



# Introduction to Modeling and Optimization of Sustainable Energy Systems

*Introduction*

André Bardow & Giovanni Sansavini



# Who are we?



Reliability and Risk Engineering  
<https://rre.ethz.ch/>

Prof. Dr. Giovanni Sansavini



Energy and Process Systems Engineering  
<https://epse.ethz.ch/>

Prof. Dr. André Bardow

# Administration

- Course dates
  - Lecture Wed 16:15 p.m. – 18:00 p.m. in HG D 7.1
  - Exercise Thu 13:15 p.m. – 14:00 p.m. in ML F 36
- Course documents
  - Livestream of the Lecture (record provided afterward):  
<https://video.ethz.ch/live/lectures/zentrum/hg/hg-d-7-1.html>
  - Slides, recordings, exercises, solutions, and discussion forum are provided via Moodle:  
<https://moodle-app2.let.ethz.ch/course/view.php?id=15661>
- Exam
  - Written exam
  - 120 minutes
  - No written aids allowed
  - Session examination
- Office hours: write to [moses-edu@ethz.ch](mailto:moses-edu@ethz.ch)
- Exam office hours: 1-2 weeks before the exam (tba)

# Found any mistakes?

- *Modeling and Optimization of Sustainable Energy Systems* is a new lecture in an emerging field
  - Lectures and exercise are new at ETH
  - Thus: Mistakes are unavoidable
- If you found any mistakes, please let us know: [moses-edu@ethz.ch](mailto:moses-edu@ethz.ch)
- The participant providing the best feedback will receive a prize!



# Lecture plan

No.	Date	Content	
1	29.09.	Introduction & Models	
2	06.10.	Heat integration	Applications
3	13.10.	Continuous Optimization	Methods
4	20.10.	Heat exchanger networks	Applications
5	27.10.	Discrete Optimization	Methods
6	03.11.	Life Cycle Assessment (LCA)	Metrics
7	10.11.	Thermoeconomics	Metrics
8	17.11.	Risk Key Performance Indicators for Security	Metrics
9	24.11.	Multi-energy dimension: introduction	Methods & Applications
10	01.12.	Design dimensions: technology modelling	
11	08.12.	Space dimensions: energy networks	
12	15.12.	Uncertainty in energy systems	
13	22.12.	Recap (online)	



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# After this lecture, you are able to...

- ✓ **plan your participation** in this course
- explain the **scope of this course**
- recognize tradeoffs in the **energy trilemma**
- classify **mathematical models**



# Introduction to Modeling and Optimization of Sustainable **Energy** Systems

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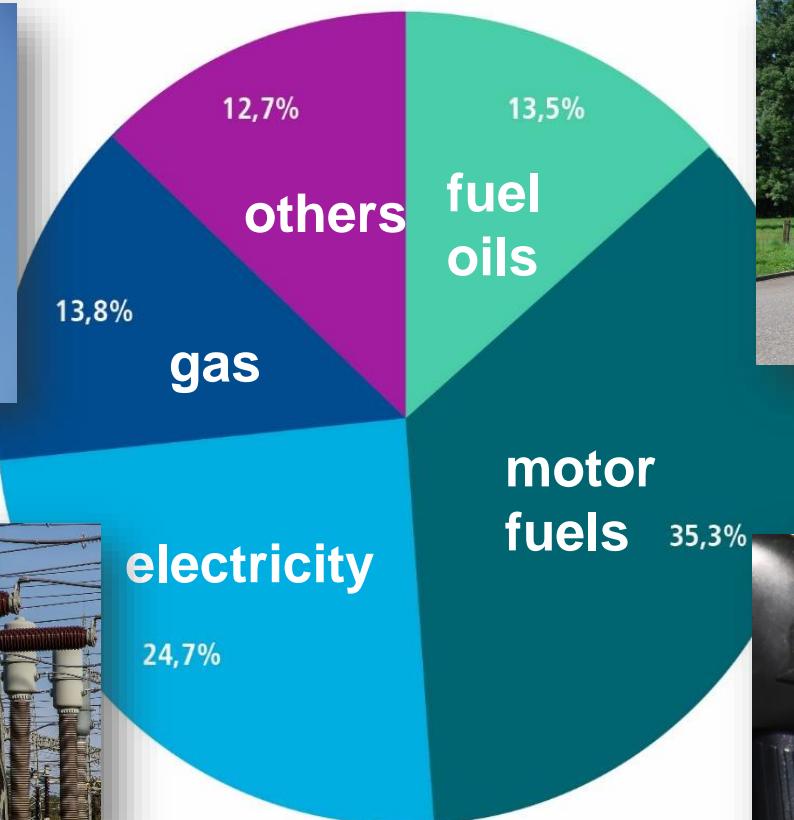


Switzerland.

# WE ARE FULL OF ENERGY

<https://www.eda.admin.ch/>

Final energy consumption in Switzerland 2019



Q BFE, Schweizerische Gesamtenergiestatistik 2019 (Fig. 2)  
OFEN, Statistique globale suisse de l'énergie 2019 (fig. 2)



Switzerland.

# WE ARE FULL OF ENERGY

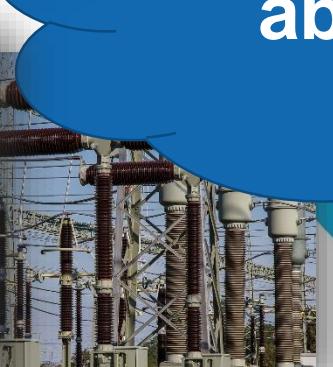
Final energy consumption in Switzerland 2019



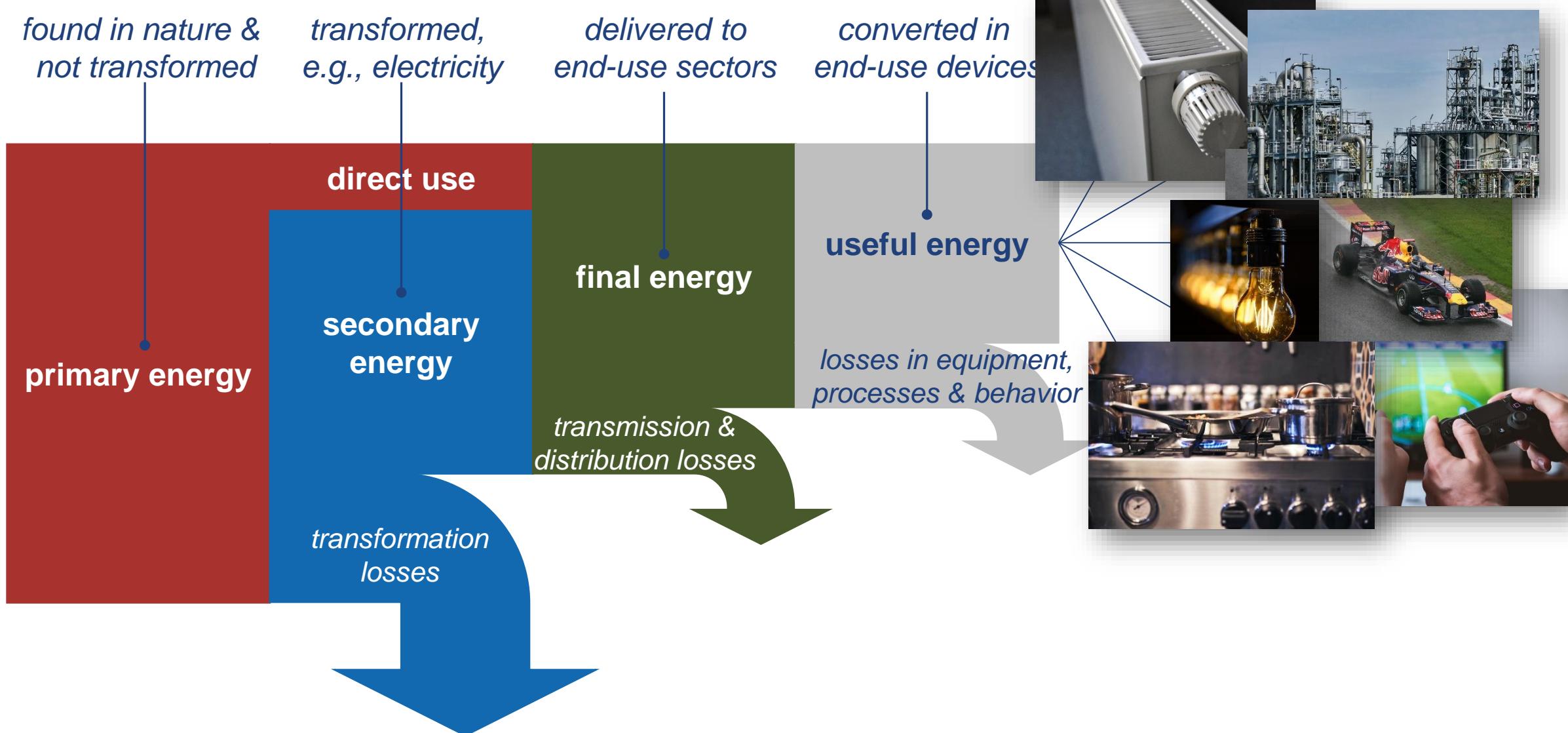
Do we really care  
about energy ?



BFE, Schweizerische Gesamtenergiestatistik 2019 (Fig. 2)  
OFEN, Statistique globale suisse de l'énergie 2019 (fig. 2)



# Useful energy, final energy, secondary energy, primary energy





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# Climate change ! Recommended video by Jeff Reimer

## ***Jeff Reimer: Our Changing Atmosphere - Evidence That Demands a Verdict***

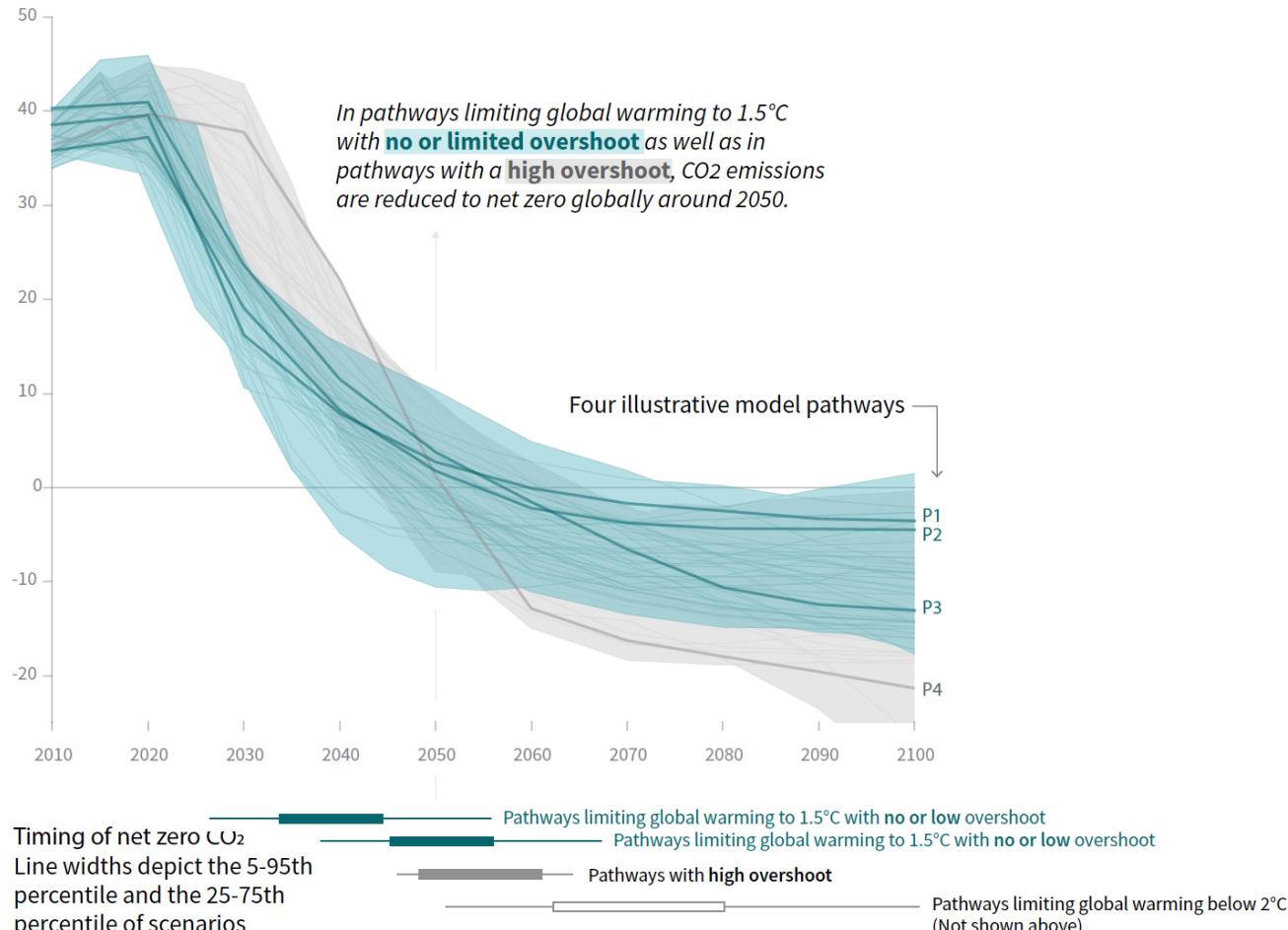


<https://youtu.be/QeqDfDD4xbg>

# Climate change targets require transition to sustainable energy systems

Global total net CO<sub>2</sub> emissions

Billion tonnes of CO<sub>2</sub>/yr



IPCC, Global warming of 1.5°C, 2018

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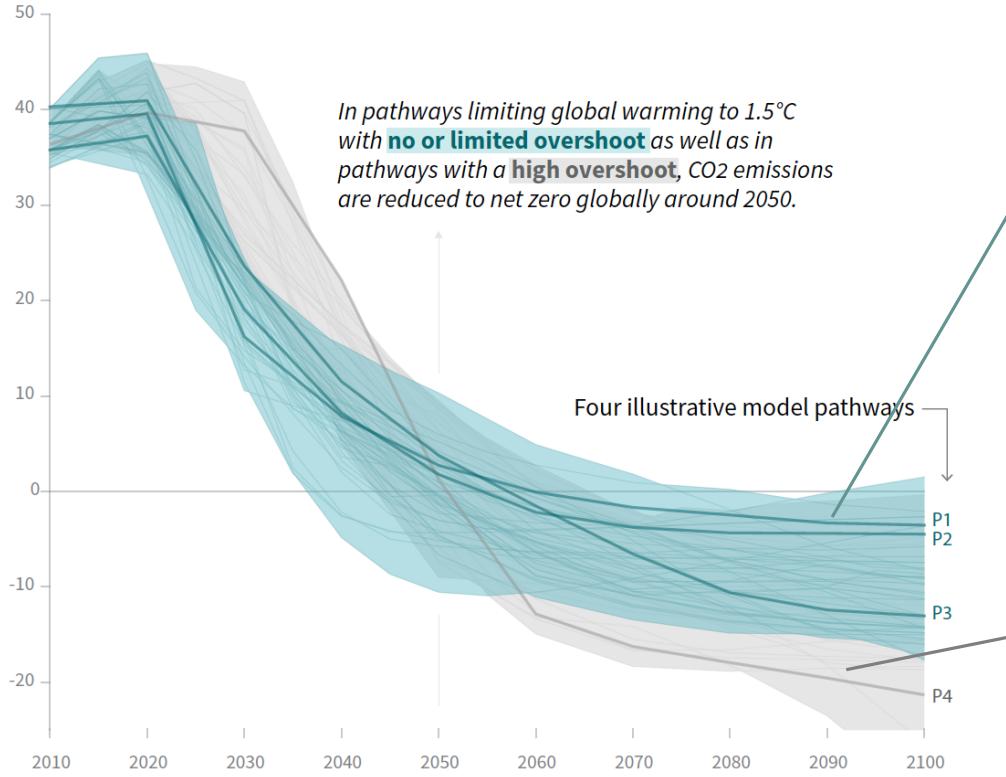
9/28/2021

15

# Climate change targets require transition to sustainable energy systems

Global total net CO<sub>2</sub> emissions

Billion tonnes of CO<sub>2</sub>/yr



Timing of net zero CO<sub>2</sub>

Line widths depict the 5-95th percentile and the 25-75th percentile of scenarios

Four illustrative model pathways

Pathways limiting global warming to 1.5°C with no or low overshoot

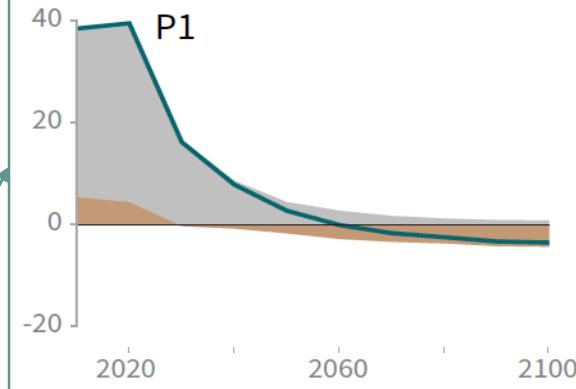
Pathways limiting global warming to 1.5°C with no or low overshoot

Pathways with high overshoot

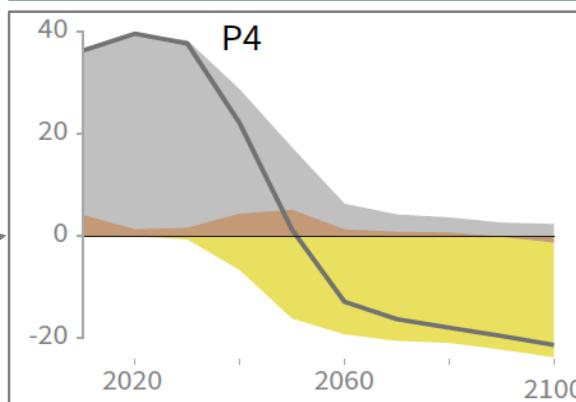
Pathways limiting global warming below 2°C  
(Not shown above)

Fossil fuel and industry   AFOLU   BECCS

Billion tonnes CO<sub>2</sub> per year (GtCO<sub>2</sub>/yr)



P1



P4

IPCC, Global warming of 1.5°C, 2018

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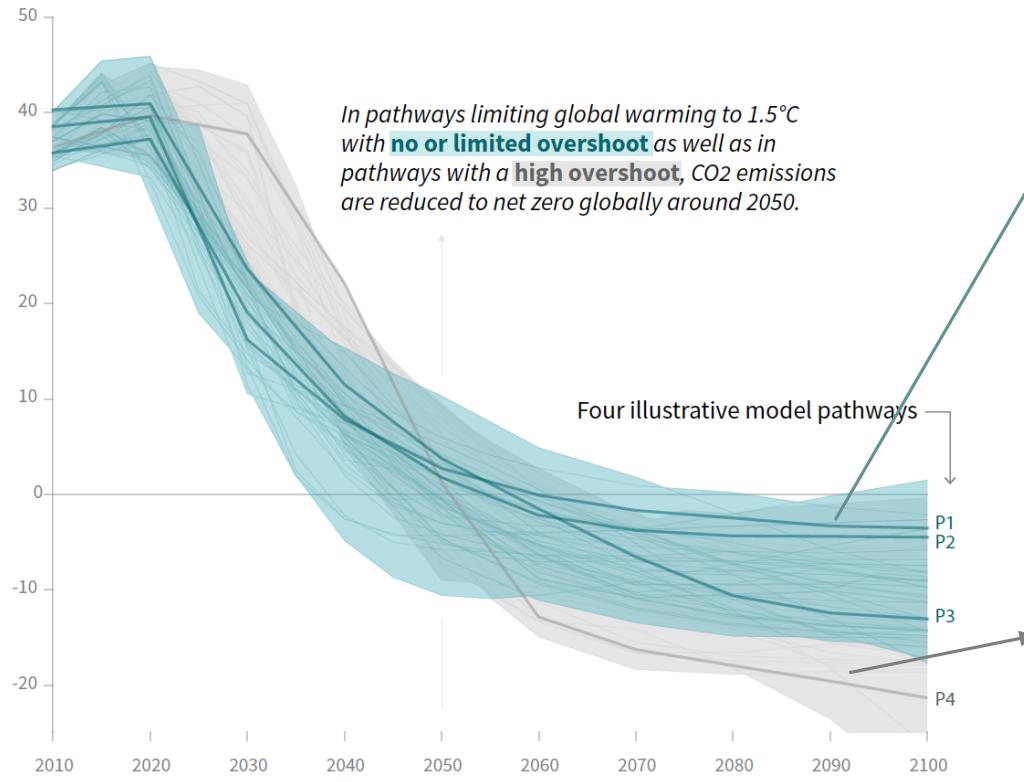
9/28/2021

16

# Climate change targets require transition to sustainable energy systems

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Pathways limiting global warming to 1.5°C with no or low overshoot

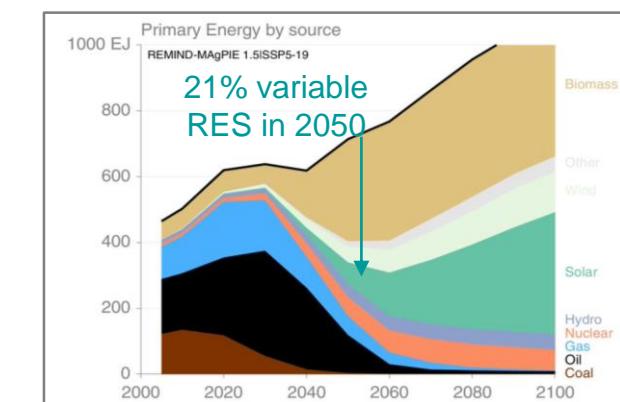
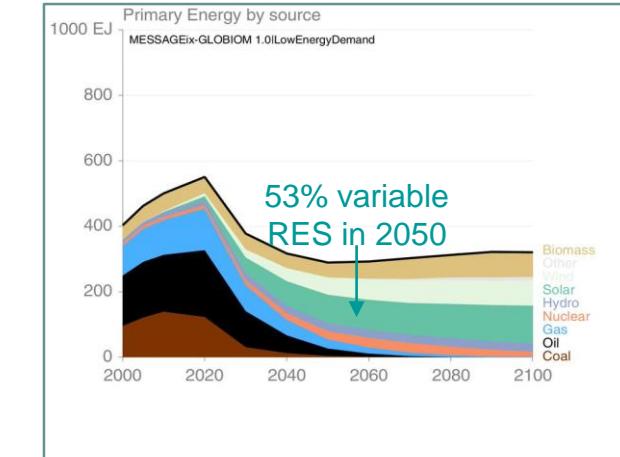
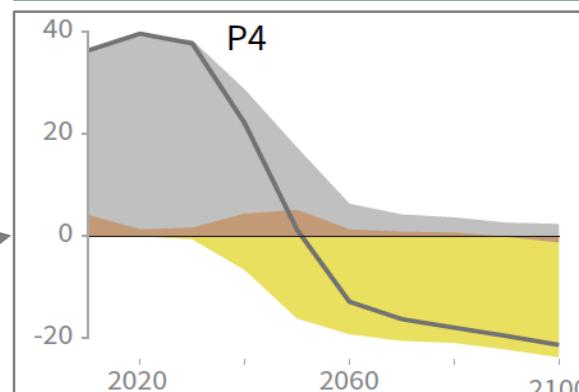
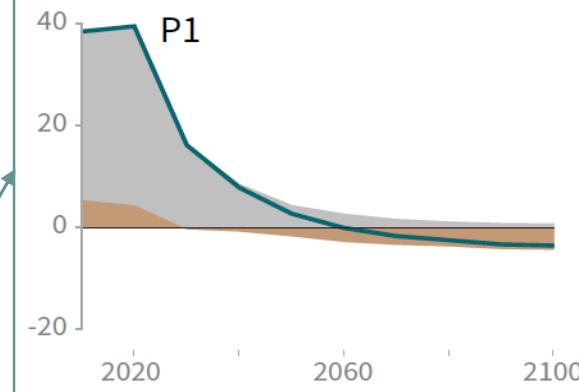
Line widths depict the 5-95th percentile and the 25-75th percentile of scenarios

Pathways with high overshoot

Pathways limiting global warming below 2°C (Not shown above)

Fossil fuel and industry AFOLU BECCS

Billion tonnes CO<sub>2</sub> per year (GtCO<sub>2</sub>/yr)



IPCC, Global warming of 1.5°C, 2018

**ETH**zürich

# Swiss greenhouse gas emissions (GHG) emissions: The role of energy

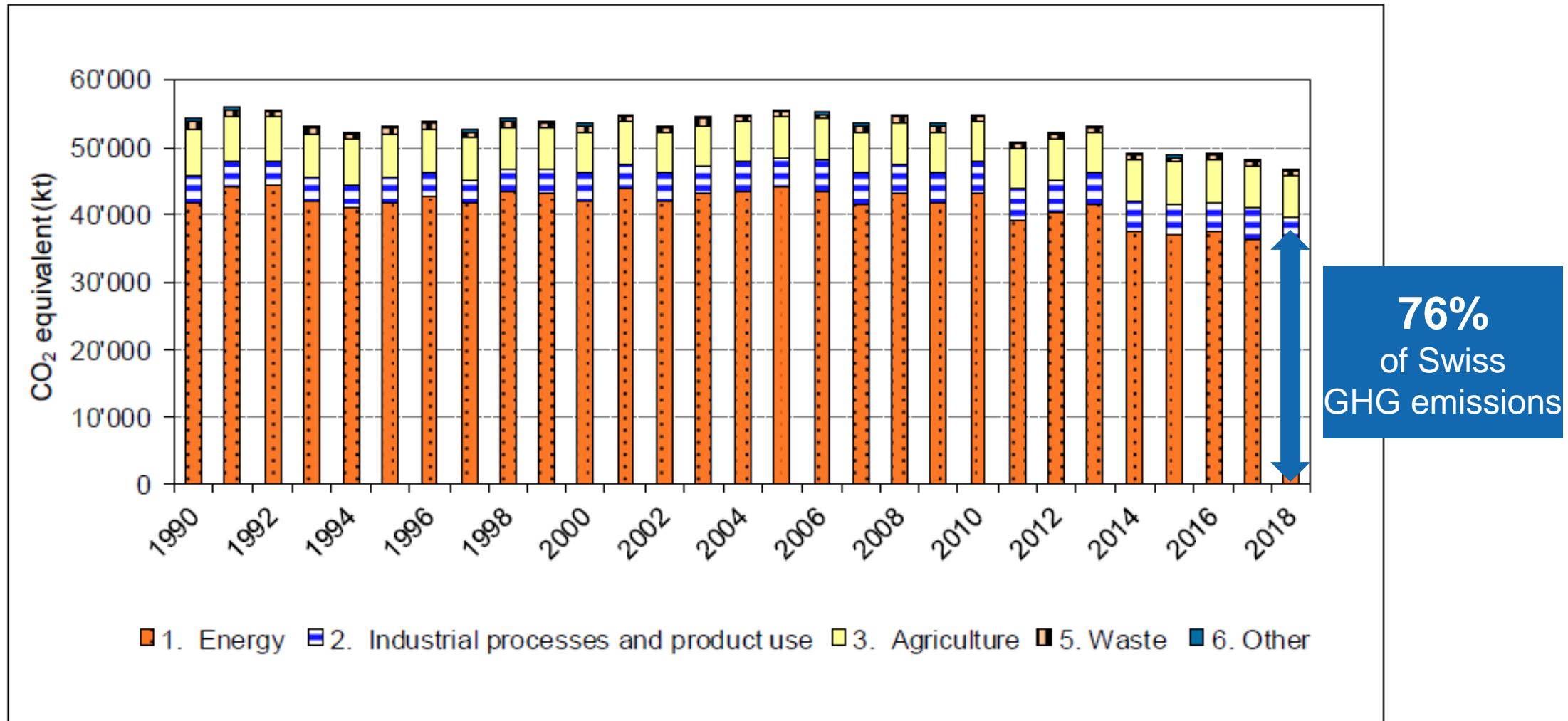
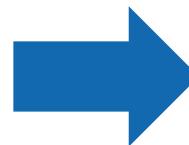


Figure 2-4 Greenhouse gas emissions in CO<sub>2</sub> equivalent (kt) by sectors (excluding LULUCF, excluding indirect CO<sub>2</sub>).

# Swiss plans for GHG emissions

- by 2030: -50% GHG emissions from 1990
- by 2050: no more net GHG emissions



achieve at least 30% in Switzerland and a maximum of 20% abroad

<https://www.admin.ch/gov/en/start/documentation/media-releases.msg-id-76206.html>

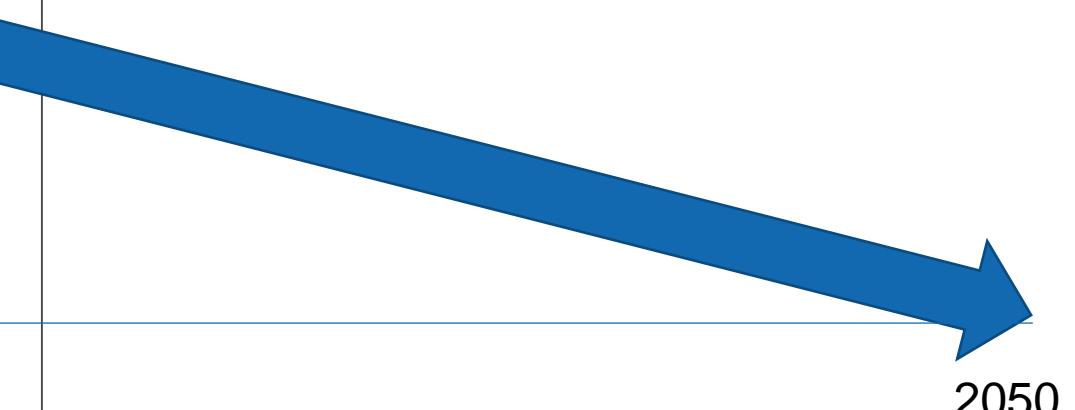
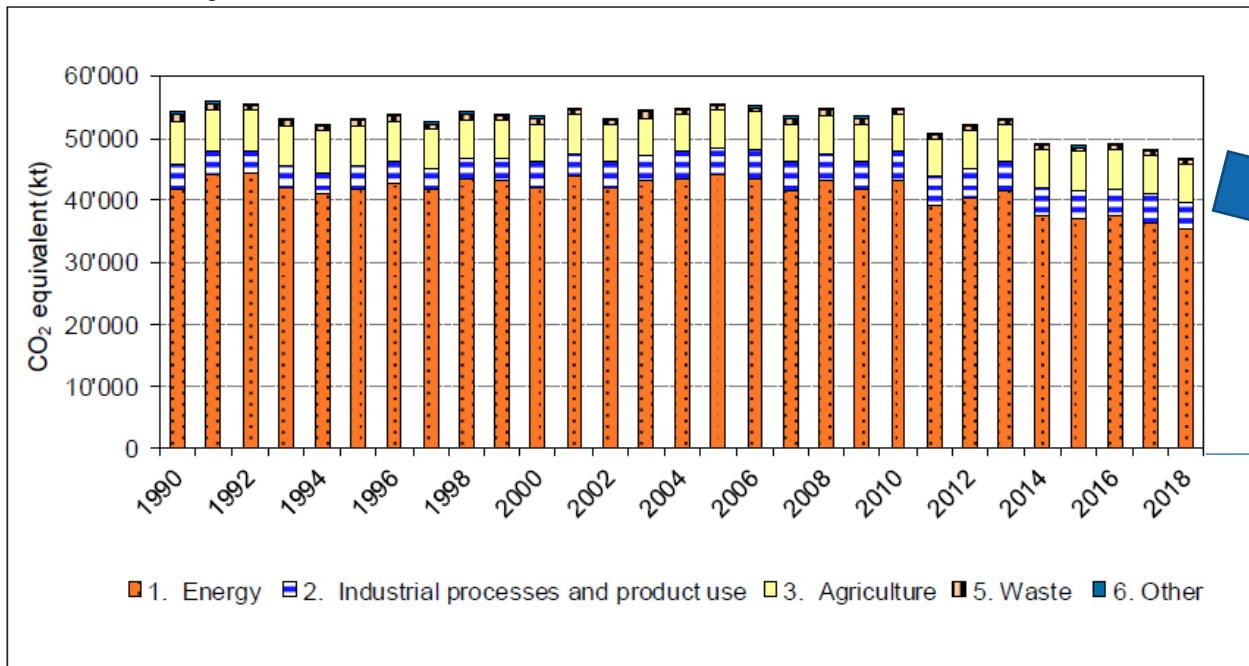


Figure 2-4 Greenhouse gas emissions in CO<sub>2</sub> equivalent (kt) by sectors (excluding LULUCF, excluding indirect CO<sub>2</sub>).



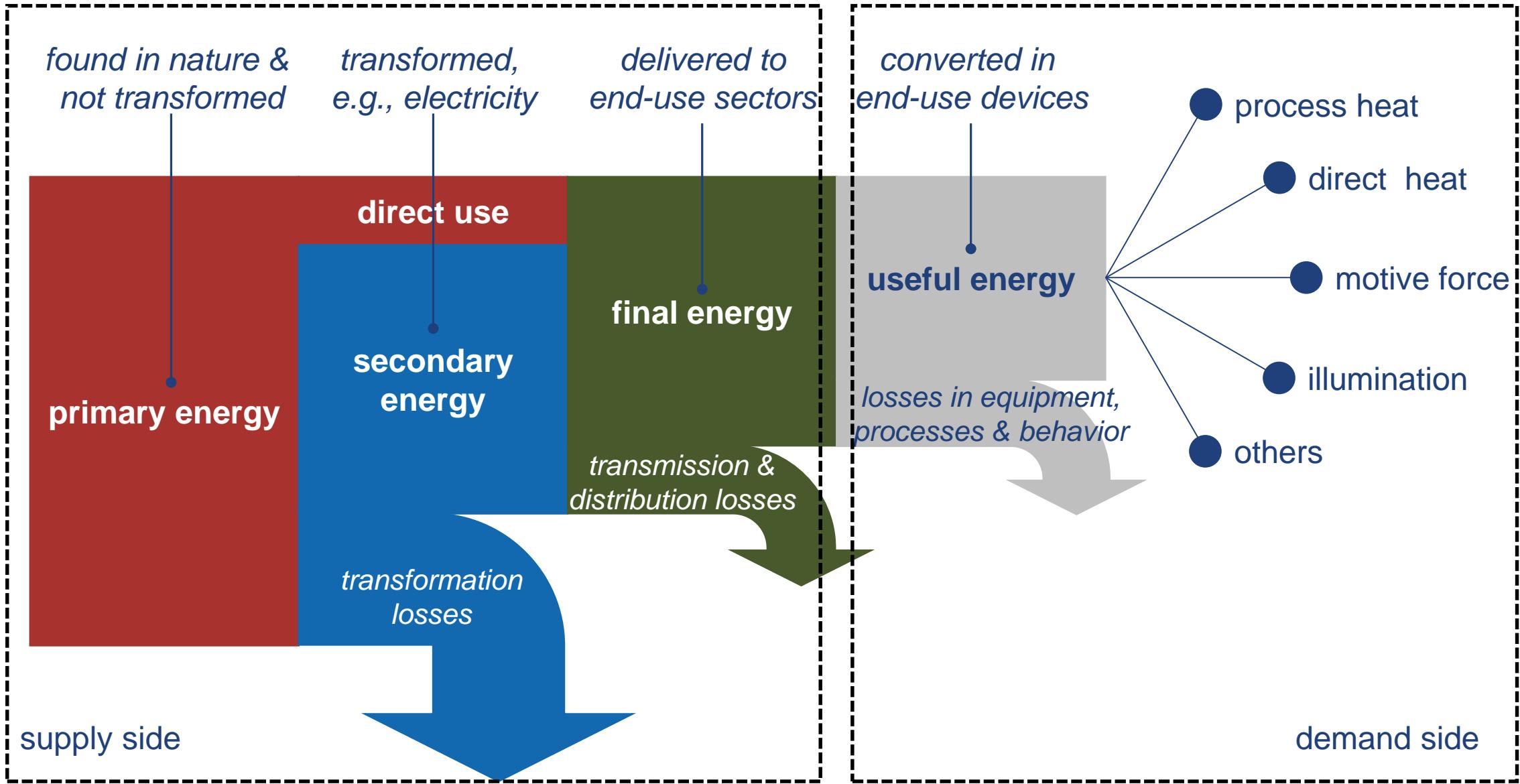
# Introduction to Modeling and Optimization of **Sustainable Energy Systems**

*Introduction*

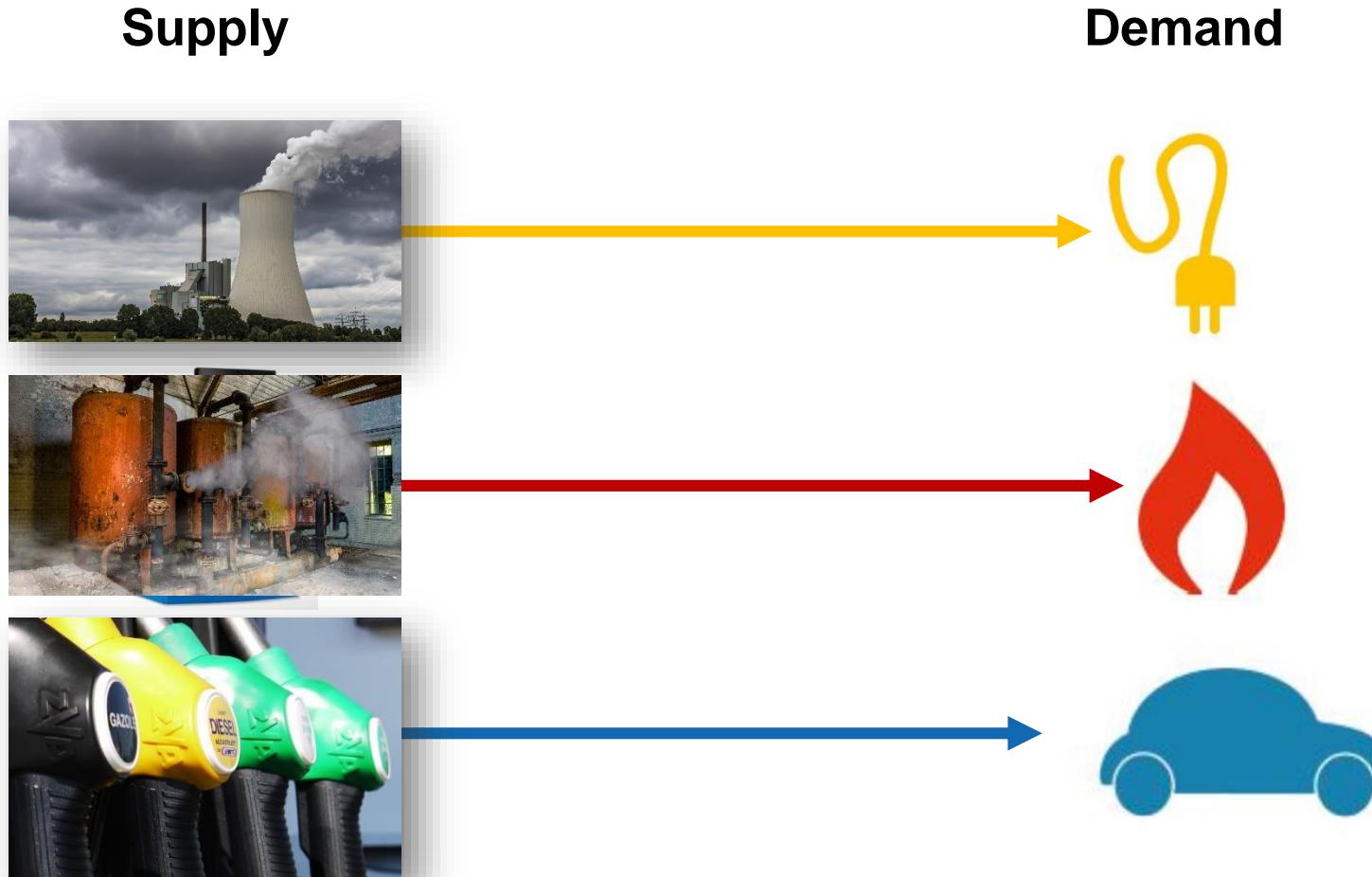
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# Towards sustainable energy systems: The actors



# Energy systems back in the day



# Energy systems today

supply



coal power



heating plant



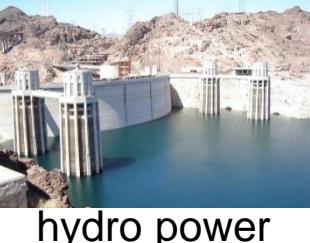
wind



PV



concentrated solar



hydro power



fuel cell



biogas

coupling



CHP



heat pump



electric heating



electrolyser

storage



Li-ion battery



heat storage



(pumped) storage



gas storage

distribution



electric grid



gas grid



heating network



telecommunication

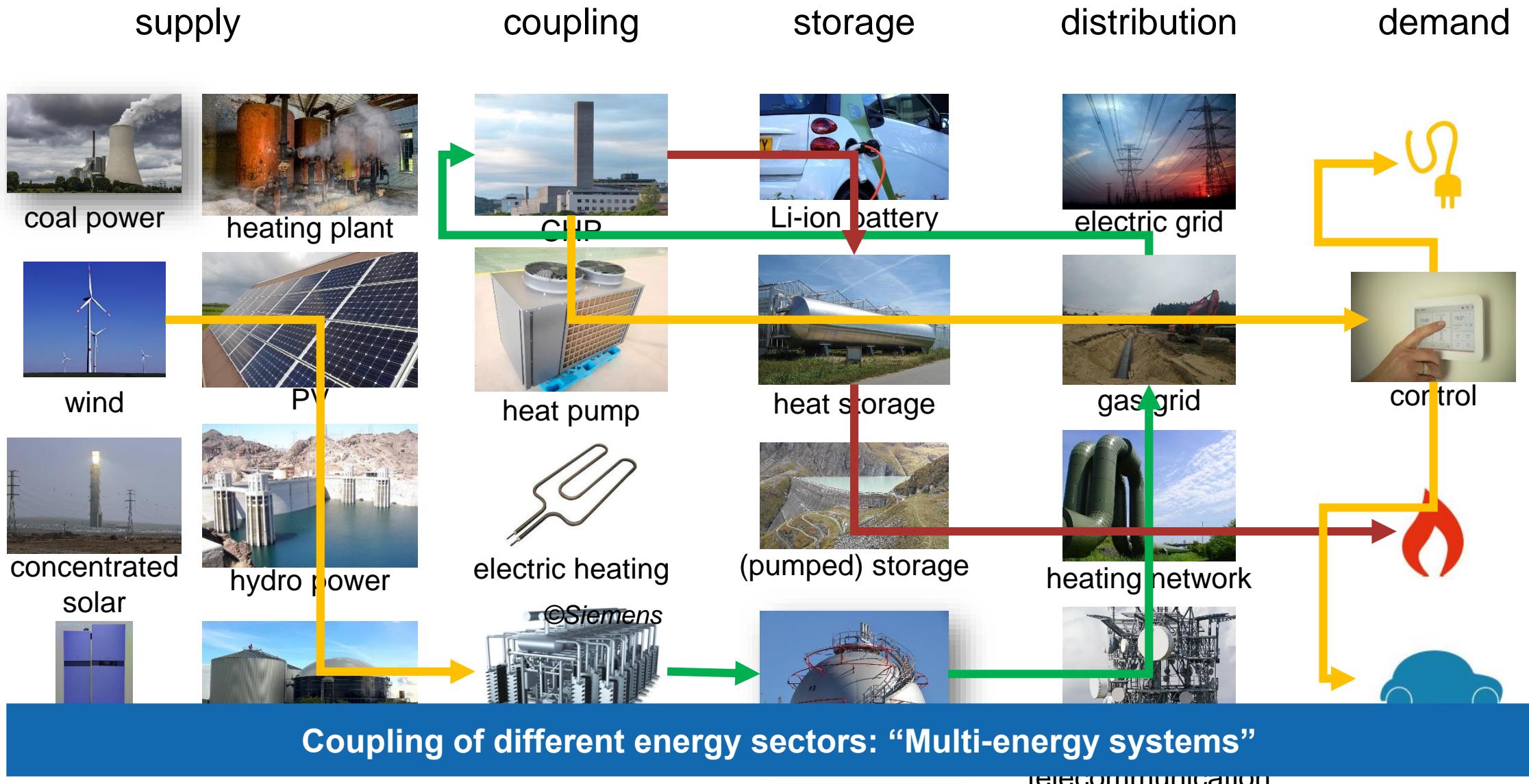
demand



control

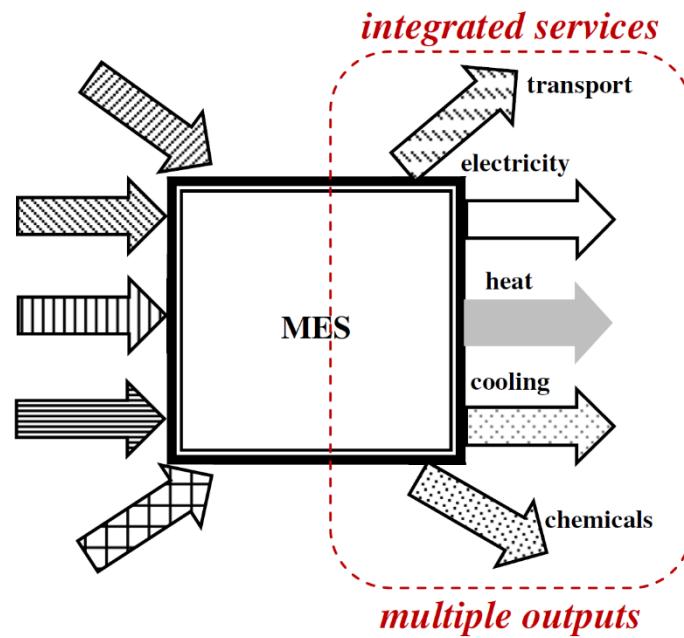


# Energy systems today: Multi-energy systems

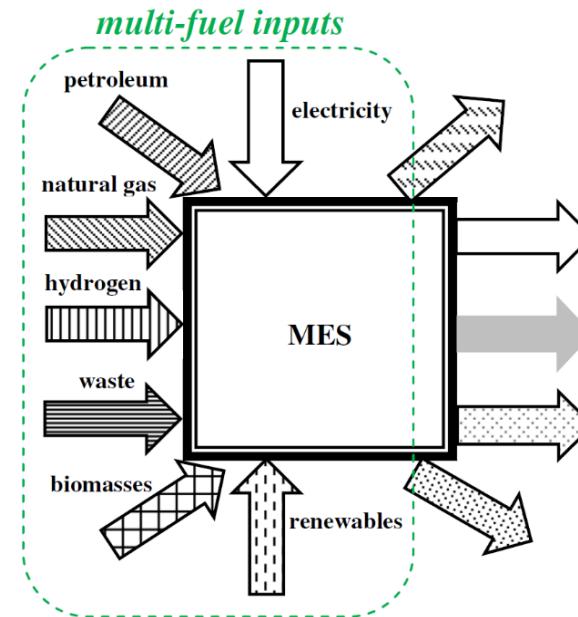


# Multi-energy systems from different perspectives

multi-service perspective

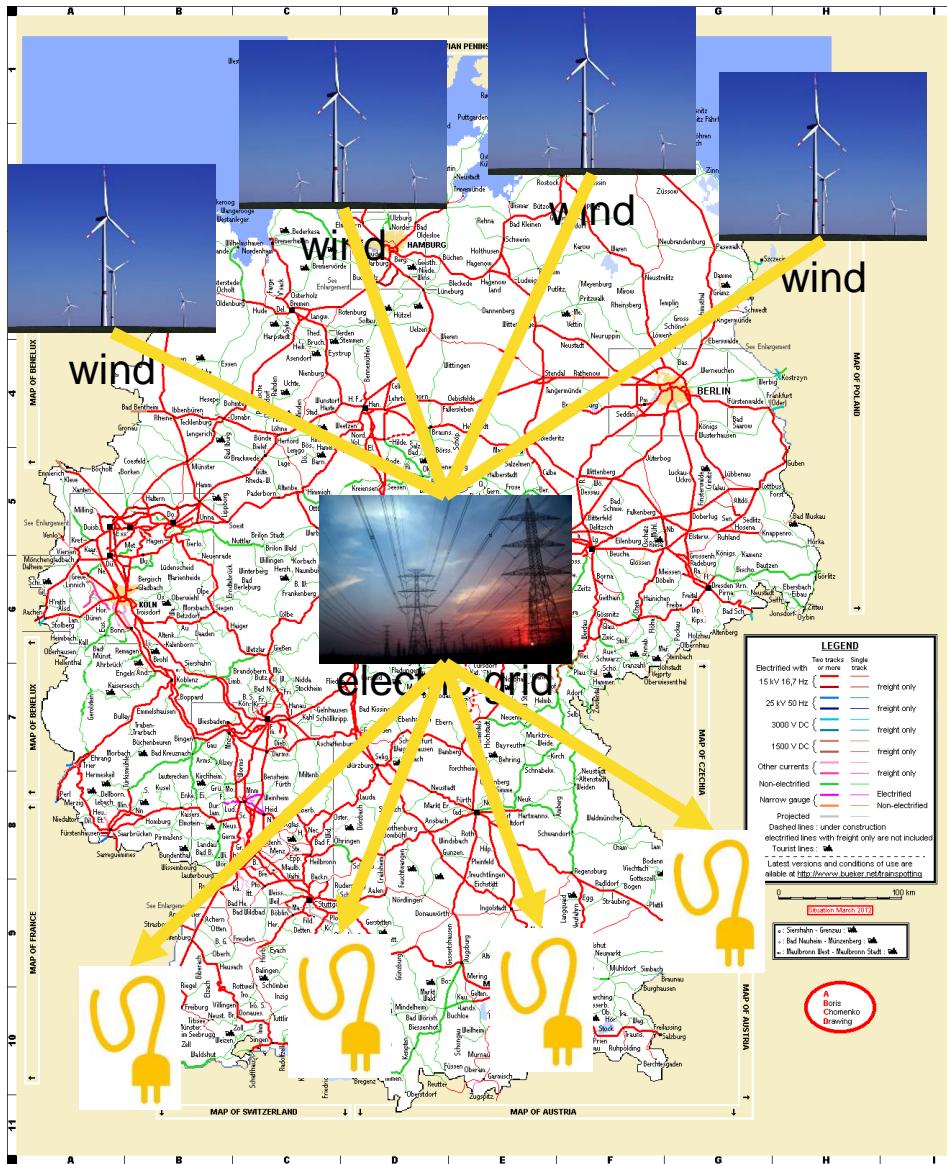


multi-fuel perspective

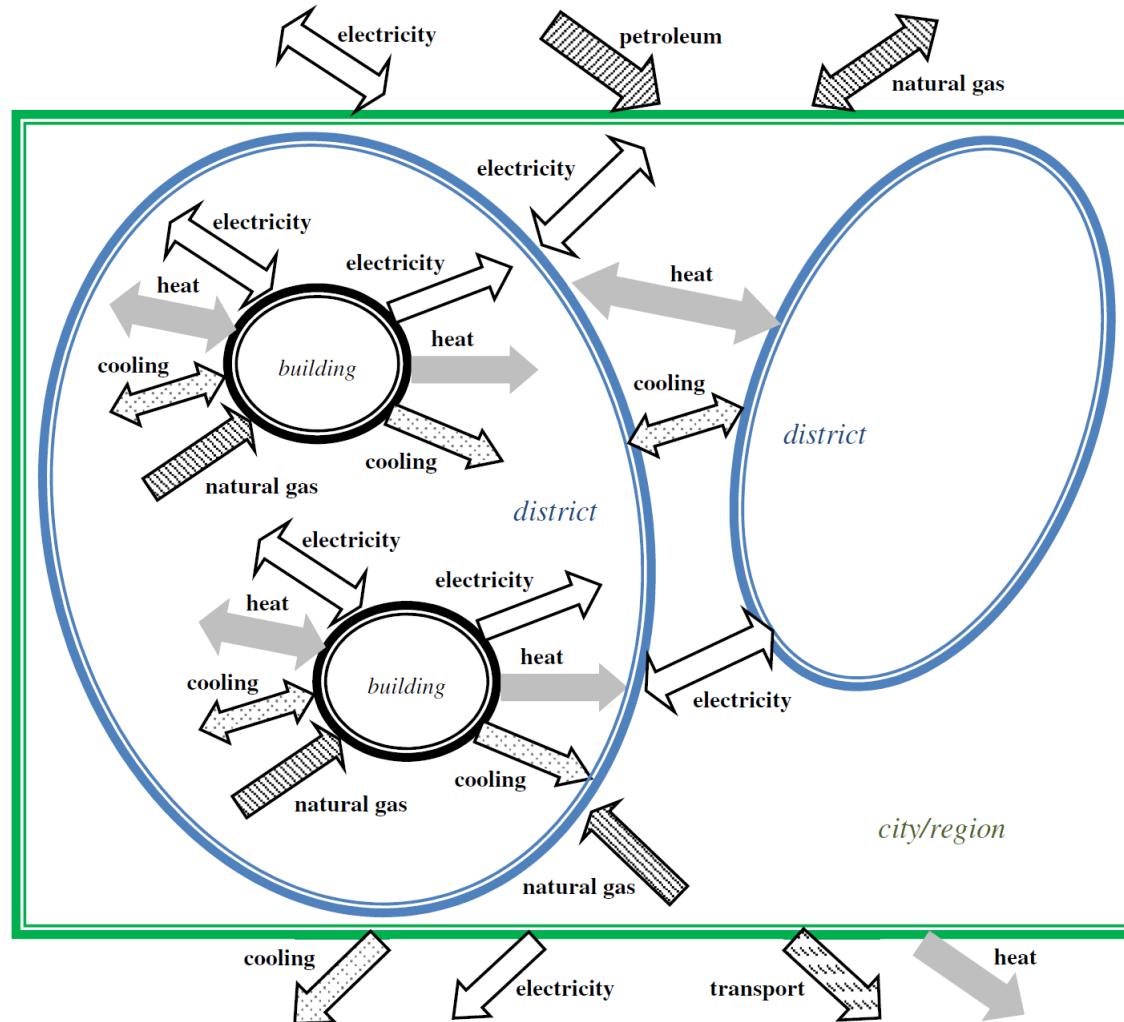


Mancarella P., 2014, MES (multi-energy systems): An overview of concepts and evaluation models P, Energy 65, 1-17.

Energy transmission and generation are **spatially distributed**

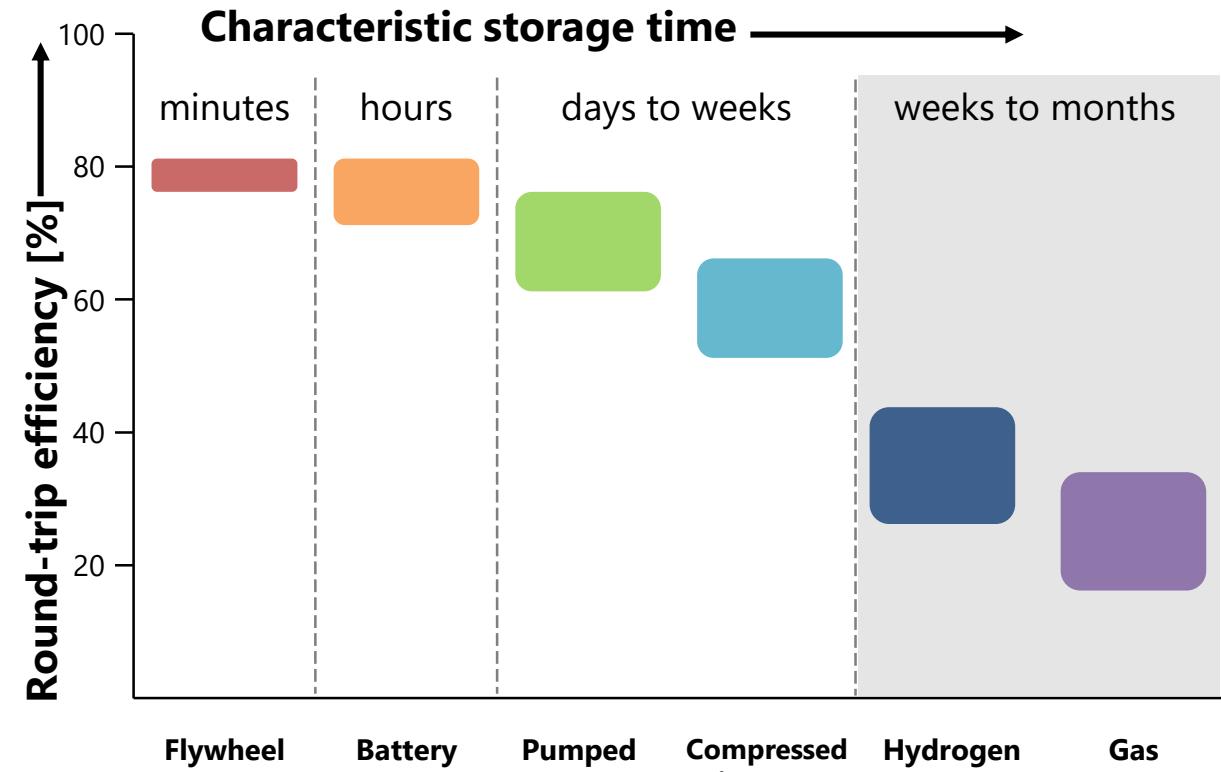
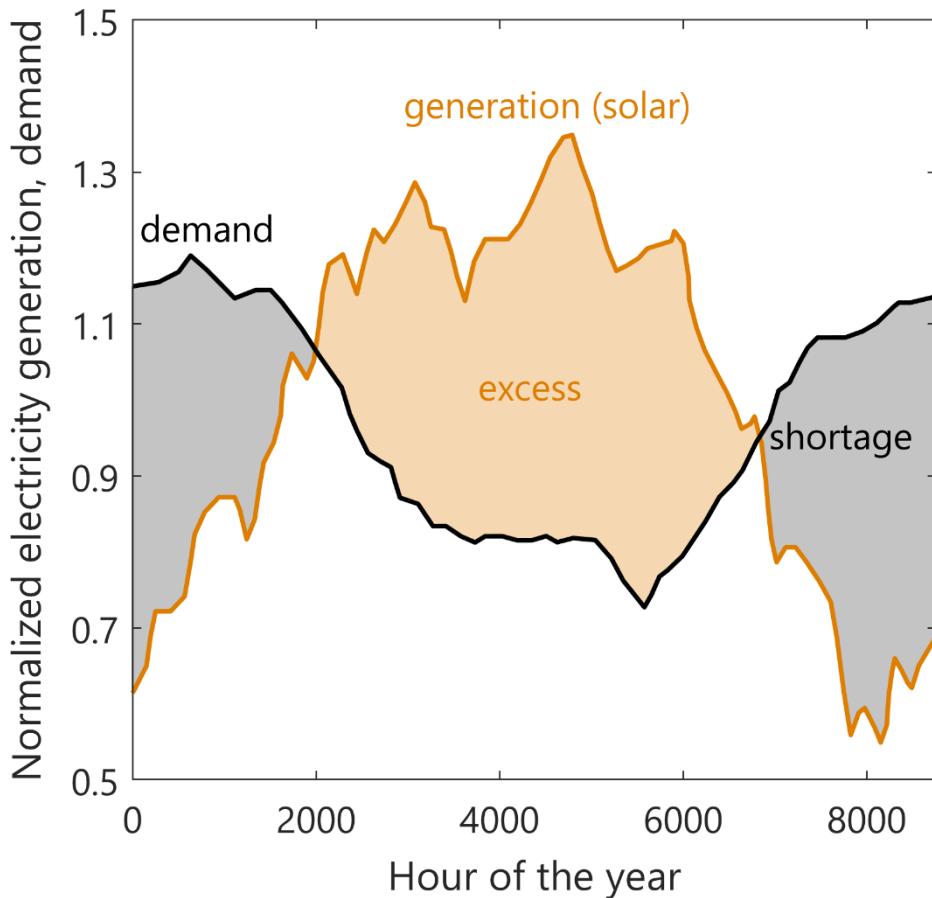


# Multi-energy systems from different perspectives: spatial perspective



Mancarella P., 2014, MES (multi-energy systems): An overview of concepts and evaluation models P, Energy 65, 1-17.

# Generation & consumption are temporally separated



adapted from: Ueckerdt et al., *Energy Econ.* **64**, 2017. Annual time series of weekly averages illustrating the time decoupling of electricity demand and solar generation for Europe (normalized over the corresponding average value).

# Challenges in operation planning of multi-energy systems

1

many **energy services** need to be supplied

2

many **energy sources** to be employed

3

interdependence increases due to **sectors-coupling**

4

demand & supply are **spatially distributed**

5

demand & supply are **temporally separated**

need for (computer-aided) decision support and therefore **models**

# After this lecture, you are able to...

- ✓ plan your participation in this course
- ✓ explain the scope of this course
- recognize tradeoffs in the **energy trilemma**
- classify **mathematical models**



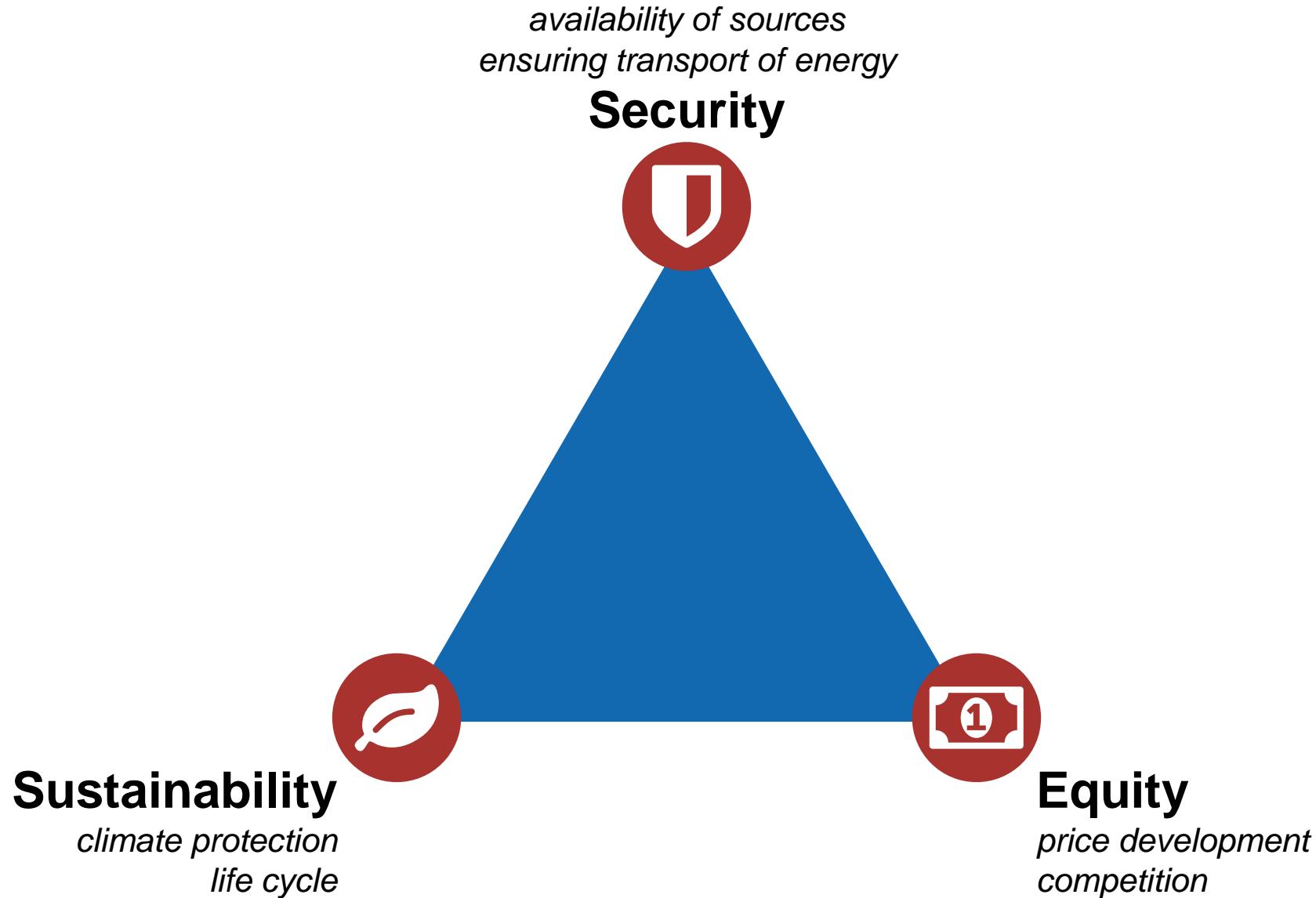
# Introduction to Modeling and Optimization of Sustainable Energy Systems

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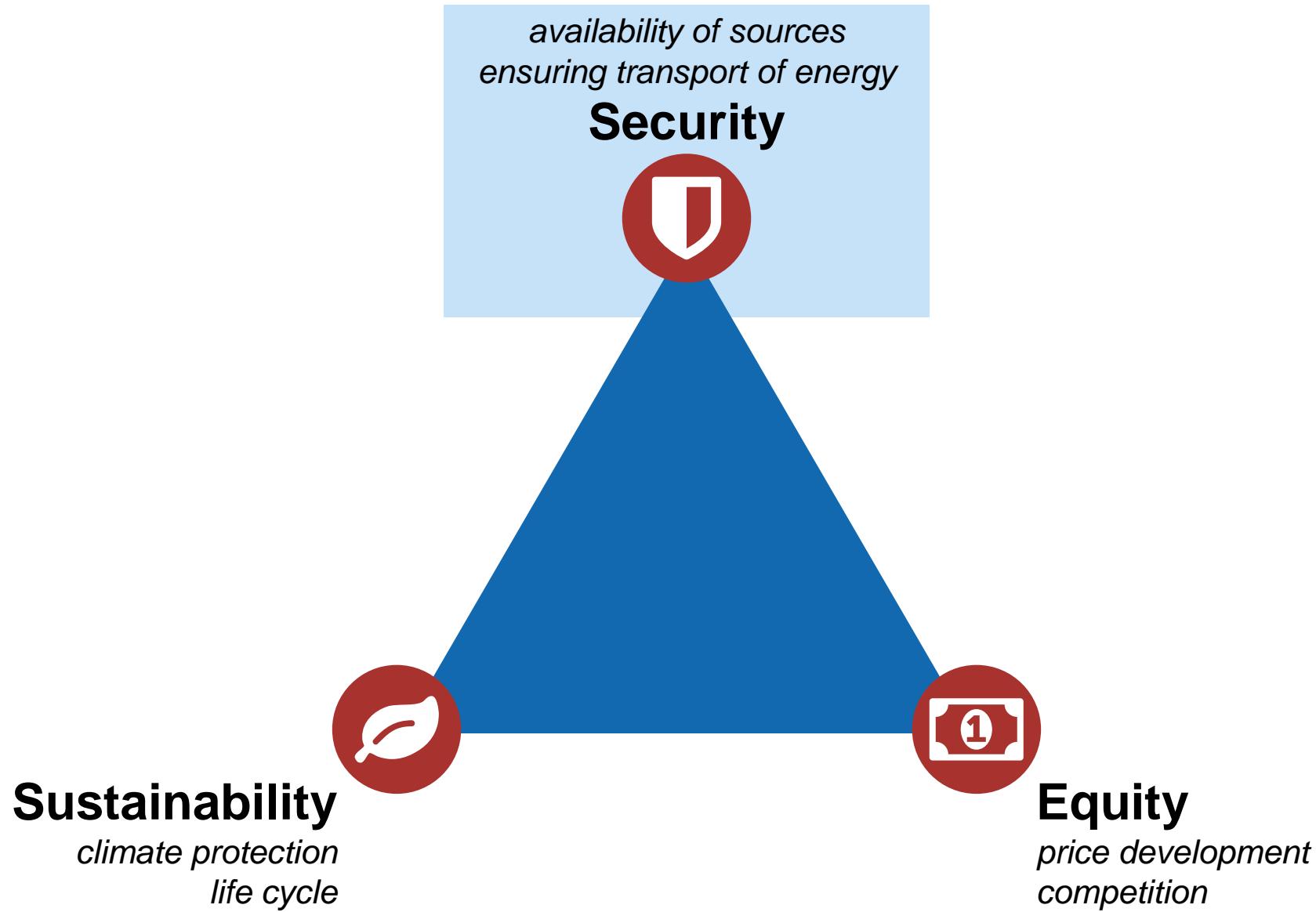
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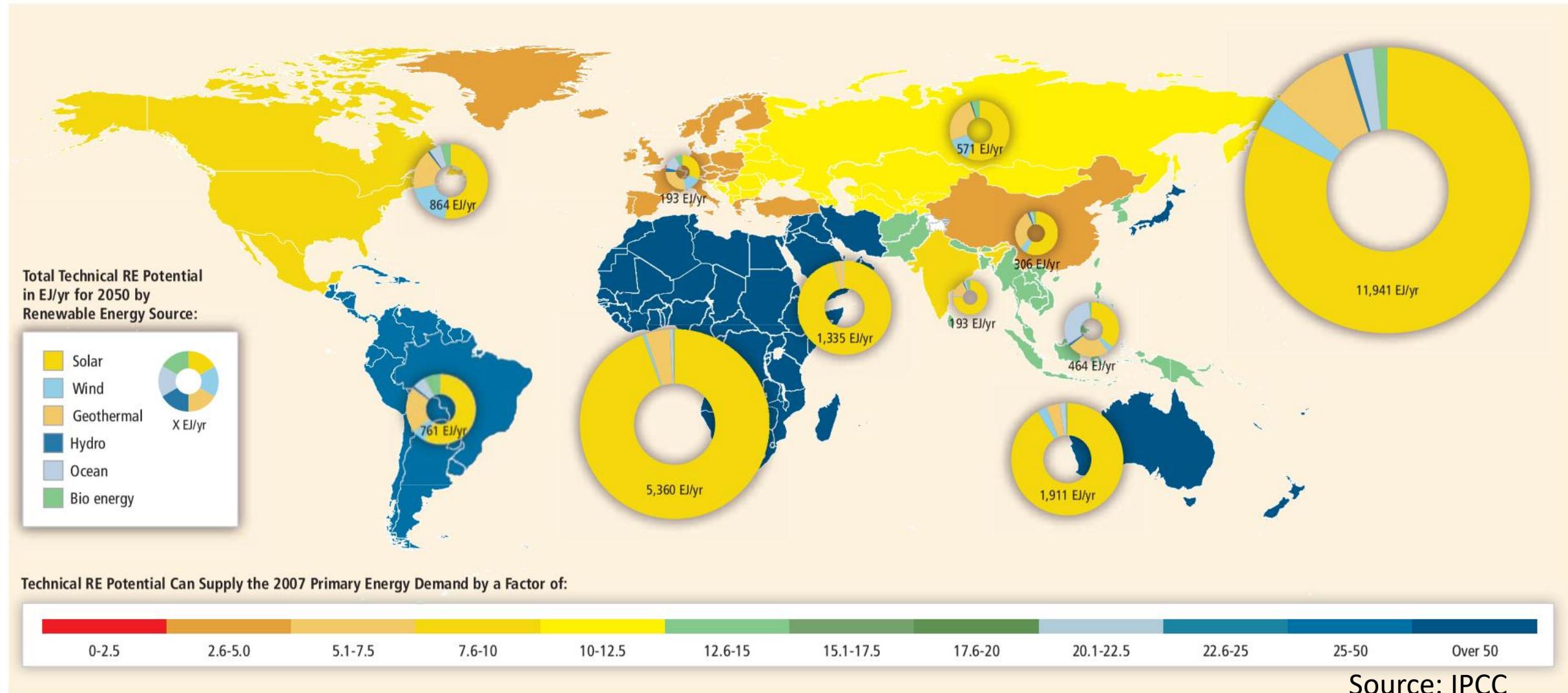
# Energy trilemma – Objectives of the energy system



# Energy trilemma – Objectives of the energy system

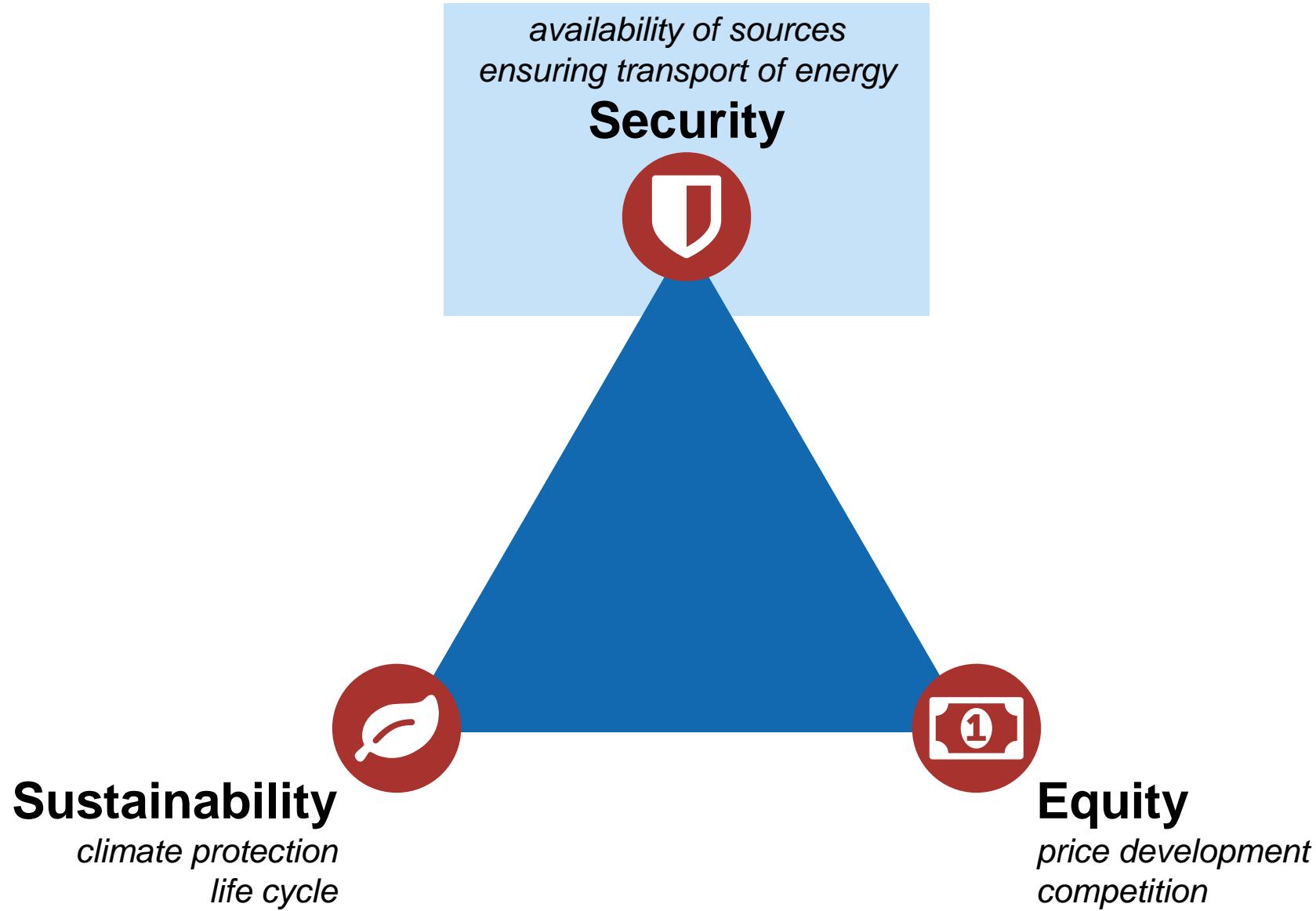


# Global technical potential of renewable energies



Source: IPCC

# Energy trilemma – Objectives of the energy system



# Characteristics of renewables

energy source / technology		power / MW	characteristic time scales for power system operation	dispatchability	predictability
Bioenergy		0.1 – 100	seasons	+	+
Geothermal		2 – 100	years	+	+
sun	Photovoltaics	0.004 – 100	minutes	-	-
	concentrated solar power with thermal storage	50 – 250	hours	+/-	+
water	run of river	0.1 - 1.500	hours	+/-	+
	reservoir	1 - 20.000	days	+	+
	tides	0.1 – 300	hours	-	+
wind		5 - 300	minutes	-	-

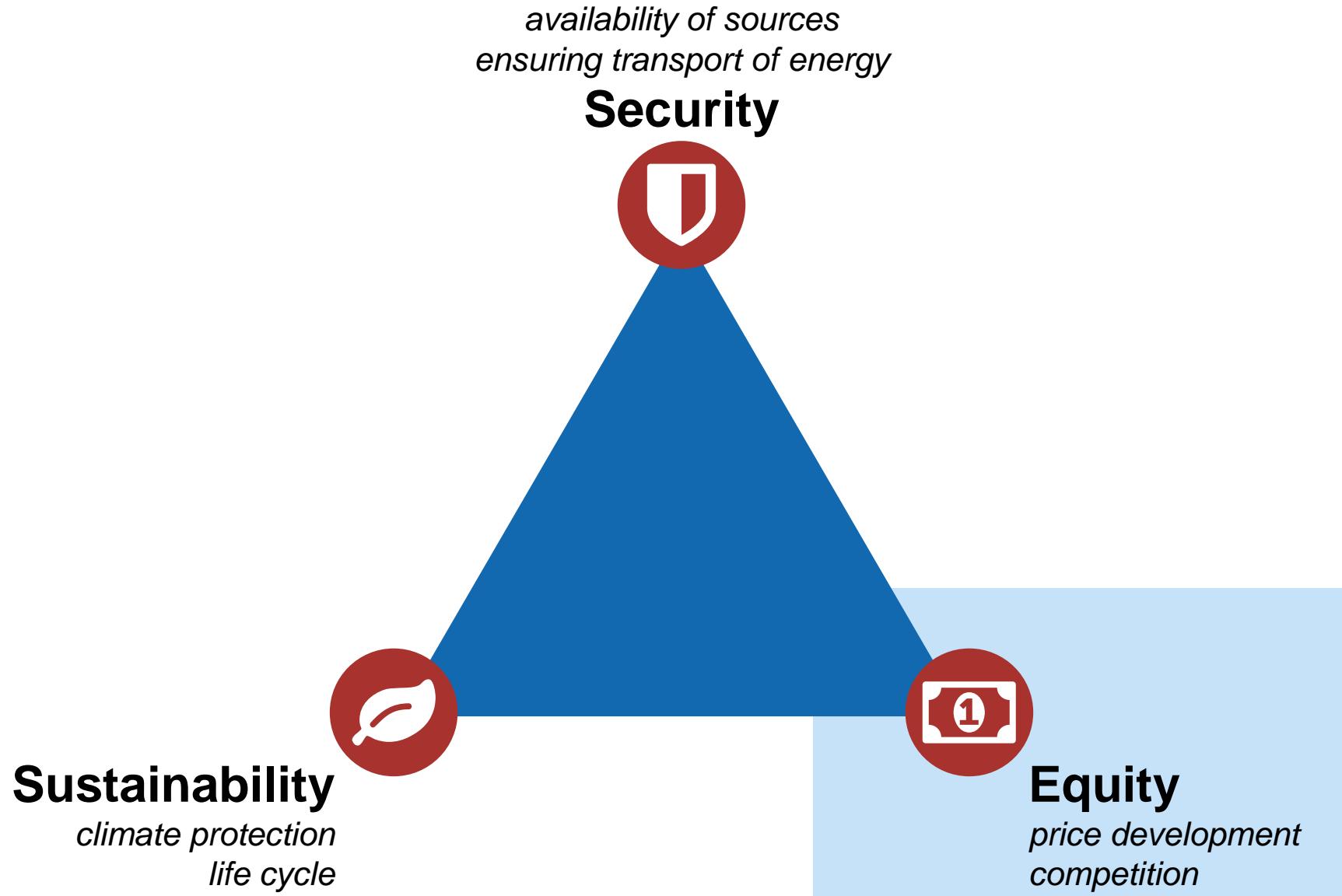
Source: IPCC

# Characteristics of renewables

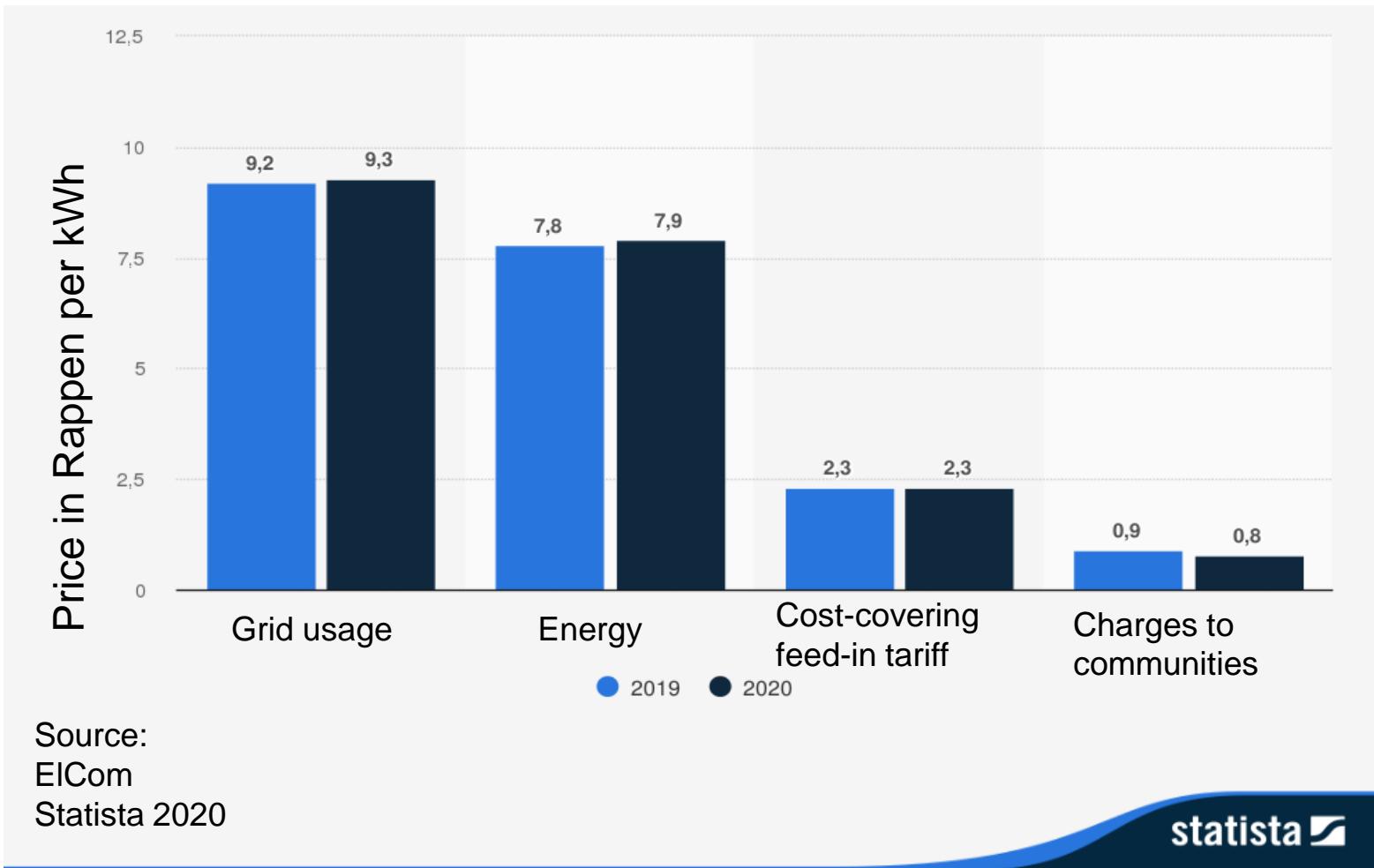
energy source / technology		power / MW	characteristic time scales for power system operation	dispatchability	predictability
Bioenergy					+
Geothermal					+
sun	Photovoltaic				-
	concentrated solar power				+
	with the sun				
			ABSTRACT		
water	run of river	0.1 - 1.500	hours	+/-	+
	reservoir	1 - 20.000	days	+	+
	tides	0.1 – 300	hours	-	+
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Source: IPCC

# Energy trilemma - Requirements of energy systems



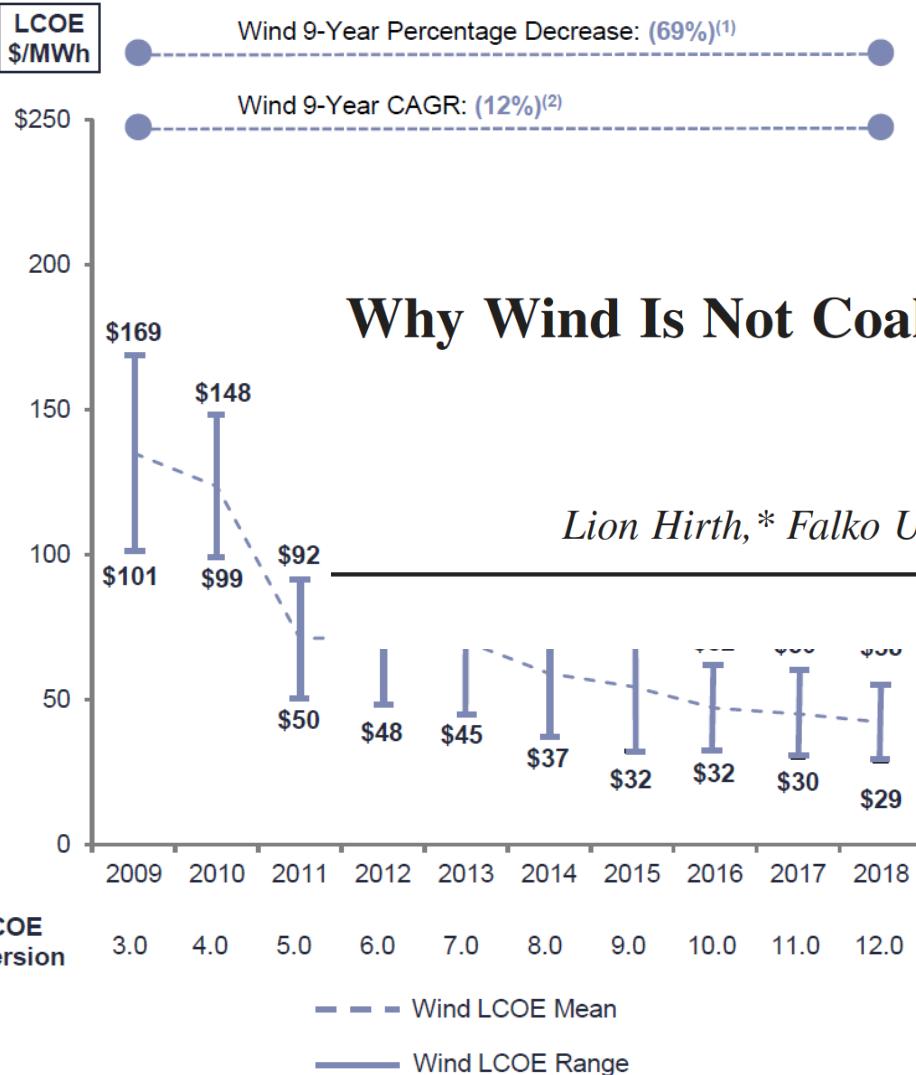
# Electricity price for households in Switzerland



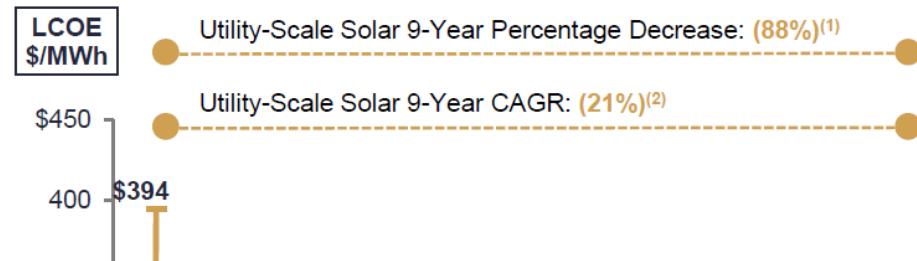
# Levelized cost of renewable Energy

<https://www.lazard.com/perspective/lcoe2019>

## Unsubsidized Wind LCOE



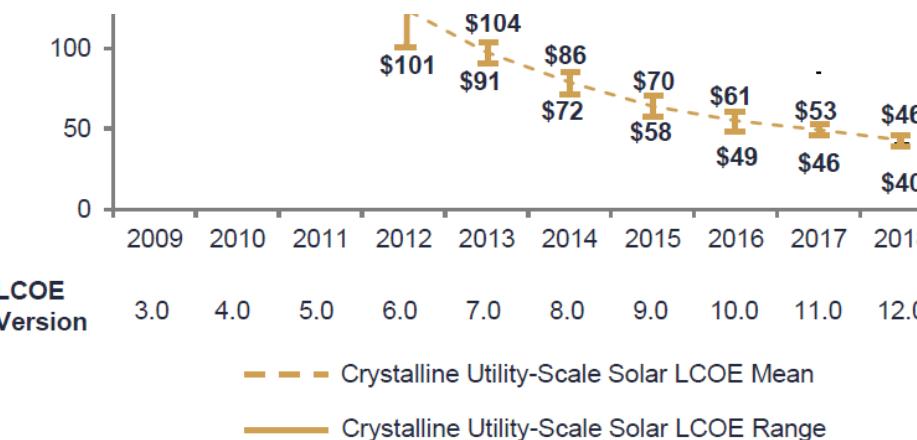
## Unsubsidized Solar PV LCOE



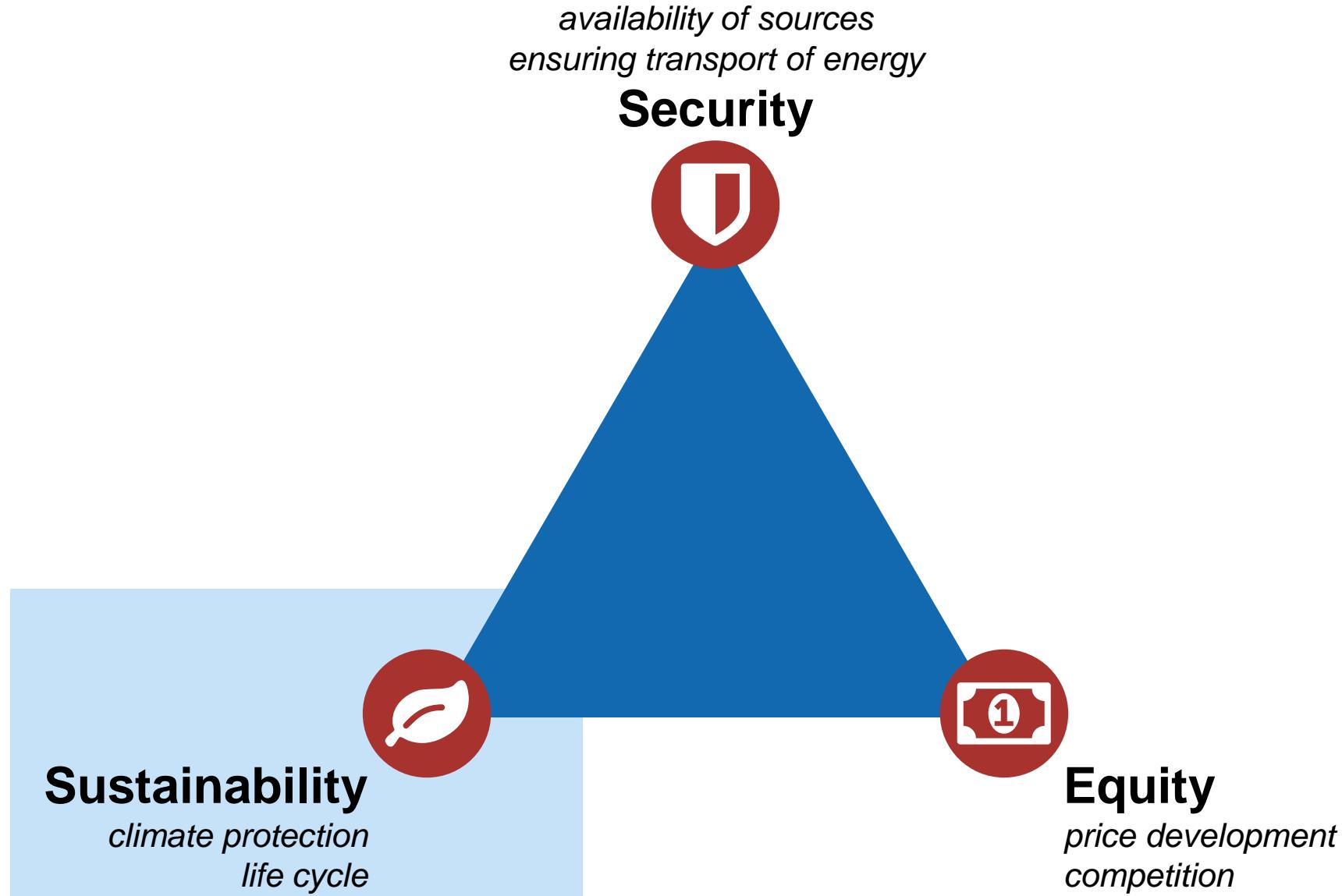
## Why Wind Is Not Coal: On the Economics of Electricity Generation

Lion Hirth,\* Falko Ueckerdt,\*\* and Ottmar Edenhofer\*\*\*

### ABSTRACT

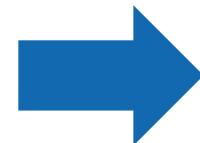


# Energy trilemma - Requirements of energy systems



# Swiss plans for GHG emissions

- by 2030: reduce GHG emissions by 50% compared to 1990
- by 2050: no more net GHG emissions



achieve at least 30% in Switzerland and a maximum of 20% abroad

<https://www.admin.ch/gov/en/start/documentation/media-releases.msg-id-76206.html>

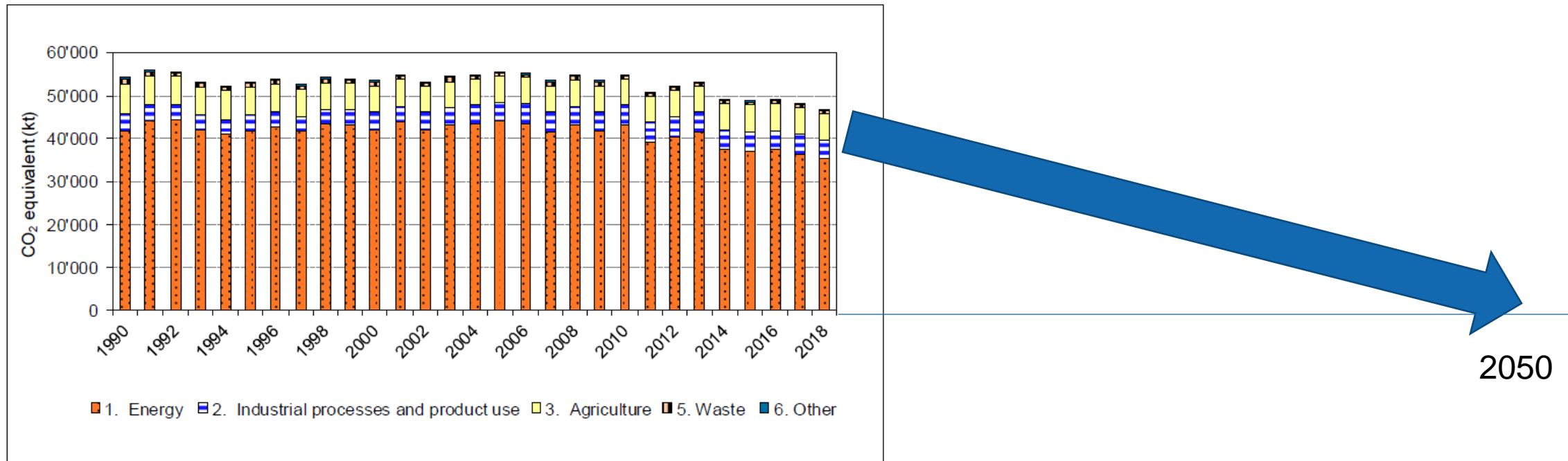


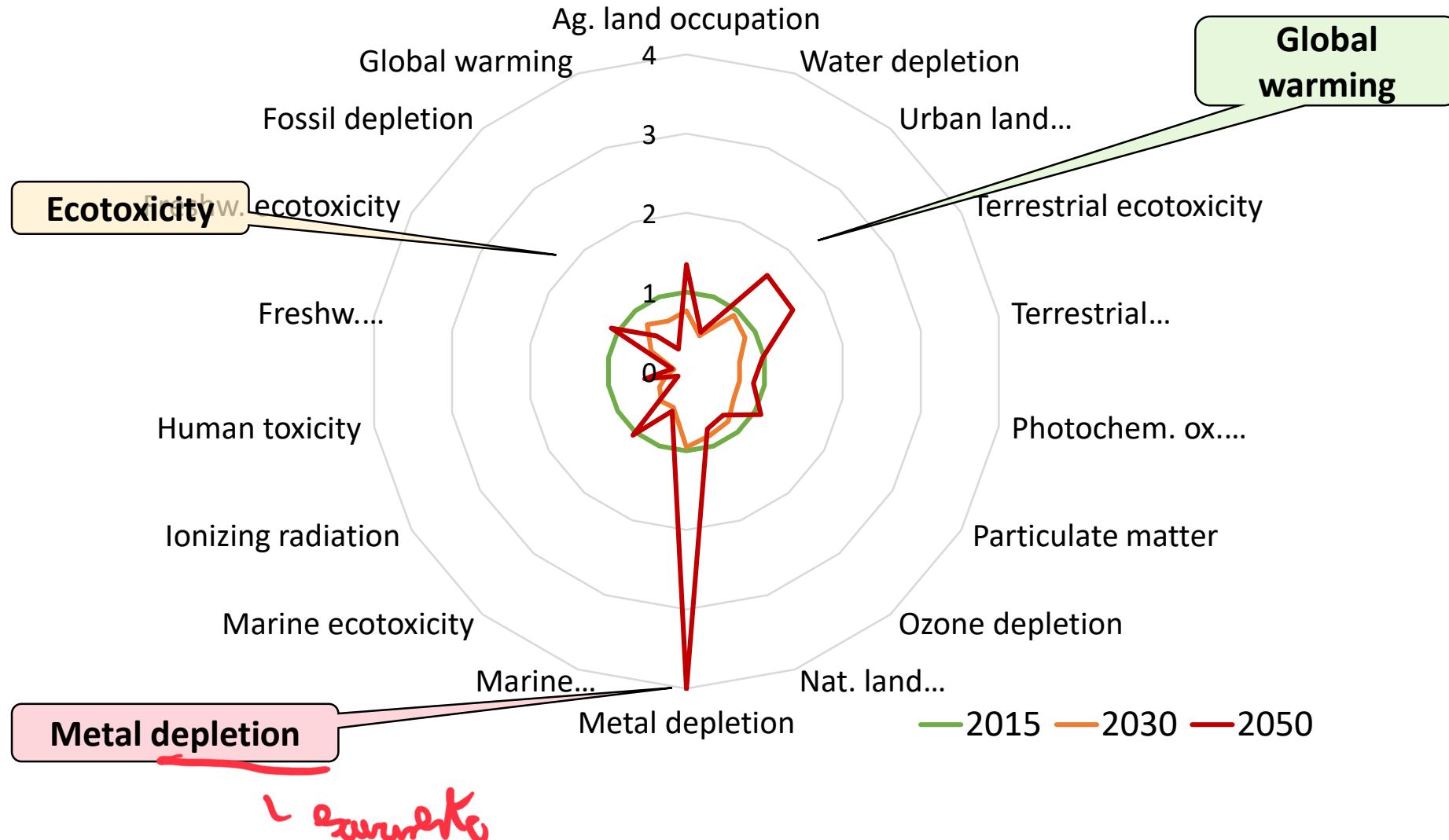
Figure 2-4 Greenhouse gas emissions in CO<sub>2</sub> equivalent (kt) by sectors (excluding LULUCF, excluding indirect CO<sub>2</sub>).

# Example of a large-scale energy system model

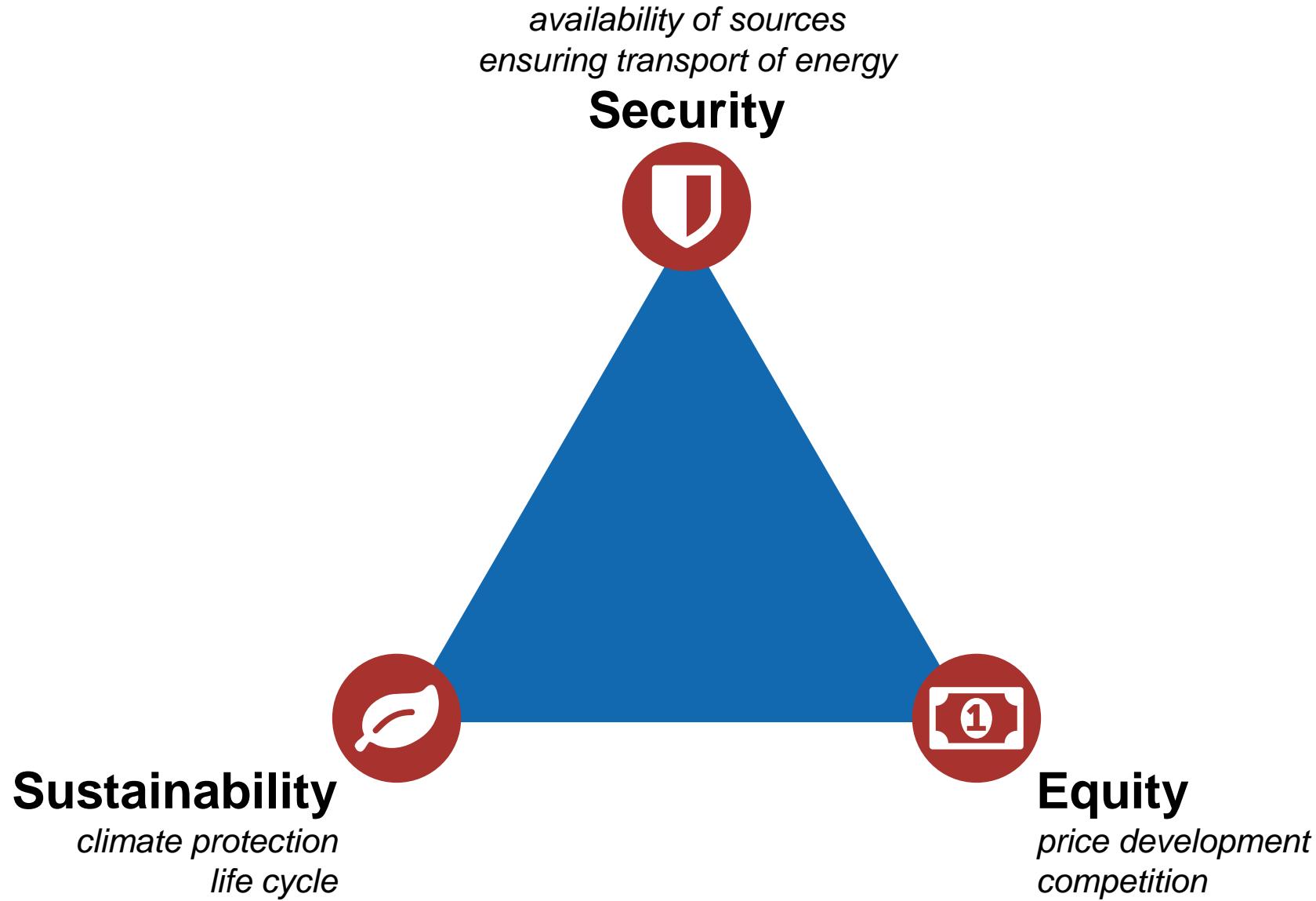


- 28 countries (EU +)
- International grid 
- Fossil and renewable **plants**
- Electricity demands
- Heating  
(Households + industry)  
*(Households + industry)*
- Transport (passenger cars) 
- Weather data

# Environmental impacts of the future energy system: Burden shifting



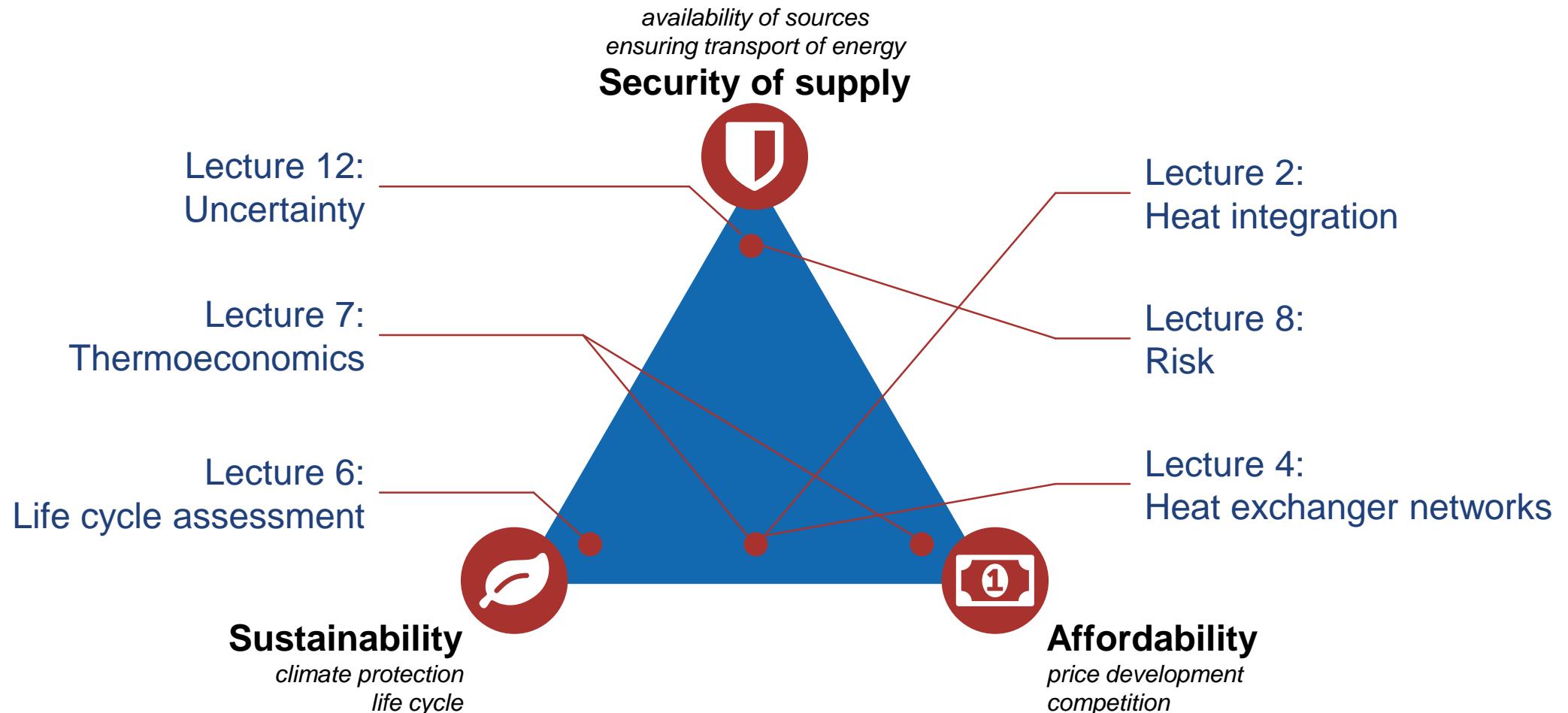
# Energy trilemma – Objectives of the energy system



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# Course content in the energy trilemma



## Methods & Models:

Lecture 3 & 5:  
Optimization

Lecture 9:  
Conversion

Lecture 10:  
Storage

Lecture 11:  
Transport

# After this lecture, you are able to...

- ✓ **plan your participation** in this course
- ✓ **explain the scope of this course**
  - ✓ name the difference between primary energy, final energy, and useful energy.
  - ✓ discuss the need for sustainable energy systems.
  - ✓ summarize sources of complexity in multi-energy systems.
- ✓ recognize tradeoffs in the **energy trilemma**
- classify **mathematical models**



# Introduction to Modeling and Optimization of Sustainable Energy Systems

*Modeling*

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# Why Modeling?

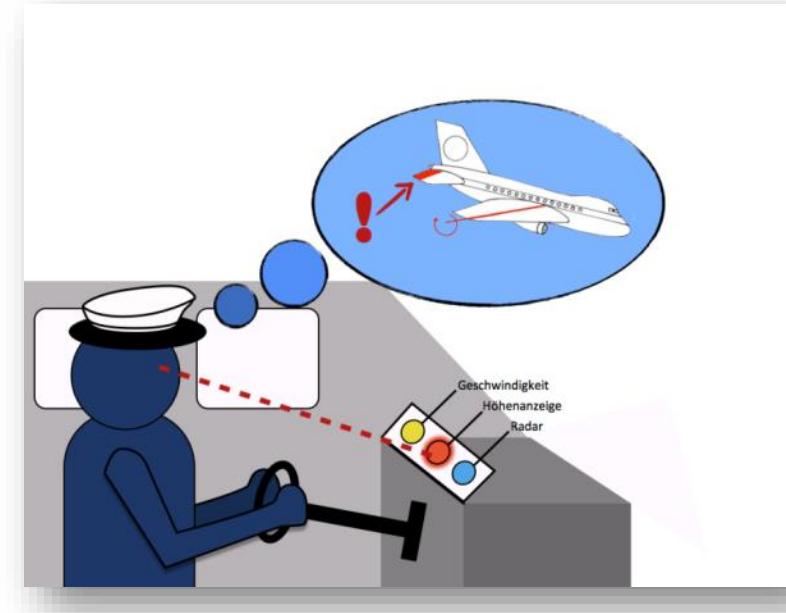
- A model allows the performance of experiments / measurements that cannot be performed on the real system.
- A model is often cheaper than an experiment.
- No damage can be caused to the real system.

# Model vs. reality



# Types of models

- mental models



# Types of models

- mental models
- physical models

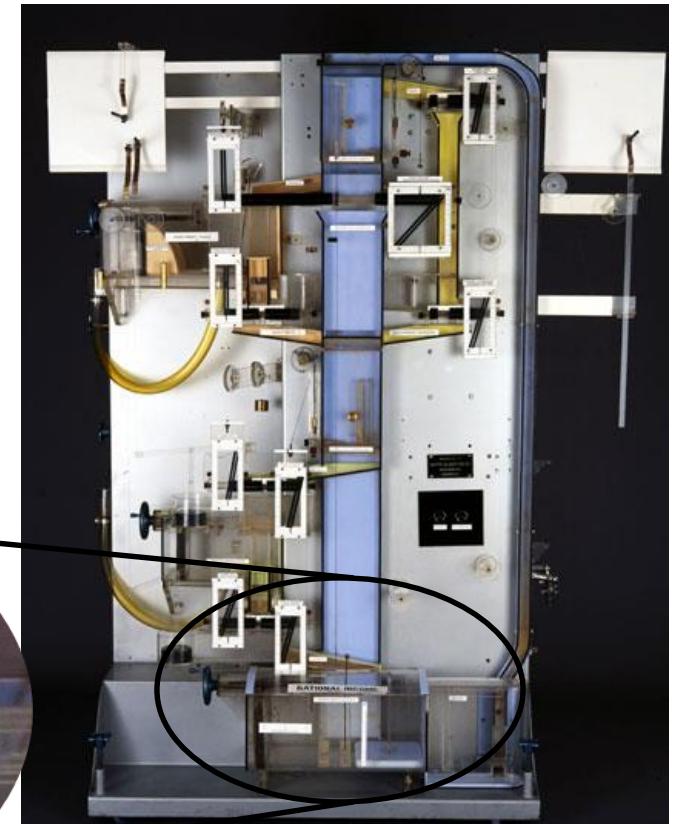


[https://de.wikipedia.org/wiki/Datei:Europaviertel\\_modell.jpg](https://de.wikipedia.org/wiki/Datei:Europaviertel_modell.jpg)

# Types of models

- mental models
- physical models
- models from analogies

MONIAC: <https://youtu.be/rAZavOcEnLg>



[collection.science museum group.org.uk/objects/co64127/phillips-economic-computer-analog-computer](http://collection.science museum group.org.uk/objects/co64127/phillips-economic-computer-analog-computer)

# Types of models

- mental models
- physical models
- models from analogies
- **Mathematical models**

$$C = \sum_{i=0}^n c_i(t) (m_B H_U)_i$$

$$(m_B H_U)_i = \int_{t=0}^T \eta_{\text{th},i}(t) \dot{Q}_{H,i}(t) dt$$

$$\dot{Q}_H(t) = \sum_{i=0}^n \dot{Q}_{H,i}(t)$$

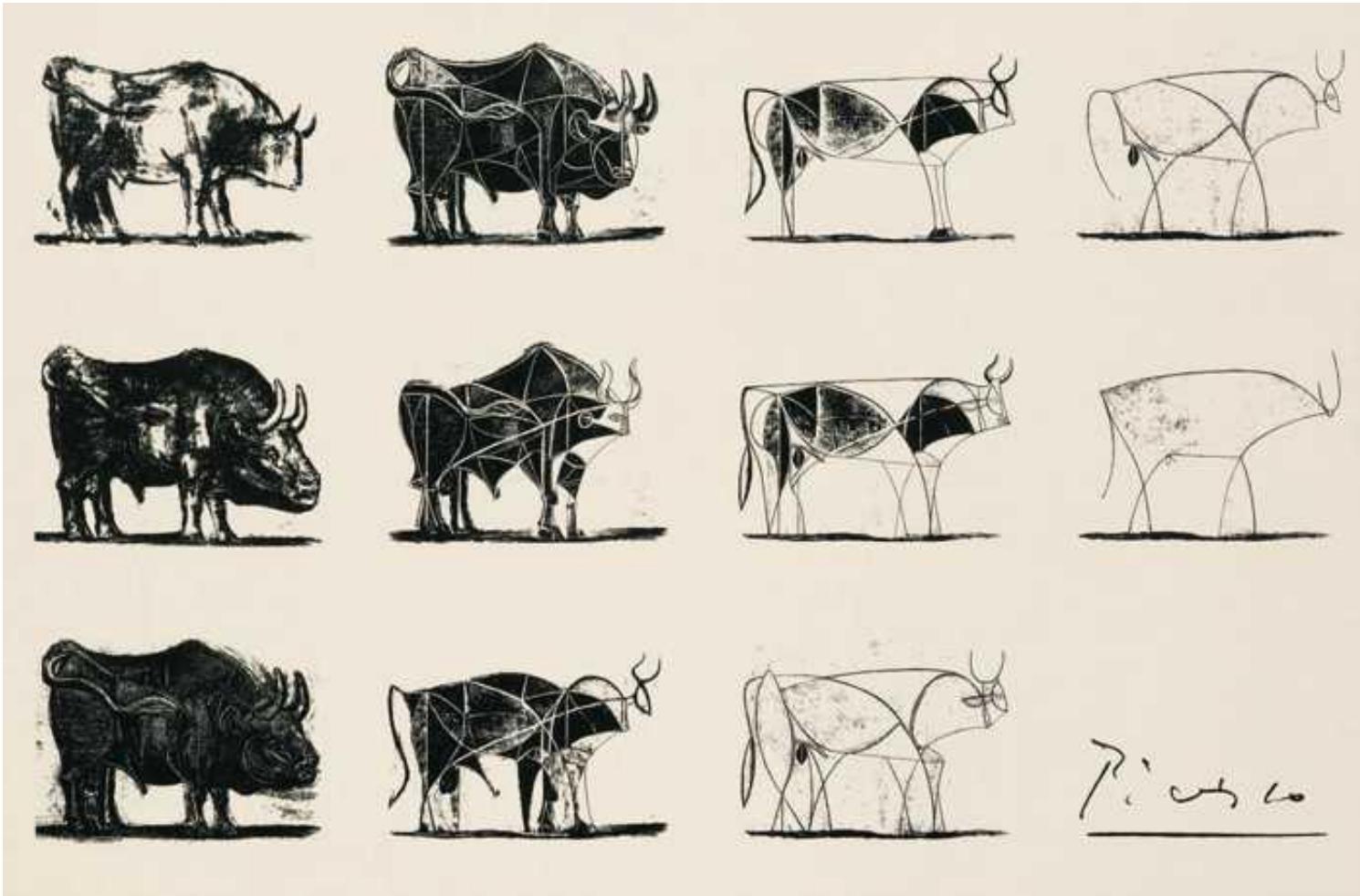
$$\dot{Q}_{H,i}(t) \leq u_i(t) \dot{Q}_{H,i}^{\text{Nenn}} \quad \forall i = 1..n$$

$$\dot{Q}_{H,i}(t) \geq u_i(t) x_{\min} \dot{Q}_{H,i}^{\text{Nenn}} \quad \forall i = 1..n$$

$$T_{\min,i} \geq \int_{t=0}^T u_i(t) dt \quad \forall i = 1..n$$

$$\eta_{\text{th},i}(t) = f(\dot{Q}_{H,i}(t)) \quad \forall i = 1..n$$

# Which model is the right model?



# Classes of mathematical models

## Example energy system

# Classes of mathematical models

Example energy system: Boiling water on a camping stove



Idea: use a model to make predictions about boiling water.

# Mathematical modeling: Steam production

How much steam do we produce when boiling?



understand the problem

Which properties are relevant?

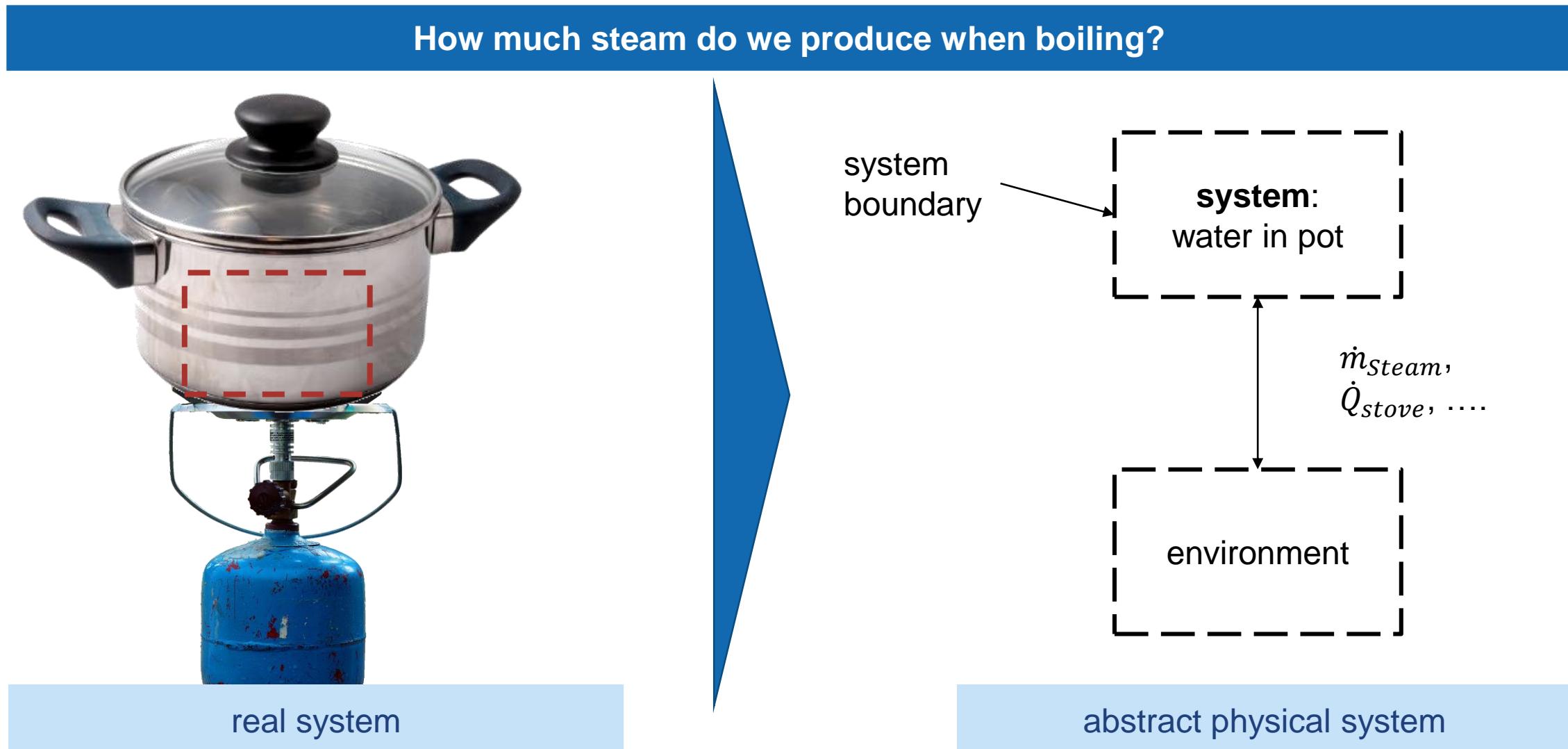
- temperature of water  $T_{water}$
- gas flow of stove  $\dot{m}_{gas}$
- geometry of pot  $r, h$
- heating supply  $\dot{Q}_{stove}$
- ...

identify relationships

heating supply  $\leftrightarrow$  gas flow of stove

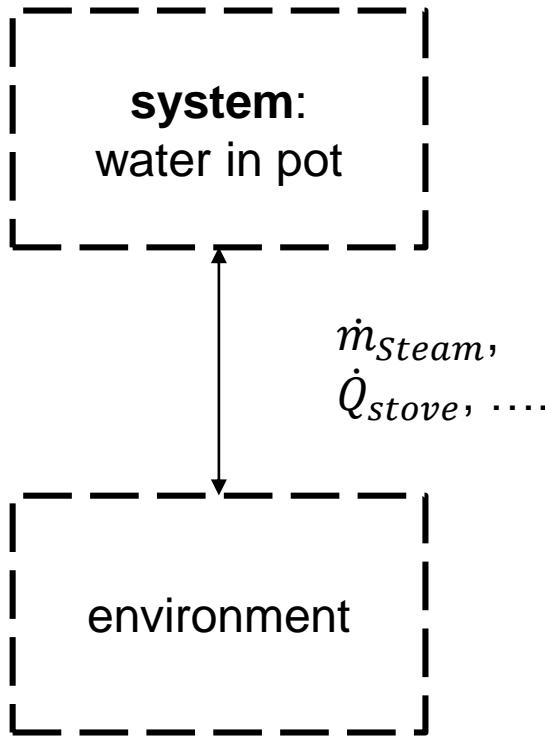
...

# Mathematical modeling: Balances



# Mathematical modeling: Steam production

How much steam do we produce when boiling?



assumptions

- ideally mixed water
- steady state
- no uncertain events

dimension

0D

time

static

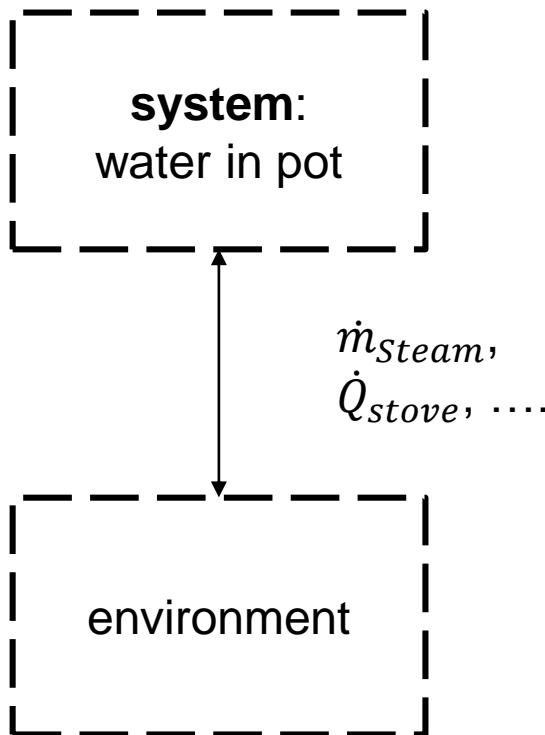
predictability

deterministic

abstract physical system

# Mathematical modeling: Steam production

How much steam do we produce when boiling?



Balance equations:

$$0 = \dot{Q}_{stove} - \dot{m}_{steam} \cdot h''(100\text{ }^{\circ}\text{C}, 1\text{ bar}) - \dot{Q}_{loss}$$

Literature

#variables > #equations  
⇒ Underdetermined system

Do we know more equations?

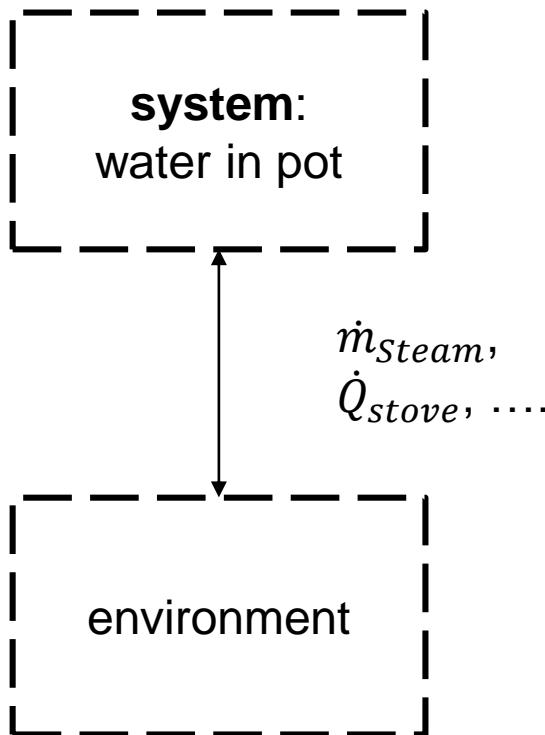
abstract physical system

unknown = variables  
known = parameters

dimension	0D
time	static
predictability	deterministic

# Mathematical modeling: Steam production

How much steam do we produce when boiling?



abstract physical system

unknown = **variables**  
known = **parameters**

Balance equations:

$$0 = \dot{Q}_{stove} - \dot{m}_{Steam} \cdot h''(100\text{ }^{\circ}\text{C}, 1\text{ bar}) - \dot{Q}_{loss}$$

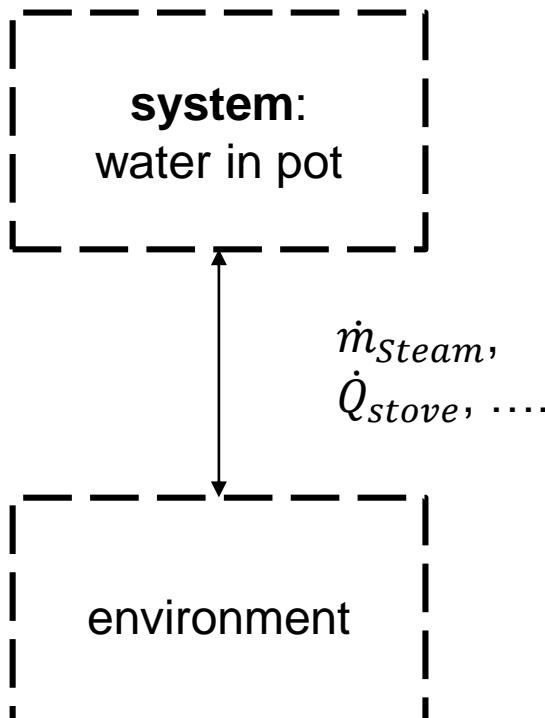
$$\begin{aligned}\dot{Q}_{stove} &= \dot{m}_{gas} \cdot \Delta h_{gas} && \text{Literature} \\ \dot{Q}_{loss} &= A_w \cdot \alpha \cdot (T_{water} - T_{envir}) && \begin{array}{l} \text{Thermometer} \\ \text{Manual of stove} \end{array} \\ & & & \text{Geometry}\end{aligned}$$

#variables = #independent equations  
→ solvable

dimension	0D
time	static
predictability	deterministic

# Mathematical modeling: Steam production

How much steam do we produce when boiling?



abstract physical system

unknown = variables  
known = parameters

Balance equations:

$$0 = \dot{Q}_{stove} - \dot{m}_{Steam} \cdot h''(100\text{ }^{\circ}\text{C}, 1\text{ bar}) - \dot{Q}_{loss}$$

$$\dot{Q}_{stove} = \dot{m}_{gas} \cdot \Delta h_{gas}$$

$$\dot{Q}_{loss} = A_w \cdot \alpha \cdot (T_{water} - T_{envir})$$

Variables are only multiplied with parameters. All equations are linear!

All variables are continuous

equations	linear
variables	continuous
dimension	0D
time	static
predictability	deterministic

# Mathematical modeling: Steam production

How much steam do we produce when boiling?



real system

increasing complexity →

dimension	0D	?
time	static	?
variables	continuous	?
equations	linear	?
predictability	deterministic	?

# Mathematical modeling: Steam production

How long does it take until the water boils?



Balance equations:

$$0 = \dot{Q}_{stove} - \dot{m}_{steam} \cdot h''(100^\circ C, 1 \text{ bar}) - \dot{Q}_{loss}$$

$$\dot{Q}_{stove} = \dot{m}_{gas} \cdot \Delta h_{gas}$$

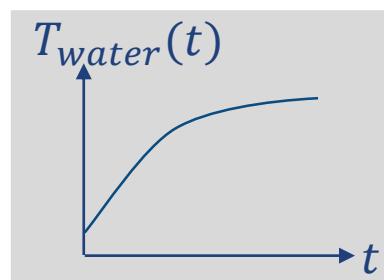
$$\dot{Q}_{loss} = A_w \cdot \alpha \cdot (T_{water} - T_{envir})$$

increasing complexity  
→

dimension	0D	
time	static	
variables	continuous	
equations	linear	
predictability	deterministic	

# Mathematical modeling: Steam production

How long does it take until the water boils?



Balance equations:

$$m \cdot c_p \cdot dT_{water}(t)/dt = \dot{Q}_{stove} - \dot{Q}_{loss}$$

$$\dot{Q}_{stove} = \dot{m}_{gas} \cdot \Delta h_{gas}$$

$$\dot{Q}_{loss} = A_w \cdot \alpha \cdot (T_{water}(t) - T_{envir})$$

increasing complexity →

dimension	0D	
time	static	dynamic
variables	continuous	
equations	linear	
predictability	deterministic	

# Mathematical modeling: Steam production

How long does it take until the water boils?



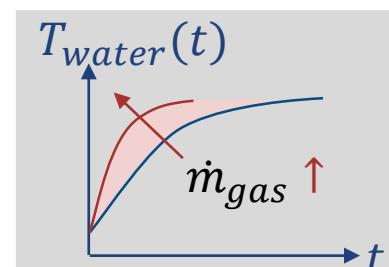
Balance equations:

$$m \cdot c_p \cdot dT_{water}(t)/dt = \dot{Q}_{stove} - \dot{Q}_{loss}$$

$$\dot{Q}_{stove} = \dot{m}_{gas} \cdot \Delta h_{gas}$$

$$\dot{Q}_{loss} = A_w \cdot \alpha \cdot (T_{water}(t) - T_{envir})$$

controllable



increasing complexity →

dimension	0D	
time	static	dynamic
variables	continuous	
equations	linear	
predictability	deterministic	

# Mathematical modeling: Steam production

How long does it take until the water boils?



Balance equations:

$$m \cdot c_p \cdot dT_{water}(t)/dt = \dot{Q}_{stove} - \dot{Q}_{loss}$$

$$\dot{Q}_{stove} = \boxed{\dot{m}_{gas} \cdot \Delta h_{gas}}$$

$$\dot{Q}_{loss} = A_w \cdot \alpha \cdot (T_{water}(t) - T_{envir})$$

controllable

increasing complexity →

dimension	0D	dynamic
time	static	
variables	continuous	
equations	linear	
predictability	deterministic	

# Mathematical modeling: Steam production

$$\alpha = \frac{k}{L} \left( 0.825 + \frac{0.387 \text{Ra}_L^{1/6}}{(1 + (0.492/\text{Pr})^{9/16})^{8/27}} \right)^2$$

$$\text{Ra}_L < 10^{12}$$

until the water boils?

$k$  is the thermal conductivity of the fluid,

$L$  is the characteristic length with respect to the direction of gravity

$$\text{Ra}_x = \frac{g\beta}{\nu\alpha} (T_s - T_\infty) x^3 = \text{Gr}_x \text{Pr}$$

where:

$x$  is the characteristic length

$\text{Ra}_x$  is the Rayleigh number for characteristic length  $x$

$g$  is

$\beta$  is

$\nu$  is

$\alpha$  is

$T_s$  is the surface temperature

$T_\infty$  is the quiescent temperature (fluid temperature far from the surface of the object)

$\text{Gr}_x$  is the Grashof number for characteristic length  $x$

$\text{Pr}$  is the Prandtl number

Nonlinear!



of

$$\text{Pr} = \frac{\nu}{\alpha} = \frac{\text{momentum diffusivity}}{\text{thermal diffusivity}} = \frac{\mu/\rho}{k/(c_p\rho)} = \frac{c_p\mu}{k}$$

where:

- $\nu$ : momentum diffusivity (kinematic viscosity),  $\nu = \mu/\rho$ , (SI units:  $\text{m}^2/\text{s}$ )
- $\alpha$ : thermal diffusivity,  $\alpha = k/(c_p\rho)$ , (SI units:  $\text{m}^2/\text{s}$ )
- $\mu$ : dynamic viscosity, (SI units:  $\text{Pa s} = \text{N s/m}^2$ )
- $k$ : thermal conductivity, (SI units:  $\text{W/m}\cdot\text{K}$ )
- $c_p$ : specific heat, (SI units:  $\text{J/kg}\cdot\text{K}$ )
- $\rho$ : density, (SI units:  $\text{kg/m}^3$ ).

Balance equations:

$$m \cdot c_p \cdot dT_{water}(t)/dt = \dot{Q}_{stove} - \dot{Q}_{loss}$$

$$\dot{Q}_{stove} = \dot{m}_{gas} \cdot \Delta h_{gas}$$

$$\dot{Q}_{loss} = A_w \cdot \alpha(T_{Water}(t)) \cdot (T_{Water}(t) - T_{Envir.})$$

Thermo II:  
Heat transfer coefficient  
is not constant

increasing complexity

dimension	0D	1D
time	static	dynamic
variables	continuous	discrete
equations	linear	
predictability	deterministic	

# Mathematical modeling: Steam production

**How long does it take until the water boils?**

**ETH** Thermodynamik II

bekannter Körper

Kartesisches Koordinatensystem

$\dot{Q}_{x+dx} = \dot{Q}_x + \frac{\partial \dot{Q}_x}{\partial x} dx + \underbrace{\left( \frac{1}{2!} \cdot \frac{\partial^2 \dot{Q}}{\partial x^2} \cdot dx^2 + \dots \right)}_{\text{Glieder höherer Ordnung}}$

$\dot{Q}_{y+dy} = \dot{Q}_y + \frac{\partial \dot{Q}_y}{\partial y} dy + (\text{G.h.O.})$

$\dot{Q}_{z+dz} = \dot{Q}_z + \frac{\partial \dot{Q}_z}{\partial z} dz + (\text{G.h.O.})$

Grösse der Quelle [W/m<sup>3</sup>]

Eintritt Austritt

**location dependent**

$\frac{dT}{dt} = \dot{Q}_{stove} - \dot{Q}_{loss}$

$\Delta h_{gas}$

$T_{water}(t) \cdot (T_{water}(t) - T_{Envir.})$

increasing complexity →

dimension	0D	1D
time	static	dynamic
variables	continuous	discrete
equations	linear	nonlinear
predictability	deterministic	probabilistic

Thermo II: Heat transfer in multiple dimensions  
→ temperature gradient in pot

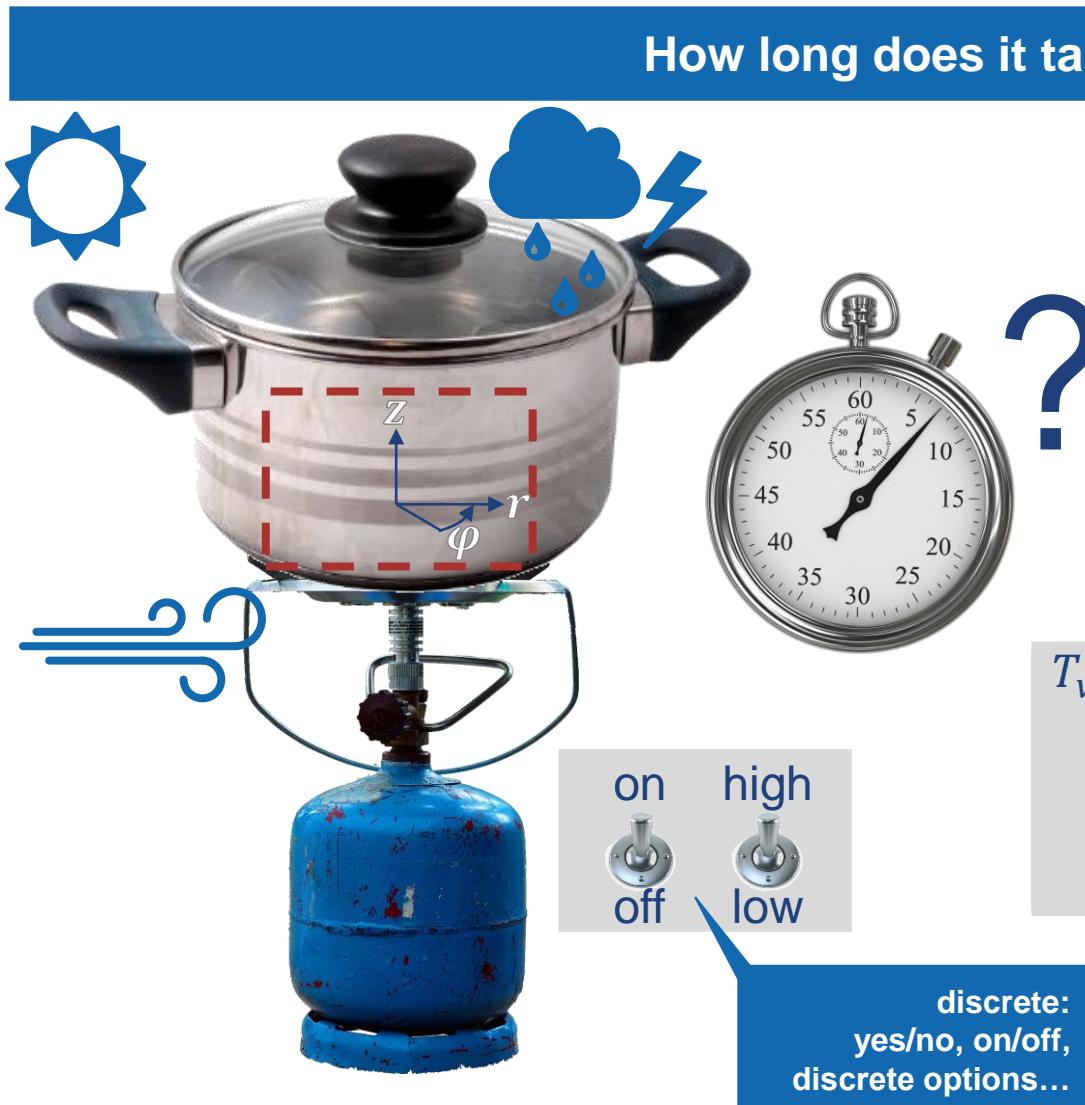
Lecture 1

9/28/2021

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# Mathematical modeling: Steam production

How long does it take until the water boils?



location dependent

Balance equations:

$$m \cdot c_p \cdot dT_{water}(t)/dt = \dot{Q}_{stove} - \dot{Q}_{loss}$$
$$\dot{Q}_{Stove} = \dot{m}_{gas} \cdot \Delta h_{gas}$$
$$\dot{Q}_{loss} = A_w \cdot \alpha(T_{water}(t)) \cdot (T_{water}(t) - T_{Envir.})$$

increasing complexity →

Stochastic changes		0D	3D
time	static	dynamic	discrete
variables	continuous	discrete	nonlinear
equations	linear	deterministic	
predictability			

$T_{water}(t)$

$\dot{m}_{gas} \uparrow$

discrete:  
yes/no, on/off,  
discrete options...

ETH zürich

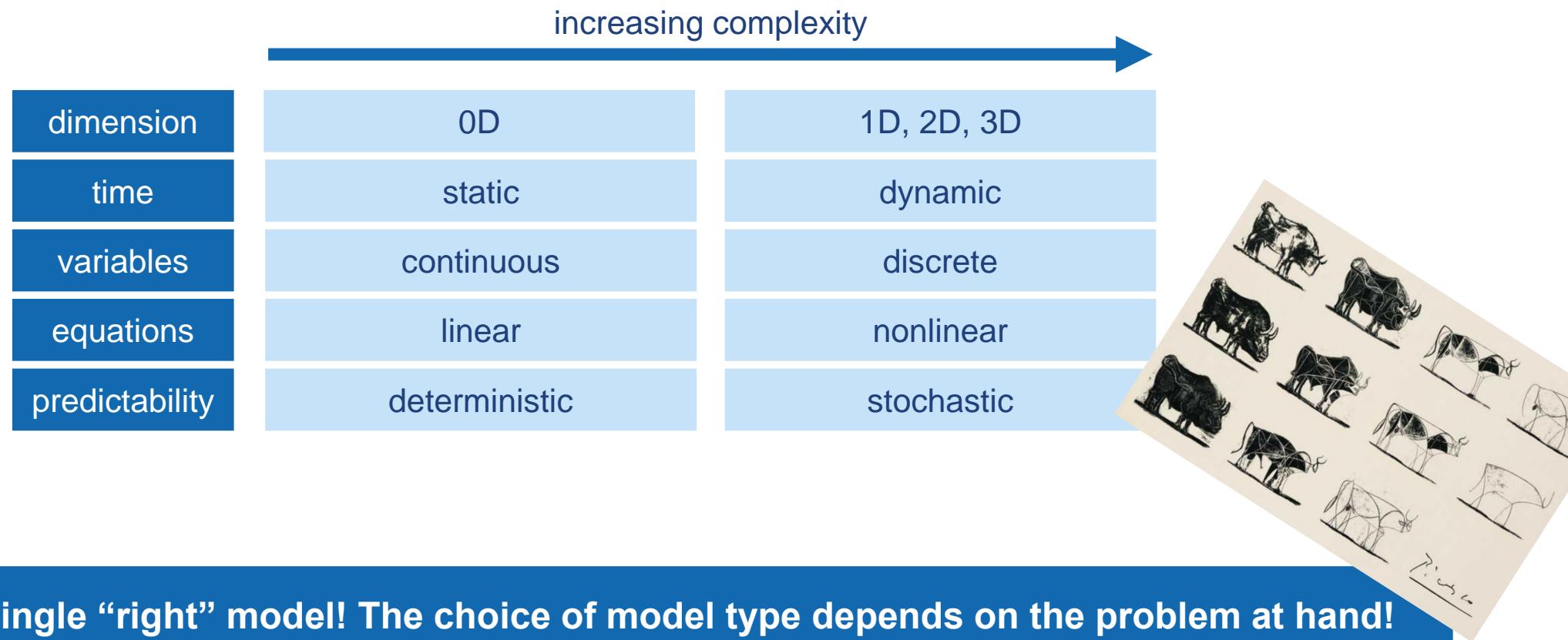
André Bardow & Giovanni Sansavini | Introduction to Modeling and Optimization of Sustainable Energy Systems | Lecture 1

9/28/2021

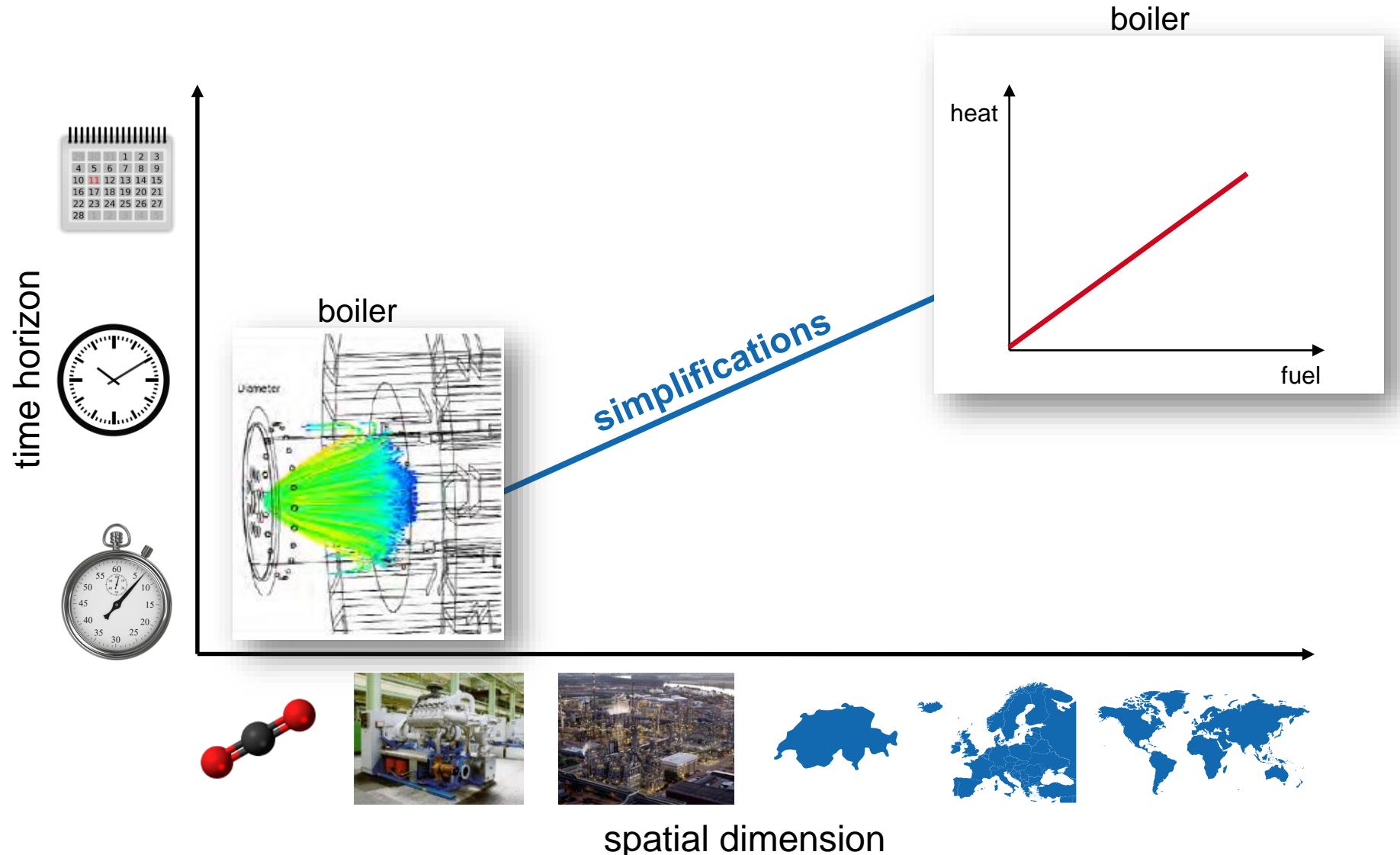
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# Mathematical model types

## Summary

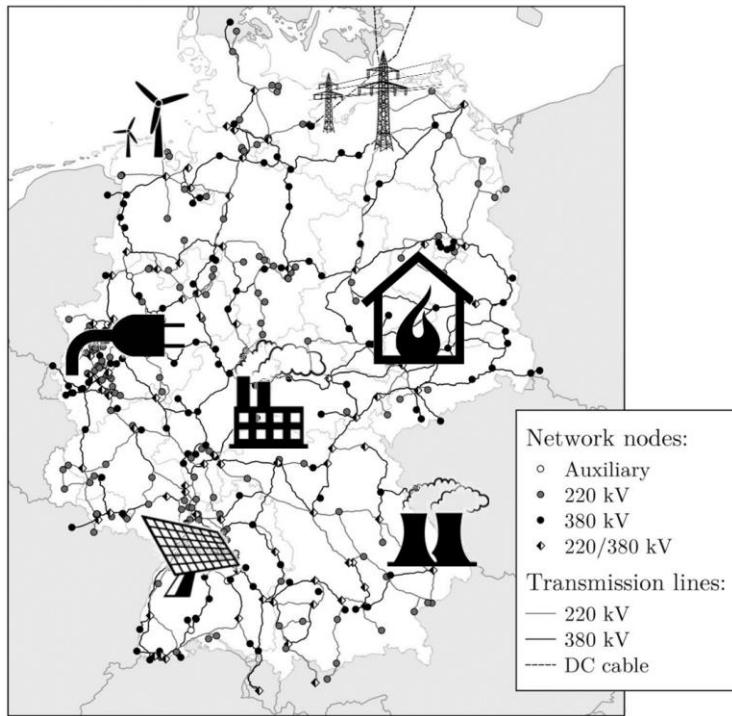


# Modeling scales



# National energy system models

## How to steer the energy transition?



dimension  
time  
variables  
equations  
predictability

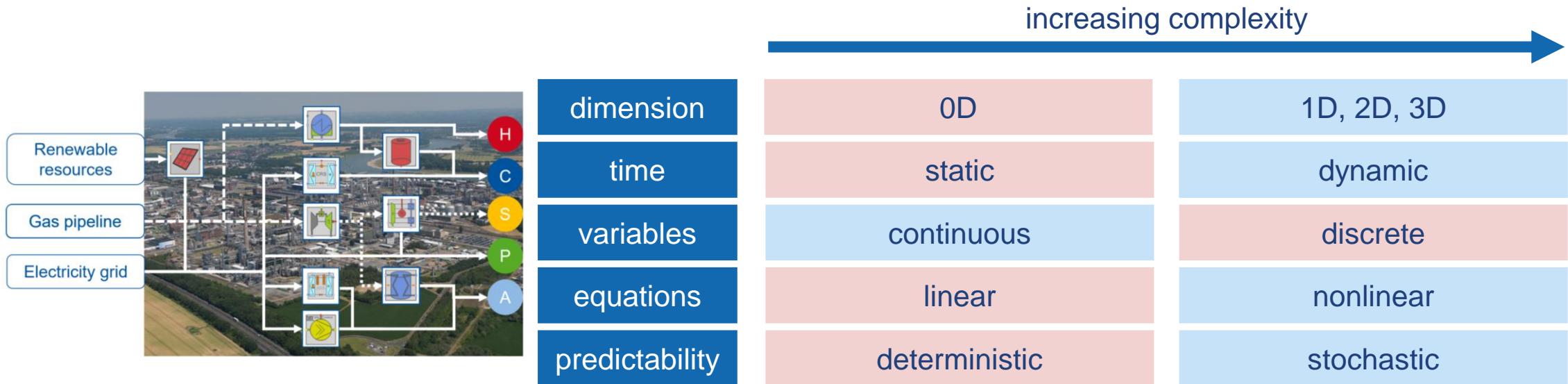
increasing complexity

0D	1D, 2D, 3D
static	dynamic
continuous	discrete
linear	nonlinear
deterministic	stochastic

Figure: Egerer, 2016, Open Source Electricity Model for Germany (ELMOD-DE)

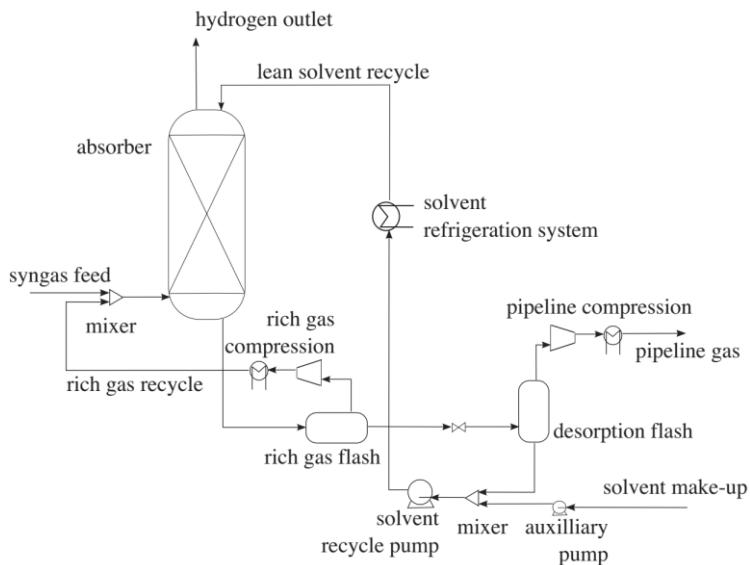
# Industrial energy system design

## How to invest into new equipment?



# Working fluid selection

Which working fluid to use to capture CO<sub>2</sub> ?

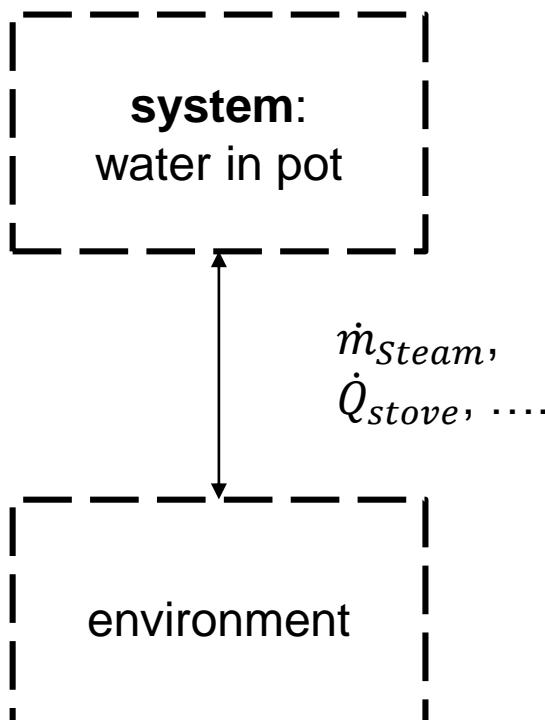


dimension	increasing complexity	
time	0D	1D, 2D, 3D
variables	static	dynamic
equations	continuous	discrete
predictability	linear	nonlinear
	deterministic	stochastic

Lampe, Matthias, et al. *Computer-aided molecular design in the continuous-molecular targeting framework using group-contribution PC-SAFT*. *Computers & Chemical Engineering* 81 (2015).

# From mathematical modeling to optimization

Before: How much steam do we produce when boiling?



abstract physical system

unknown = **variables**  
known = **parameters**

Balance equations:

$$0 = \dot{Q}_{stove} - \dot{m}_{Steam} \cdot h''(100 \text{ }^{\circ}\text{C}, 1 \text{ bar}) - \dot{Q}_{loss}$$

$$\dot{Q}_{stove} = \dot{m}_{gas} \cdot \Delta h_{gas} \quad \text{Literature}$$

$$\dot{Q}_{loss} = A_w \cdot \alpha \cdot (T_{water} - T_{envir})$$

#variables = #independent equations  
→ solvable

dimension	0D
time	static
predictability	deterministic

# Degree of freedom analysis

Degree of freedom  $d$  of a model  
is the difference of number of variables  $n_x$   
and number of independent equations  $n_e$ .

$$d = n_x - n_e$$

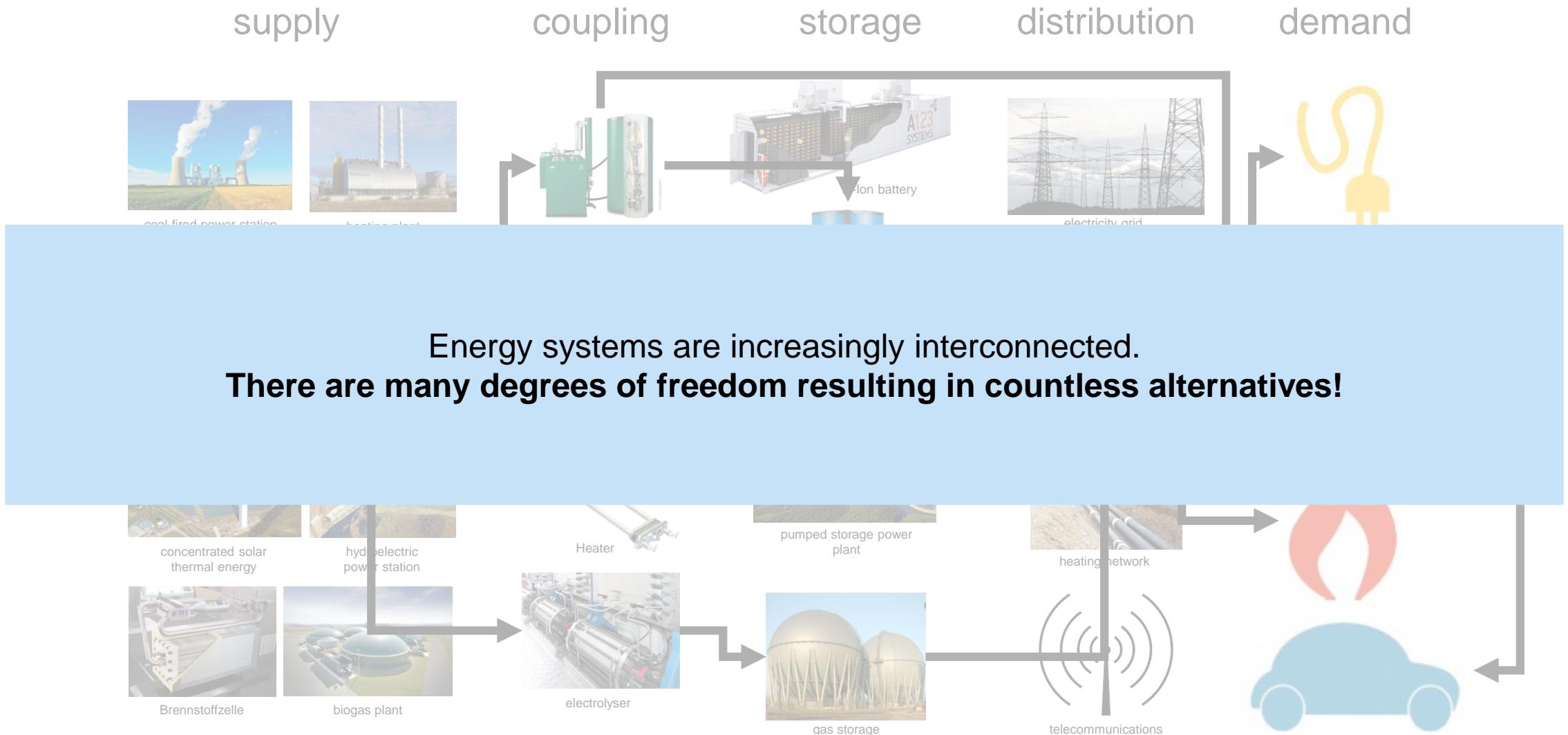


$$d > 0:$$

There is no unique solution!

**Which one of many solutions is the best?**

# Energy systems today: Which one of many solutions is the best?



# After this lecture, you are able to...

- ✓ explain the **scope of this course**
- ✓ explain **your participation** in this course
- ✓ recognize tradeoffs in the **energy trilemma**
- ✓ classify **mathematical models**