Flow And Heat Transfer Simulations As A Development Tool For A Novel Microcalorimeter

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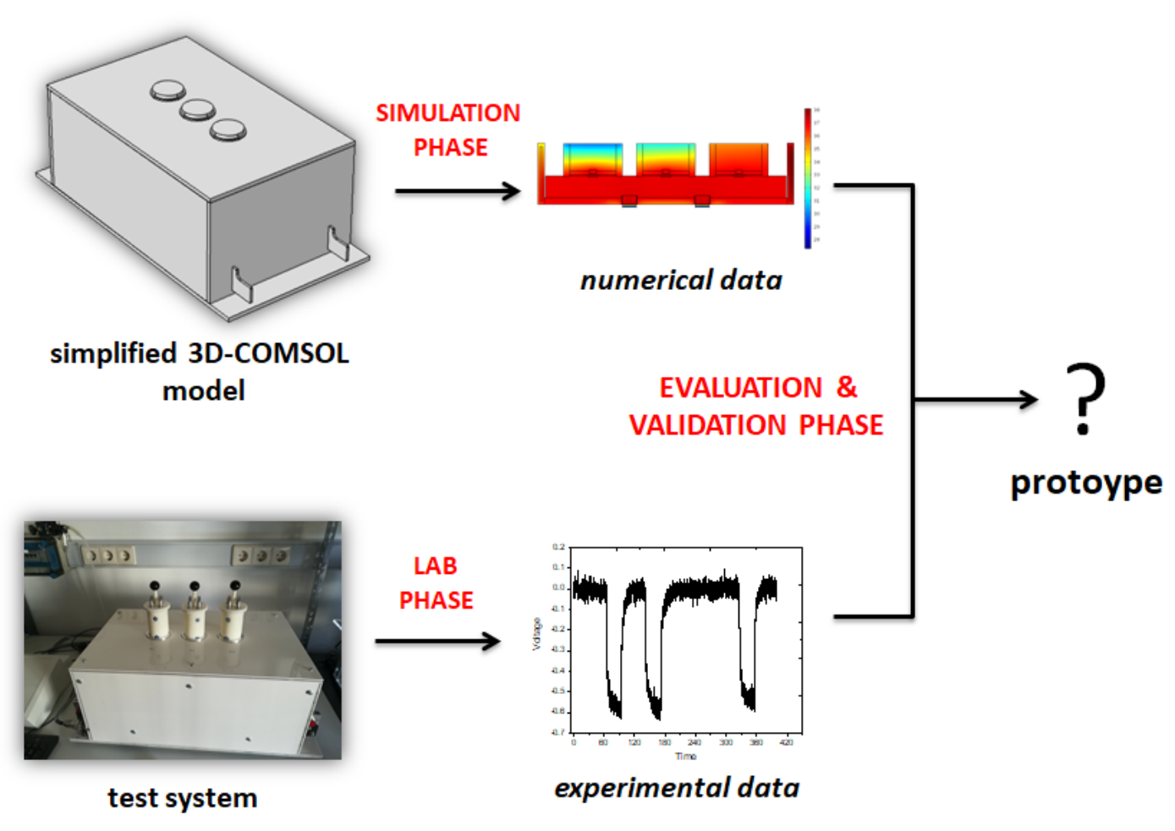
INTRODUCTION

In this study, we used version 5.3a of the simulation software COMSOL Multiphysics® as a development tool for a novel microcalorimeter. Our simulation results give us a comprehensive insight into the 3D-temperature distribution of the entire system. As a result, we can comprehend all heat flow pattern that cannot be measured experimentally. In this way, we cannot only improve the performance of the microcalorimeter but also expand our understanding of heat transfers within microcalorimeter.



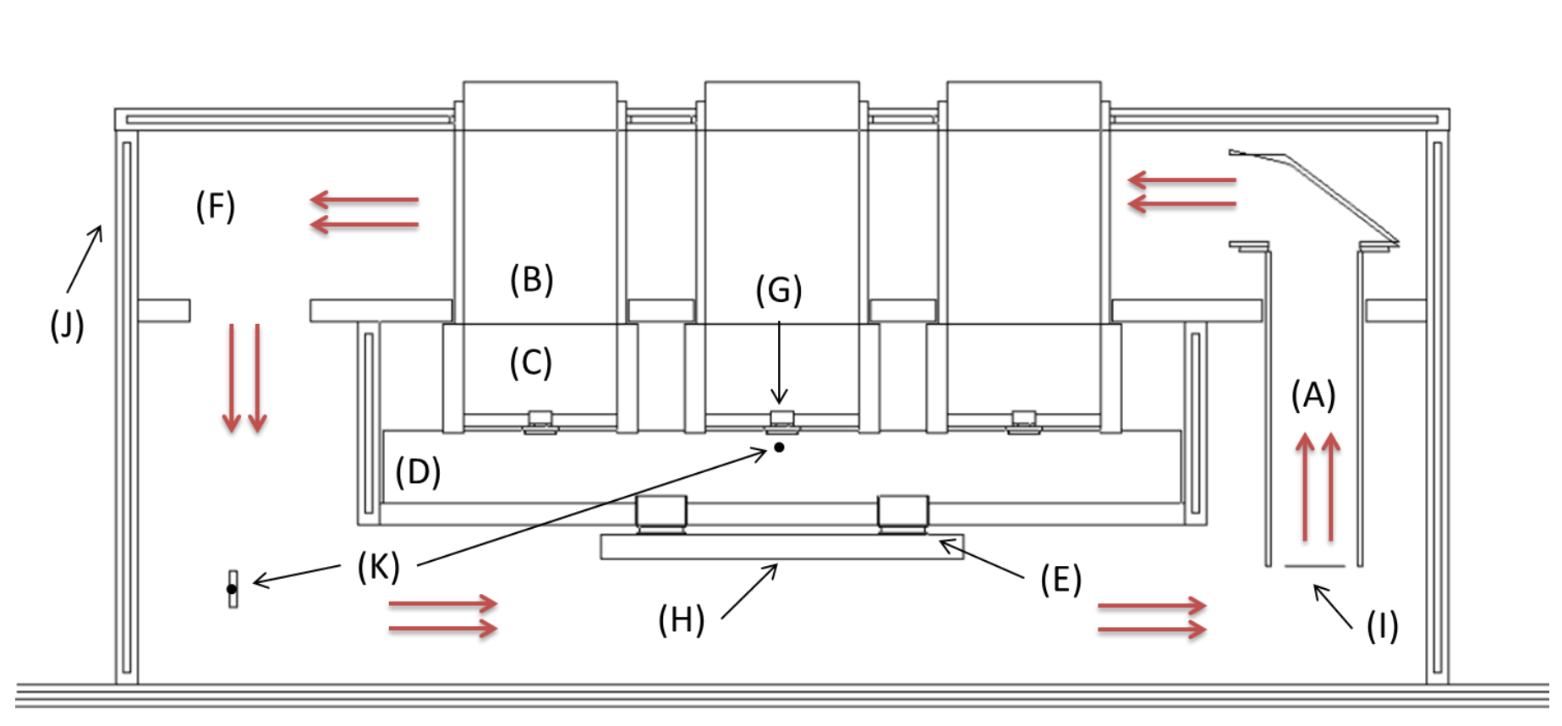


Figure 1: Cross-section of the 3D-COMSOL model.
A: air heater. **B:** upper channel part. **C:** lower channel part. **D:** primary heat sink. **E:** thermoelectric cooler (T.E.C). **F:** interior air domain. **G:** heat flow sensors (HFS). **H:** auxiliary heat sink. **I:** interior fan. **J:** housing. **K:** temperature probes.
Red arrows - flow direction. Not shown here are the two heating foils below the heat sink D.

COMPUTATIONAL METHODS

The simplified 3D-model simulates in a first stationary study step the laminar flow caused by an interior fan. Subsequently, the heat transfer is simulated in a time-dependent study step. Both interfaces are connected via the nonisothermal multiphysics interface. Additionally, ODE and DAE interfaces (Events and Global ODE and DAE Interface) are applied to simulate the temperature control unit.

laminar flow

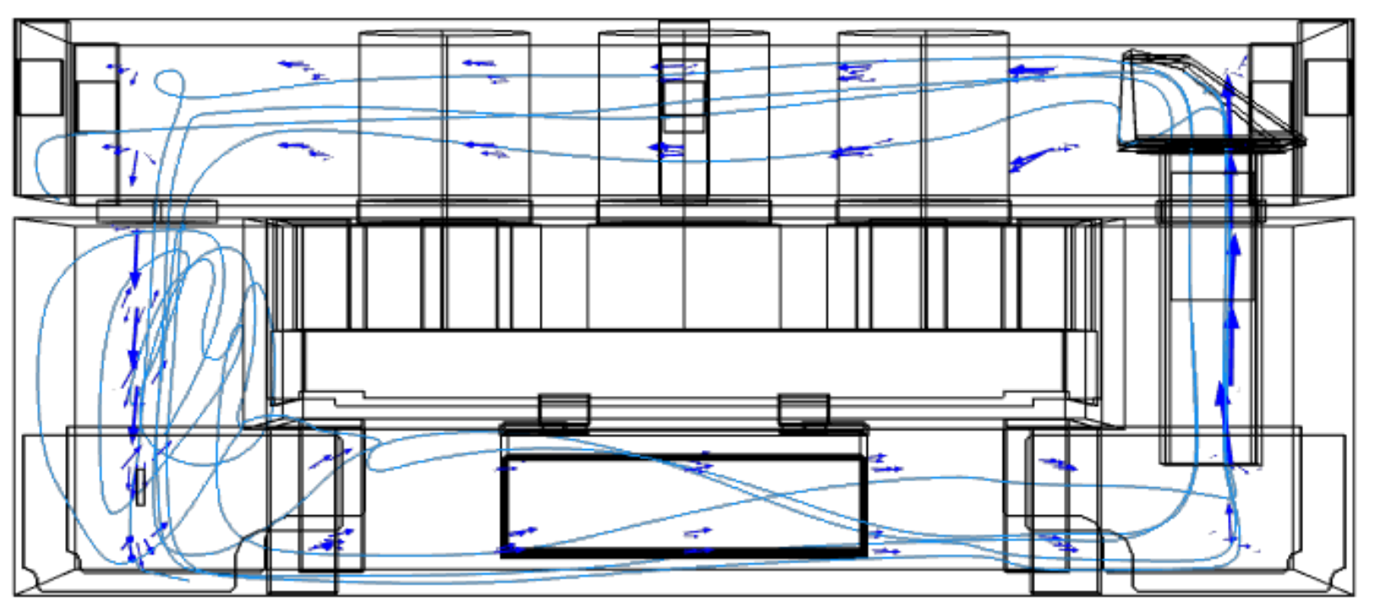


Figure 2: 3D-volume plot of the air domain. Blue arrows - flow direction; blue lines - streamlines of the velocity field.

Governing equations laminar flow

$$\left.\begin{aligned}&\rho(\mathrm{u}\cdot\nabla)\mathrm{u} = \\ &\nabla\cdot\left[-p\mathrm{I}+\mu\left(\nabla\mathrm{u}+(\nabla\mathrm{u})^{T}\right)-\frac{2}{3}\mu(\nabla\cdot\mathrm{u})\mathrm{I}\right]+\mathrm{F}\end{aligned}\right\}\ \textbf{Navier-Stokes equation}$$

$$\nabla\cdot(\rho\mathrm{u}) = 0 \qquad \textbf{continuity equation}$$

Boundary conditions

$$\left.\begin{aligned}&[\rho\mathrm{u}\cdot\mathrm{n}]_{-}^{+} = 0\\ &\left[p-\mathrm{n}^{T}\left[\mu(\nabla\mathrm{u}+(\nabla\mathrm{u})^{T})-\frac{2}{3}\mu(\nabla\cdot\mathrm{u})\mathrm{I}\right]\mathrm{n}\ldots\right.\\ &\left.+\rho(\mathrm{u}\cdot\mathrm{n})^{2}\right]_{-}^{+} = \Delta p_{\mathrm{pc}}\\ &\Delta p_{\mathrm{pc}} = f(p_{\mathrm{nf}}, V_{0,\mathrm{fd}})\end{aligned}\right\}\ \textbf{interior fan}$$

$$\mathrm{u} = 0 \qquad \textbf{wall (no slip)}$$

temperature regulation

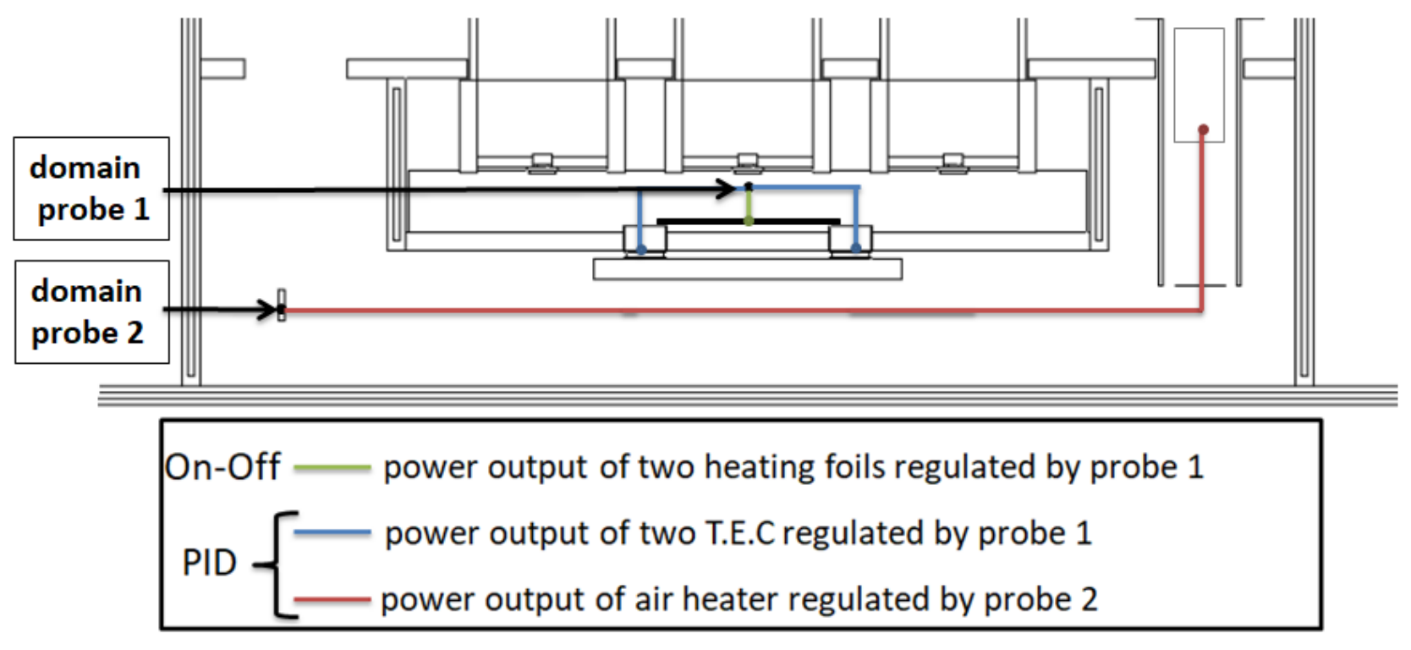


Figure 3: Schematic description of the temperature feedback system.

Governing equations PID controller

$$P = \mathrm{nojack}(\mathrm{K_P}\cdot(\mathrm{T_{mp}}-T_{\mathrm{set}})+\mathrm{K_I}\cdot\mathrm{I}[\mathrm{K}\cdot\mathrm{s}]+\mathrm{K_D}\cdot\mathrm{Tt_{mp}}$$

$$\mathrm{I} = \mathrm{It}[\mathrm{s}] - (\mathrm{T_{mp}}[\mathrm{K}^{-1}]-T_{\mathrm{set}}[\mathrm{K}^{-1}]) \qquad \textbf{integral function}$$

Boundary conditions

$$\left.\begin{aligned}P_{\mathrm{ctrl}} = \mathrm{if}(&P < Q_{\mathrm{min}}, Q_{\mathrm{min}},\\ &\mathrm{if}(P > Q_{\mathrm{max}}, Q_{\mathrm{max}}, P))\end{aligned}\right\}\ \textbf{lower and upper limit}$$

heat transfer

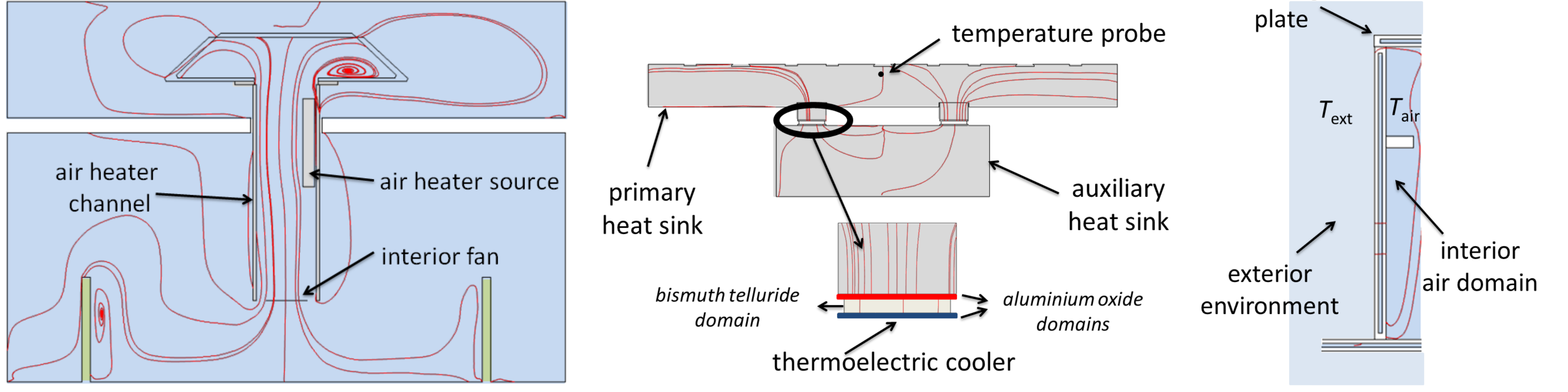


Figure 4: Cross-sections of different areas within the 3D-COMSOL model. **Left:** xz-plane through the air heater. Air domain is heated by an air heater source (electrical resistor). **Center:** temperature of the primary heat sink has to be kept constant (T_{set} = 310.22 K). This temperature is regulated by two thermoelectric coolers (T.E.Cs) via a PID controller, using the temperature probe as input. **Right:** the interior air domain is surrounded by housing plates. The external temperature (T_{ext}) is 293.15 K and the heat transfer coefficient (h) is 5 W/(m^2·K). Blue area - interior air domain. Red lines - heat fluxes in the respective plane.

Governing equations heat transfer

$$\left.\begin{aligned}\rho C_p\frac{\partial T}{\partial t}+\rho C_p\mathrm{u}\cdot\nabla T+\nabla\cdot\mathrm{q} &= Q+Q_{\mathrm{ted}}\\ \mathrm{q} &= -k\nabla T\end{aligned}\right\}\ \textbf{heat transfer in solid}$$

$$\left.\begin{aligned}\rho C_p\frac{\partial T}{\partial t}+\rho C_p\mathrm{u}\cdot\nabla T+\nabla\cdot\mathrm{q} &= Q+Q_p+Q_{\mathrm{vd}}\\ \mathrm{q} &= -k\nabla T\end{aligned}\right\}\ \textbf{heat transfer in fluid}$$

Boundary conditions

$$T = 293.15\ \mathrm{K} \qquad \textbf{initial values}$$

$$Q_{\mathrm{min}} = 0\ \mathrm{W}, Q_{\mathrm{max}} = 62.3\ \mathrm{W} \qquad \textbf{air heater source}$$

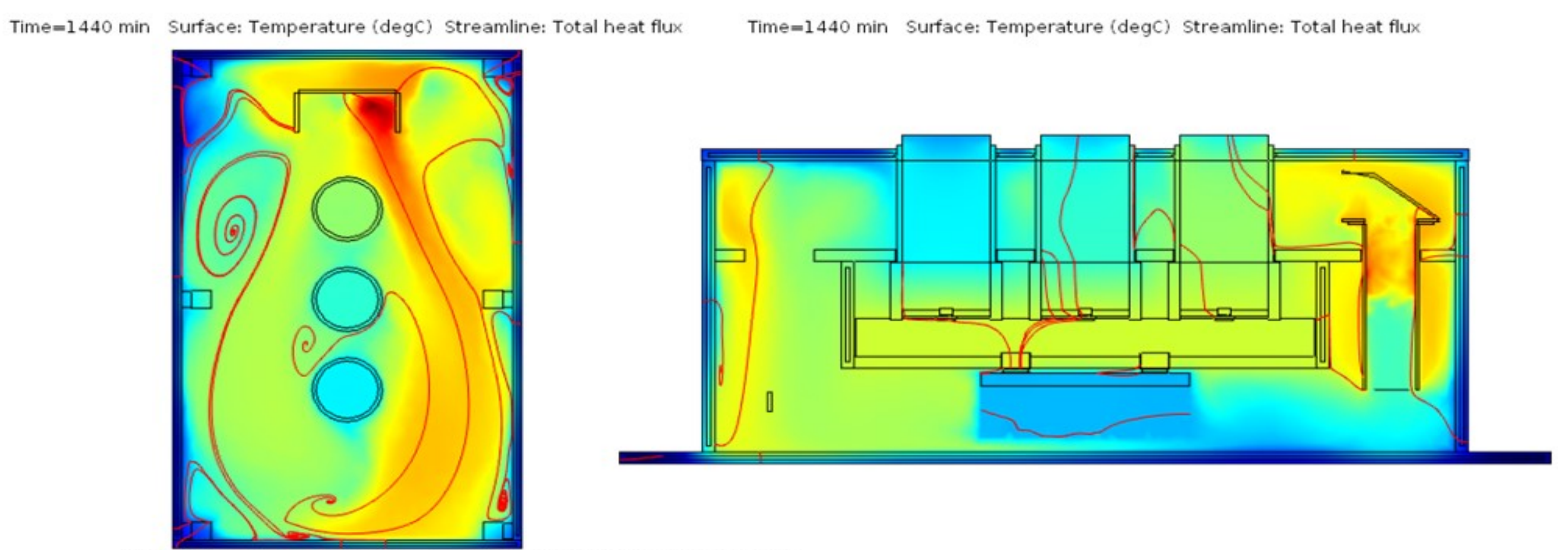
$$\left.\begin{aligned}-\mathrm{n}\cdot\mathrm{q} &= q_0\\ q_0 &= h(T_{\mathrm{ext}}-T)\end{aligned}\right\}\ \textbf{heat flux}$$

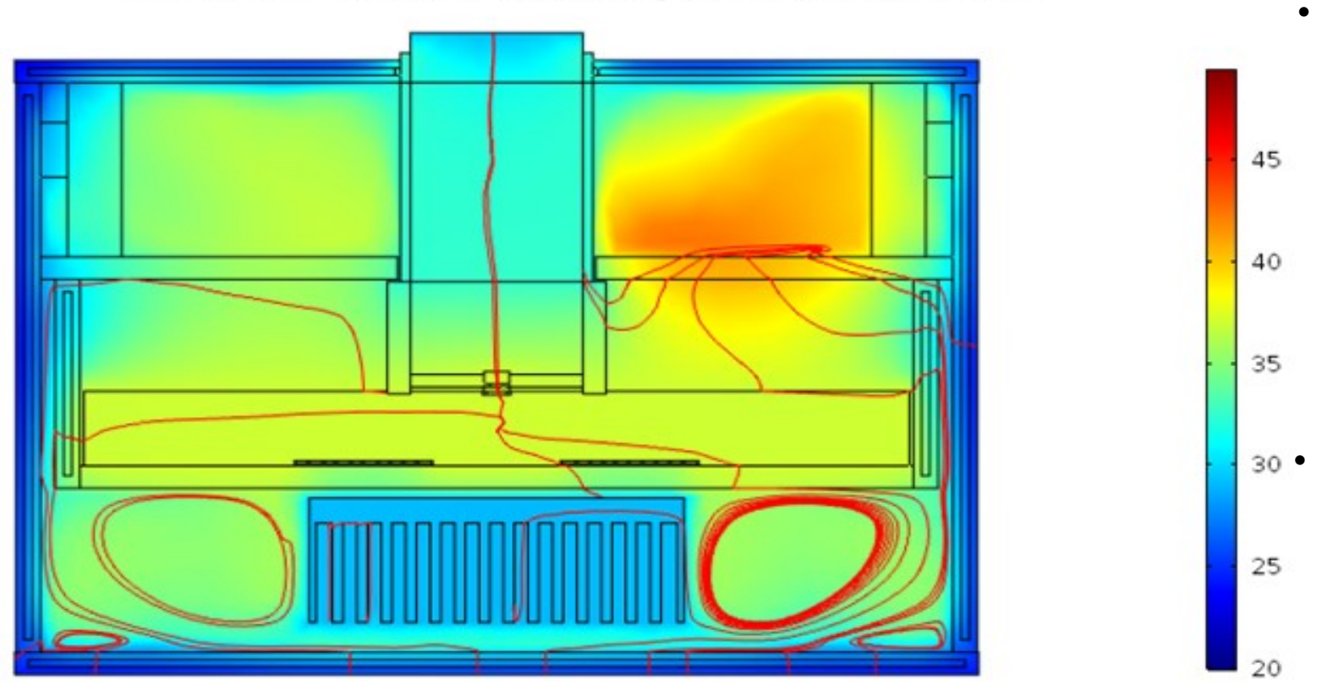
$$Q_{\mathrm{min}} = -7.6\ \mathrm{W}, Q_{\mathrm{max}} = 7.6\ \mathrm{W} \qquad \textbf{T.E.C heater source}$$

$$\left.\begin{aligned}-\mathrm{n}\cdot\mathrm{q} &= Q_{\mathrm{b}}\\ Q_{\mathrm{min}} &= 0\ \mathrm{W}, Q_{\mathrm{max}} = 14.85\ \mathrm{W}\end{aligned}\right\}\ \textbf{boundary heating foil source}$$

RESULTS

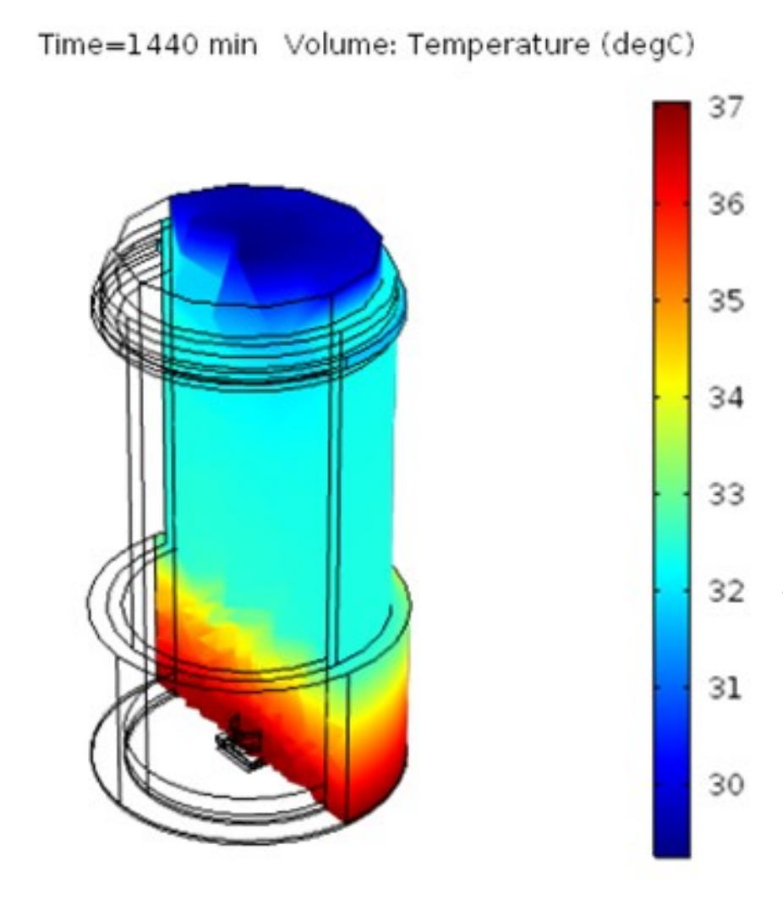
Figure 5: 2D surface (T in °C) and streamline (heat flux) plots of different cross-sections (xy-, xz- and yz-plane) through the 3D-COMSOL model.



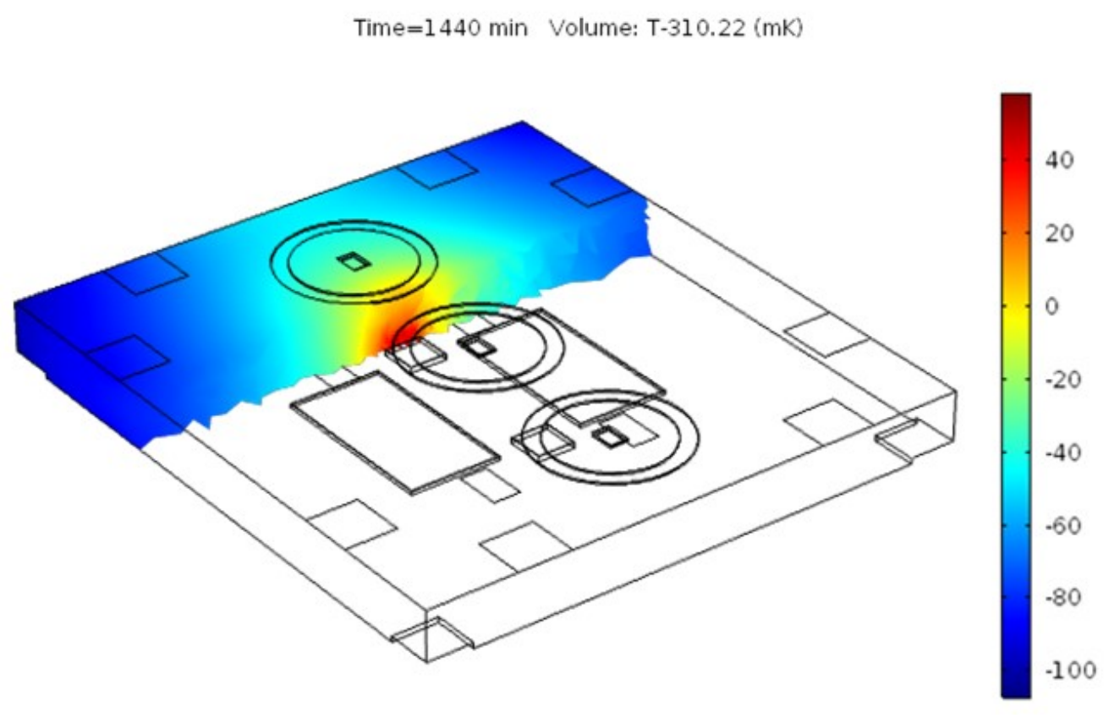


- 2D-plots showed hot and cold spots in temperature throughout the system.
- Red streamlines revealed thermal bridges in our test system.
- Both aspects, which are not easily accessible experimentally, help us to further improve the test system.

Figure 6: 3D-volume plots of the primary heat sink (above, ΔT in mK) and the middle channel (below, T in °C).

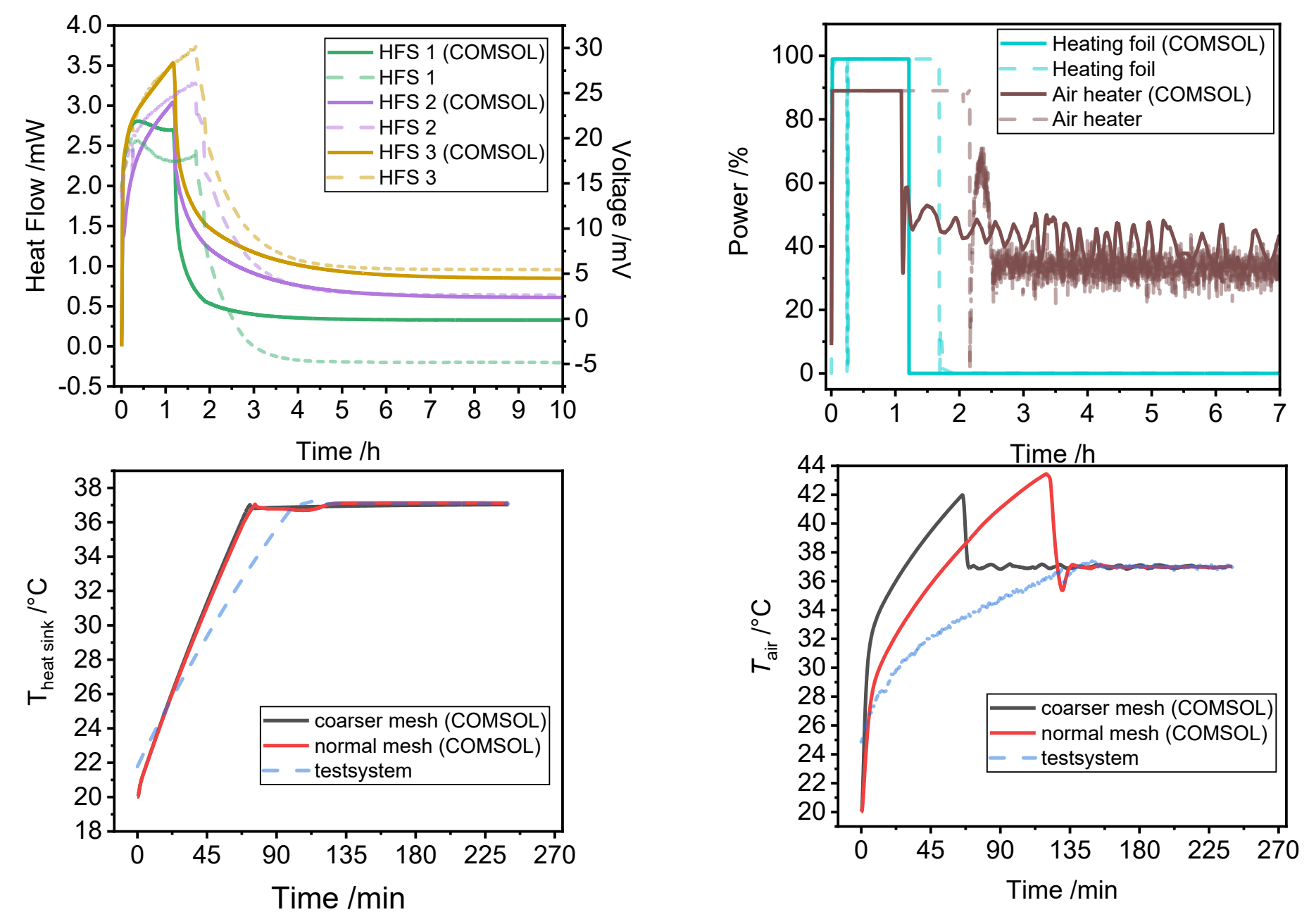


- Using the element filter tool in post-processing allows a comprehensive insight into individual components of the calorimeter.
- Observed spatial temperature gradients on the primary heat sink and the measuring channels that negatively influence the performance of the heat flow sensors (HFS).



- This information is useful to improve the overall system performance during the development phase.

Figure 7: Comparison between simulation of (solid lines) and experimental data (dashed lines) from the test system.



- Qualitatively, simulation data is in strong agreement with experimental data obtained from our test system.
- Deviations can be attributed to **a)** unconsidered lab conditions (temperature fluctuations), **b)** different control behavior of the systems PID controllers and **c)** mesh quality.

CONCLUSION

- Results obtained greatly aided us in the devices construction process and provide us with valuable information about the overall system performance.
- Simulation results were confirmed by experimental data obtained from our test system under laboratory conditions.
- Further interfaces including e.g. chemical reactions can easily be applied and the generated heat can be monitored.

Acknowledgement

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