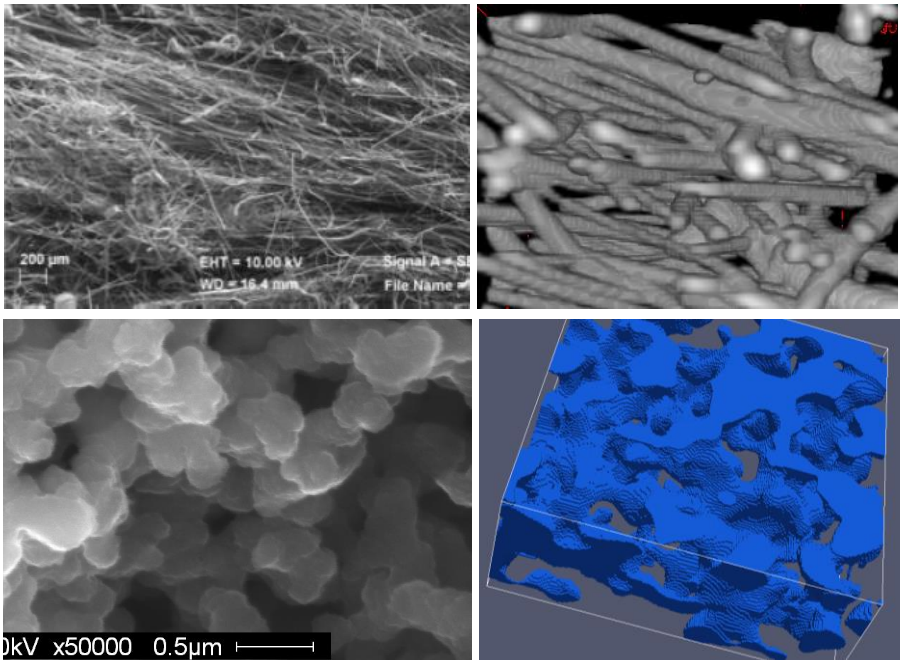
Modelling of Thermal Transport Properties of Advanced Porous Materials

Dr. Sandra Galmarini, Dr. Matthias M. Koebel
Building Energy Materials and Components, Empa, CH-8600 Dübendorf (Switzerland)

Dr. David Geissbühler, Prof. Heinrich Hofmann
Powder Technology Laboratory (LTP), EPFL, CH-1005 Lausanne (Switzerland)

Motivation

High-performance insulation materials are invariably porous materials with complex microstructures. This complicates the prediction of the thermal transport properties of these materials based on the materials properties. The existing analytical tools do not sufficiently take into account the characteristics of each material. Although the influence of general characteristics, such a the total amount of porosity, can be estimated, the influence of more subtle changes, such as changes in the orientation of the fibres in a fibre network, as well as the thermal transport properties of more complex composite microstructures, cannot be easily predicted at present. A better understanding of the influence of the materials properties and the microstructure on the thermal behaviour would however be of invaluable help in the development and improvement of the next generation of super-insulating materials. The development and implementation of a tool capable of predicting the thermal transport properties of complex porous materials, based on previous work looking at conductive and radiative heat transport separately, is therefore the aim of this project.



Scanning electron microscopy images (left) and 3D tomography data (right) of mineral wool (top) and carbon based aerogels (bottom)

Objectives

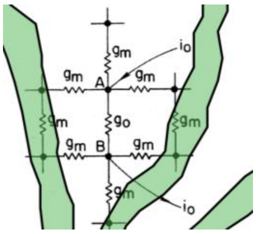
The computational tool to develop should be capable of estimating the thermal transport properties of both:

- Real 3D microstructures as measured by e.g. x-ray tomography: In order to better understand the thermal transport properties in porous insulations, it should be possible to calculate the thermal conductivity of real microstructures of well-characterised materials.

- Proposed new microstructures: Often the possibility to evaluate the thermal properties of e.g. new composite materials before doing any experiments would help guide future developments of high-performance materials. Consequently it is important to be able to look not only at measured 3D microstructures, but also at new imaginary microstructures.

Two different contributions to the thermal transport in the materials will be taken into account:

- Conductive heat transport: One way to describe the conductive thermal properties of a porous microstructure is by representing it as a network of resistors with different resistivities, as described by e.g. Kirkpatrick [1]. Such a model has been implemented at the Powder Technology Laboratory in Lausanne. The model is capable to describe any geometry, if the structure can be represented by a resistor network with a reasonable number of resistors.



- Radiative heat transport: For insulation for ambient temperatures the characteristic wavelength of the radiation (~ µm) is often similar in size as the microstructure. This means that geometric ray tracing is no longer applicable. Instead generally solutions to the Maxwell equation for regular waves are used to estimate the scattering and adsorption of the microstructure [2]–[4]. The Maxwell equation can only be solved for geometrically simple geometries and often only for one scattering body. Consequently Larkin [5] developed a relatively simple two flux model that makes it possible extrapolate the radiative heat transport properties based on the scattering properties of a single scattering body. While several solutions to the Maxwell equation have already been implemented in a previous project the application of the two flux model has so far not yet been automated.

During this project the student will implement the two flux model and combine the different pre-existing programs for calculating the conductive and radiative conductivity of microstructures into a single extensible tool, capable of modelling both real and proposed novel porous microstructures. The computational tool will then be validated based on a range of experimentally fully characterised mineral wool fiber networks. Once the validation is complete, the tool is then used to estimate the thermal transport properties of different microstructures, such as carbon or silica aerogels. Finally, based on the previous results, some new microstructures will be looked at to determine some general rules and guidelines for the design of porous insulation materials. The work will be carried out at Empa in close collaboration with EPFL Lausanne.

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[2] K.-N. Liou, "Electromagnetic scattering by arbitrarily oriented ice cylinders," *Appl. Opt.*, vol. 11, no. 3, pp. 667–674, 1972.

[3] H. E. Bussey and J. H. Richmond, "Scattering by a lossy dielectric circular cylindrical multilayer numerical values," *IEEE Trans. Antennas Propag.*, vol. 23, no. 5, pp. 723–725, 1975.

[4] P. W. Barber and S. C. Hill, *Light Scattering by Particles: Computational Methods*. World Scientific, 1990.

[5] B. K. Larkin, "A study of the rate of thermal radiation through porous insulating materials," University of Michigan, 1957.

Contact

Dr. Sandra Galmarini, sandra.galmarini@empa.ch, +41 58 765 4066

Dr. Matthias Koebel, matthias.koebel@empa.ch, +41 58 765 4780