Numerical study of thermal evaporation unit for phase change of liquid hydrogen peroxide to vapor

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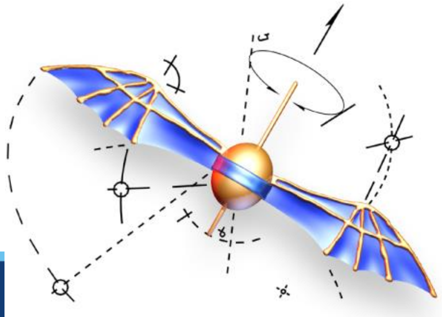

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Outline

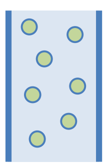
- Introduction and motivation
- Physical background
- Numerical model
- Results
- Conclusions

Introduction and motivation

- Hydrogen peroxide (H_2O_2)
  - Strong antimicrobial properties
  - Commonly applied in the form of gas/vapor for package sterilization in aseptic filling machines
  - Gaseous or vapor form is produced by evaporating and subsequent heating of an **aerosol** mixture of aqueous H_2O_2 and air

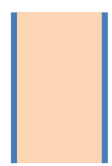
@ inlet

Heterogeneous mixture of air and droplet of aqueous H_2O_2

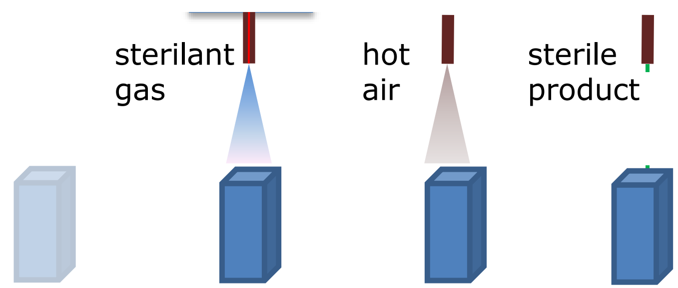


@ outlet

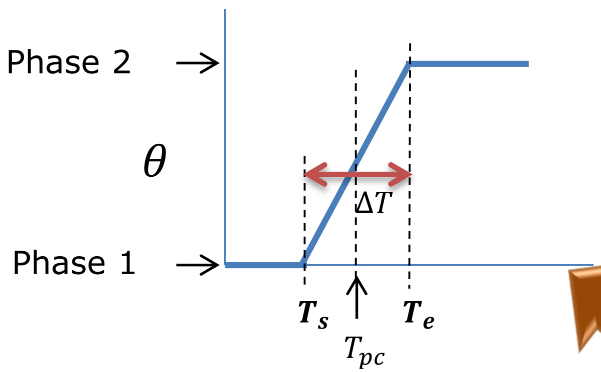
Homogeneous mixture of air, steam and H_2O_2 gas



- ➢ Involve high energy and material costs
- ➢ Little knowledge about the process
- ➢ Slow development



Physical background



Phase fraction: $\theta = \begin{cases} 0: T_{pc} - {}^{\Delta T}/_{2} & \rightarrow \boldsymbol{T_s} \\ \downarrow & \\ 1: T_{pc} + {}^{\Delta T}/_{2} & \rightarrow \boldsymbol{T_e} \end{cases}$

The equivalent (effective) material properties defined as a function of phase fraction

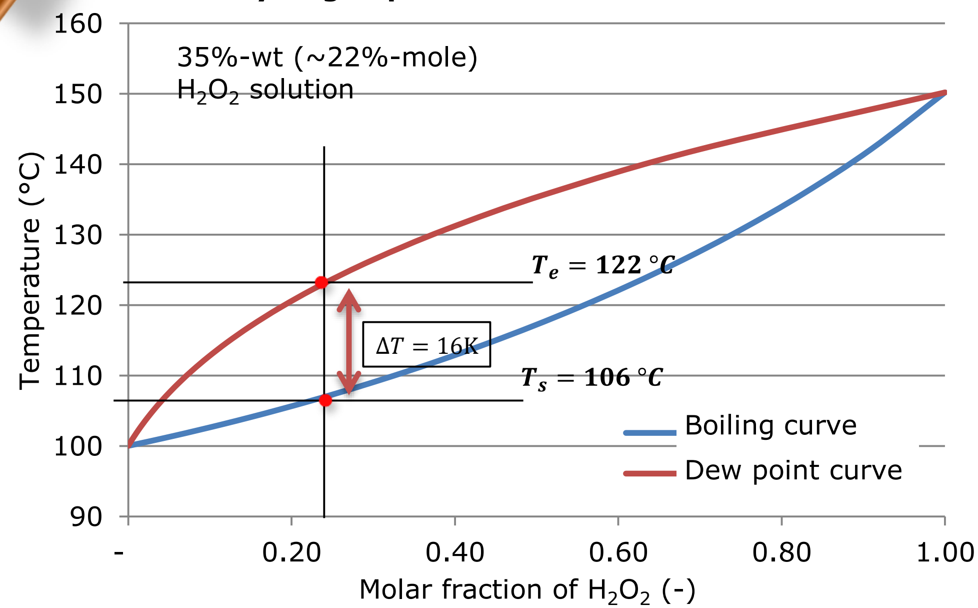
Aqueous H_2O_2 (35%-wt) solution

35% H_2O_2 65% H_2O

Binary mixture

100°C **150°C**

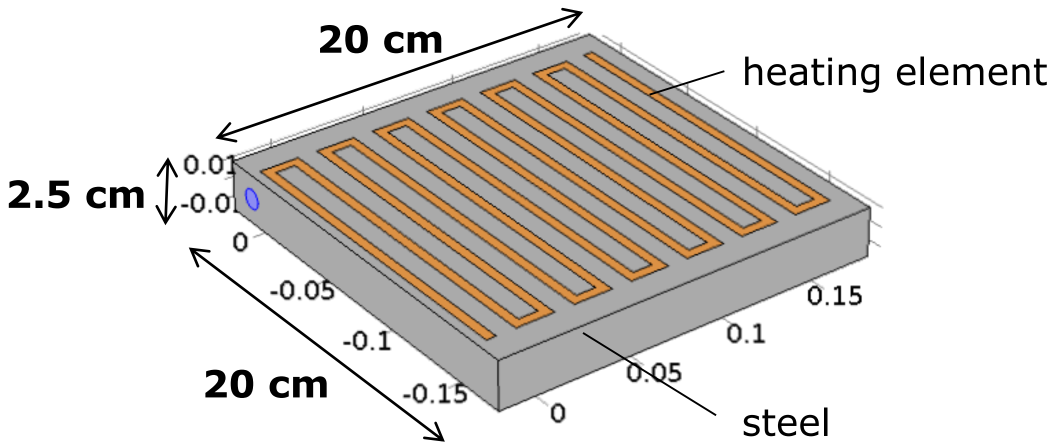
Binary isobaric phase change diagram of aqueous hydrogen peroxide solution at 1 atm

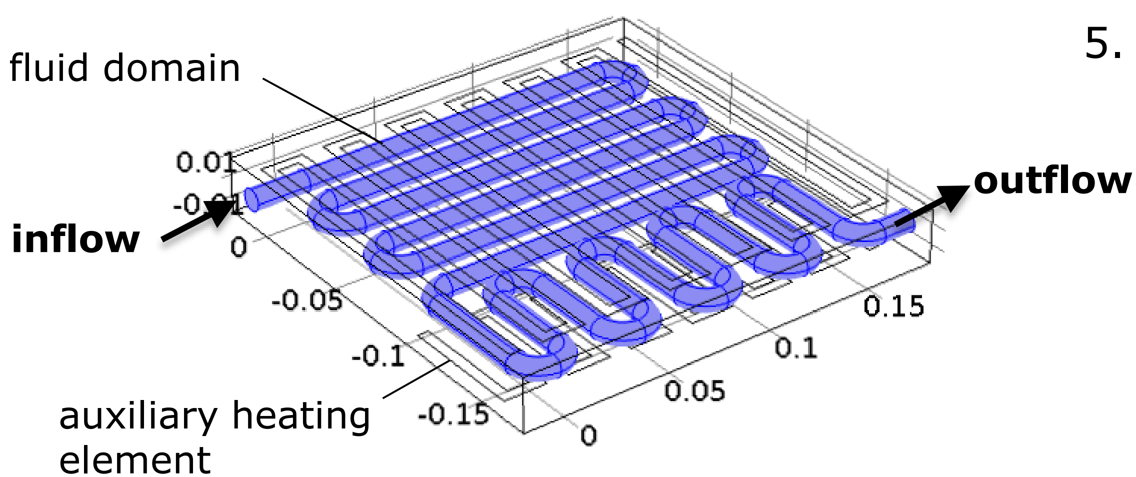


→ Figure based on the formulations published by Scatchard et al. (1952), Keyes (1947) and corrections from Manatt and Manatt (2004)

1. Phase change of aerosol mixture
2. Material properties → molar basis
3. Constant H_2O_2 concentration

Numerical model:
Geometry and parameters

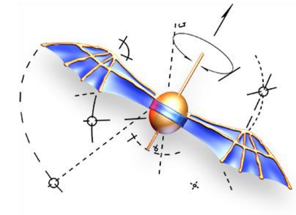




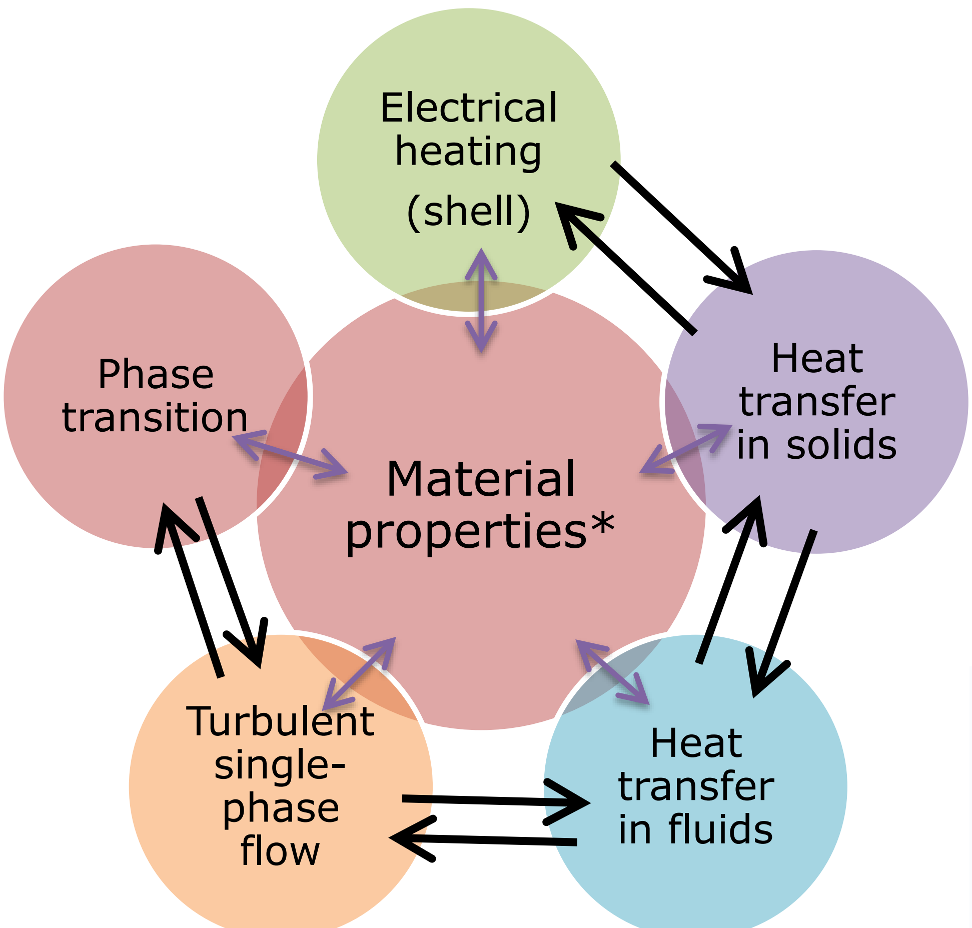
Model parameters:

1. Electric current value
2. H2O2 concentration
3. Volumetric flow rate of H2O2
4. Volumetric flow rate of air
5. Stop criterion for parametric solver (temperature)

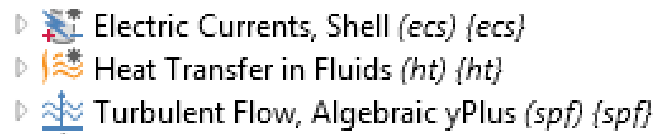
Numerical model:
Physical interfaces



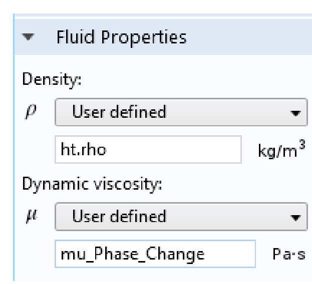
The interdependencies:



* Aerosol was assumed as an ideal mixture.



- $Q_s = \mathbf{J} \cdot -\nabla \mathbf{V}$ → surface joule heating
- $\nabla_t \cdot (d_s \kappa_s \nabla_t T) = Q_s$ → boundary heat source
- Heat transfer to fluid domain
- Temperature change → phase fraction (θ) change
- Temperature and phase fraction change
  → flow properties change using:

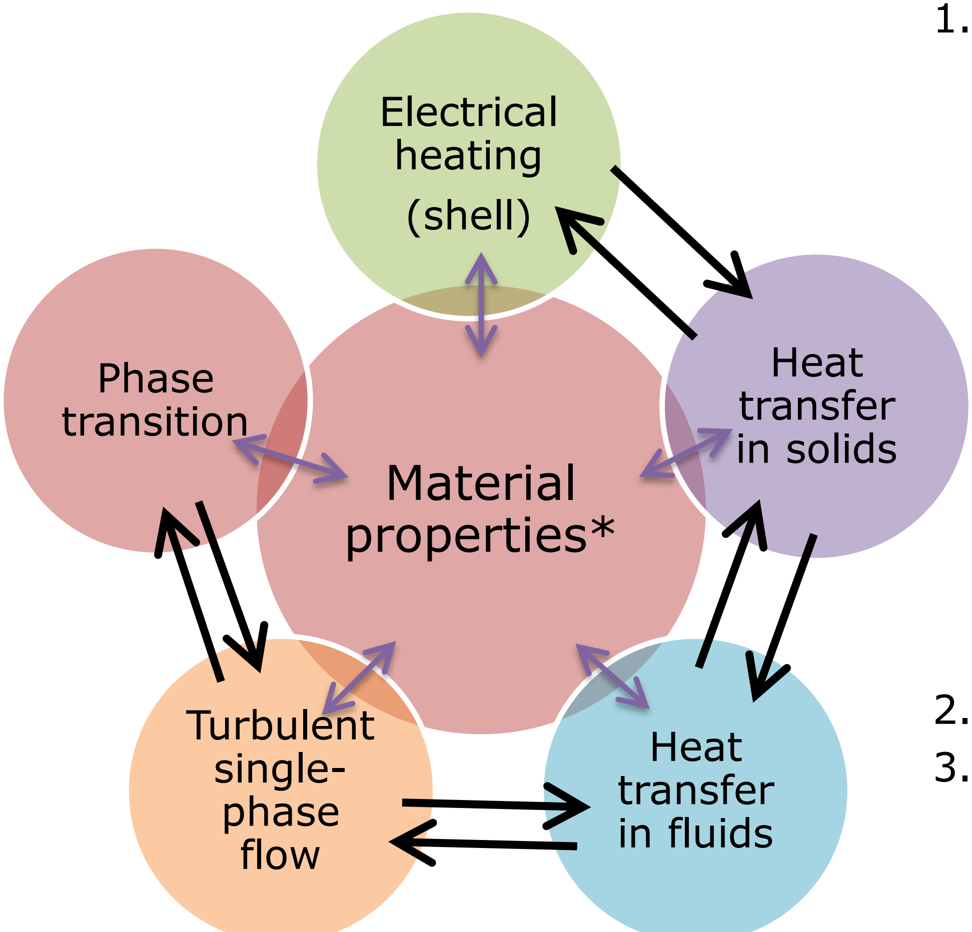


$$\rho = \theta\rho_1 + (1-\theta)\rho_2$$

$$\mu = \theta\mu_1 + (1-\theta)\mu_2$$

Numerical model:
Mesh and study

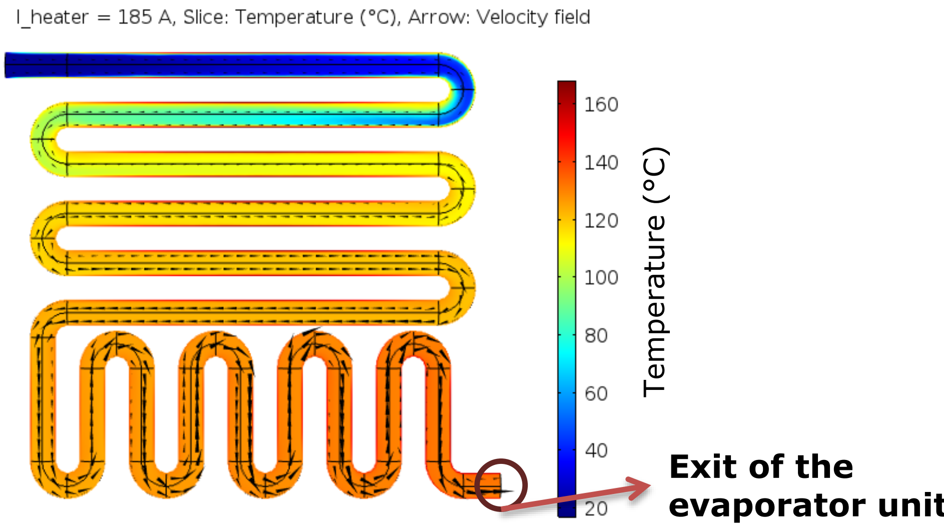
The interdependencies:

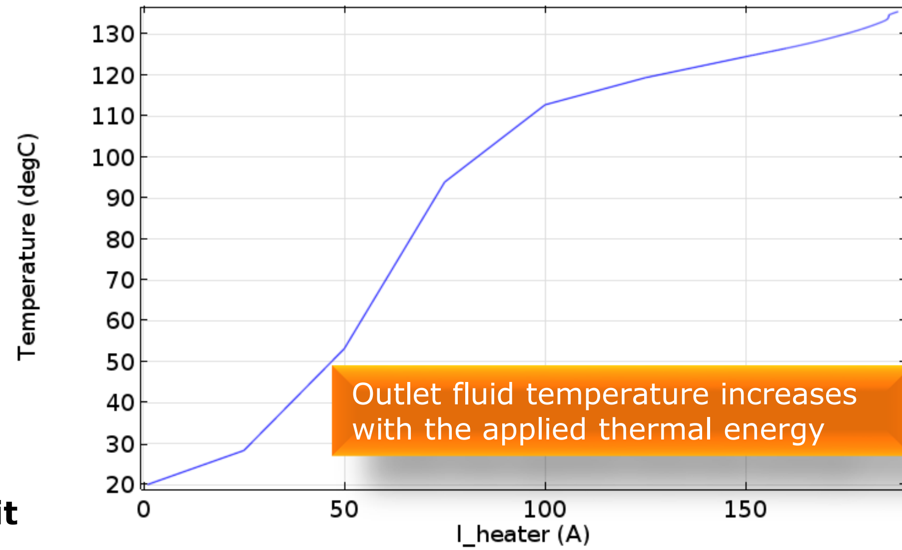


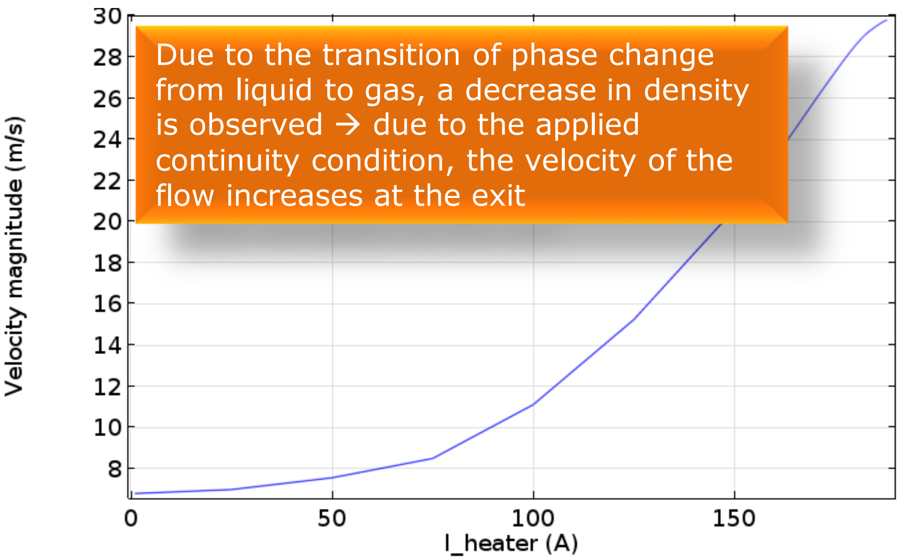
* Aerosol was assumed as an ideal mixture.

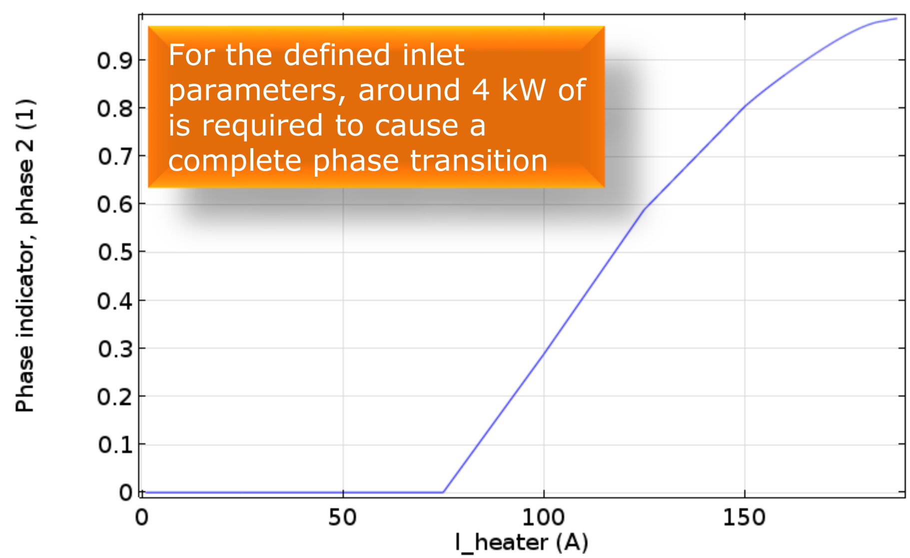
1. Steady state solution
    - **Study 1:** Initial guess → isothermal flow defined at the inlet temperature
    - **Study 2:** Auxiliary parametric solver (with continuation) for the electric current (coarse values), while plotting the average phase indicator of fluid 2 at the outlet.
    - **Study 3:** Using last converged value from Study 2 as initial condition for fully coupled solver and a small range for the parametric solver
2. Direct solvers are used → robustness
3. Coarse mesh with quadratic discretization level for heat transfer was used → faster convergence

Results:
Phase change

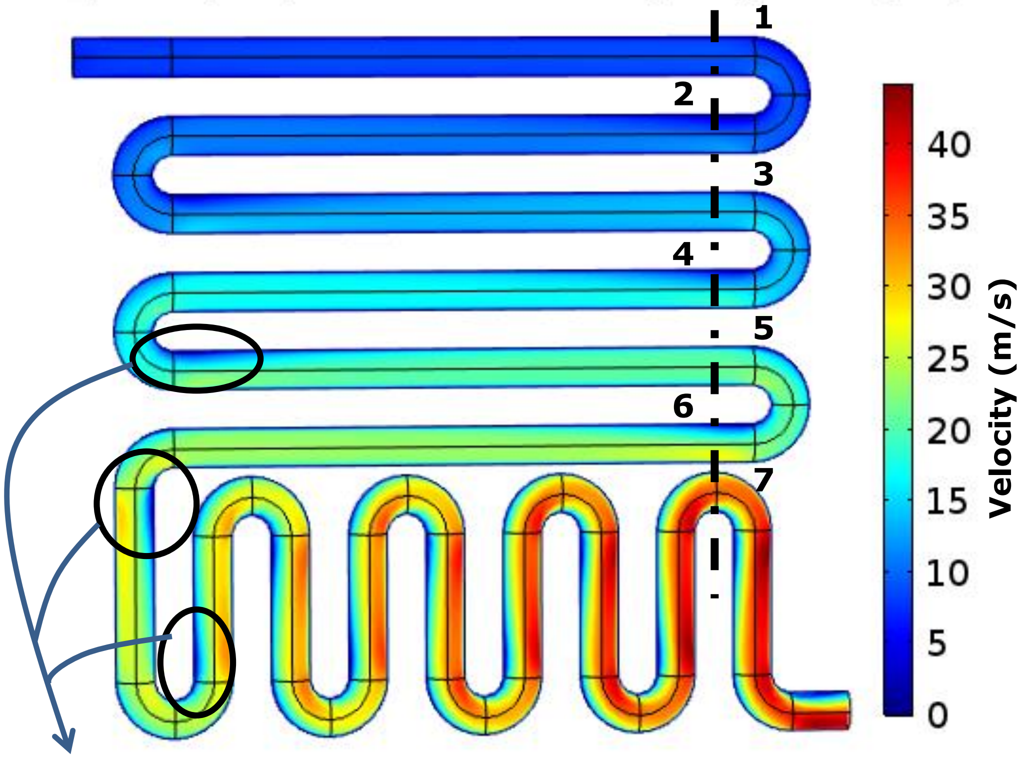




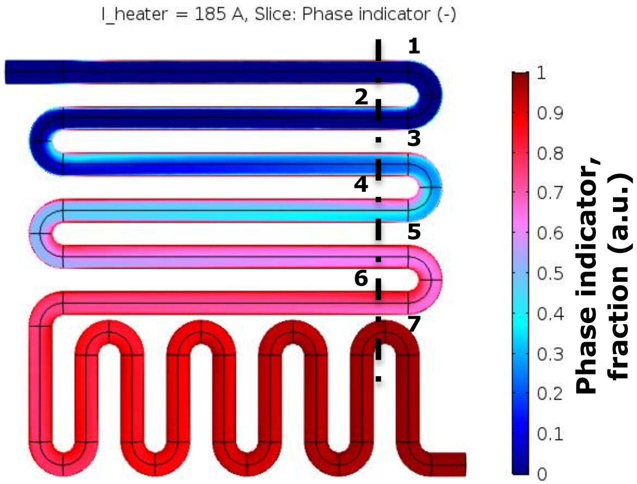


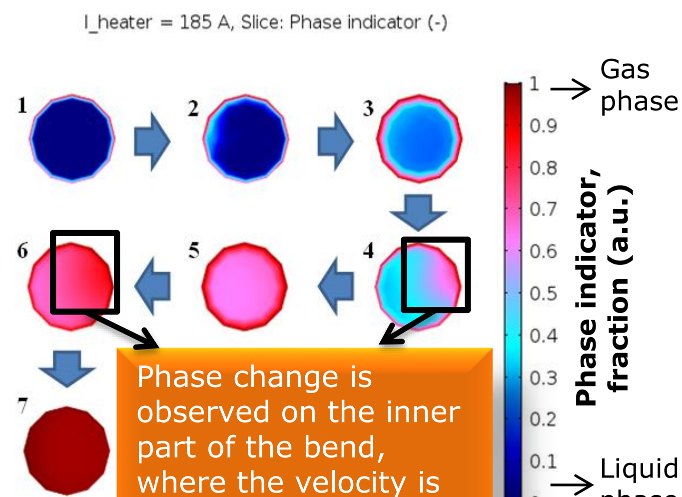


Results:
Fluid flow



Pressure drop around a bend → velocity difference.
Heat transfer to the fluid increases with lower velocity → phase transition is observed more around bends





Phase change is observed on the inner part of the bend, where the velocity is lowest

Conclusions

- Multiphase flow was approximated as a single flow
- Modeling concept was created for the phase change behavior of an aerosol containing a binary mixture using apparent heat capacity formulation.
- Effective material properties of the aerosol is defined and integrated in the model as molar basis.

- Serpentine meander channels ensure aerosol mixing (homogeneity) and increase the heat transfer
- Due to phase change and the poor thermal conductivity of aerosol gas, more heat and/or mixing is required near phase change region

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Thank you
for your attention

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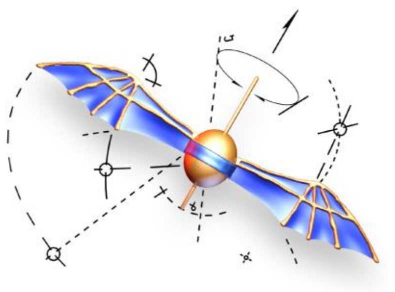

Parameters

- **Fluid properties:**
  - Volumetric flow rate of $H_2O_{2(aq)}$ (35%): 1000 µL/s
  - Volumetric flow rate of air: 2 m³/h
  - Inlet fluid velocity: 7 m/s
  - Inlet fluid temperature: 20 °C

- **Heating element:**
  - Set current: 1-185 A
  - Thickness of the heating element: 0.1 mm

Heating

Two-stage heating strategy was adopted:

1. Initial heating from main current 0-150 A (equivalent to: 0-1700 W) → initial phase change is observed
2. Low thermal conductivity of aerosol gas after phase change → an auxiliary heating switched around 150 A