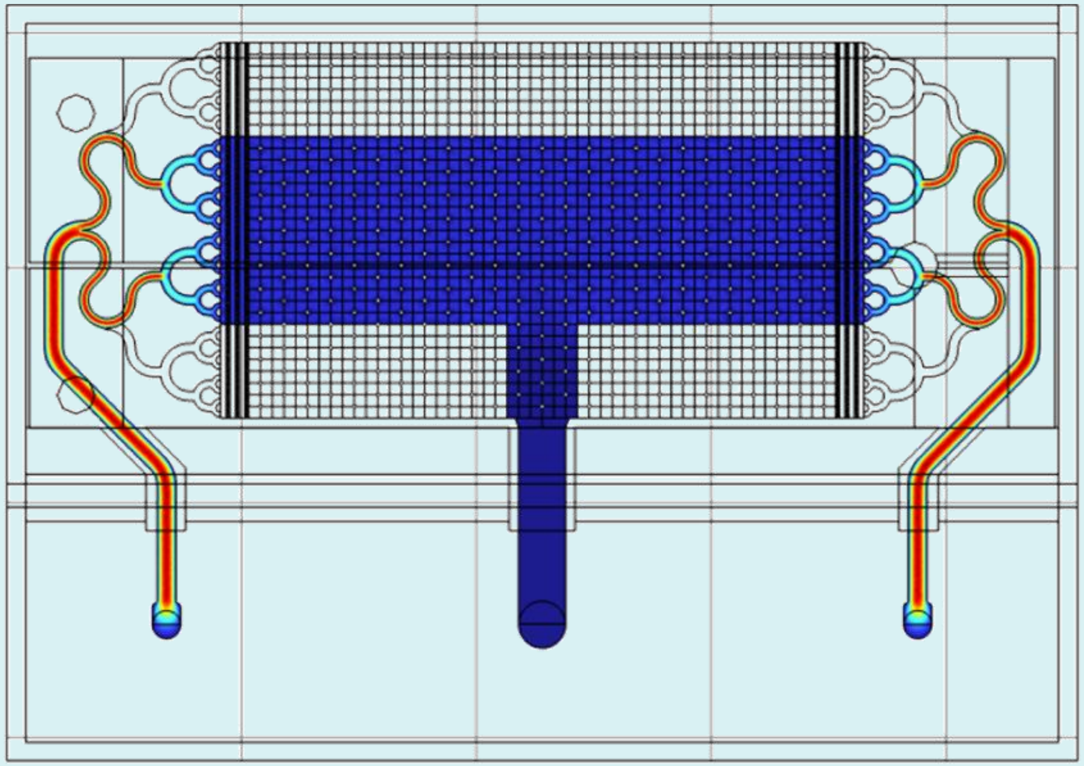

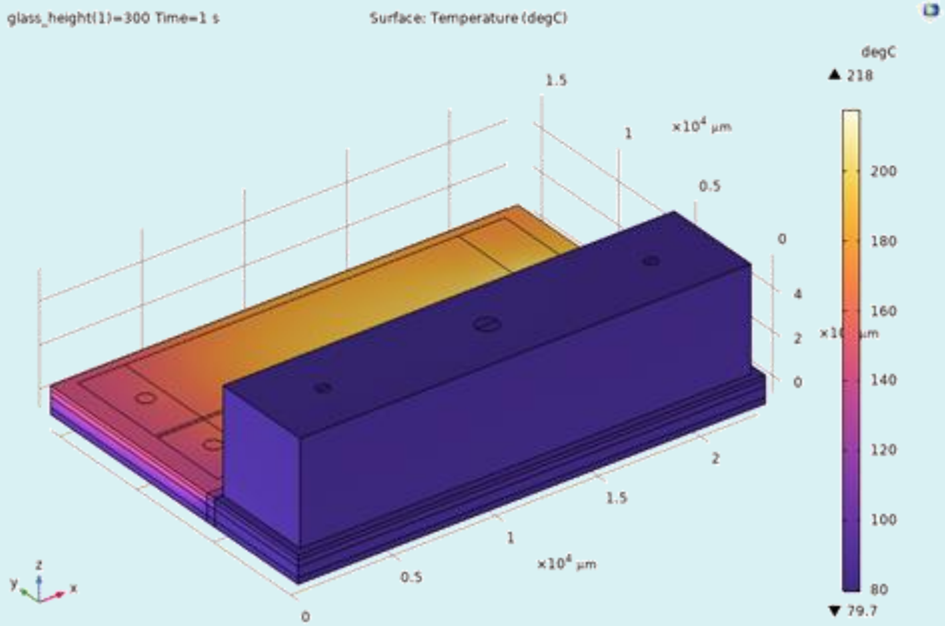

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October 2024

MEMS GAS-CHROMATOGRAPH PRE-CONCENTRATOR MULTI-PHYSICS SIMULATION

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CSEM AT A GLANCE

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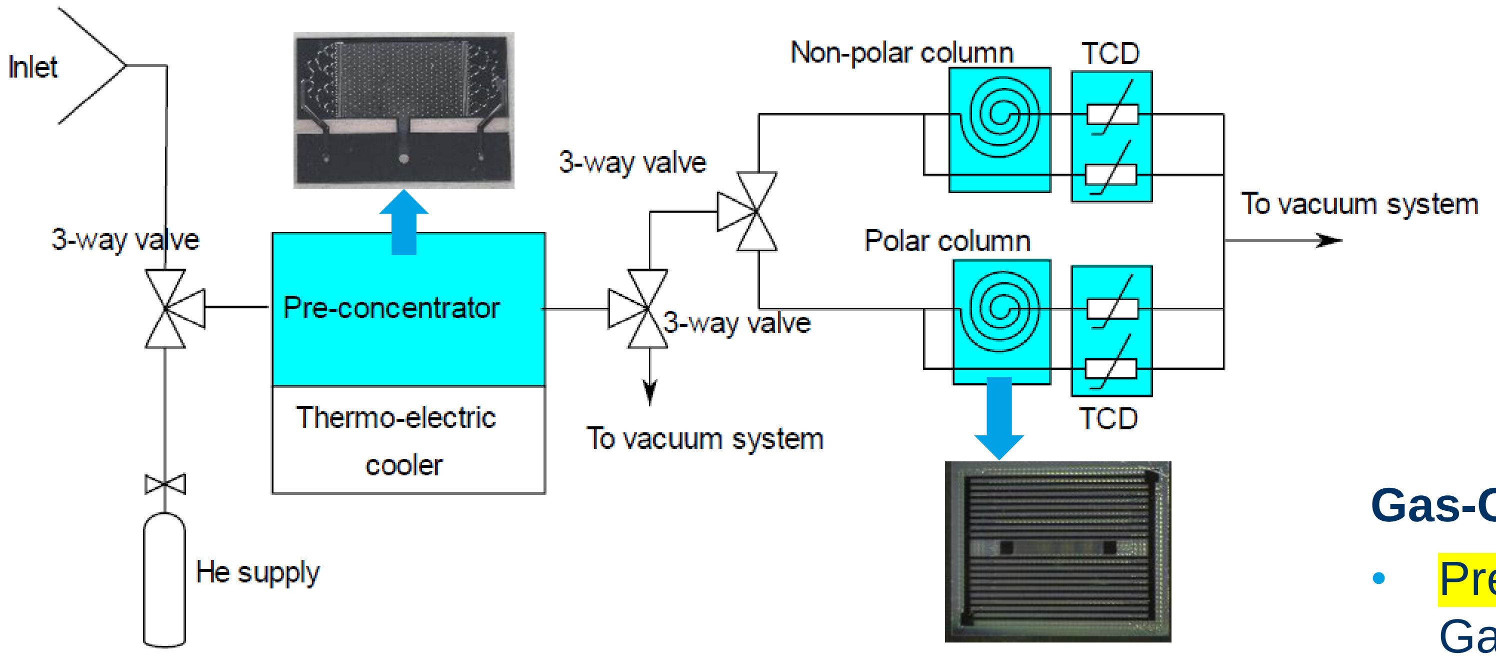
INTRODUCTION: WHAT'S A MEMS GAS-CHROMATOGRAPH (MS-GC)?



Source: wikipedia

Mems Benefits (in blue)

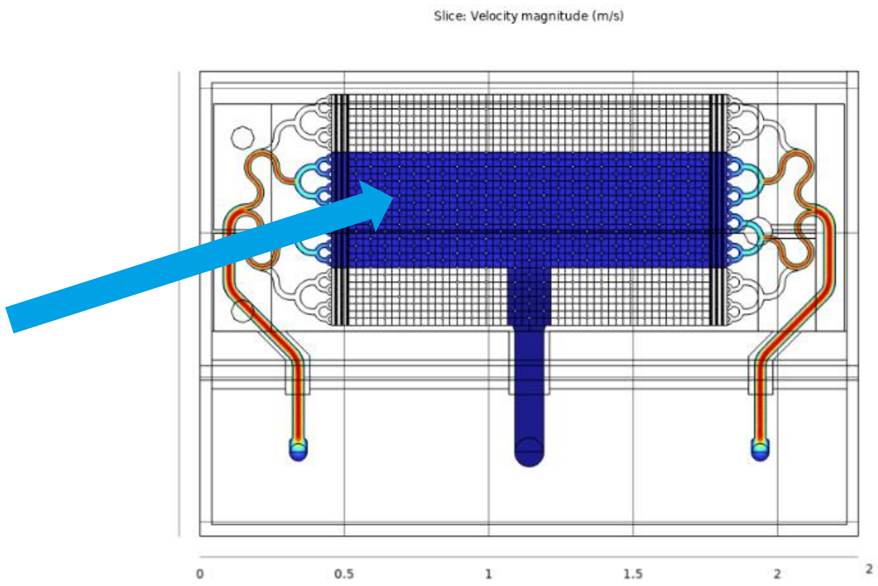
- System size reduction from 50cm to 5cm i.e. 10X
- Large Volume/weight reduction i.e. ~1000x
- Heater Power consumption reduction
- Sensing Speed increased

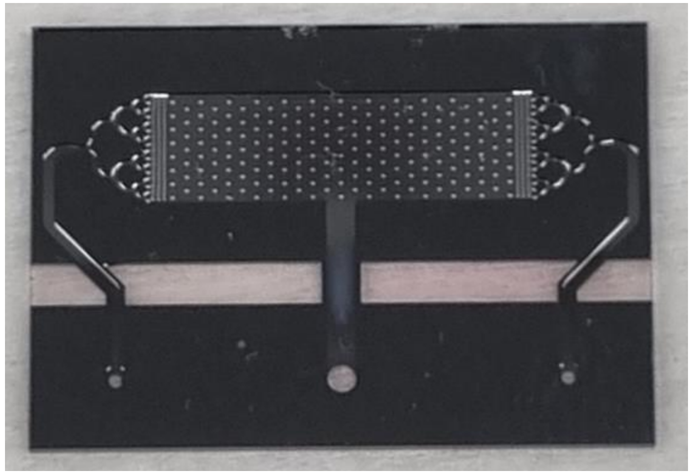
Gas-Chromatograph working principle

- Pre-concentrator absorbs/fast-desorbs Gas impurities (VOCs) in carrier gas (He) to increase pulse VOCs concentration
- Gas impurities pulse time delay is generated in a long column μ-channel
- Thermal conductivity variation detector measures VOCs type and amount

PRE-CONCENTRATOR DESIGN CHALLENGES

- **CHIP SIZE**
  - limited due to yield & costs issues
- **FLOW FIELD**
  - Uniform gas speed in **porous material (Tenax®)** to improve **VOCs absorption uniformity** and **speed**
- **THERMAL FIELD**
  - Peltier for controlling absorption in Tenax®
  - Tenax® temperature uniformity during fast heating
    - 280-300°C in <5s in >70% volume: target specifications
  - Thermal mass connected to the MEMS
- **HERMETICITY**
  - System interconnects carried out with invar block bonding.
- **HEATER DESIGN**
  - voltage is limited to 28V (space application)
  - current lower than electro-migration limit <1E7A/cm^2





GOAL OF SIMULATION TASKS

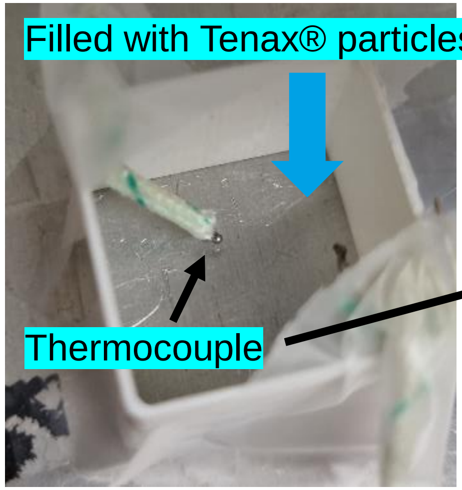
- Simulation to extract material properties of Porous material (Tenax®)
- Flow uniformity check with defined tree-geometry
- Check thermal resistance to Peltier is acceptably slow during cooling to perform VOCs absorption in Tenax® porous material
- Heater thermal design optimization to achieve fast heating
  to perform fast VOCs desorption in Tenax® porous material (pre-concentrator)

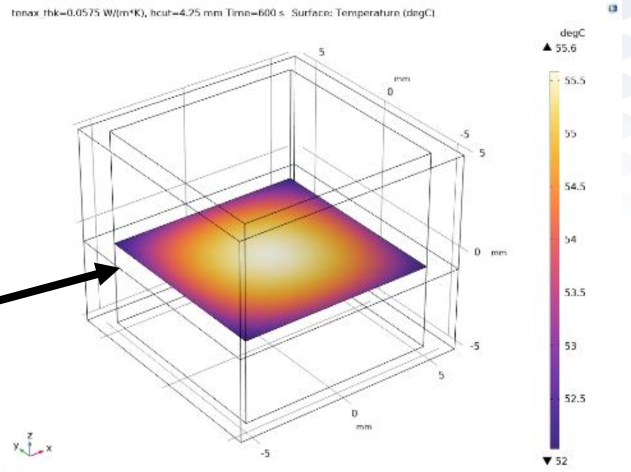
POROUS MATERIAL – THERMAL PROPERTIES

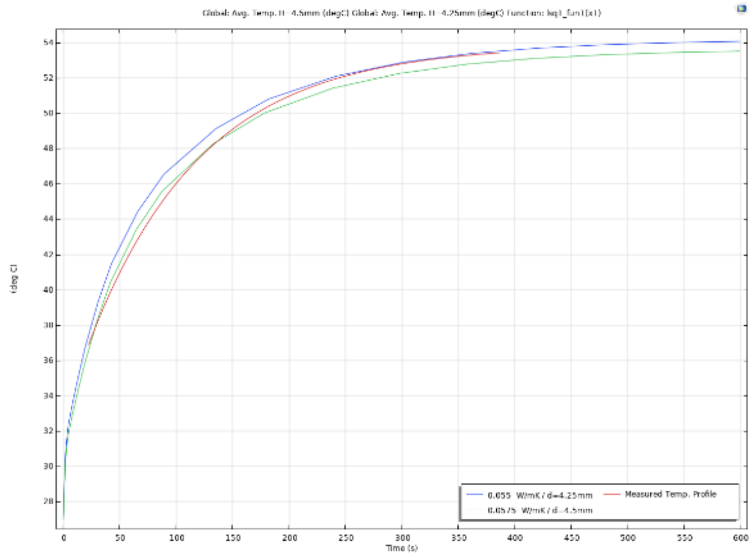
- Thermal conductivity estimated from heating of a 1cm^3 cube filled with Tenax®. The assumptions are:

  1. Tenax® porosity of 60% and around
  2. 30% of air around the Tenax® pellets (~packed spheres)
  3. Density estimated from datasheet
  4. Heat capacity estimated from literature and porosity assumption

- Good fit of Tenax® polymer heating curve measured in the middle section of the reference cube with simulated curve.
  - thermal conductivity estimated to be 0.0575 W/m*K
    - Lower limit is bound by air 0.0257 W/m*K
    - Error is most likely underestimated value. This leads to higher values, improving speed & uniformity of heating







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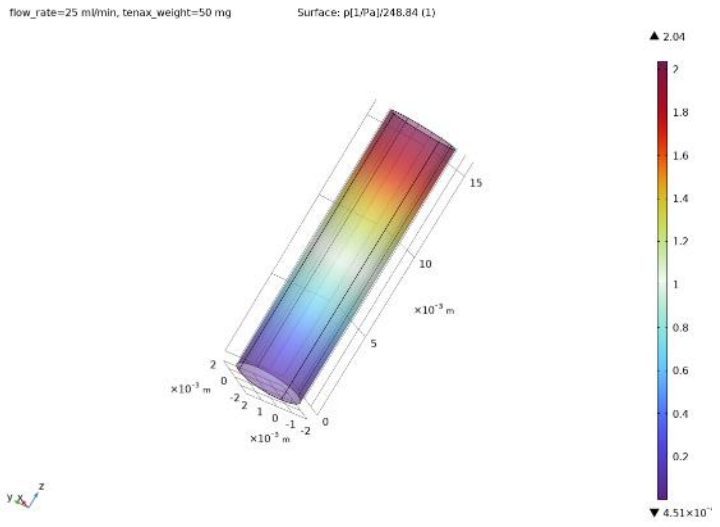
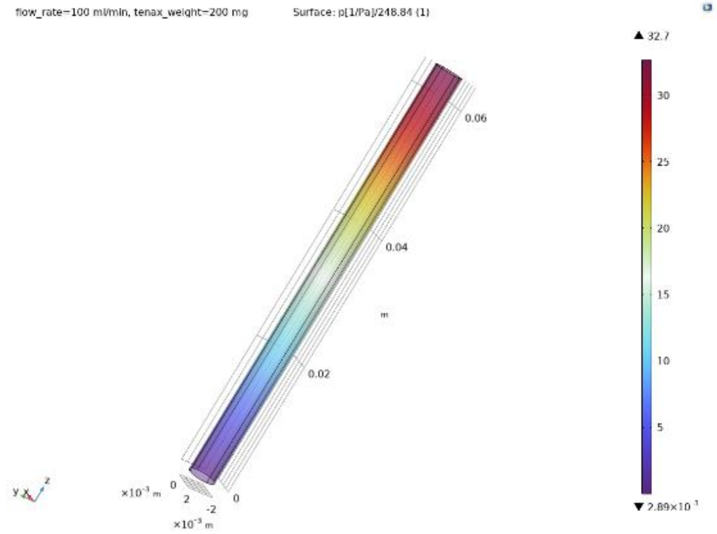
POROUS MATERIAL – FLOW PROPERTIES

- A parametric COMSOL model is set-up to simulate the porous flow with defined tube diameter & flow-rate
- Permeability parameter of Tenax® is estimated to be: $k = 1.9e\text{-}11 m^2$
  - back-pressure is within 10% in accordance with the calibration data.
  - The flow speed is also in accordance with flow ranges of selected Darcy porous flow model.

Tenax TA Back Pressures for 4.0 mm I.D. Desorption Tubes

mg Tenax TA	25 ml/min	50 ml/min	75 ml/min	100 ml/min	125 ml/min	150 ml/min	175 ml/min	200 ml/min
50	2	4	6.5	8	10.5	12	14	16.5
100	3.5	7	10.5	13.5	17	20	23.5	27.5
150	5	10	15	19	24	28.5	31.5	39
200	7.5	14.5	21.5	29	35.5			
250	10	20	30.5					





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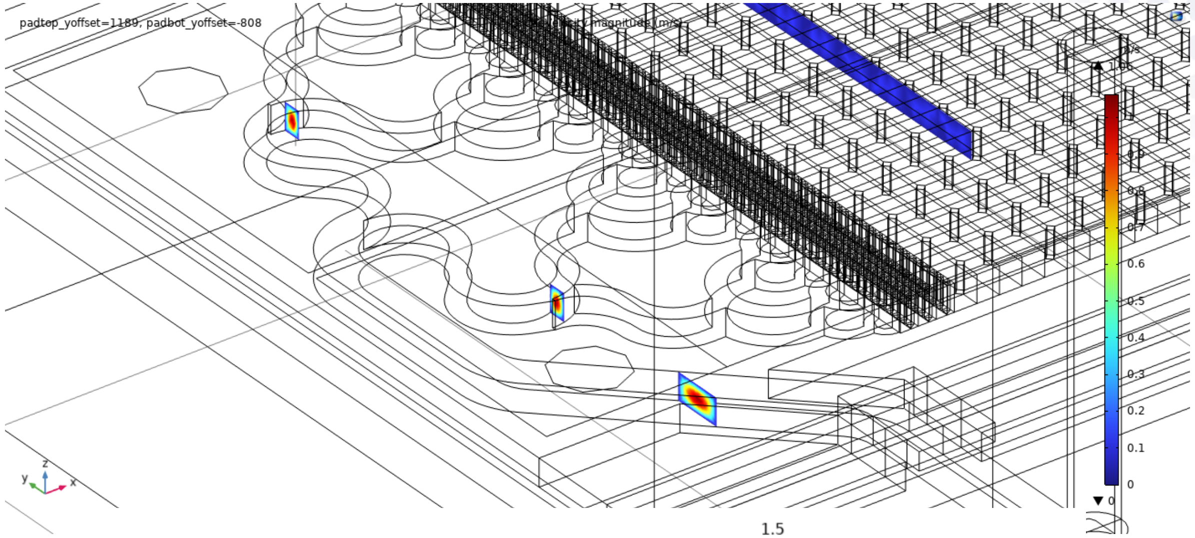
MULTI-PHYSICS COUPLED MODEL DESCRIPTION

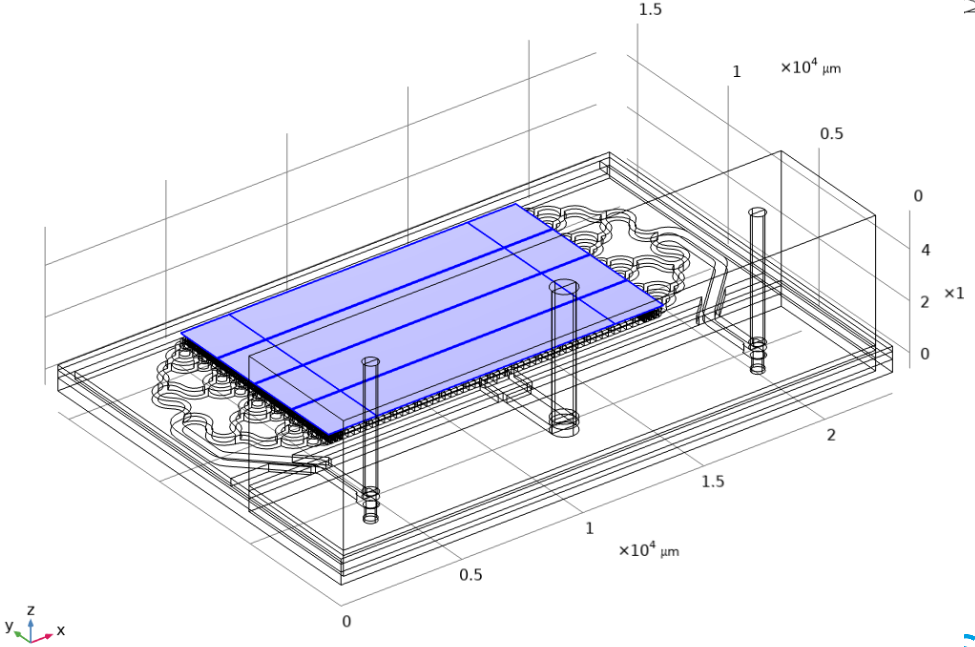
Selected Physics

- heat transfer in solid and fluids
- laminar flow, including porous flow (Tenax®)
- electrical current in shells (2D-layer) to model the pre-concentrator heater.

Multi-physics coupling

- Electrical – thermal
  - Modeling of ohmic losses in the heater
- Fluidic - thermal
  - Modeling of non-isothermal flow

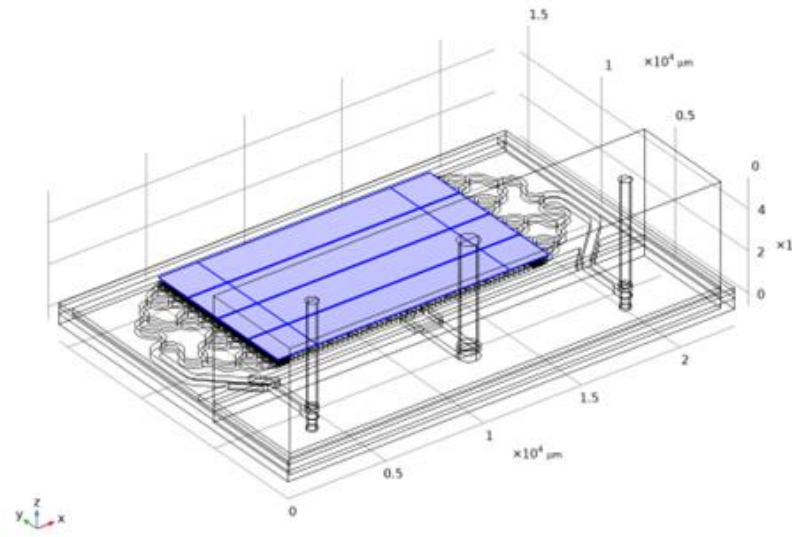


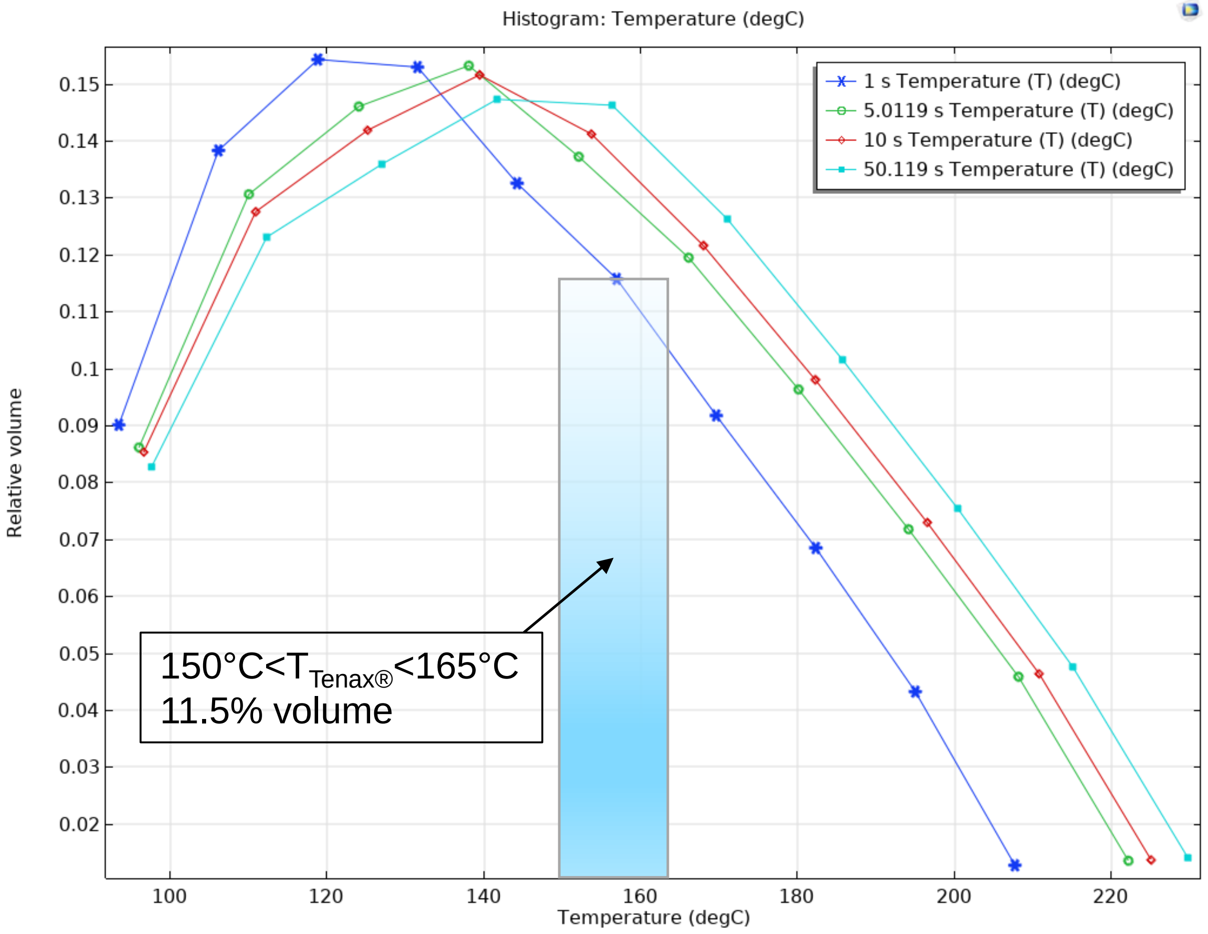


POST-PROCESSING STRATEGY

- **Initial test with not optimized heater**
  - Heater geometry caused non-uniformity of temperature across Tenax® volume
  - Heater reached high voltage limit

- **Post-processing based on histogram**
  - **Temperature** plot divided in bins of **volume %** to check for uniformity





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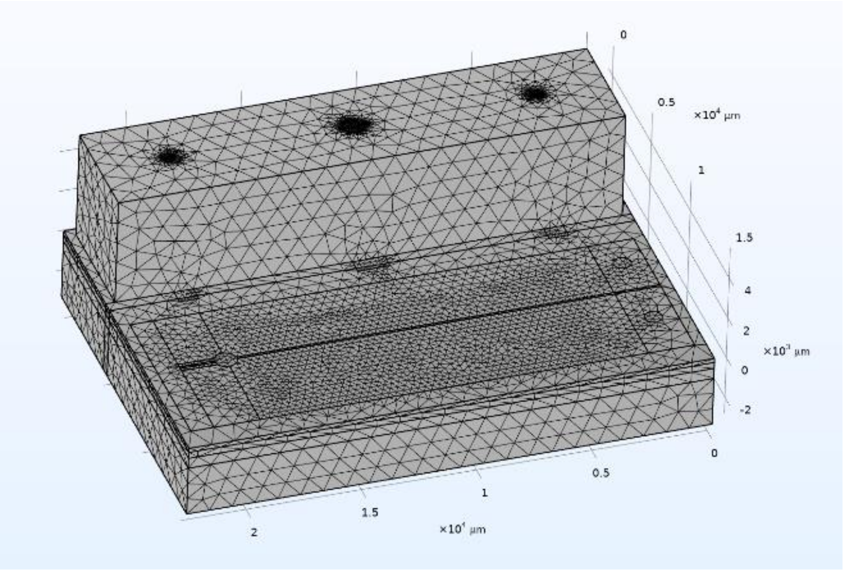
MEMS PRE-CONCENTRATOR PARAMETRIC OPTIMIZATION

- Flow speed impact analysis
- Size of heater (length, width)
- Folding and symmetry of heater analysis
- Insulation thickness towards Peltier
- Starting temperature of Tenax® before heat pulse (VOCs de-sorption step)



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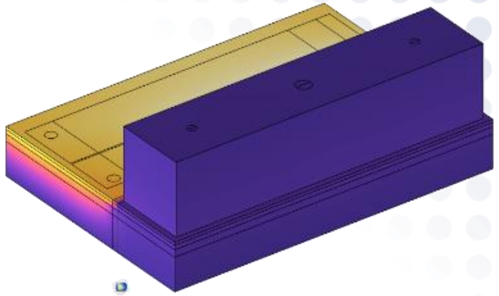
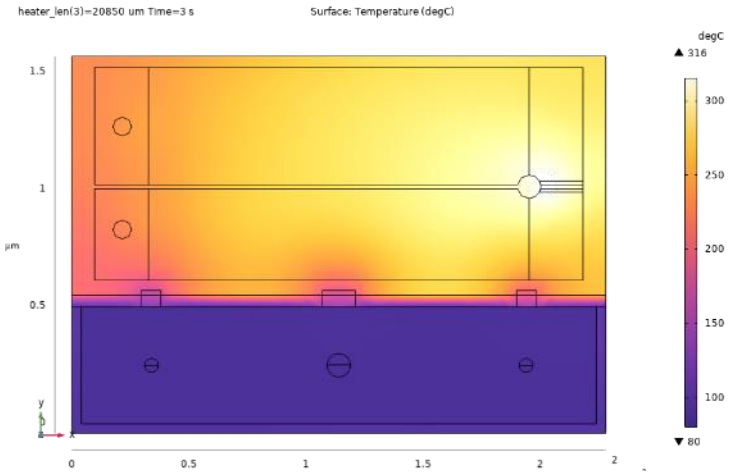
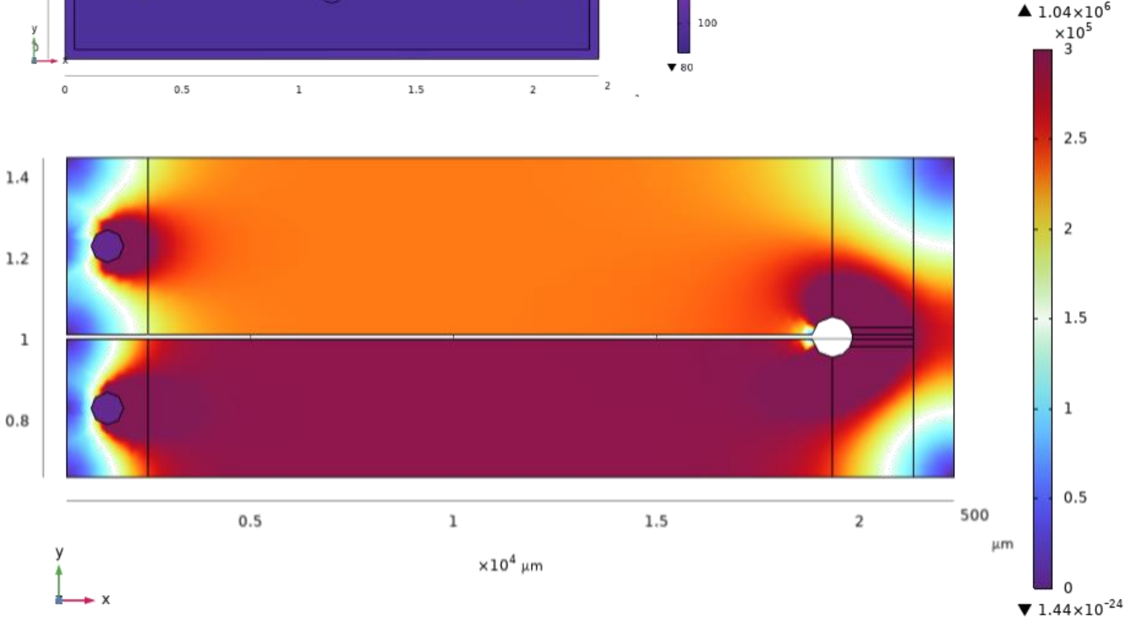
RESULTS SUMMARY – TEMPERATURE PLOTS



- Large heater provides max temperature above 300°C while keeping below 300°C in Tenax® cavity
- Strong gradient from Invar block can be partially requires asymmetric heater to compensate
- Glass block below chip helps to insulate from Peltier. Cooling from +80°C to -10°C takes 100s
- Heater voltage is ~13.5V
- Heater current density peaks at ~3E5 A/cm^2





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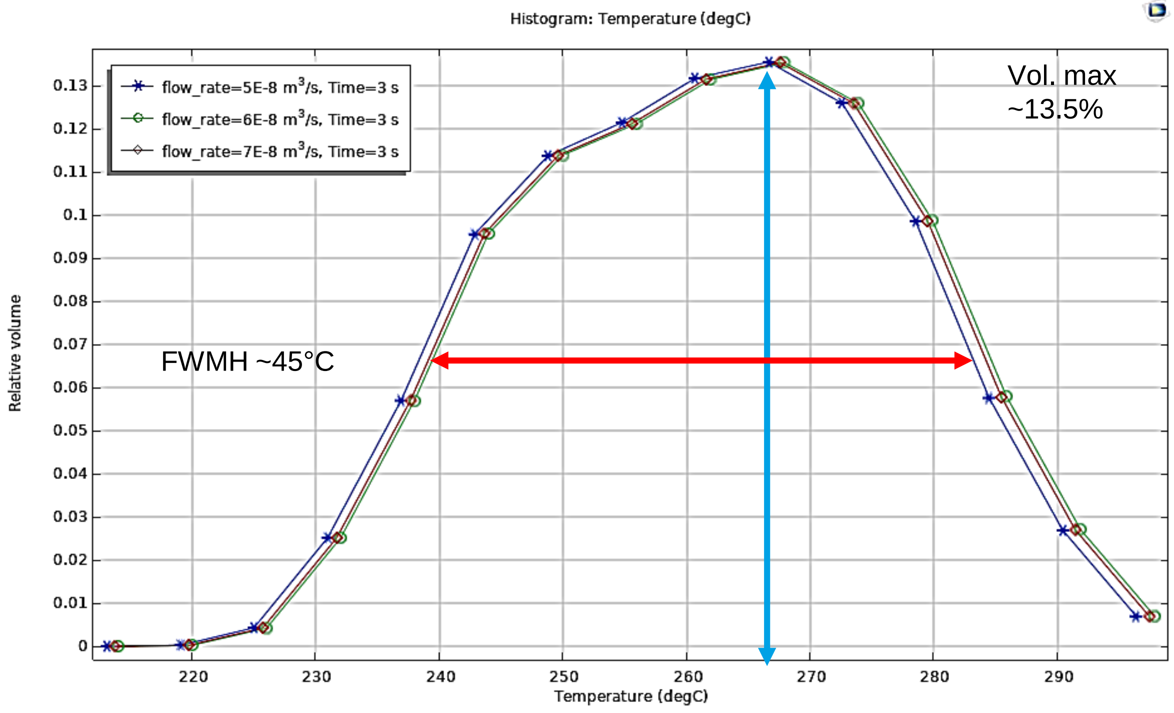
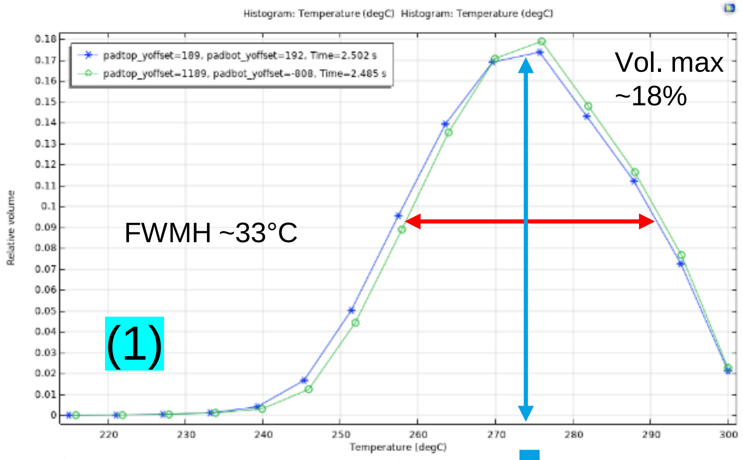
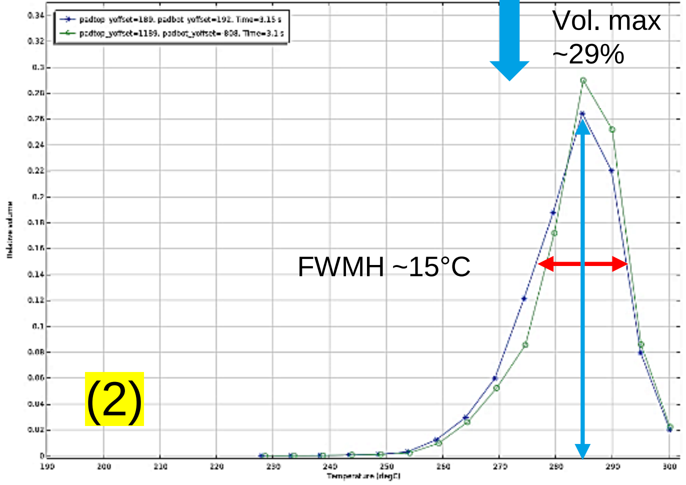
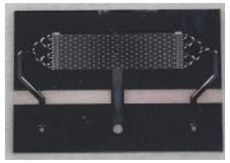
RESULTS SUMMARY – TEMPERATURE HISTOGRAMS

- Flow speed impact is minimal on heating pulse
- Optimized heater: Tenax® reaching 265-285°C in ~2.5s within >64% volume at ~23W (1)
- Second configuration yields Tenax® reaching 275-295°C in ~3.1s within >84% volume (1-mask change) (2)









CONCLUSIONS & SIMULATION BENEFITS

CONCLUSION

- Tenax® thermal/flow properties validated with experimental values and literature data
- A multi-physics model was implemented including flow, porous flow, heat transfer and electric current analysis
- Parametric investigation was done and took for each simulation case 1h40m to solve
- Optimized heating in Tenax®: reaches 265-285°C in ~2.5s within >64% volume at heating power of ~23W
- Second configuration yields Tenax® reaching 275-295°C in ~3.1s within >84% vol. (1-mask) change

SIMULATION BENEFITS

- Non-trivial design optimization of on-chip asymmetric heater design
- Chip analysis of temperature rise time & volume % i.e. transient and spatially impacting factors
- System estimate and optimization of time constant of cooling with the Peltier

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