G_1\,(T_1 - T_i) = G_2\,(T_i - T_2)$$

Thermal conductance [W/K]:

$$G = \frac{A}{L}\lambda$$

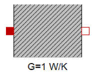
Conservation of energy:

$$\dot{Q}_1 = \dot{Q}_2 = \dot{Q}$$

Component-based modelling

Instead of rewriting equations each time, an instance of the needed physics law component is added.

Thermal components

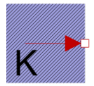


thermalConductor
Models heat linear heat flow between two ports determined by a constant thermal conductance G

$$\dot{Q} = G\,(T_a - T_b) \quad ; \quad \dot{Q} = \frac{\lambda \cdot A}{L}$$

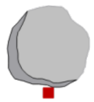
fixedHeatFlow
A source that injects a constant heat flow into the connected component

$$port.\dot{Q} = -\dot{Q}_{\text{component}}$$



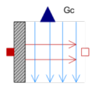
fixedTemperature
Defines a constant temperature boundary condition (acting like an infinite heat reservoir).

$$port.T = T_{\text{parameter}}$$



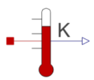
heatCapacitor
Thermal mass that stores energy, where temperature changes based on heat flow and heat capacity C.

$$C \cdot \frac{dT}{dt} = m \cdot c_p \cdot \frac{dT}{dt} = \dot{Q}$$



convection
Models the heat transfer between a solid surface and a moving fluid based on a convection coefficient G_{conv}.

$$\dot{Q} = \alpha \cdot A \cdot \Delta T = G_{\text{conv}} \cdot (T_{\text{solid}} - T_{\text{fluid}})$$



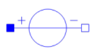
temperatureSensor
Measures the absolute temperature at the thermal port and outputs that value as a real signal.

$$y = T_{port} \quad ; \quad \dot{Q} = 0$$

Electrical components

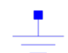
resistor
Resists the flow of electric current, creating a voltage drop proportional to the current.

$$U = R \cdot I \quad ; \quad \dot{Q} = P = U \cdot I$$



constantVoltage
An ideal voltage source that maintains a constant voltage difference between its positive and negative pins.

$$u_{port} = U_{\text{const}}$$

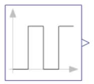


ground
Defines the reference potential (zero voltage) for an electric circuit.

$$u_{port} = 0$$

Signal components

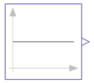
pulse



Generates a signal that alternates between two values (amplitude and offset) with a defined period and pulse width.

$$y = \begin{cases} \text{offset + ampl.}, & \text{if} \in \text{pulse width} \\ \text{offset}, & \text{otherwise} \end{cases}$$

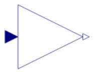
constant



A signal source that outputs a fixed numerical value.

$$y = k$$

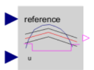
gain



A signal block that multiplies the input signal u by a constant parameter k to produce the output signal y.

$$y = ku$$

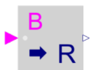
onOffController



A logical controller that switches its output between true and false based on comparing a measured signal u to a reference value.

$$y = \begin{cases} \text{true} & \text{if } u < (\text{reference} - \frac{\text{bandswitch}}{2}) \\ \text{false} & \text{if } u > (\text{reference} - \frac{\text{bandswitch}}{2}) \end{cases}$$

booleanToReal



Converts a Boolean signal into a Real float number.

$$y = \begin{cases} \text{realTrue} & \text{if input is True} \\ \text{realFalse} & \text{if input is False} \end{cases}$$

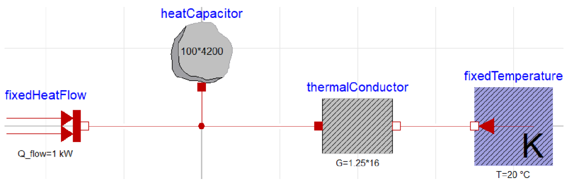
Dynamic systems

Two things can lead to time-varying behavior:

1. Transient boundary conditions
2. A dynamic system starting from a non-eq. state

First-order thermal model

A mass is heated by a constant source while simultaneously losing heat to a cooler environment



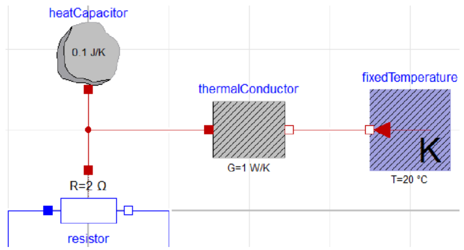
Conservation of energy at the central node:

$$C \cdot \frac{dT}{dt} = Q_{in} - G\,(T - T_{\text{sink}})$$

Multi-domain modelling

Multi-domain model

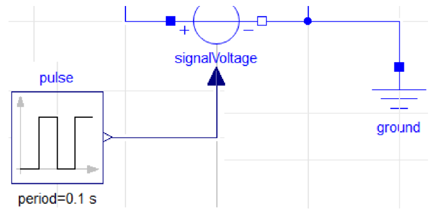
Allows representing different physical domains such as electrical, mechanical, thermodynamic, and fluid dynamics in a single model.



Resistor heat interacts with the thermal system

Cyber-physical model

A model combining physical domains with a software.



One-dimensional model

Simulation technique used to calculate spatial distribution by discretizing a continuous object into multiple discrete, lumped segments.

About Modelica

Definition and structure

Open source, equation-based, non-casual language for modelling dynamic behavior of multidisciplinary systems. Component-based (graphical connection), object oriented (inheritance), and hierarchical.

Equation-based / non-casual modelling

- Component diagram: topological (physical) structure;
- Equation-based: no fixed input/output direction;
- Connections: represent physical wiring/piping;
- Pros: reusable, multi-domain, closer to physics.

Casual modelling

- Block diagram: represents computational data flow;
- Assignment-based: fixed input/output;
- Connections: represent signal flow variables;
- Cons: prone to errors when modifying structure.

Hierarchical structure

Components are built from connected subcomponents and/or equations, allowing complex systems to be broken down into reusable parts.

Object-oriented

Allows creating general base definitions (superclasses) that specific components extend, rather than defining every component from scratch.

Physical mapping

Icons represent physical components, connections represent actual physical couplings.

Application examples

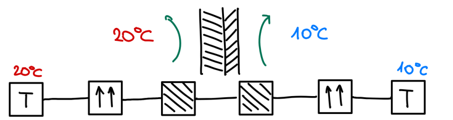
- Multiphase flow: refrigeration systems;
- Multi-domain: Pneumatic piston pump;
- Compressible media: Medical pulse wave analysis.

Examples wrap-up

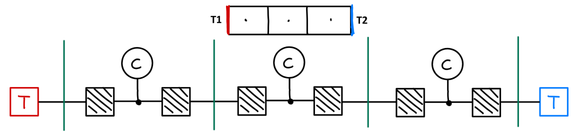
Thermal circuit

$$\frac{dE}{dT} = \frac{dU}{dT} = m \cdot c \cdot \frac{dT}{dt} = \dot{Q}$$

Heat flow



Heaten up rod



Physical units

Heat flow	$\dot{Q}$	$[W]$	Heat capacity	C	$[J/K]$
Thermal conductivity	λ	$[W/mK]$	Thermal conductance	G	$[W/K]$
Specific heat capacity	c_p	$[J/kgK]$	Convection coefficient	α	$[W/m^2K]$

SW11: Model and control energy systems