When simple models fail

CT-FEA simulations of metal foams

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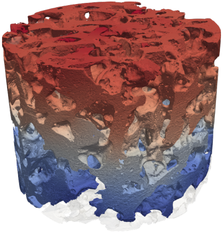
Background

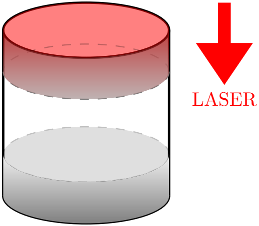
Fourier's law

Heat flux: $\mathbf{q} = -\lambda \nabla T$,

where λ – thermal conductivity [W/(m·K)], T – temperature.

Consequently: $\frac{\partial T}{\partial t} = a \Delta T + f(\mathbf{r}, t)$, where a – thermal diffusivity.





Can heat conduction in a porous solid be reduced to a 1D problem?

Experimental

LFA: Netzsch LFA 457

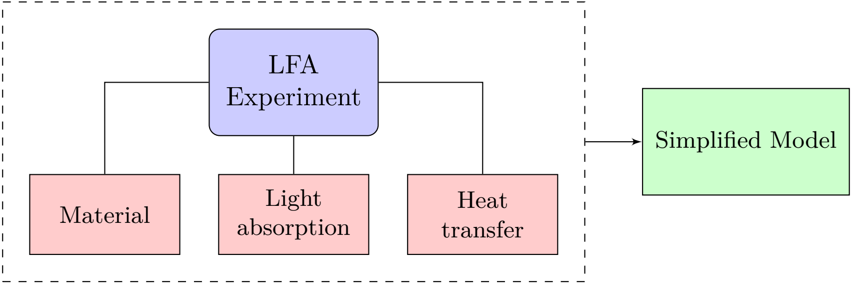
CT: Nikon XTEK XTH 225

EXXENTIS

Samples: metal foams

- Al-Mg-Si
- Diameter: 12.5 mm
- Porosity 60%
- Small, medium and large pores
- Thickness: 2.0 – 10.0 mm

Conventional Paradigm



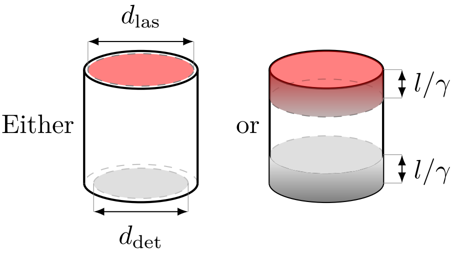
LFA Experiment

Material

Light absorption

Heat transfer

Simplified Model



$$\begin{aligned} \theta_{\text{Fo}} &= \theta_{yy} + \Phi(\text{Fo})\Psi(y), \\ \theta_y|_{y=0} &= \text{Bi}\cdot\theta|_{y=0}, \\ -\theta_y|_{y=1} &= \text{Bi}\cdot\theta|_{y=1}, \\ \theta(y,0) &= 0. \end{aligned}$$

Conventional Paradigm

Problems:

- Classical LFA requires homogeneous samples
- Porous samples combine two phases (pores and matrix)
- Samples are heterogeneous!
- Assume microgeometry changes $a \equiv \lambda/(C_p\rho)$ while same equations are valid
- An effective medium is analysed

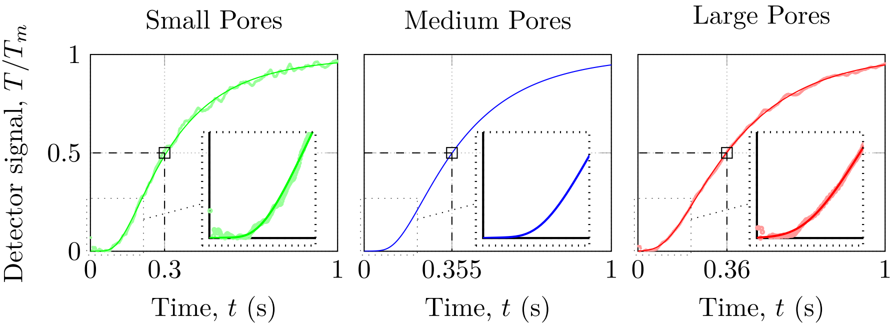
Use Beer-Lambert law to introduce:

- a distributed heat source $\Psi(y) \propto \gamma \exp\left(-\gamma y\right)$
- a distributed temperature detection $V \propto \int_0^1 \theta(y) \exp(-\gamma y) \mathrm{d}y$

... this leads to the “Penetration model”.

LFA Heating Curves

$l = 10$ mm, open pores



- Curves processed with the PULsE software
- Optimised parameters: a, Bi, T_{inf}, γ
- BFGS/Wolfe optimiser robust to outliers (least absolute deviations)

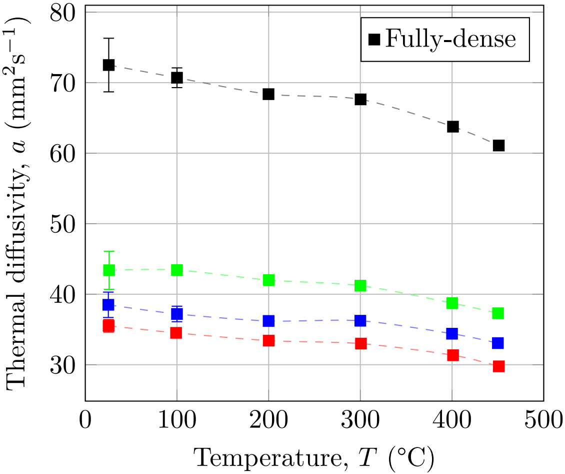
Thermal diffusivity in $l = 10$ mm metal foams

Open surface pores, Penetration model

🟩 Small Pores

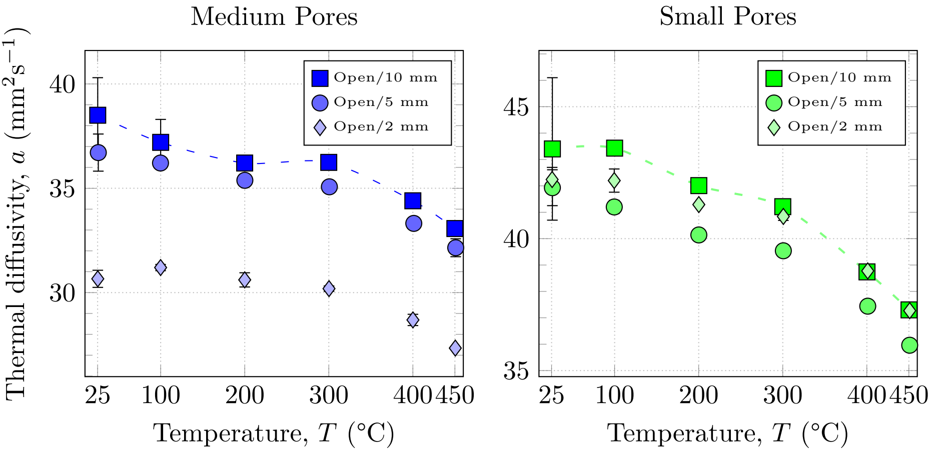
🟦 Medium Pores

🟥 Large Pores



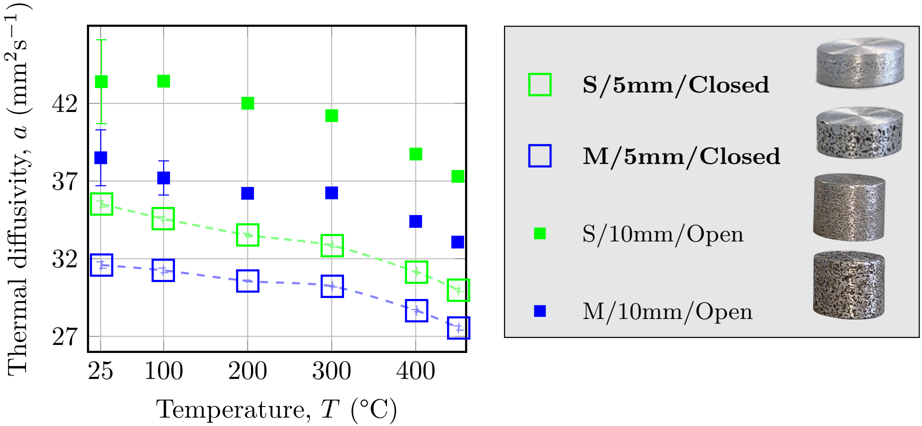
Thermal diffusivity: size dependence

Open surface pores, Penetration model

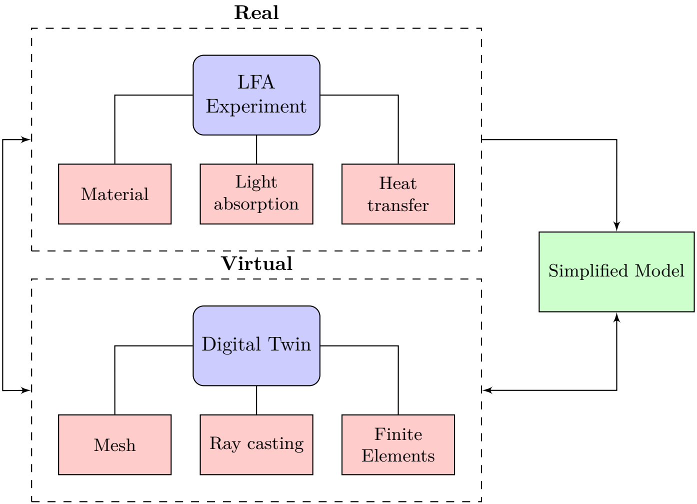


Thermal diffusivity in $l = 5$ mm metal foams

Closed surface pores, Standard model



Change of Paradigm



Real

LFA Experiment

Material

Light absorption

Heat transfer

Virtual

Digital Twin

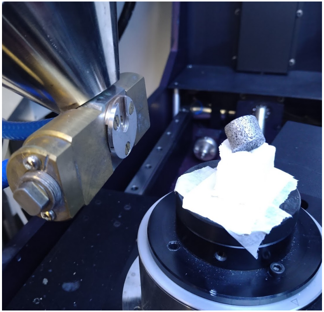
Mesh

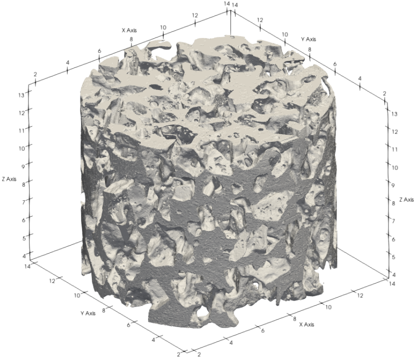
Ray casting

Finite Elements

Simplified Model

Constructing meshes





Exposure time	708 ms	no pre-filtration
Projections	3142	2 frames per projection
Acquisition time	2 h 30 min	per sample
Voxel size	9.71 μm	CT Pro
Processing	ThermoFisher Avizo v2019.2	

Mesh parameters

All meshes consist of 4-nodal tetrahedral elements.

The VTK software was used to estimate:

- the aspect ratio, $\eta = 12(3V)^{2/3} / \sum_e l_e^2$
- the typical edge length $l_{\mathrm{typ}} = \sqrt{2\langle \eta^{-1} \rangle}[3\langle V \rangle]^{1/3}$

Pores (mm)	Nodes ($\times 10^6$)	Elements ($\times 10^6$)	Element characteristics			
			mean volume ($\times 10^{-6}$ mm^3)	volume s.d. ($\times 10^{-6}$ mm^3)	l_{typ} (mm)	quality, $\langle \eta^{-1} \rangle$
0.6 - 4.00	3.30	11.4	43.5	65.3	0.22	1.99
0.4 - 1.00	10.9	35.3	14.3	22.6	0.071	2.06
0.2 - 0.35	27.7	88.2	5.58	8.20	0.050	1.89

Given the above:

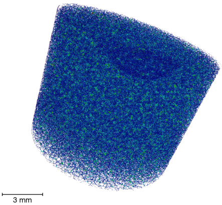
- the mesh quality is reasonable: $\eta^{-1} \approx 2$
- l_{typ} is smaller than the average pore diameter

Therefore, the segmentation is adequate.

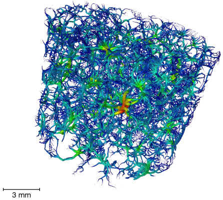
Pore analysis

Avizo and Reactive'IP IPSDK

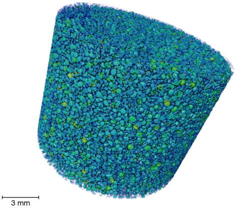
(a) Skeletonization (small)

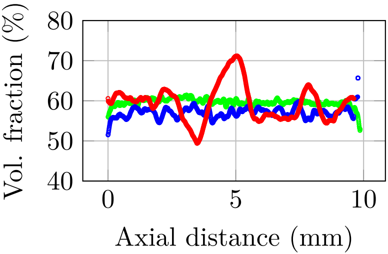


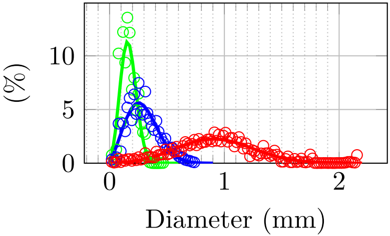
(b) Skeletonization (large)



(c) Sphere fitting

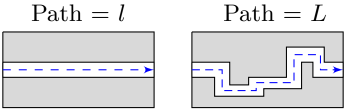






Tortuosity calculation

Tortuosity is defined as: $\tau = L/l$, where L is the curved path and l is the Euclidean distance between two points (bee-line).



Two methods were used to calculate tortuosity:

- Centroid path (Avizo) – traces a path using centroids of planar slices
- Geodesic vs Euclidean distance maps – each voxel contributes equally to the statistics

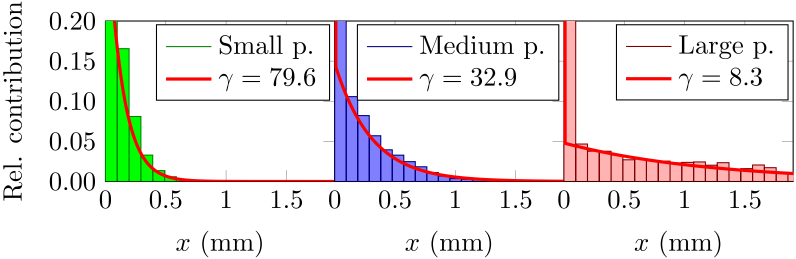
Method			Pore size
	Large	Medium	Small
Centroid (metal)	1.459	1.385	1.508
Distance maps	1.095 ± 0.117	1.077 ± 0.069	1.076 ± 0.060

Light penetration

Light assumed to illuminate visible surfaces only. Algorithm:

- identify boundary between matrix and pores
- select cells with $\mathbf{n} \cdot \mathbf{n}_l > 0$, where $\mathbf{n}_l$ is the direction of the laser beam
- cast ray from cell centre toward the source direction $-\mathbf{n}_l$
- test intersection with other surfaces (Möller–Trumbore algorithm)
- assume side is illuminated by the laser if test passes

Same procedure identifies surfaces visible by the detector. Finally, the attenuation coefficient γ was extracted from the absorption profiles below.



Three-dimensional heat conduction

Let $\theta = (T - T_0)/\delta T_m$, where δT_m is the maximum adiabatic heating. Additionally, $\mathrm{Fo} = a_m t/l^2$.
Solve the heat equation with the boundary conditions

$$\begin{aligned} \phi(\mathbf{r})\frac{\partial\theta}{\partial\mathrm{Fo}} &= l^2\nabla(\phi(\mathbf{r})\nabla\theta), \\ \textit{illuminated} \quad \textit{surfaces:} \quad l(\mathbf{n}\cdot\nabla\theta) &= \frac{1}{\mathrm{Fo}}(\mathbf{n}\cdot\mathbf{n}_l)f(\mathrm{Fo}), \\ \textit{other} \quad \textit{surfaces:} \quad (\mathbf{n}\cdot\nabla\theta) &= 0, \end{aligned}$$

where $\phi = 1$ inside the matrix and nil elsewhere; $\mathbf{n}$ is the inward normal vector; $f(\mathrm{Fo})$ is the pulse shape function.
Boundary conditions are formulated at the matrix-pore interface and at the external surfaces.
Detector signal:

$$J(\mathrm{Fo}) = \int_{\text{visible}} (\mathbf{n}\cdot\mathbf{n}_d)\theta(\mathrm{Fo})\,dA$$

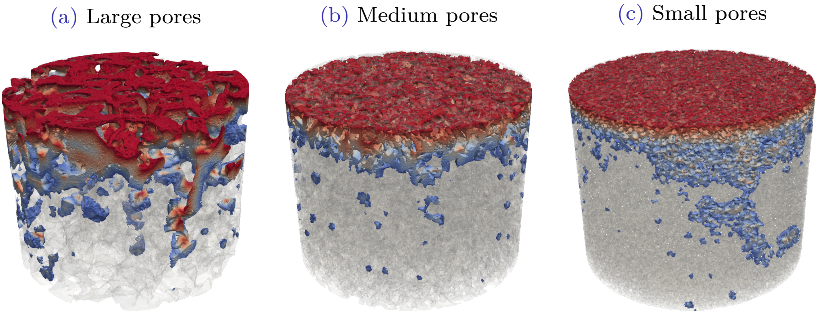
Finite element modelling

The system of equations reduces to a sparse linear system $\mathbf{H}\mathbf{y} = \mathbf{f}$ with a symmetric positive-definite matrix $\mathbf{H}$.

- $\mathbf{H}$ depends on sample geometry and time step.
- $\mathbf{H}$ is used to calculated the solution at every time step. The linear system is solved with the Intel MKL PARDISO package using multicore shared memory system.
- The matrix $\mathbf{H}$ is factorised only at the first time step
- Subsequent factorisations are performed only after a change of time step
- A simulation of the LFA experiments consists of 84 time steps and only 5 changes in time steps, hence 5 factorisations.
- The performance of solution is limited by the amount of available RAM and CPUs.
- For example, the mesh corresponding to the sample with small pores requires about 160 GB of RAM (other meshes have smaller requirements).
- Calculations done on Google VM instances.

Heat diffusion

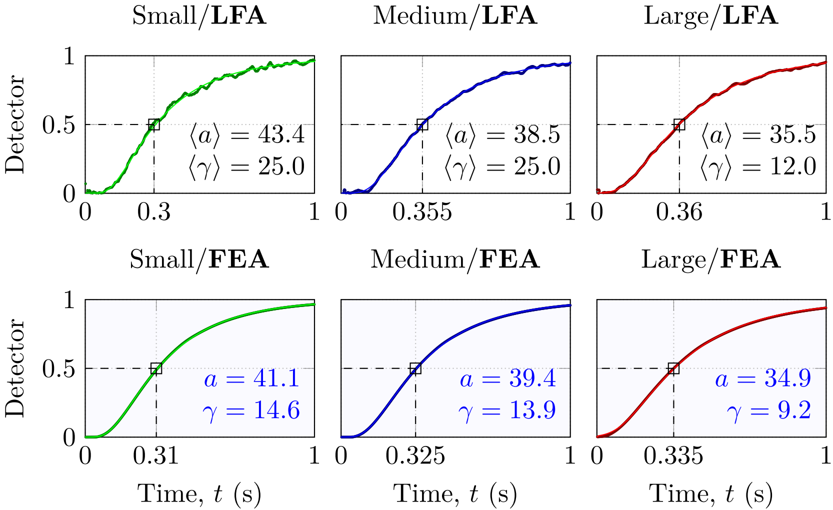
in samples with light penetration


(a) Large pores (b) Medium pores (c) Small pores

- Logarithmic θ scale (5×10^{-3} – 20)
- Visualised in ParaView
- Open this pdf in Acrobat Reader or Okular to watch the animation

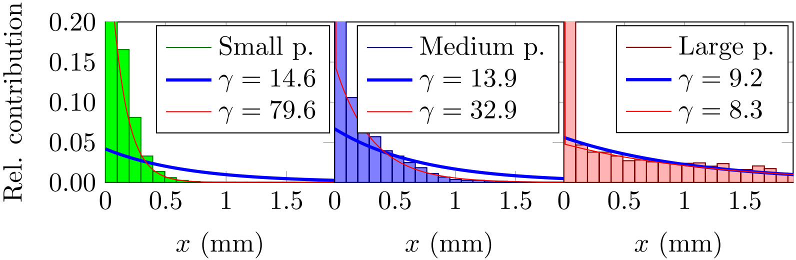
LFA vs FEA comparison

Open pores



LFA vs FEA comparison

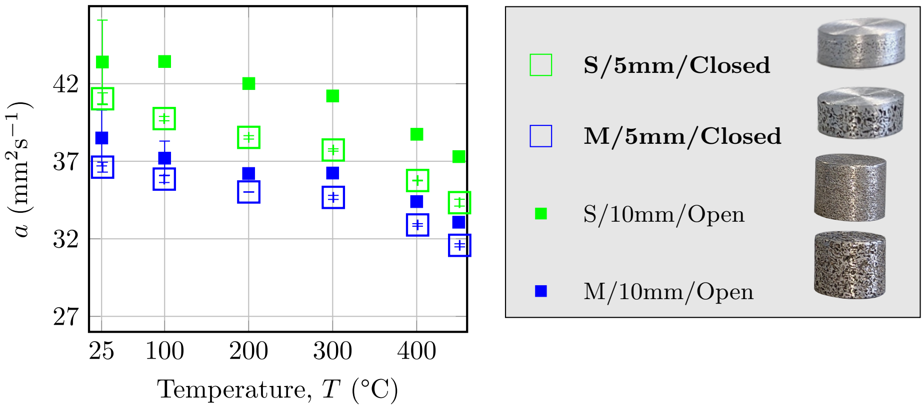
Open pores



- Blue – γ extracted from time-temperature profile optimisation
- Red – true absorption profiles
- In both cases, the Beer-Lambert law is used
- “**Model mimicry**”!

Thermal diffusivity in $l = 5$ mm metal foams

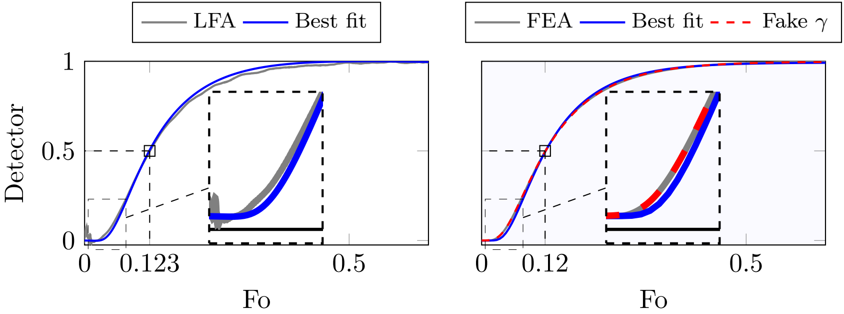
Closed surface pores, Standard model – *tortuosity correction*



Better results – but deviation still significant. Why?

FEA vs LFA

Opaque 5 mm thick samples with medium pores



- Opaque faces and tortuosity correction
- Model treating foams as solid cylinders produces time lag
- Introducing “fake” absorption profile “solves” the problem
- Sample heterogeneity defies classical models

Conclusions

1. If direct CT-informed FEA calculations are possible, they should be given priority over misinformed LFA experiments
2. Existing coarse-grained models fail to describe temperature transients in metal foams
3. This leads to size dependence in LFA measurements
4. The Fourier law is not strictly applicable to porous media
5. Effecitve-medium models still needed to validate complex installations combining multiple levels of detail

To be continued...

Acknowledgements

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Further reading:

- Digital twin of a laser flash experiment helps to assess the thermal performance of metal foams
- Experimental evidence of gas-mediated heat transfer in porous solids measured by the flash method

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Other misconceptions in laser/light flash analysis

There are examples of other materials and experimental conditions making classical analysis non-straightforward.

Some interesting cases are summarised in the articles below:

- Lunev, A. (2022). Applied Physics Letters, 121(9), 096101.
- Lunev, A. (2022). Advanced Functional Materials, 2205076.
- Lunev, A., Zborovskii, V., & Vilkhivskaya, O. (2022). Revisiting transient heat transfer in coated transparent media.