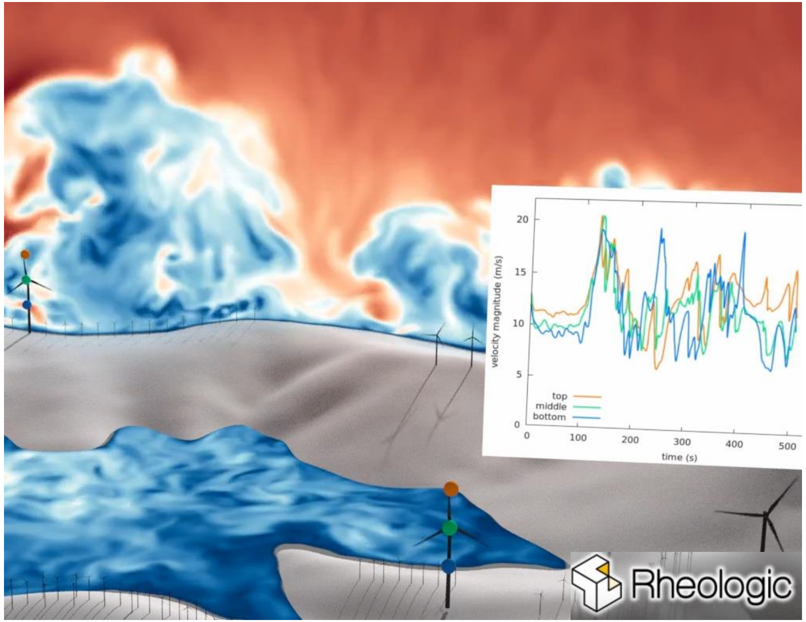
KEB-45250
Numerical Techniques for Process Modeling

Spring 2018

Antti Mikkonen
Kaj Lampio
Niko Niemelä

What is the course about?

- Industrial applications
  - Heat transfer
  - Fluid flow
  - Reacting systems
- Numerical modeling
  - Flexible
  - Custom codes
  - Software packages

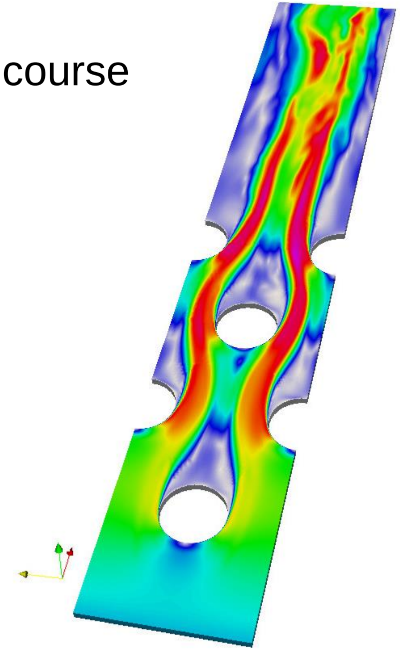


General information

- **First implementation**, all plans are preliminary
- Lectures
  - Wednesday 13-15 K1241
- Exercises
  - Thursday 10-12 SB202 – Computer lab
- Intensive course on ANSYS Fluent
  - Tuesday 30.1. 9-16 SB202
  - Wednesday 31.1. 9-15 RG100C

CFD software

- ANSYS Fluent
  - Computational Fluid Dynamics (CFD) software on this course
  - Easy to learn
  - Commercial and expensive
  - Intensive course
    - Tuesday 30.1 9-16 SB202
    - Wednesday 31.1. 9-15 RG100C
- OpenFOAM
  - More popular at TUT
  - Slow to learn
  - Free and open source
- Many others

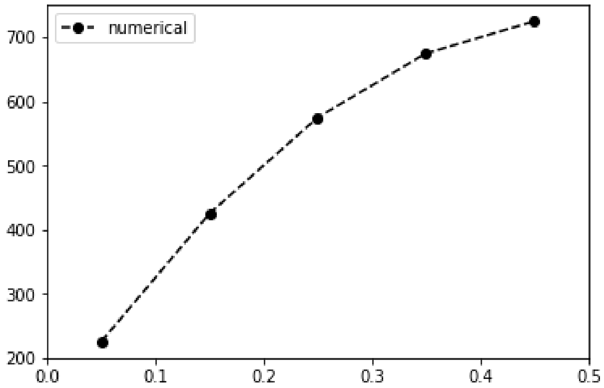


Programming language

- Python 3.6
  - Most students familiar with
  - One of the most popular languages in the world
  - Extensive **liberties** for engineers
- If you want to use something else, for example Matlab, just ask

```
# Solution
T = sp.linalg.solve(A,b)

# Plot numerical and exact solution
x = sp.linspace(dx/2,L-dx/2,n)
plt.plot(x, T, "k--o", label="numerical")
plt.legend()
```



Mandatory steps to pass

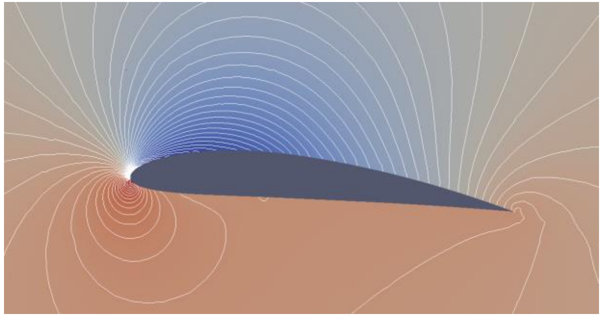
- Exam
  - 60% of total points
  - Must be passed
- 2 assignments with reports
  - 40% of total points
  - Must be passed

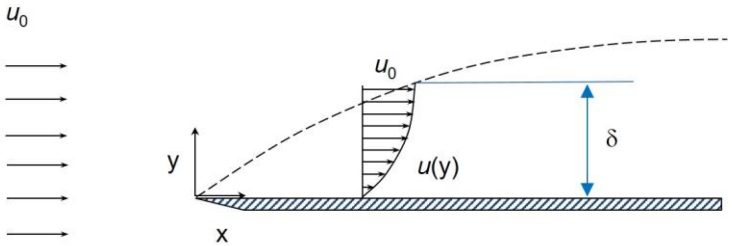
Exam, 60%

- 11.05.2018, time: 17-20
- Preliminary plan
  - 5 questions
  - ~ 2.5 about Computational Fluid Dynamics
  - ~ 1.5 about numerical modeling in general
  - ~ 1 about reacting systems

Assignment 1, 25%

- Two options
  - Calculate a 2D case with CFD software
    - Probably wing
    - Ansys Fluent/OpenFOAM
    - Industry oriented
  - Own code
    - Probably flat plate
    - Python/other language
    - Deeper understanding
  - You can also do both
    - 5-10% extra





Assignment 2, 15%

- Own numerical code (Python)
  - Custom code is better for some applications
  - Combination of analytical models and numerical modeling
- Maybe geothermal energy

https://commons.wikimedia.org/wiki/File:Impjanti_Gjeotermik.jpg

Course material

- CFD part
  - Lecture notes
    - Writing in process
  - Additionally:
    - H. Versteeg & W. Malalasekera:

      "An introduction to computational fluid dynamics: The finite-volume method", 2nd ed.
- Lecture slides for the rest

Preliminary plan

Month	Week	Day	Lectures	Day	Exercises
1	1	3		4	
	2	10	Introduction	11	Python basics and libraries
	3	17	Basics. Matrix, NS,…	18	Lecture topic
	4	24	CFD Basics	25	Lecture topic
2	5	30	ANSYS intensive course	31	ANSYS intensive course
	6	7	Heat convection, FVM	8	Lecture topic with Python
	7	14	Advection	15	Lecture topic with Python
	8	21	Navier-Stokes	22	Navier-Stokes with ANSYS
	9	28	Mesh	1	Mesh with ANSYS
3	10	7	Turbulence	8	Turbulence with ANSYS
	11	14	Differential equations	15	Lecture topic
	12	21	Linear systems	22	Lecture topic
	13	28	Easter Holiday	29	Easter Holiday
4	14	4	Linear/Non-linear systems	5	Lecture topic
	15	11	Non-linear systems	12	Lecture topic
	16	18	Reacting systems	19	Lecture topic
	17	25	Reacting systems	26	Lecture topic

Example Cases

- Glass tempering
  - Antti Mikkonen
- Fin optimization (separate slides)
  - Kaj Lampio
- Combustion modelling (separate slides)
  - Niko Niemelä

Tempered Glass

Safety Glass Door
by Wei Min Chan,
https://www.youtube.com/watch?v=aQ902DfWILs

John Hancock Panorama, Chicago
by RhythmicQuietude, CC BY-SA 3.0
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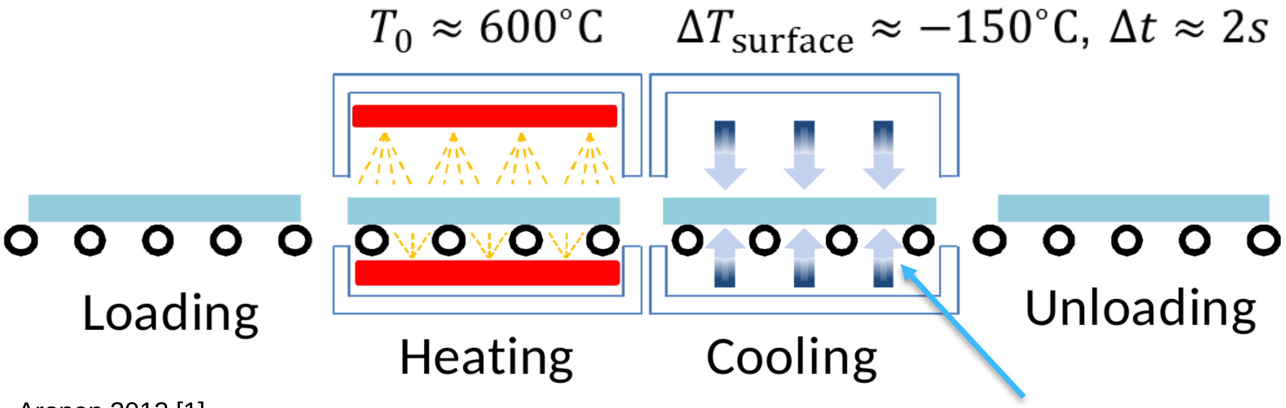
Production



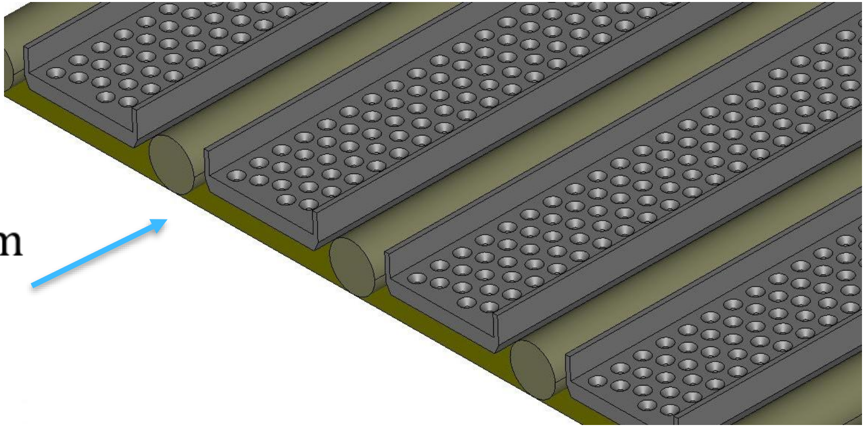
Aronen 2012 [1]

Cooling Jets

$\mathrm{Ma} \approx 0.85$

$d_{\mathrm{nozzle}} \approx 1 - 3\ \mathrm{mm}$

$\bar{h} \approx 1000\ \mathrm{W/m^2K}$

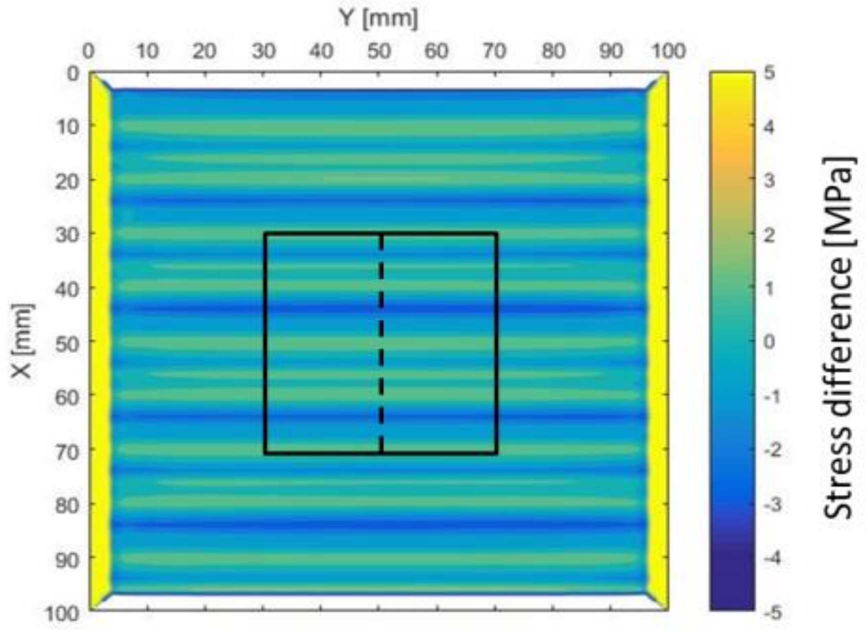


Visual issues


Figure 1.3. Roller waves (Henriksen & Leosson 2009).

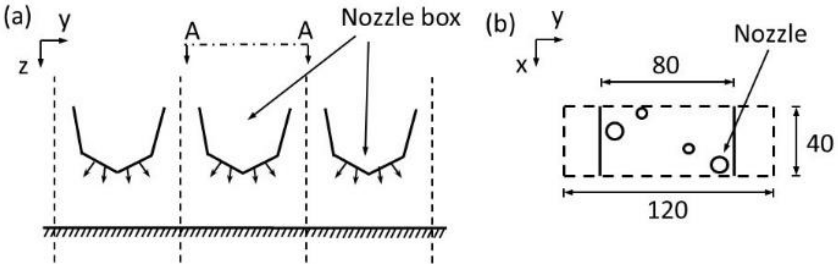

Figure 1.4. Longitudinal patterns (Henriksen & Leosson 2009).

Residual stress

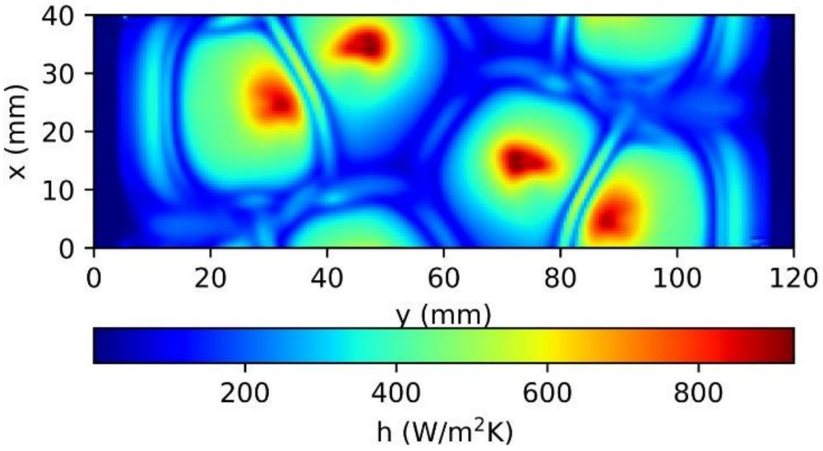


Antti Aronen

Heat transfer modeling

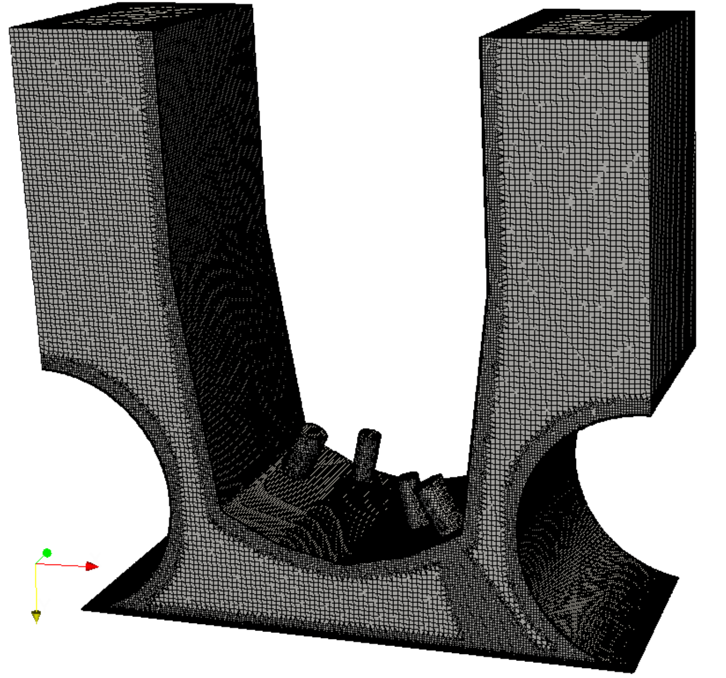


Schematic of the nozzles (a) and locations in nozzle plate (b).

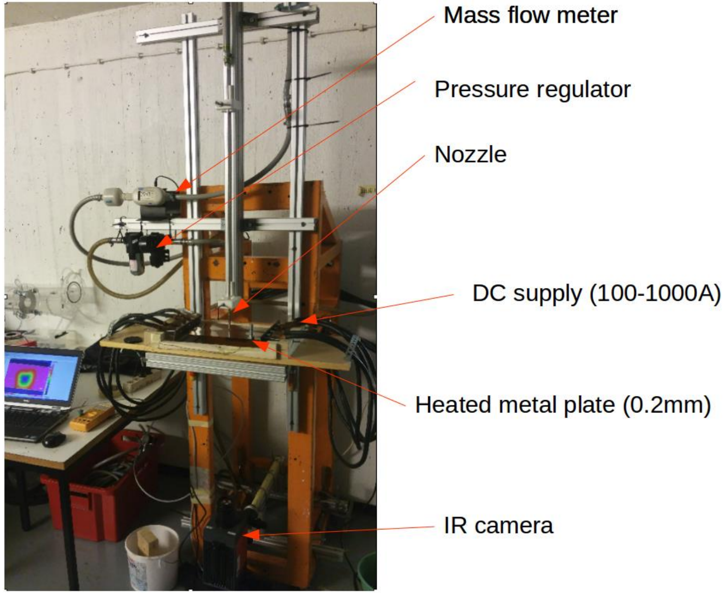


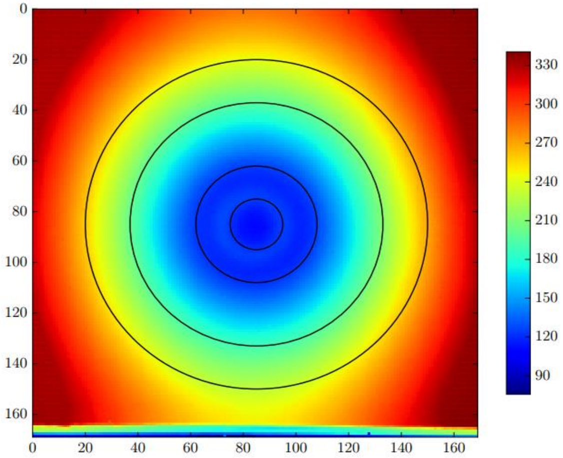
Distribution of heat transfer coefficient

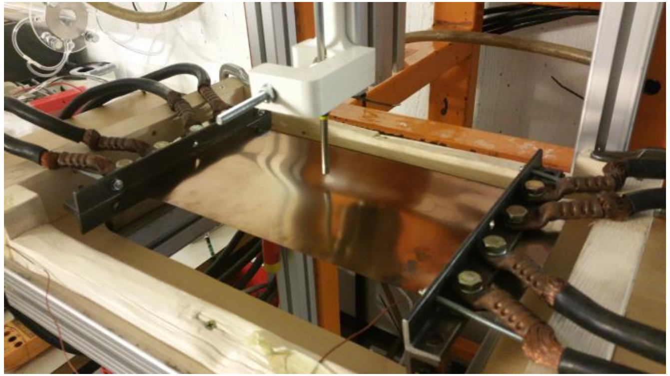
Mesh



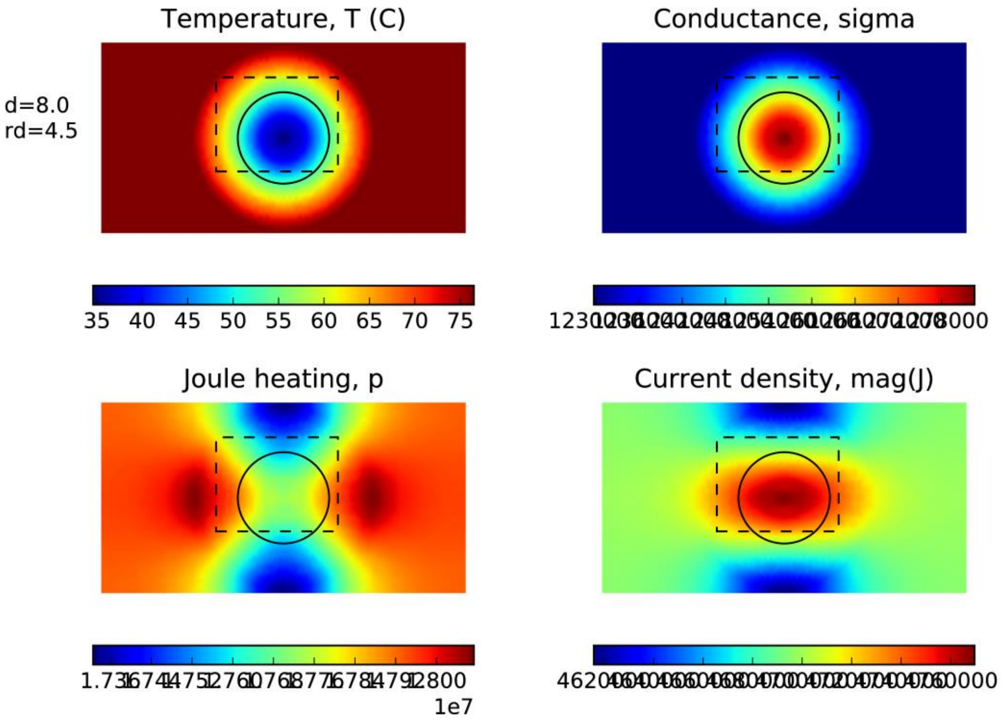
Measurements



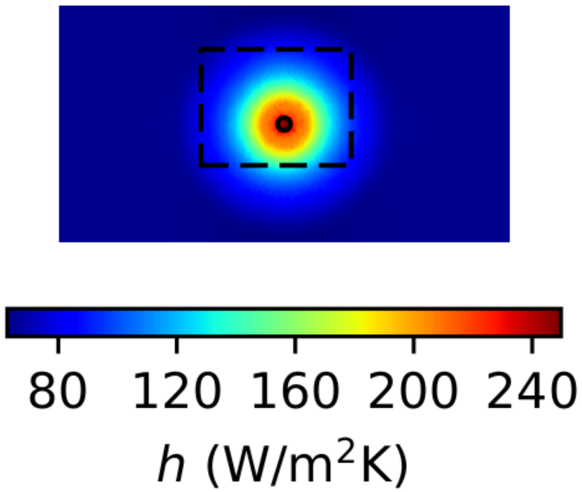


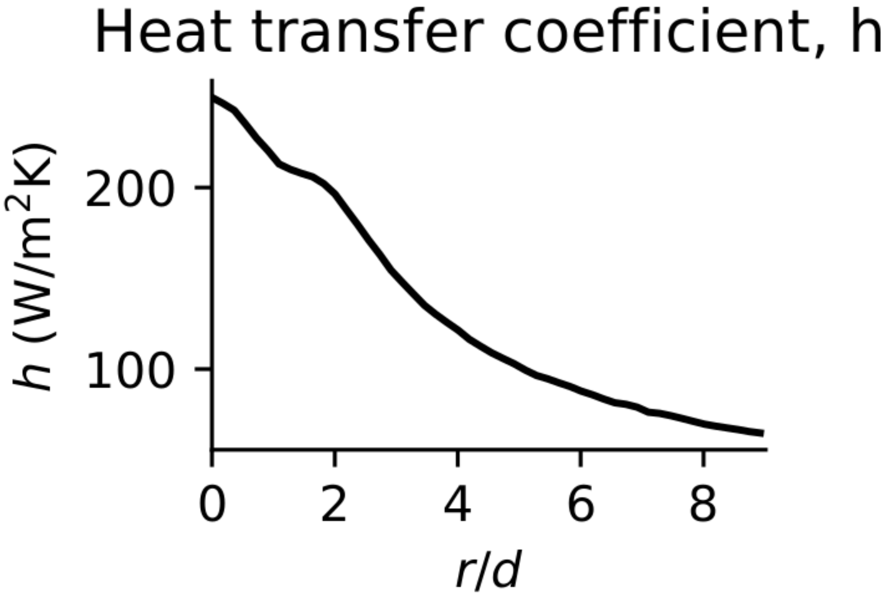


Joule heating



Heat transfer





OpenFOAM, Open Source

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho U_j k)}{\partial x_j} = \tilde{P}-\beta^{*}\rho k\omega + \frac{\partial}{\partial x_i}\left[(\mu+\sigma_k\mu_t)\frac{\partial k}{\partial x_i}\right]$$

```
    // Turbulent kinetic energy equation
    tmp<fvScalarMatrix> kEqn
    (
        fvm::ddt(alpha, rho, k_)
      + fvm::div(alphaRhoPhi, k_)
      - fvm::laplacian(alpha*rho*DkEff(F1), k_)
     ==
        min(alpha*rho*G, (c1_*betaStar_)*alpha*rho*k_*omega_)
      - fvm::SuSp((2.0/3.0)*alpha*rho*divU, k_)
      - fvm::Sp(alpha*rho*betaStar_*omega_, k_)
      + kSource()
      + fvOptions(alpha, rho, k_)
    );
```

Full address:
https://github.com/OpenFOAM/OpenFOAM-dev/blob/master/src/TurbulenceModels/turbulenceModels/RAS/kOmegaSST/kOmegaSST.C

Electric heating with FEniCS

$$\nabla \cdot \sigma \nabla \phi = 0$$

$$\boldsymbol{E} = -\nabla \phi$$

$$\boldsymbol{J} = \sigma \boldsymbol{E}$$

$$p = \frac{dP}{dV} = \boldsymbol{J} \cdot \boldsymbol{E} = \boldsymbol{J} \cdot \boldsymbol{J} / \boldsymbol{\sigma} = \frac{\mid \boldsymbol{J} \mid^{2}}{\boldsymbol{\sigma}}$$

```
# Define variational problem
    u = TrialFunction(V)
    v = TestFunction(V)
    F = sigma*dot(grad(u), grad(v))*dx
    a, L = lhs(F), rhs(F)
    u = Function(V)
    solve(a == L, u, [bcL, bcR])

    J = -sigma*grad(u)
    p = project(dot(J,J)/sigma, V)
```

KEB-45250
Prosessien numeerinen mallinnus

Kevät 2017

Luento 1

Tohtorikoulutettava
DI Niko Niemelä
niko.p.niemela@tut.fi

PhD topic

- ***Research topic:*** Determining biomass reaction kinetics and using them in pulverized fuel combustion modeling
- Reaction modeling is done by coupling experimental data and CFD modeling
- Research topic involves chemistry, fluid dynamics, heat transfer and numerical modeling

Pulverized fuel (PF) combustion

- Used in power plants for heat and electricity generation
- Fuel is pulverized and fed through a specifically designed burner
- Challenges related to industrial boilers:
  - Unburned fuel → poor combustion efficiency
  - Variable fuel properties → burner needs tuning depending on the fuel
  - Slagging and fouling of heat transfer surfaces

→ ***Modeling important for solving these problems***

Coal vs. Biomass in PF Combustion

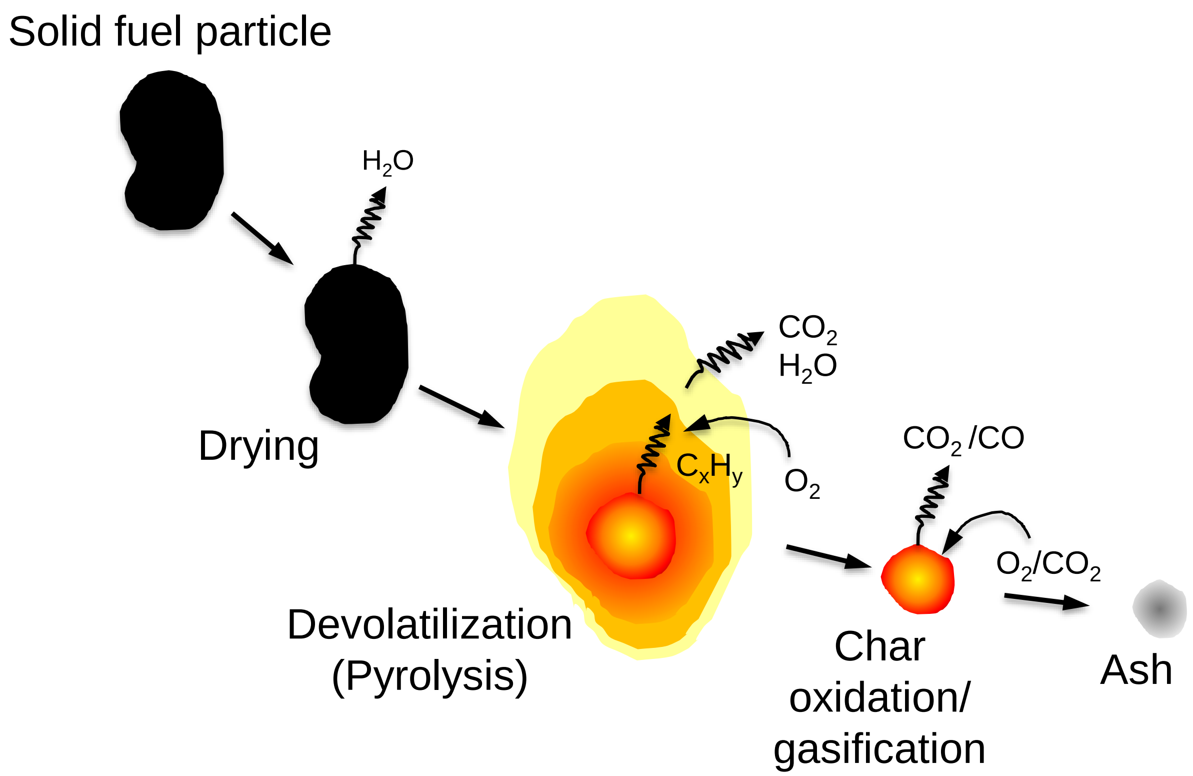
Coal

- Volatile content typically between 30% to 60% (dry)
- Very fine particles, most below 0.5 mm
- Spherical particle shape

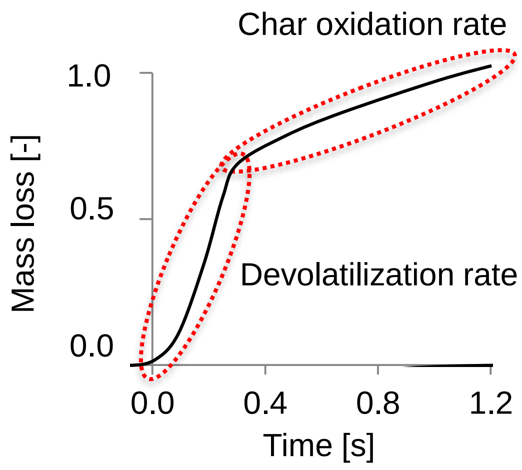
Biomass

- High volatile content, up to 95% (dry)
- Relatively large particles, up to 2-3 mm
- Non-spherical particle shape

Particle Combustion Stages

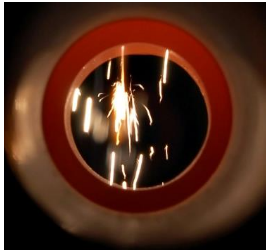


$$-\frac{dm_p}{dt} = Ae^{-\frac{E_a}{R_u T_p}}[m_p(t) - m_{vol,0}]$$



Modeling Strategy

Experimental Tests (DTR)



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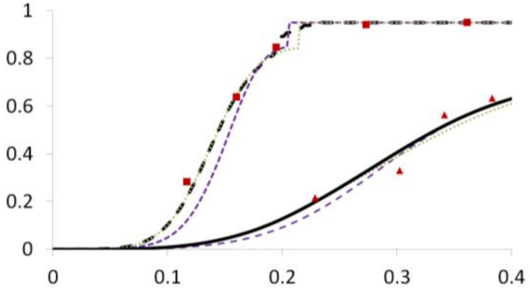
Kinetic Modeling (MATLAB) ⟷ CFD Model of the DTR



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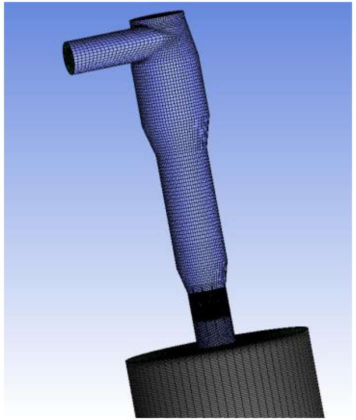
Verified Reactivity Parameters

↓

Larger Scale CFD Modeling



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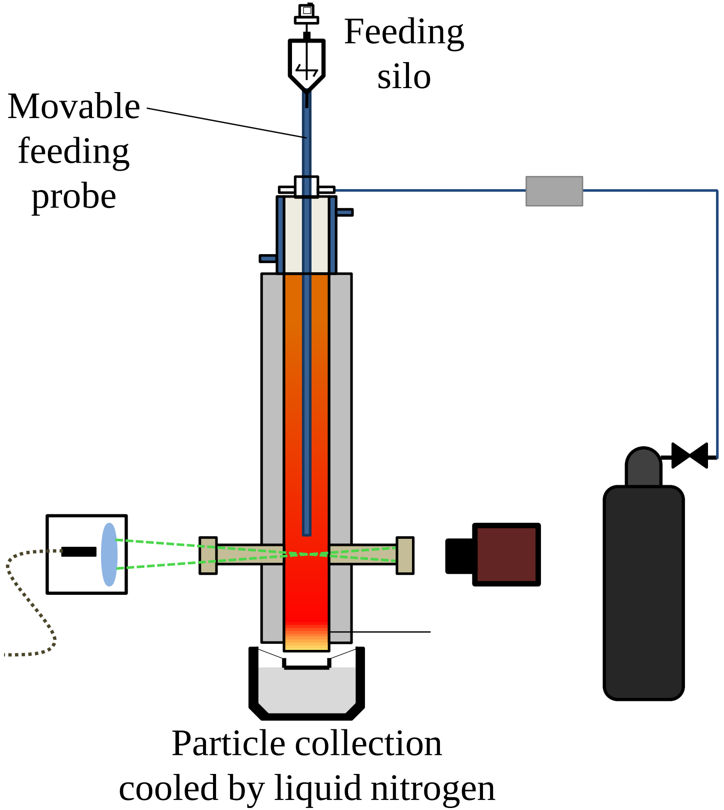
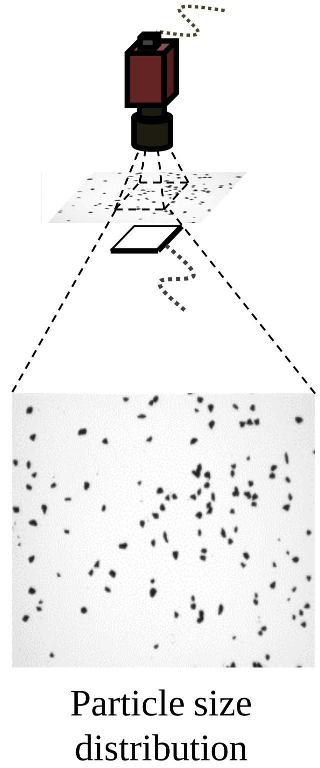
Validated Reactivity Parameters

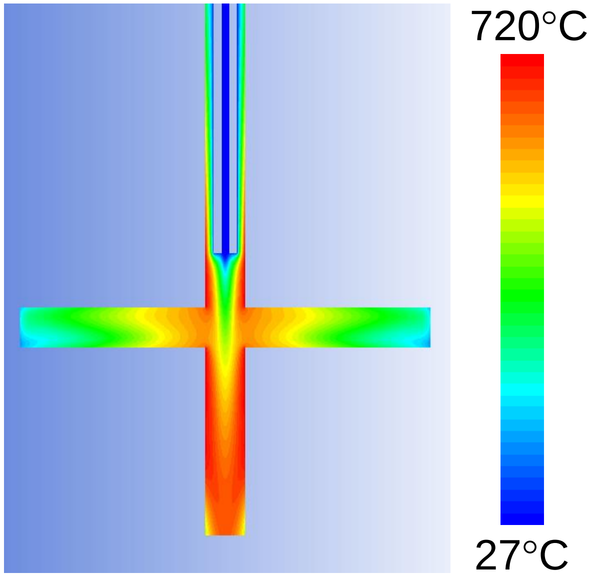
Drop-Tube Reactor (DTR)



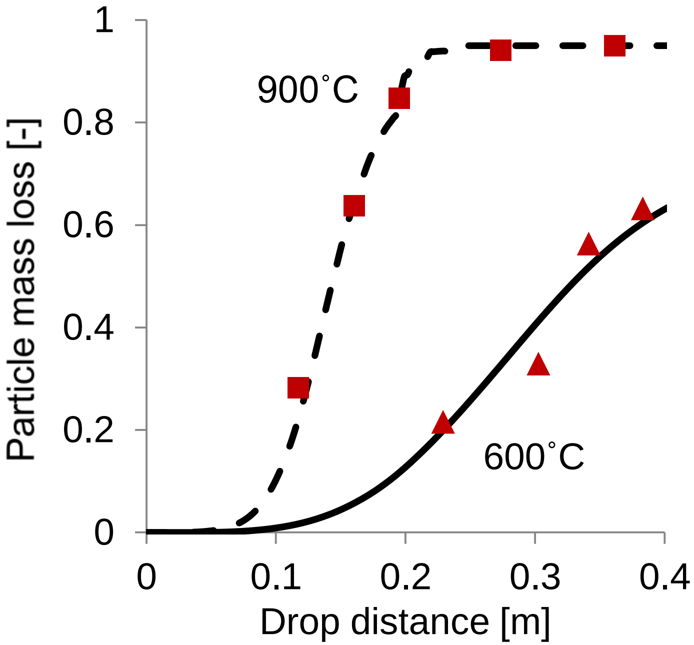


Drop-Tube Reactor Modeling

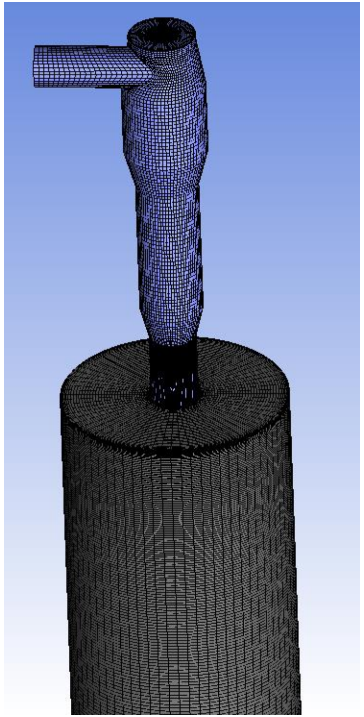
Reactor temperature



Pyrolysis mass loss

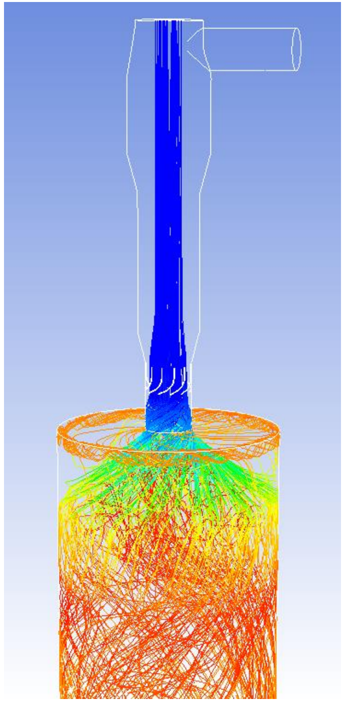


CFD Model of a 50kW Test Reactor

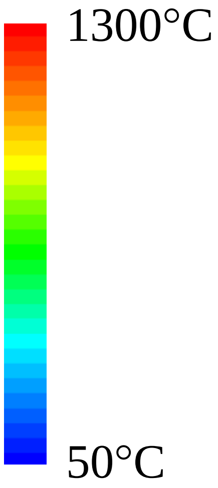


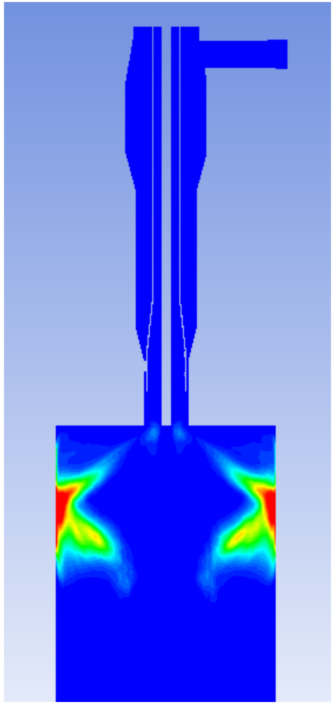
Comparison between lignite (brown coal) and woody biomass combustion

Results from 50kW reactor simulations

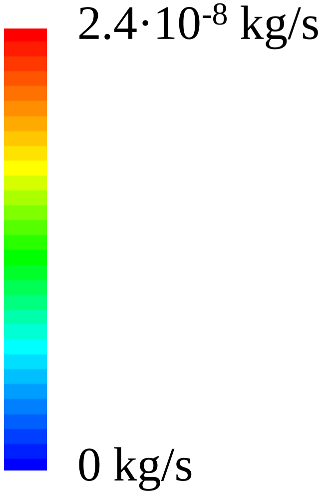


Trajectories and temperature histories of 50μm lignite particles

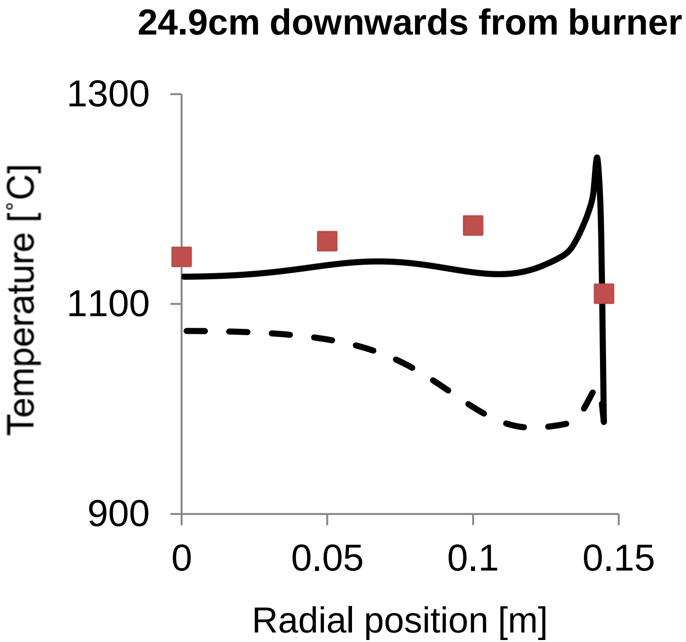


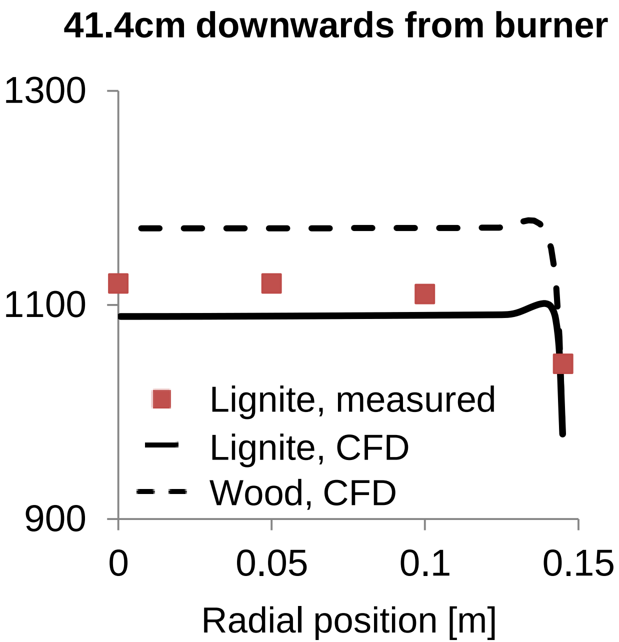


Formation rate of pyrolysis gases



Results from 50kW Reactor Simulations





	Lignite	Wood Pellet
Burnout efficiencies:	98.5%	93.1%

Summary of course objectives

- Choosing the right modeling technique case specifically
  - Own codes are often superior for solving a specific problem, and for saving computational time
  - Software packages and CFD are often better in more complicated problems
- Understanding the strengths and weaknesses of certain models and numerical techniques
- Analyzing the results and solving industrial problems
- Presenting the results clearly and comprehensively

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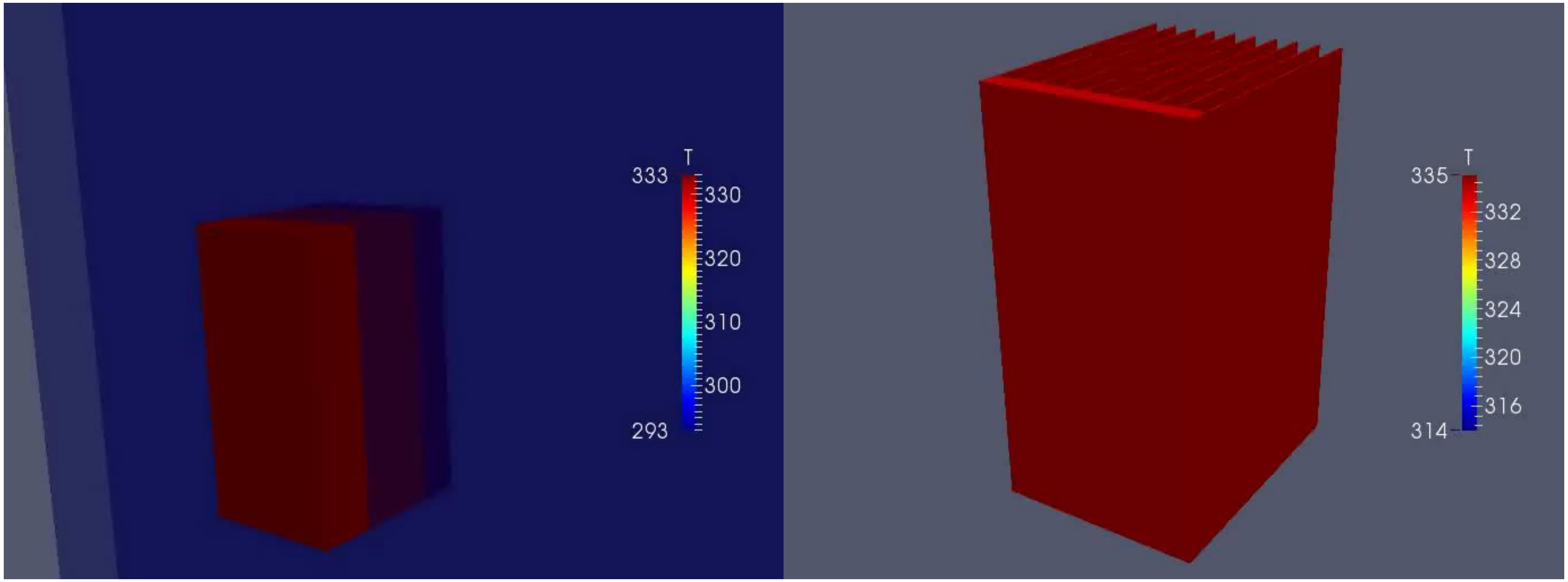
KEB-45250 Numerical Techniques for Process Modelling

Lecture 1

Kaj Lampio

Tampere University of Technology

Introduction

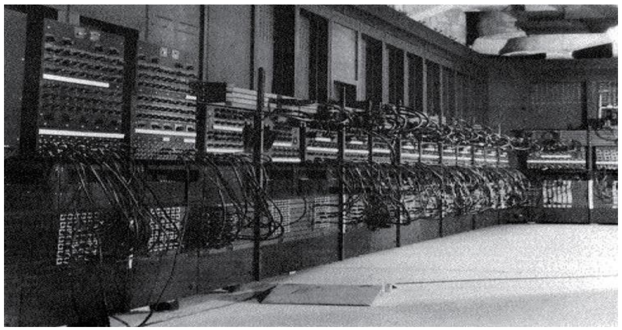


Dissertation

Optimization of fin arrays cooled by forced or natural convection

- Calculation model
- Optimization algorithm

Electronics cooling



- 1940s (ENIAC) ~170kW
- 1950s (IBM Mark 2)
- 1980s (IBM System 360)

Electronics cooling

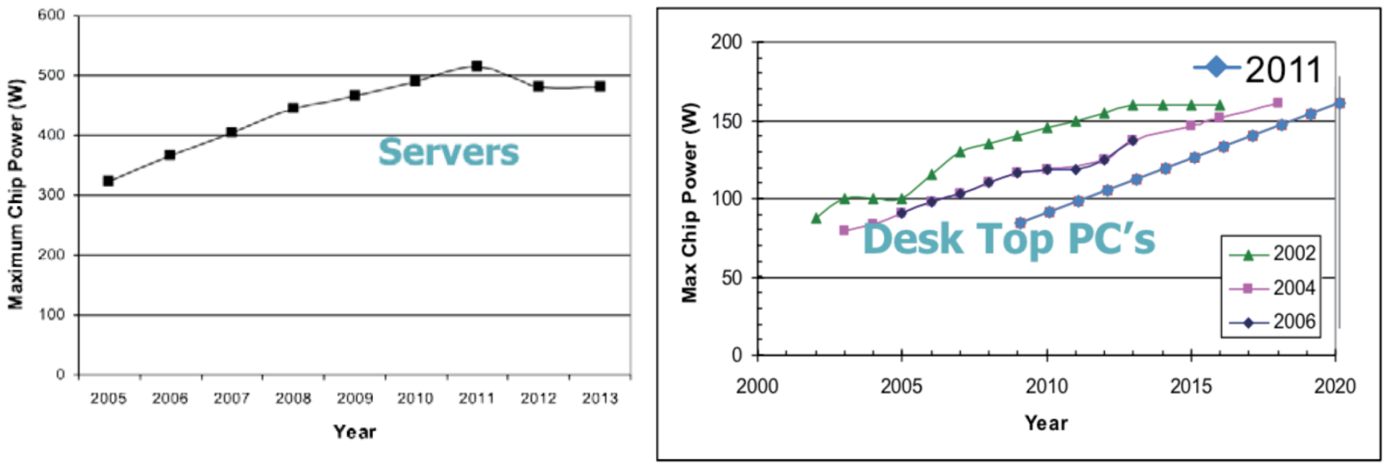
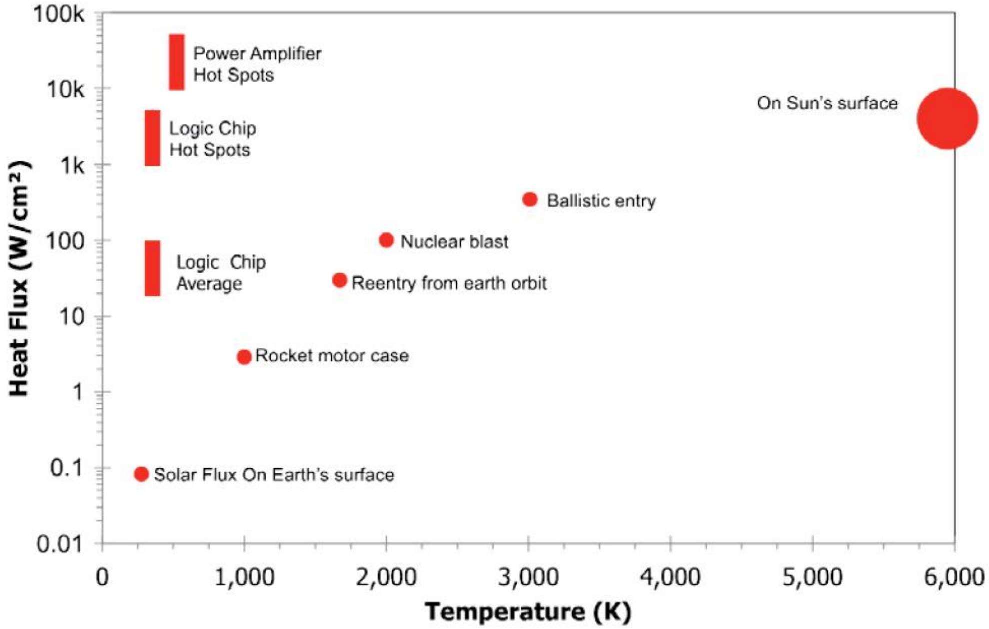


Figure. iNEMI Roadmap 2013, chip power dissipation

- Modern chips produce a lot heat
- Their size is relatively small
  – Heat dissipation per surface area large

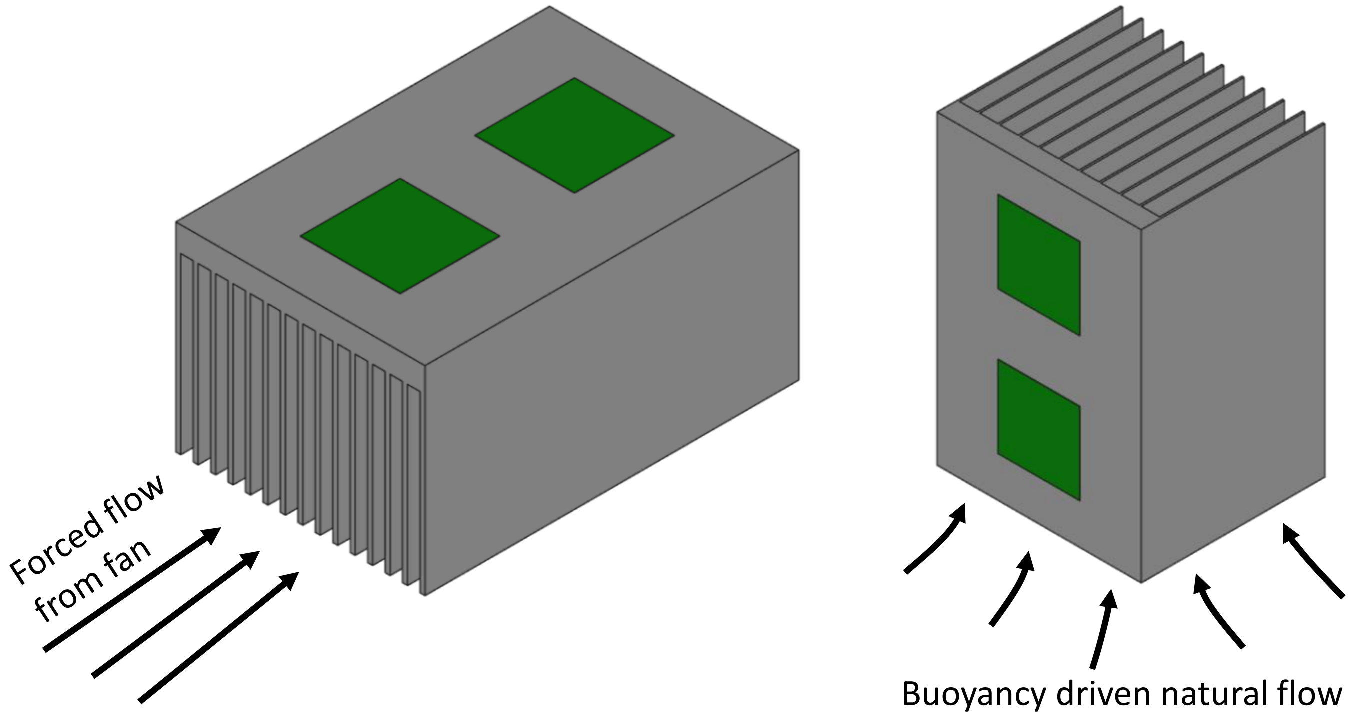
Electronics cooling



- Chips produce a lot of heat
- Operating temperatures close to room temperature

Heat sink

- Usually aluminum array
- Components attached to base plate surface



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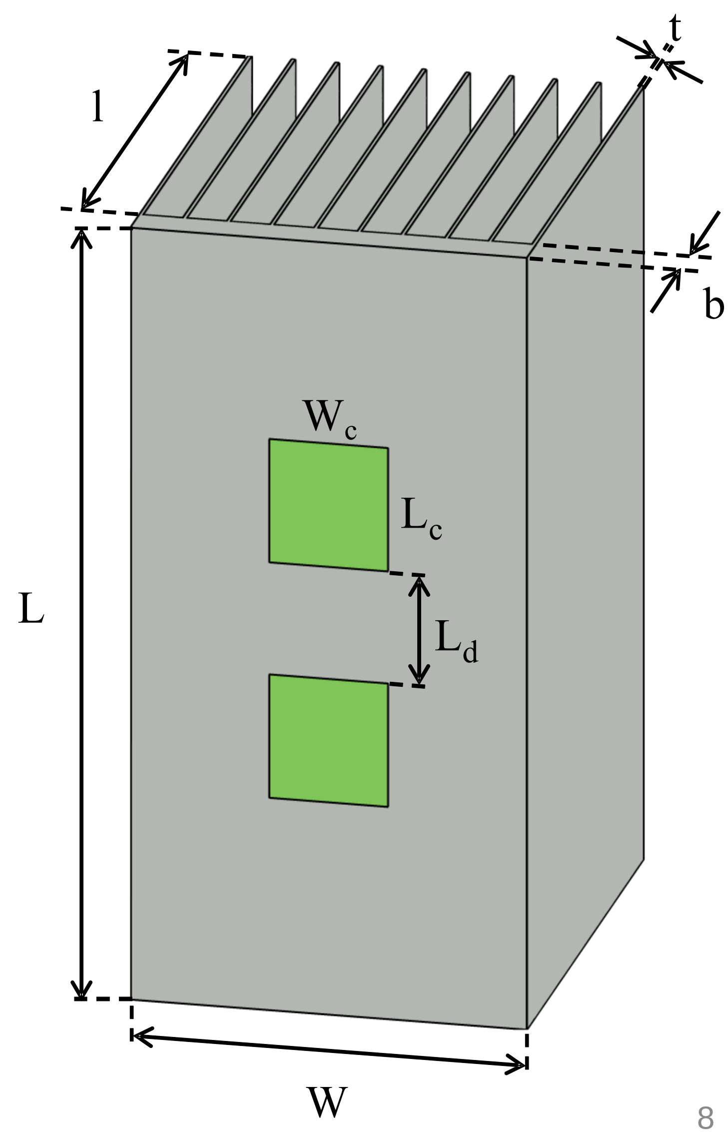
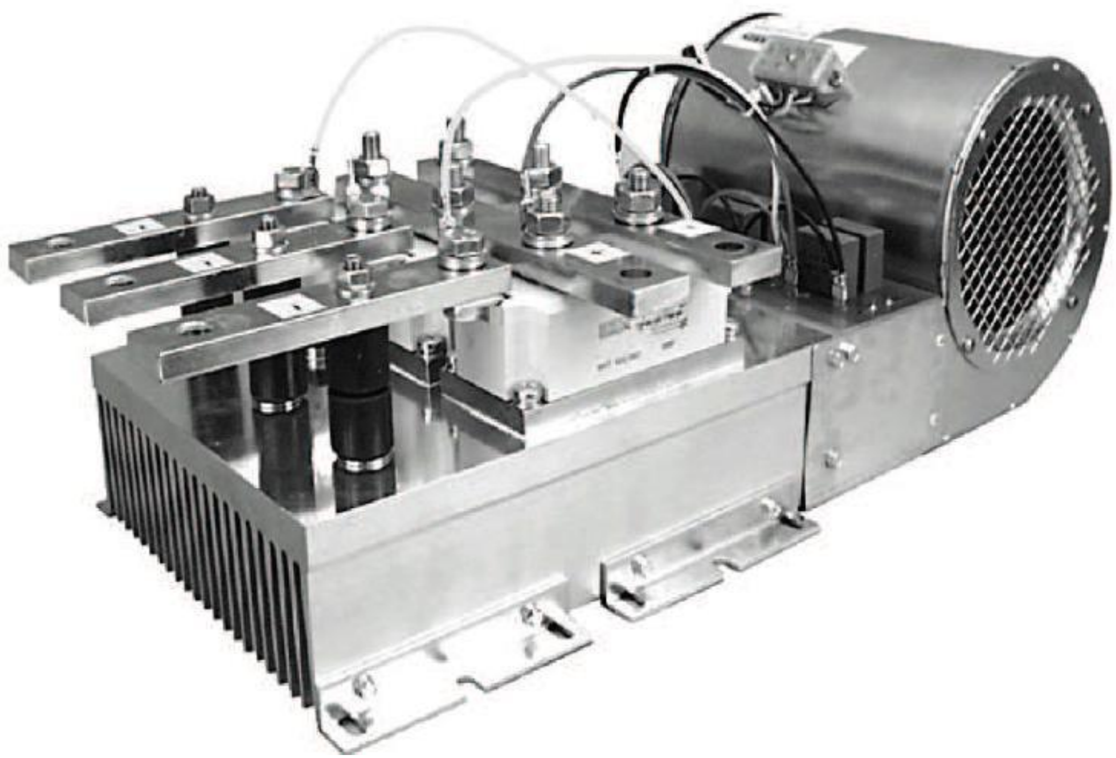
Heat sink design

- Limiting factor T_{max}
- Mass and volume should be small



Forced cooling: CPU

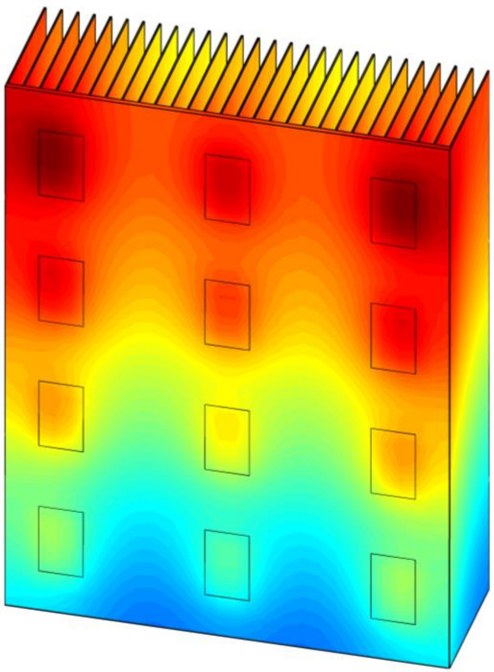
Forced cooling: Power electronics



Natural cooling: Base stations

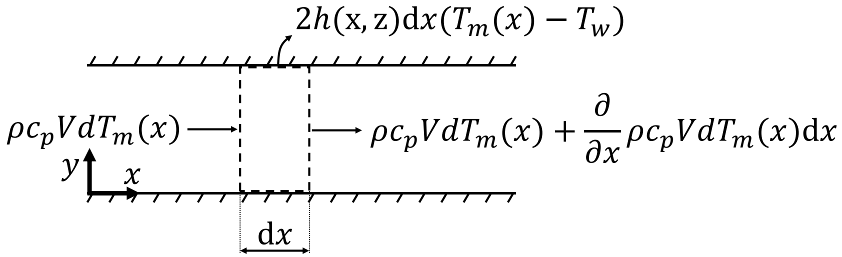
Obtaining temperatures

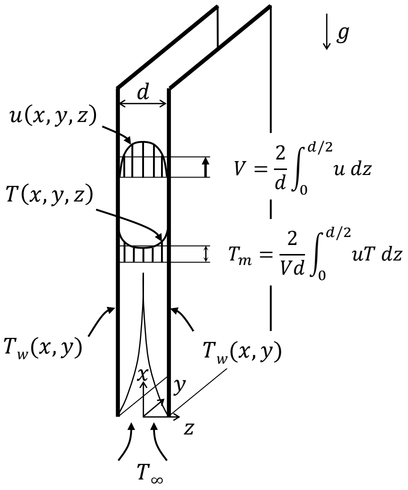
- Commercial CFD methods too time consuming for optimization
- A custom calculation model was created



Calculation model

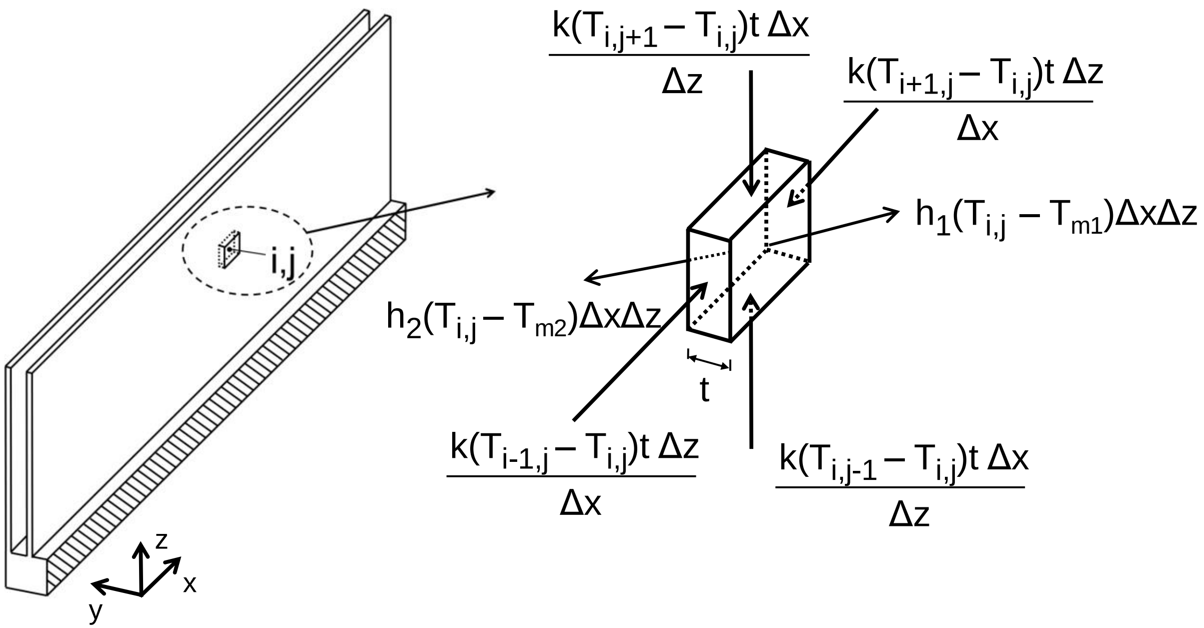
- Design method for engineers
- Target: engineering accuracy (+- 10%)
- Convective heat transfer analytically





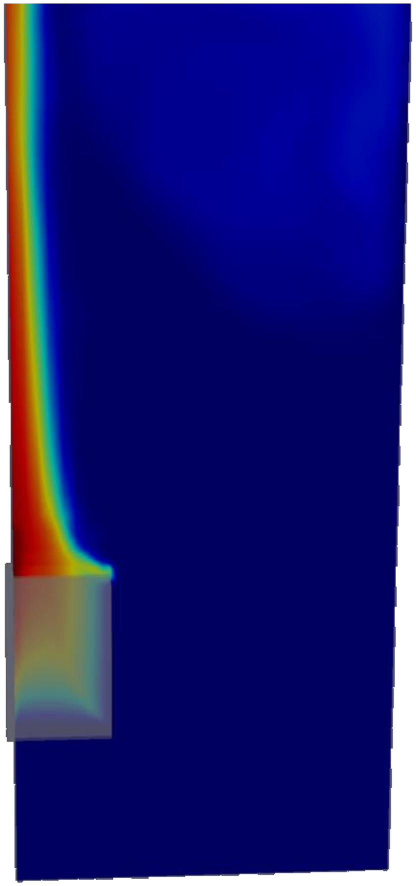
Calculation model

- Solid temperature field numerically



Testing calculation model

- Tested in forced flow test against experimental results
- Tested in natural flow test against calculated CFD results



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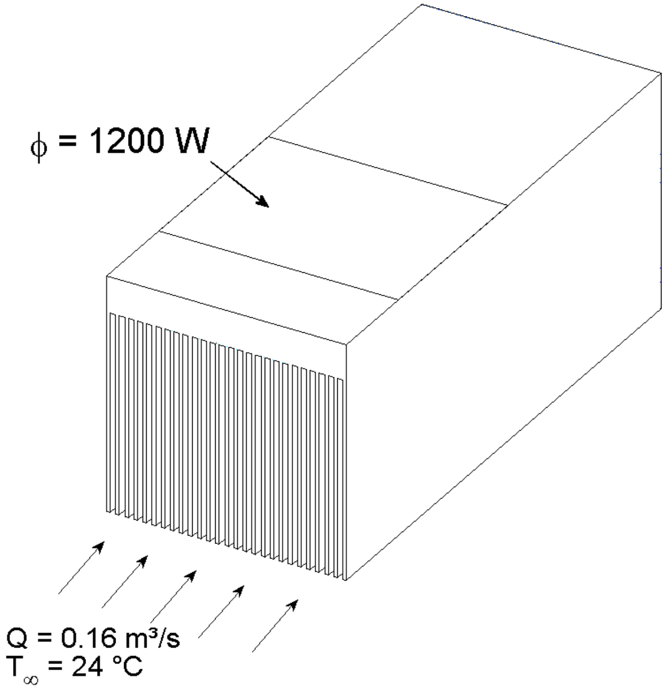
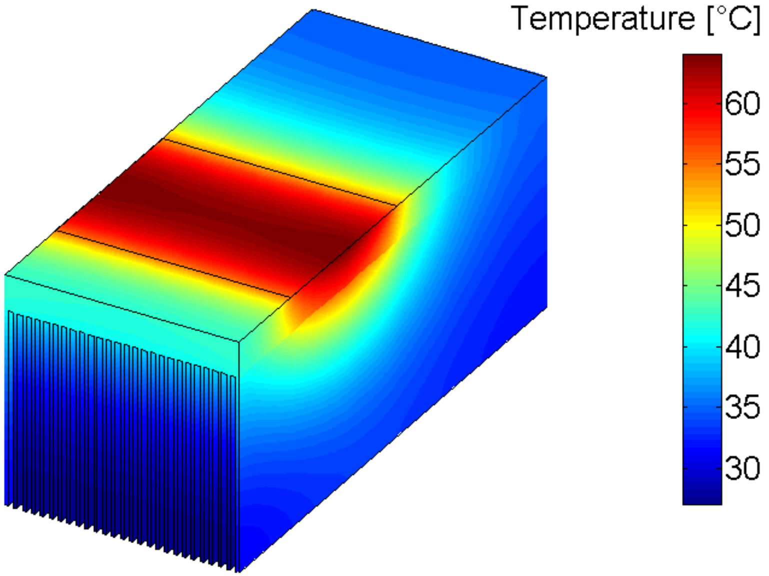
Forced flow test

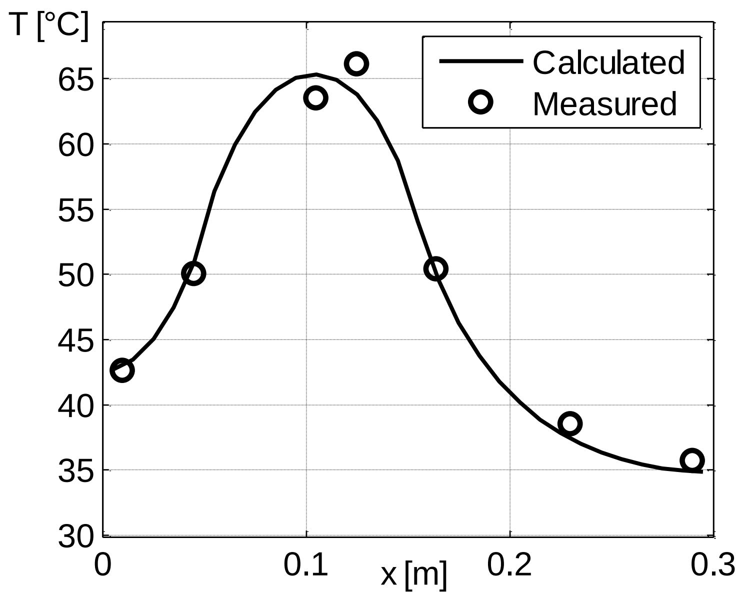
- One heat dissipating component (1200 W)
- Fixed volumetric flow

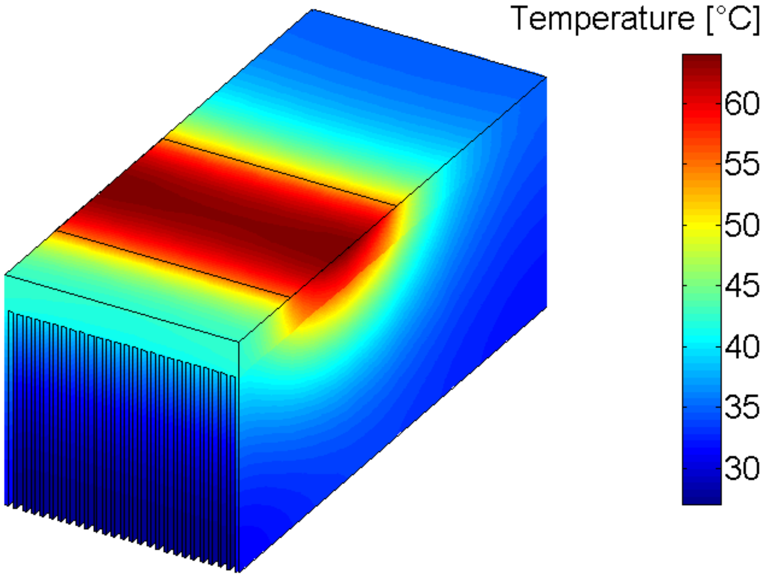


Forced flow test



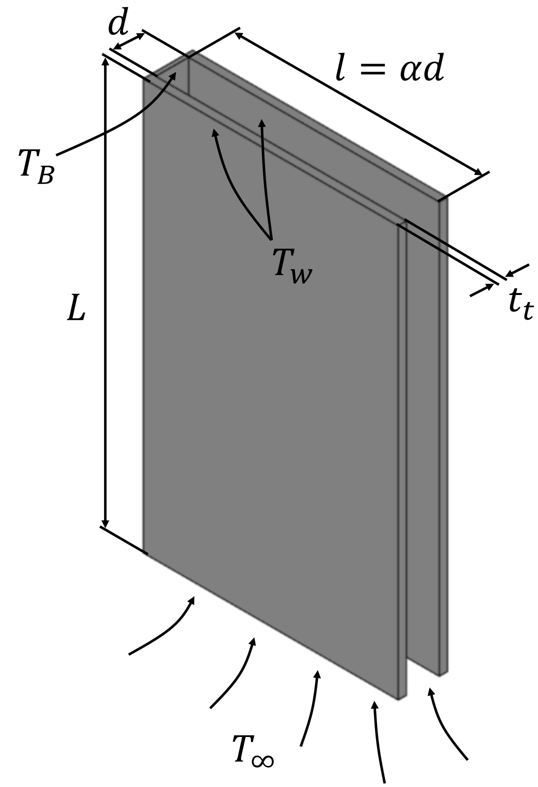
Forced flow test





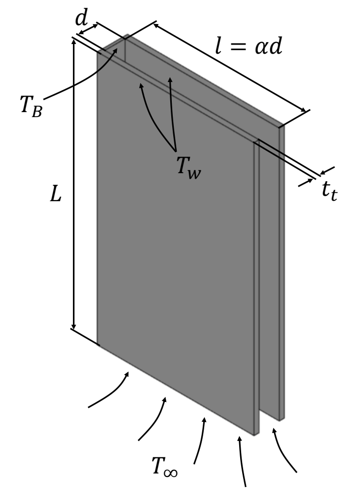
Natural convection test 1

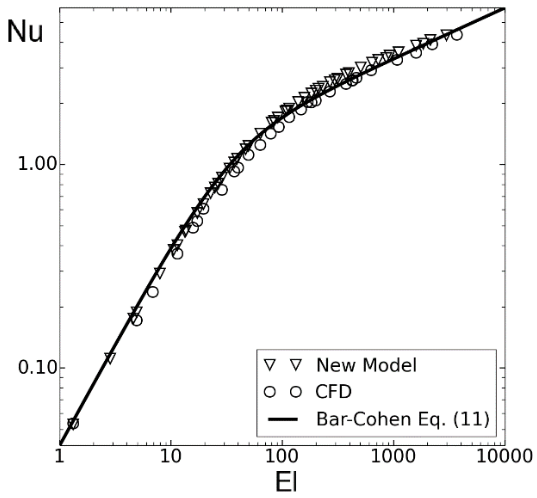
- Testing one channel
- Isothermal walls
- 144 different geometries



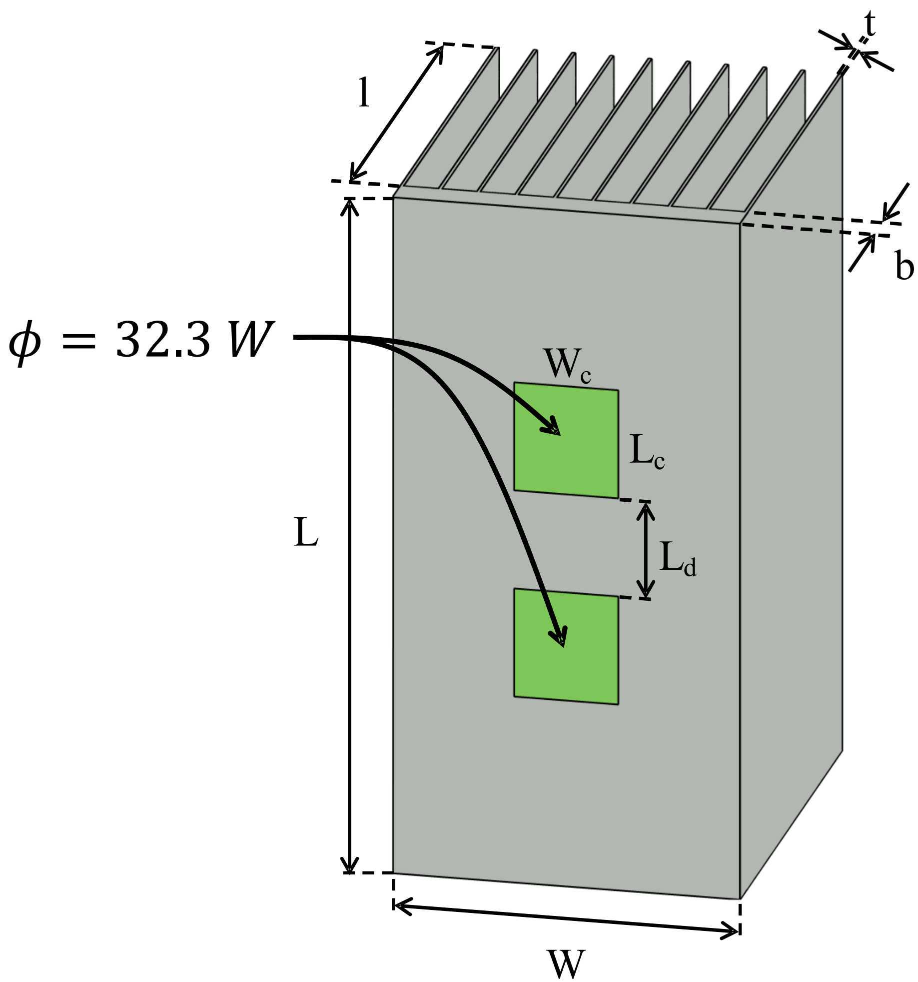
Natural convection test 1

- Good agreement between calculation model, CFD and analytical results



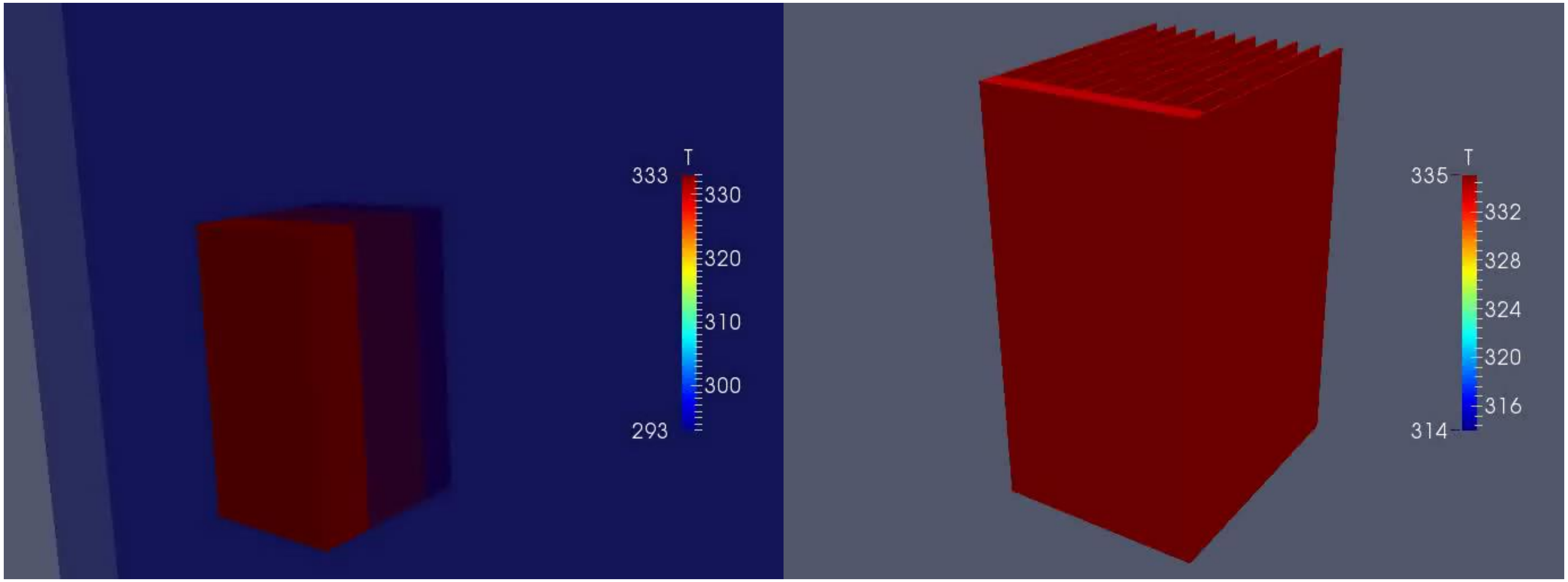


Natural convection test 2

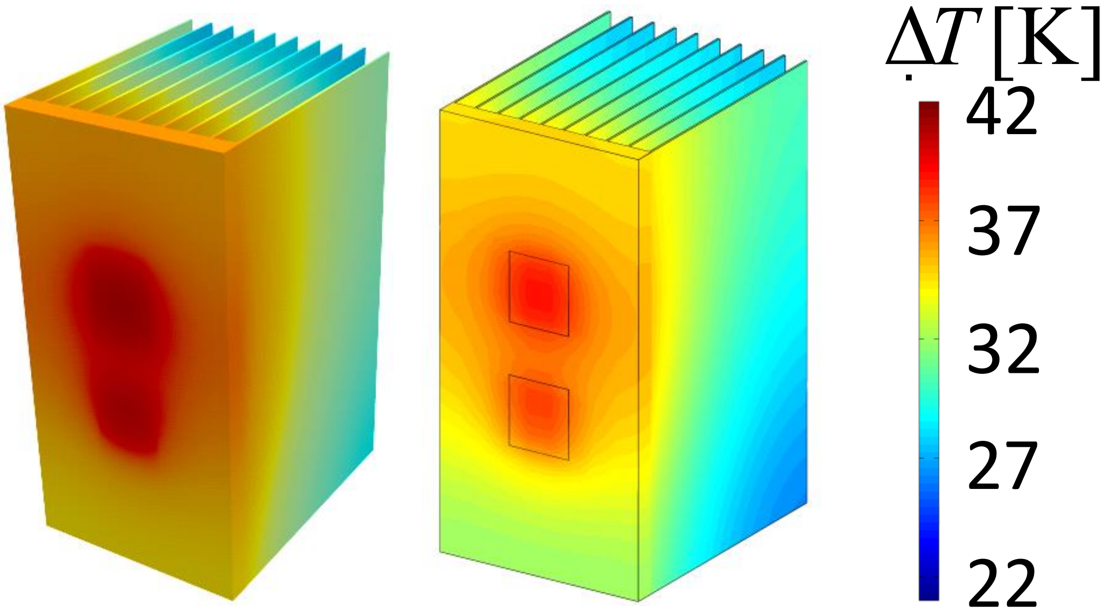


Dimension	Value [mm]
L	200
l	120
W	100
b	10
t	1
L_c	32
W_c	30
L_d	24

Natural convection test 2 - CFD



Natural convection test 2 Comparison



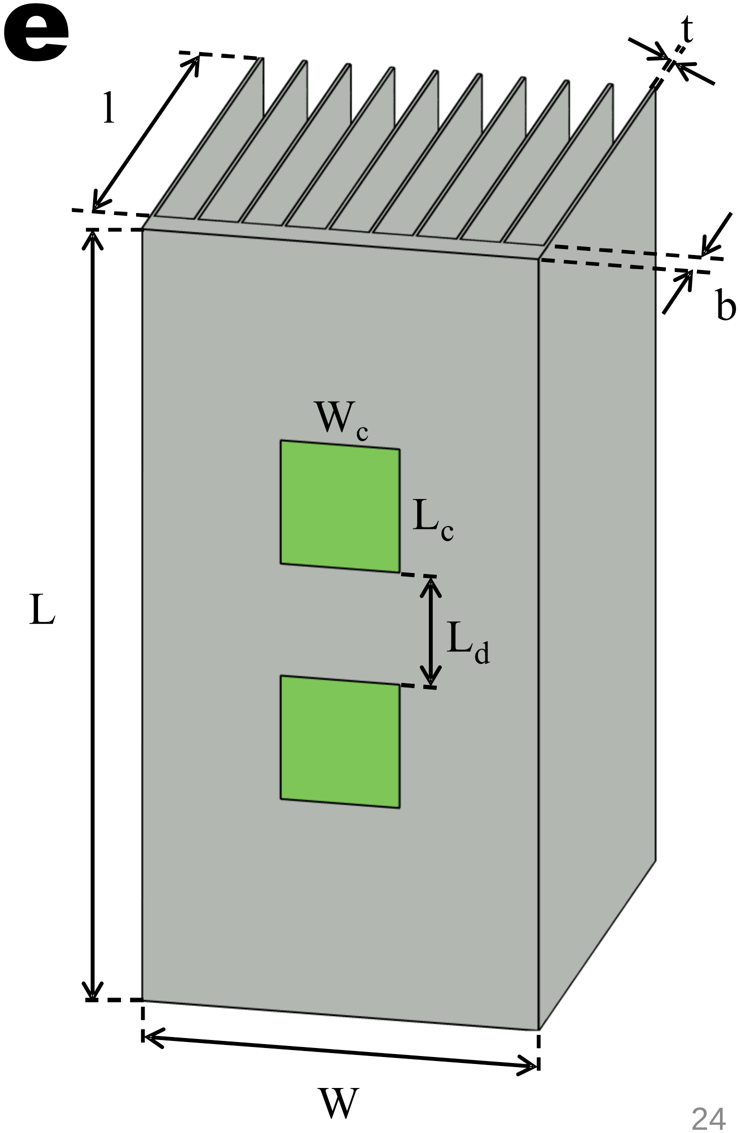
	CFD	New method	Difference
ΔT_{min}	23.5	21.4	-8.9 %
ΔT_{max}	41.7	38.9	-6.7 %

Natural convection optimization case

$$\min \begin{cases} T_{max} \\ m \\ V \end{cases}$$

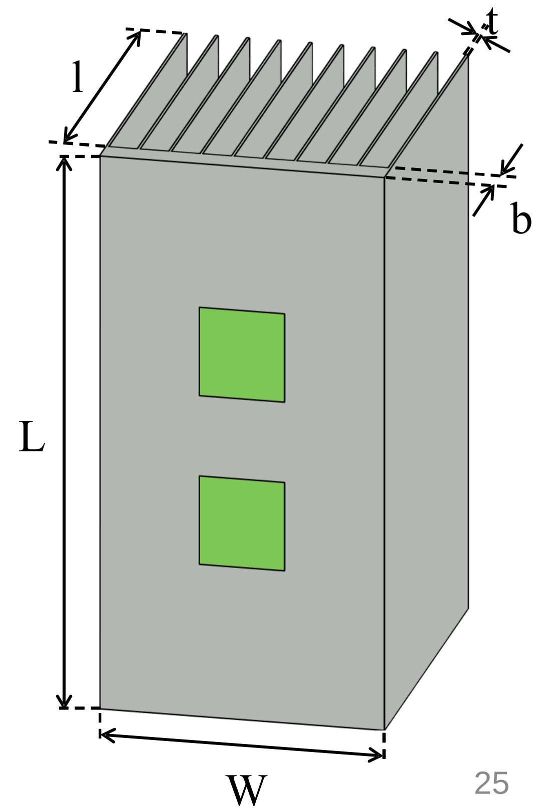
Design variables

- Geometry (L,W,l,t,b,N)
- Component locations

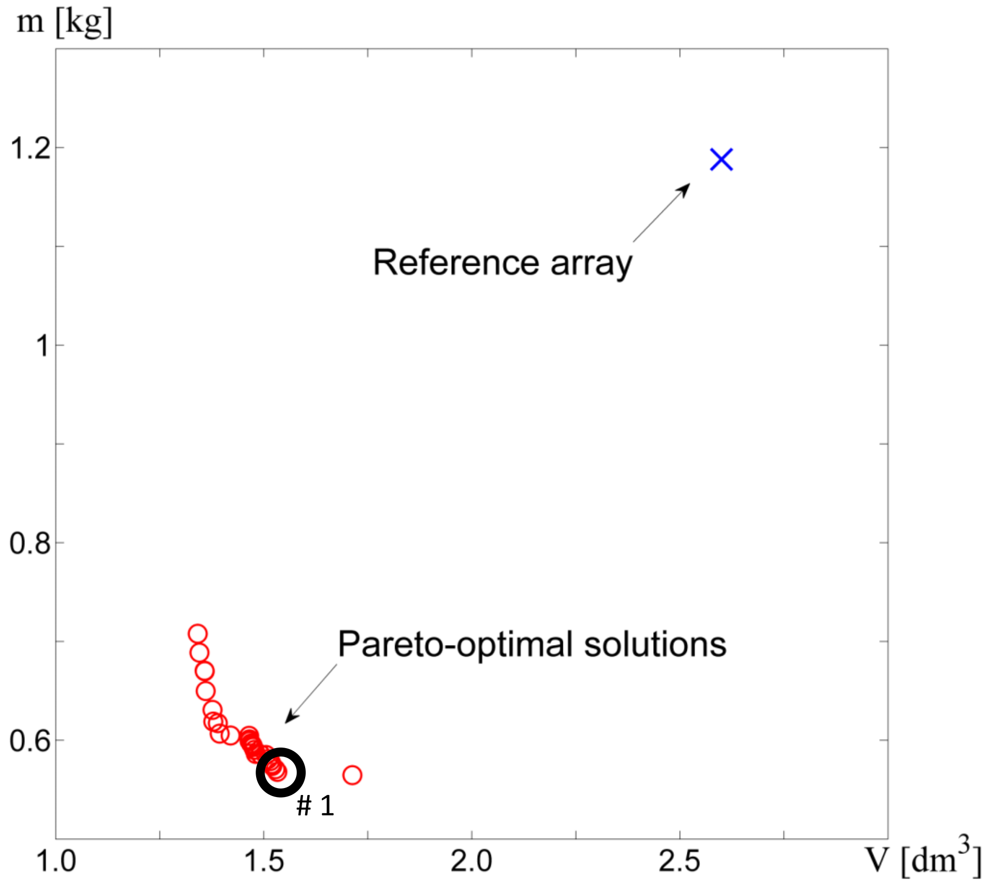


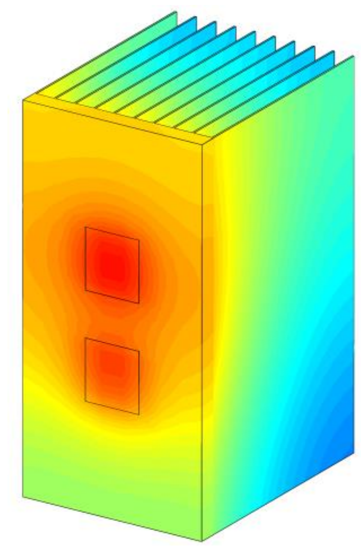
Multi-objective optimization

- Minimize V (volume) and m (mass)
- Design variables:
  - Geometrical variables (L, W, b, N, l, t)
  - Location of components ($\boldsymbol{X}$, $\boldsymbol{Y}$)
- Limiting factor T_{max}

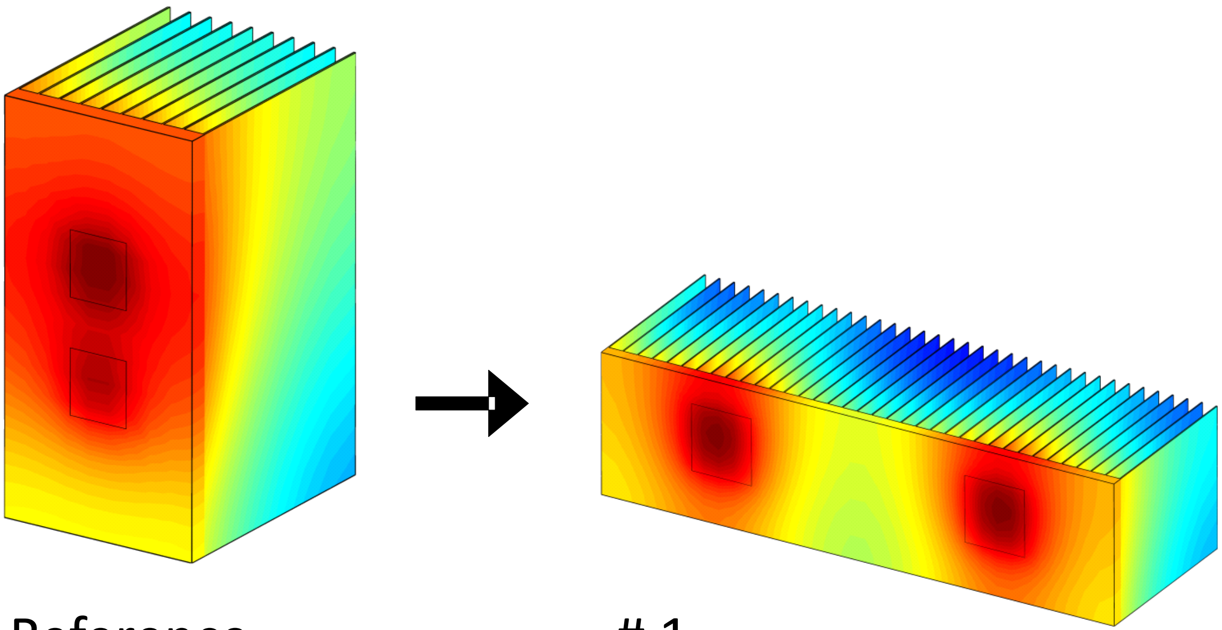


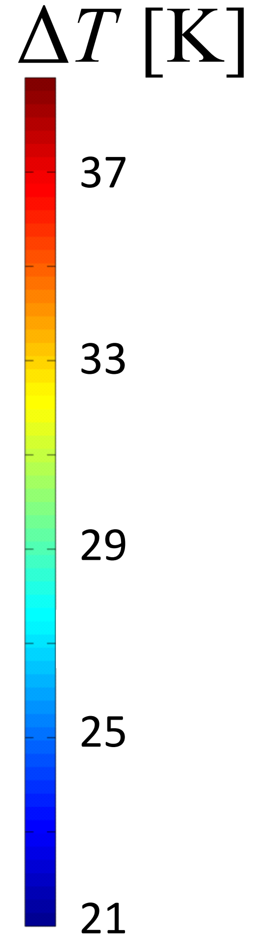
Optimization results





Reference
m = 1.19 kg
V = 2.6 dm³
T_{max} = 331.9 K



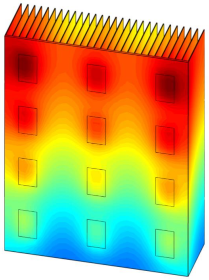


Reference
m = 1.19 kg
V = 2.6 dm³
ΔT_{max} = 38.9 K

1
m = 0.57 kg
V = 1.53 dm³
ΔT_{max} = 38.9 K

Conclusions

- New calculation model for forced and natural convection fin arrays
- Analytical and numerical solutions
- Tested with simple test cases
- Can be used in optimization of practical fin arrays where CFD is too time consuming



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Thank you for attention

Kaj Lampio

Tampere University of Technology