

## Dynamic system modeling for control and diagnosis



Energy system modeling, Fundamentals of thermodynamics and the model equations



#### Contents

- Introduction to thermodinamics
  - System and environment
  - Isolated system
    - Description of the system, statevariables
    - Extensive and intensive quantities
    - Ideal and real gas laws
  - Properties of water
  - Interactions
  - The internal energy
  - 1st law of thermodynamics
    - Work types in thermodinamics
  - Heat capacity, specific heat, enthalpy
  - Heat transfer
- Energy systems
  - A nuclear power plant
  - Lumped parameter models os the system
    - Heated solid pipe
    - Water pipe
    - Steam generator
    - Steam collector

## Introduction to thermodynamics (thermostatics)

- Concerns heat, energy, work, interaction between bodies, cycles
- Describes the *macroscopic* behaviour of the processes
- Fenomenological desciption
- Very common laws (energy conservation, dircetion of spontaneous processes) – widely reusable (in economics, black holes ...)
- Macroscopic variables:
  - Temperature, pressure
  - Density, specific heat,
  - Inner energy, enthalpy,
  - Entropy
  - etc



#### Introduction

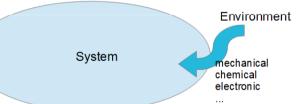
- Thermodynamic fields:
  - Engines, cycles (Carnot cycle), efficiency
  - Phase transitions
  - Chemical reactions
  - Transport (fluids, heat, mass, energy...)

Statevariables

#### ISOLATED SYSTEM DESCRIPTION

#### System and environment

- System and environment
  - We have to define them
  - Usually the system does not change the state of the environment
- Macroscopic description
  - Much larger than an atom
  - Not sensible by senses
- Physical state description
  - Measurable physical quantities
  - 2 groups: extensive and intensive quantities





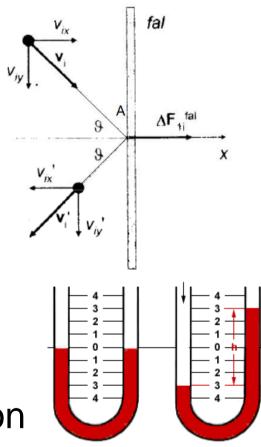
### System and equilibrium

- System in an environment
  - Ususally there are interaction between them
- Isolated system:
  - No interaction between the system and its environment
  - System will be in *equilibrium*:
    - The state does not change any more
  - States (állapotjellemzők):
    - Describes the system in equilibrium
    - Any two equilibrium can be distinguished by the state variables



#### Description of the system statevariables

- Pressure:
  - Pa (SI), 1 Pa = 1 N/m<sup>2</sup>
  - 1atm, 1bar, 10<sup>5</sup>Pa
  - Collisions of molecules and the wall
  - Absolute and overpressure
  - The pressure is independet of the direction





#### Statevariables

- Temperature
  - Measurement units: ℃ (Celsius), K (Kelvin)
  - Absolute zero (0 K = -273,15℃)
  - Measurement is complicated:
    - Needs a zero point and a linear scale
    - The thermometer has heat capacity
  - The temperature change has different effects, which can be used to measure
    - Heat expansion coefficient:

$$\frac{1}{V}\frac{\partial V}{\partial T} = \beta$$



#### Statevariables

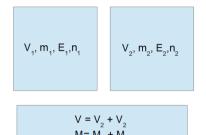
- Amount of substance (anyagmennyiség mólszám)
  - Measurement unit is: mol
  - 1 mol is the number of atoms in 12g C-12 isotope
  - 1 mol = 6.022e23 molecules or atom (Avogadro's number)
  - Number of atoms (N)
- Further properties:
  - Density and specific volume  $\rho = \frac{1}{\nu}$
  - Specific heat capacity



## Extensive and intensive

#### quantities

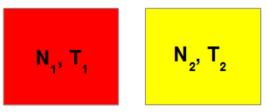
- Extensives:
  - Additivity
  - If you divide the system into two half, the quantity will be the half in each
  - Volume, energy, mass, number of molecules etc.

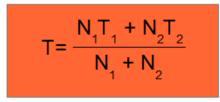






- Intensives:
  - Non-additive
  - Locally can be defined
  - Inhomogenity cause flows
  - Pressure, density, temperature ...

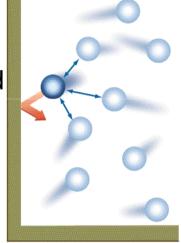




#### • IDEAL AND REAL GAS LAW'S

#### Basic system – ideal gas

- Ideal gas properties:
  - Gas molecules are small balls, the diameter of which can be neglected comparing to the *free path* (average distance between two collisions)
  - The only interaction between the molecules and between the molecules and vessel's wall is the elastic collision.
  - The movement direction of the molecules are random.
- Mass (m) / amount of substance (n), volume (V), pressure (p), temperature (T) describes the gas state.





### Ideal gas law

- Boyle-Mariotte law:
  - $p_1V_1 = p_2V_2 = const.$  if the temperature is const.
- Gay-Lussac law: • I.:  $\frac{V_1}{T_1} = \frac{V_2}{T_2} = const.$  if p is constant • II.:  $\frac{p_1}{T_1} = \frac{p_2}{T_2} = const.$  if V is constant
- Avogadro's law: •  $\frac{n_1}{V_1} = \frac{n_2}{V_2} = const.$  if p and T const.

#### Combined gas law:

 $^\circ~pV=nRT$  , where the universal gas constant R=8.31 J/mol/K



#### Real gas laws

- Van-der-Waals state equation:
  - In real gases there exist an attraction force between the particles which results higher pressure than in the ideal gas:

$$p + \frac{n^2 a}{V^2} = p_{id}$$

 In real gases the volume of the particles cannot be neglected, so there is smaller space in the vessel, than in the ideal case:

$$V - nb = V_{id}$$

• Substitute into the ideal gas law:  $(p + \frac{n^2 a}{V^2})(V - nb) = nRT$ 



#### Real gas laws

- Van der Waals
  - describes better the gases than the ideal gas law, but there are dozens of state-equations for various gases under different conditinos

#### Steam tables

- contains the properties of water and steam in different regions
- This are the most accurate source of information

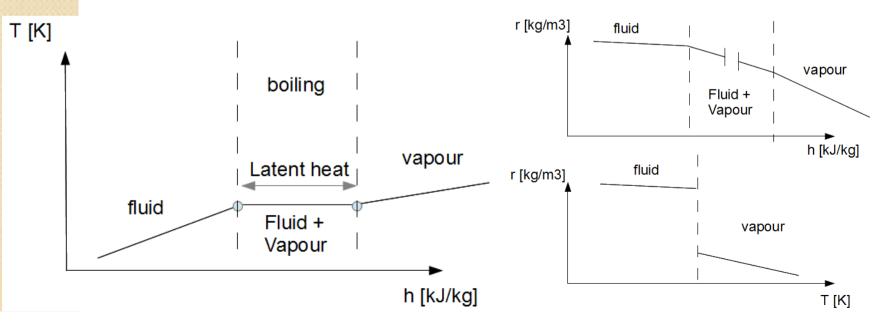
#### • THE WATER

#### The water and steam

- Most important media
  - Most frequently used material in the industries
- Accurate properties in steam tables
- 3 free parameter:
  - Pressure, temperature, volume
  - Pressure and enthalpy, volume
  - Etc.
- 2 parameter + saturated condition
  - o p\_sat = p\_sat(T\_sat)

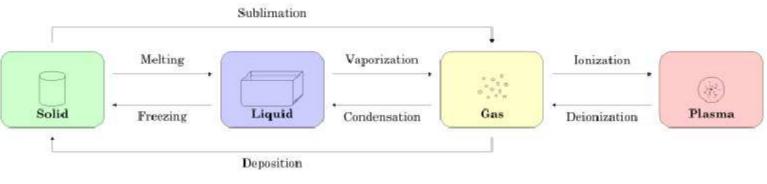
#### How to choose the state variables?

- Usual choice of intensive state variables:
  - In case of phase transition:
    - Pressure and enthalpy
    - Temperature is constant during the transition
  - In case there is no phase-transition
    - Pressure and temperature



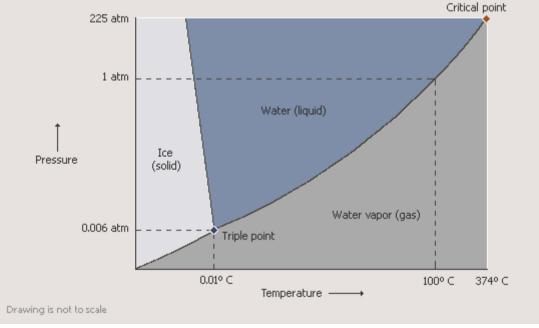
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### Phase transitions



Enthalpy of the system

#### Phase diagram of the water





#### Freezing and melting

• Transferred mass during melting:

$$\Delta M = \frac{\Delta Q}{L_m}$$

- The transferred heat does not change the temperature during the melting
- The melting temperature is depends on the pressure
  - Higher pressure cause lower melting point
  - Experiment with an icecube and a string
- Latent heat (L\_m [kJ/kg]):
  - The heat which is absorbed during the melting of 1 kg matter

### **Boiling and condensation**

• Transferred mass in phase transition:

$$\Delta M = \frac{\Delta Q}{L_v}$$

- The temperature does not change during the phase transition
- Why not to try to cook gulasch on Mont Everest?
  - The pressure affects the boiling point
  - Higher pressure cause higher boiling point
- The latent heat disappears approaching the critical point
- Above the critical point the vapour and fluid cannot be distinguished

#### • SZÜNET?



# Interactions – not isolated systems

- Mechanical interaction
  - Deformation
  - pressure difference (intensive)
  - Volume change (extensive)
- Electrostatic interaction
  - Different electrostatic potential (int.) cause the flow of the charge (ext.)
- Matterial interaction:
  - Mass transition (ext.)
  - Different concentration (chemical potential), (int.)



#### Equilibrium

- Processes goes to the equilibrium state (pressure and temperature differences disappears in time)
- Equilibrium necessary condition:
  - Spacial homogenity of all intensive quantity

#### System description

- As much number of statevariable as the number of interaction takes place is needed.
- Only extensive variables can be used for the description of the system, but only intensive variable is not enough – minimum one extensive variable is needed (what is the extent/size of the system?)
- Usually more statevariable then interaction => there are algebraic dependencies between them:
  - Stateequations
- Example:
  - Homogeneous system(statevariables: p,V,n,T) 4
  - Interactions: mechanic, thermic, matterial 3
  - F(p,V,T,n)=0, ideal gas: pV = nRT



## Energy exchange between the system & environment

- Experiences:
  - Mechanical work disappears bouncing ball
  - Warm bodys can exert mechanical work
- Let's do some work on a system what happens?

Joule's experiment:

- Adiabatic insualted system (fluid)
- Mechanic energy with a mixer
- The temperature increased
- Same ammount of work same amount of temperature increase
- Electonic work produce the same phenomena





#### Internal energy

- Adiabaticly insulated system in state A
- The same ammount of work (mechanical, electric, chemical etc...) is needed to bring the system to state B.
- There must be some "property" of the system which change during this interaction!
- Internal energy can be introduce:

 $\Delta U = U_B - U_A = W_{adiabatic}$ 



#### First law of TD

- The internal energy is a *statefunction:* 
  - Depends only on the statevariables

$$U = U(p, V, n)$$
  $U = U(T, V, n)$   $U = U(p, T, n)$ 

- Not only work can change the internal energy
  - Contact to body with different temperatures heat transfer
- First law of thermodynamics:

$$dU = \delta Q + \delta W$$

- U is the internal energy
- Q is the transferred heat
- W is the work
- This energy balance equations works in every heatexchange and in whatever macroscopic work is considered

#### Internal energy change

 $dU=\delta Q+\delta W$ 

- The equation defines only the change of the internal energy
- Is there a zero point, where U(x) = 0?
- The zero point is arbitrary defined:
  - E.g. water, 300 K and 1 atm
- U is determined by the statevariables
- Example: cycle process
  - Internal energy musst be the same at the beginning and the end:  $\Delta U = 0$
  - Work became heat:

$$\Delta Q = -\Delta W$$



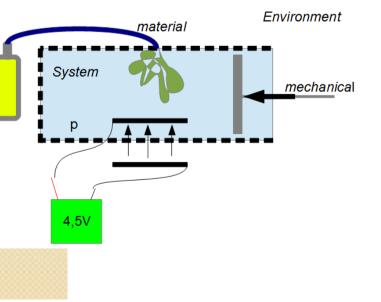
#### The work in general

- Different kind of work according to the interaction of the system with the environment.
- General form of work:

 $\delta W_i = X_i \cdot d\xi_i$ 

• Where  $X_i$  is a thermodynamic force

 $\xi_i$  is the extensive quantity



0

- Mechanical interaction
  - The volume of the system changes  $\delta W_{mach} = -n \cdot dV$

$$f_{mech} = -p$$
.

- Electrostatic interaction
  - Charges in the system change

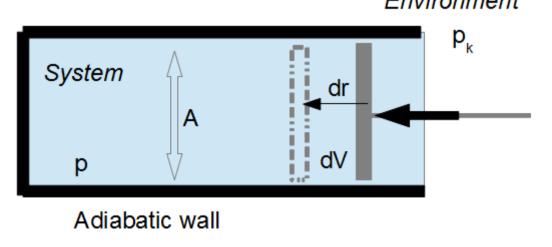
 $\delta W_{el} = \phi \cdot dq$ 

- Material interaction
  - The mass change in the system  $\delta W_{el} = \mu \cdot dn$

#### The mechanical work

- Work (def.):  $dW = \{force\} \cdot \{displacement\} = F \cdot dr$
- Pressure (*def.*):  $p = \frac{\{force\}}{\{area\}} = \frac{F}{A}$
- So the environment work done on this system:

• 
$$dW = F \cdot dr = (p_k \cdot A)dr = p_k \cdot (Adr) = -p_k dV$$





### Enthalpy

- TD. I. principle:  $dU = \delta Q + \delta W$
- If only mechanical work acts:  $\delta W = -p \cdot dV$

• 
$$dU = \delta Q - pdV$$

- Enthalpy definition:
  - Enthalpy is the inner energy of the system and the energy which is needed to constract a system in its environment
- Enthalpy change:

 $\begin{aligned} dH &= dU + d(pV) = dU + dp \cdot V + dV \cdot p = \delta Q - pdV + dp \cdot V + dV \cdot p \\ dH &= \delta Q + V dp \end{aligned}$ 

- Advantege in case of open tank:  $dp = 0 \rightarrow dH = \delta Q$
- Specific enthalpy:
  - Intensive quantity

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

Measurment unit: kJ/kg



### Heat transfer

#### • Forms:

- Heat radiation (Sun, furnace, flame...)
  - Very complicated
  - Stefan-Boltzmann law
- Conduction (thermal diffusion)
  - why put a spoon into the hot tee?
  - Temperature inhomogenity in a material cause heat flow
  - Distributed parameter systems
- Convective heat transfer:
  - transfer of heat from one place to another by the movement of fluids

#### Convective heat tranfer

• Fourier's law:

$$\frac{dQ}{dt} = \lambda \cdot A \cdot (T_A - T_B)$$

- Q: heat [J];
- $\lambda$ : heat transfer coeff. [W/m2/K]
- A: surface [m2]
- T: temperature [K]
- Heat transfer coeff. depends on the circumstances:
  - Geometry
  - Temperature of the wall and fluid
  - Pressure
  - Type of convection (laminar flow or turbulent)
- Can be calculated from steady state measured data or semi-empirical formulas

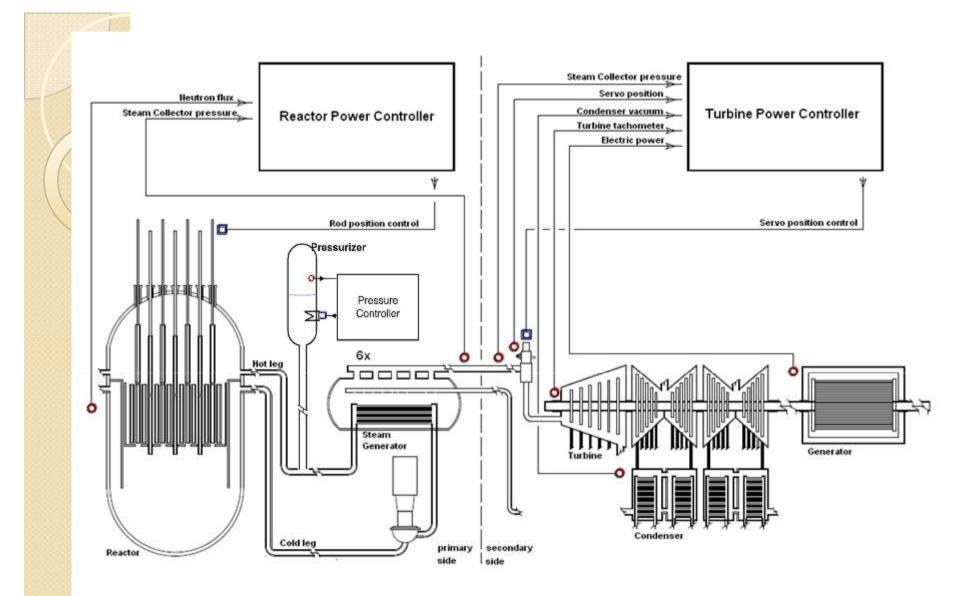
#### Need a break?

0



model equations

# • ENERGY SYSTEMS



# Parts of energy systems -

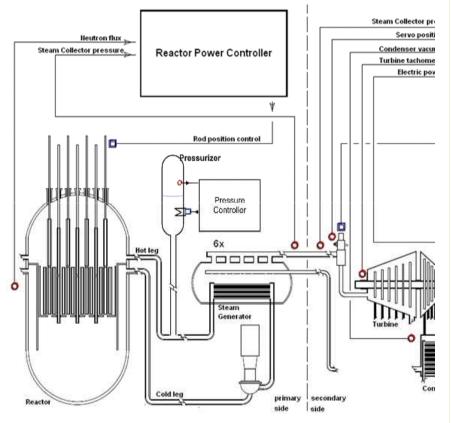
#### Primary circuit

Aim:

- fresh steam production for the turbines
- Quantity (m) and quality criterions efficiency
- Parts in a nuclear power plant:
- · Reactor vessel, active zone, reactor core
- Hot-leg, and cold-leg (pipes)
- Main coolant pumps
- Steam genereators produce steam
- Pressurizer
- Parts in a thermal power plant
- Coal hopper, conveyor, pulverizer (tartály, szállítószalag, porlasztó/örlő)
- Furnace
- Boilers generate steam

#### Thermal energy production:

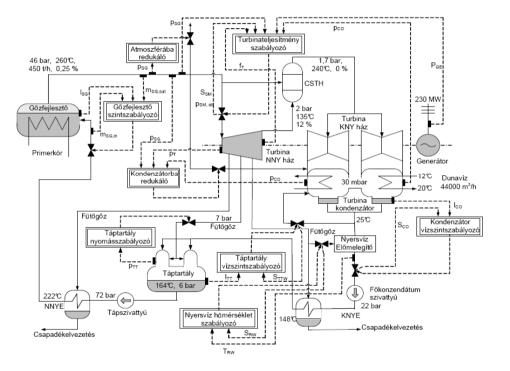
- burning (coal, oil, wood, energy-grass ...) in furnace
   Chemical reaction: exotherm, C -> CO, CO2
- Alternative source nuclear fission in active zone
   Nuclear reaction, Uranuim, Plutonium
- Results:
  - Hot water or air
- Heat transfer and/or radiation



# Parts of energy systems 2

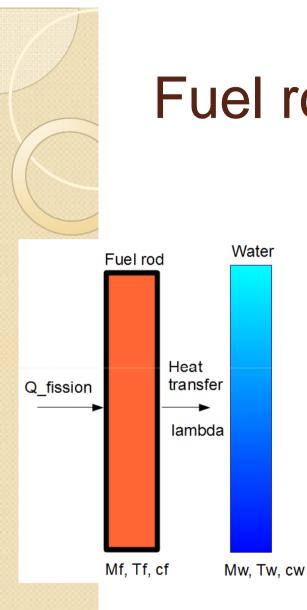
#### Secondary circuit

- Aim:
  - Electricity production
- Parts:
  - Steam control valve
  - Steam turbines (high and low pressure turbines)
  - Super-heaters
  - Condenser
  - Feed water tanks
  - Feed water heaters
  - Water pumps
  - Generators



2. ábra. A szekunder kör felépítése.

# • Lumped parameter Model equations



## Fuel rods Modeling goal:

Water

- Compute the average temperature of the fuel rods
- Fuel rods:
  - 123\*350 piece in the reactor core 0
  - UO2 fuel and zirconium clad
- Modeling assumptions:
  - Mixed fuel and clad
  - All fuel rods is modelled as one rod
  - Same temperature 0
  - Homogenen heat generation
  - Constant properties (source of information): 0
    - Density (tables)
    - Volume (geometry)
    - Specific heat (tables)
    - Heat transfer parameter (steady state calculation / par. est)
    - Surface (core geometry)
- Main phenomena: •

1

JT

- nuclear fission heat production given (model input) 0
- Heat transfer to the coolant, which temperature is known 0 (model input)

$$\frac{dT_f}{dt} = \frac{1}{M_f c_f} (Q_{fission}(t) - A\lambda(T_f - T_w))$$

# Simulink model

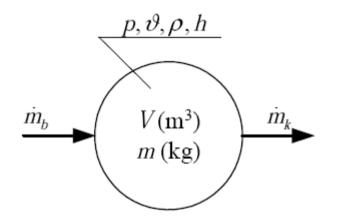
- Heated\_body.mdl:
  - Electrically heated pipe
  - Constant water temperature (80°C) and heat transfer parameter \*A = 200 W/K
  - Initial condition:
    - 150 ℃ body temperature
    - No heating power
  - 150 s:
    - Turn on heating (2 kW)
  - Facts:
    - Exponentially decreasing temperature to the equilibrium
    - The system is stable
    - After heating is switched on -> new equilibrium state (exp.)
  - Try:
    - Change the water temperature
    - Change the body mass
    - Change the heat transfer coefficiant
    - Compare the results

# Description of the coolant water

- In solid matter
  - Phenomena:
    - Heat conduction
    - Heat transfer
    - Radiation
    - Heat production
    - No mass transfer  $\rightarrow$  mass balance is not needed
- In liquid matter:
  - Displacement of the matter cause the displacement of its energy aswell
    - Convective heat transport
    - Mass transport

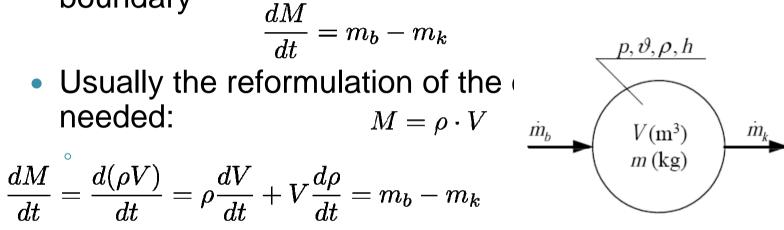
# Mass balance equation in generality

- Lumped parameter description
  - Same condition (par.) in the control volume
  - Transport phenomena on the boundary is important
- Notations:
  - m mass transfer [kg/s]
  - M mass [kg]
  - V volume [m<sup>3</sup>]
  - p pressure [Pa]
  - $T(\vartheta)$  temperature [°C]
  - $\rho$  density [kg/m<sup>3</sup>]
  - h specific enthalpy [J/kg]



# Mass balance equation in generality

• Mass balance: mass transprot through the boundary dM



- Simplification can be used in special cases
  - Is the volume or density constant?
  - 3 cases: volume, density or both can change



#### 1. Density and volume can change

$$\rho \frac{dV}{dt} + V \frac{d\rho}{dt} = m_b - m_k$$

 If the media is *fluid* (water, oil, etc.) we usually want to know its volume-change (*water in furnace's vessel*):

$$\frac{dV}{dt} = \frac{1}{\rho}(m_b - m_k - V\frac{d\rho}{dt})$$

• If the media is *gas or vapour*, we usually want to know its pressure • Using:  $d\rho = \frac{\partial \rho}{\partial T} dT + \frac{\partial \rho}{\partial p} dp$ 

• After substitution and rearrangement:

$$\frac{dp}{dt} = \frac{1}{V(\partial \rho/\partial p)} \left( m_b - m_k - \rho \frac{dV}{dt} - V(\frac{\partial \rho}{\partial T}) \frac{dT}{dt} \right)$$



## 2. The density is constant

$$ho rac{dV}{dt} + V rac{d
ho}{dt} = m_b - m_k$$

$$\rho = const.$$
 $d\rho = 0$ 

• If the vessel is open, usually we want to know the water level in the tank

$$\rho \frac{dV}{dt} = m_b - m_k$$

 If the crossection (A) is constant, then the level can be computed as (V = A \* H):

$$\frac{dH}{dt} = \frac{1}{\rho A}(m_b - m_k)$$



#### 3. The volume is constant

$$ho rac{dV}{dt} + V rac{d
ho}{dt} = m_b - m_k$$

$$V = const.$$
  $dV = 0$ 

• A fully filled tank, where the density can change.

$$V\frac{d\rho}{dt} = m_b - m_k$$

• If we interested in pressure:  

$$d\rho = \frac{\partial \rho}{\partial T} dT + \frac{\partial \rho}{\partial p} dp$$

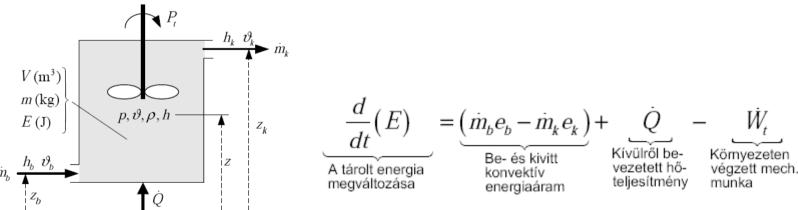
• using the relationship:

$$\frac{dp}{dt} = \frac{1}{V(\partial \rho / \partial p)} \left( m_b - m_k - V(\frac{\partial \rho}{\partial T}) \frac{dT}{dt} \right)$$

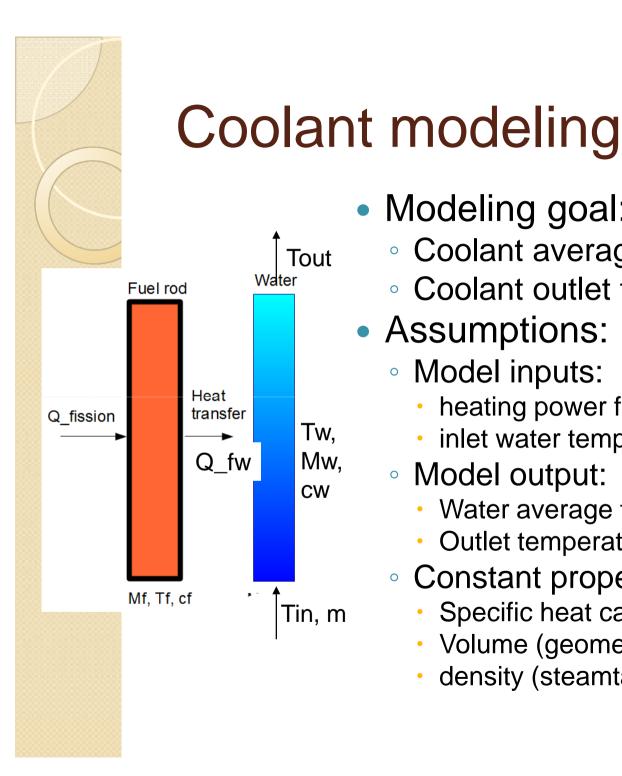


# **Energy Balance Equation**

- Control volume boundary of the system
- TD. II. principle:
  - Heat transfer
  - Mass transfer
  - work on environment



2-15. ábra. A koncentrált energiatárolás jellemzői

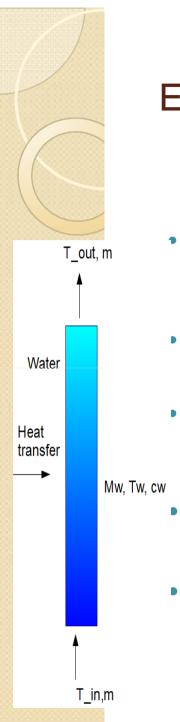


Tw.

Mw,

CW

- Modeling goal:
  - Coolant average temperature
  - Coolant outlet temperature
- Assumptions:
  - Model inputs:
    - heating power from the fuel rod (Qfw)
    - inlet water temperature (Tin)
  - Model output: 0
    - Water average temperature (Tw)
    - Outlet temperature (Tout)
  - Constant properties: 0
    - Specific heat capacity (steamtable)
      - Volume (geometry)
      - density (steamtable)



#### Energy balance equation for a heated pipe

$$\frac{dE}{dt} = m_b h_b - m_k h_k + Q$$

- If there is no phase-change, using the temperature is more convenient
  - Linear relationship between the temperature and enthalpy: h = cT
- Rewriting the left side:  $\frac{dE}{dt} = \frac{d(cMT)}{dt} = cM\frac{dT}{dt} + cT\frac{dM}{dt}$
- The mass balance is needed:

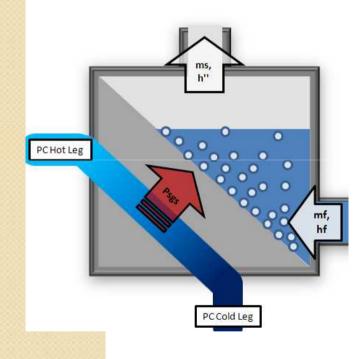
- $rac{dM}{dt} = m_b m_k$ Finally:  $\frac{dT}{dt} = \frac{1}{Mc}(m_b c(T_b - T) - m_k c(T_k - T) + Q)$
- What is T k?
  - $T_ave = (T_b + T_k)/2$  Not correct during dynamics, why?
  - $cm(T_k T_ave) = cm(T_k T_b)/2 = Q/2 \text{ or}$
  - Delayed:  $T_ki(t) = T_b(t-T) + T_ave(t-T/2)$



# Pipe modell

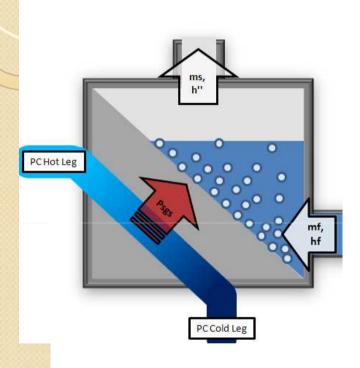
- Matlab Simulink
  - heated\_pipe.mdl
- Inital condition:
  - No heating
- Steady state: what flows in that flows out
- 150s heating turned on:
  - New equilibrium point
  - In new steadytate: dT\_ave = dT\_out/2
- Try:
  - Mass transfer changes
  - Change the volume of the pipe
  - Inlet temperature changes
  - Compare the results

# Steam generator secondary side model



- Steam generator
  - Ca. 5500 heated pipe
- Primary side
  - cooled pipe
- Secondary side
  - saturated water and steam
- Modelling goal:
  - Compute the pressure on the SC
  - Compute the temperature on the SC
- Assumptions:
  - Saturated water and steam in one control volume
    - V = Vw + Vs mass of water and steam
  - Model inputs:
    - Feed water enthalpy and mass flow
    - Fresh steam mass flow
    - Heating power from the PC
  - Model outputs:
    - Pressure, temperature

# Steam generator model



• Mass and energy balance equations:

$$\frac{dM}{dt} = m_f - m_s$$
$$\frac{dU}{dt} = P_{sgs}/6 + m_f h_f - m_s h''$$

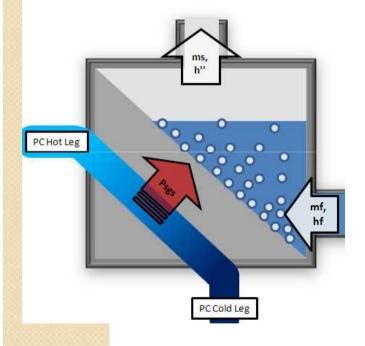
• Mass to water volume:

$$\frac{dV_w}{dt} = \frac{1}{\rho_w - \rho_s} \left( m_f - m_s - \left( V_s \frac{d\rho_s}{dp} + V_w \frac{d\rho_w}{dp} \right) \frac{dp_{sg}}{dt} \right)$$

- The volume depends on the pressure because the density depends on the pressure
- Pressure from energy balance:

$$\frac{dp_{sg}}{dt} = \frac{(1 - \frac{\rho_s}{\rho_w})\frac{P_{sgs}}{h'' - h'} + m_f(\frac{\rho_s}{\rho_w}\frac{h'' - h_f}{h'' - h'} - \frac{h' - h_f}{h'' - h'}) - m_s}{V_w a(p_{sg}) + (V - V_w)b(p_{sg})}$$

## Steam generator Simulink modell 1



- steamGenerator.mdl
- initSteadyState.m
- Initial condition
  - Constant heating (1375MW/6)
  - Constant mass flow (123 kg/s)
- Facts:
  - Non-stable model output
    - Not feedback to the heat transfer!

### Steam generator Simulink modell 2

PC Hot Leg

- Steam generator modell + primary circuit pipe
- Not the transferred heat, but the primary side temperature is the model input
  - Higher pressure -> higher SC temperature -> smaller temp.
     Difference → smaller heat transfer, which stabilize the system!

# Steam collector modell

- Steam collector connects the steam generator to the turbine
- Modeling goal:
  - Compute the pressure in the collector
- Model inputs:
  - Turbine steam consumption (m\_tu)
  - Mass flow into the collector (m\_s)
- Model output:
  - Steam collector pressure
- Modeling assumptions:
  - Constant temperature (no need of Energy balance equation)
  - Only steam in the collector
  - Steam density depends only on the pressure
- Mass balance equation:

$$\frac{dM_c}{dt} = m_{sg} - m_{tu}$$

• Mass balance to pressure:

$$\frac{\frac{dp_{c}}{dt}}{\frac{dp_{c}}{\frac{d\rho_{c}}{dp_{c}}}} = \frac{m_{sg} - m_{tu}}{\frac{d\rho_{c}}{dp_{c}}} V_{c}$$

# Steam collector Simulink Model

- Collector.mdl
- Initial condition
  - m\_in = m\_out = 123 kg/s
- Step function in m\_in (123→120 kg/s)
  - Pressure constantly decreasing
    - Non-stable...
    - Solution:
      - mass transfer depends on the pressure!
      - Bernouilli's law