Computational analysis of the thermal behavior on a silica (SiO$_2$) aerogel coating for applications in the construction industry

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Abstract. A mathematical model was developed to describe the thermal behavior of the aerogel SiO$_2$ material, which can be used as an architectural surface coating film. These types of materials allow temperature conservation within a panel so that a controlled environment is achieved. Conditions for modeling were considered, such as: porous material properties, microstructure, boundary conditions, etc. From the study of the material’s micrometry, an image processing was made, and regular grids of 6192 nodes were built. Algorithms were implemented using Matlab to describe the thermal flow within the porous material. The results obtained indicate the thermal distribution across the pores of the material and showed the zones with greater incidence and thermal conservation in the panel. This research contributes towards the thermal analysis of special insulating materials as alternatives of applications in the construction industry.

1. Introduction
In the construction sector, various types of materials are being implemented to meet specific design and thermal behavior conditions, specifically, there are few materials that gather all the conditions to perform notoriously as a thermal insulator [1]. The current needs for buildings’ construction demand a migration from traditional thermal insulators, with their relatively high thermal conductivities being one of the reasons for this change as these thermal conductivities require the insulating films to be thicker in colder seasons [1]. As thermal insulation correlates with energy use of buildings [2], seeking of new insulating materials were thoroughly carried out [3–5], not only to study their viability but also to model and characterize materials according to their thermal performance, more specifically, grasping of silica aerogel heat transfer behavior is an issue of scientific-industrial interest [6,7].

Numerical and experimental results have been presented, showing that aerogel coatings applied to buildings’ walls perform better than other insulating materials [6]. Some researches were also developed with regards to the use of aerogels in window glazing taking advantage of both thermal conductivity and transparency properties [8–10]. All of these to achieve the same objective, reducing energy consumption of buildings due to indoor environmental control. It is also worth to be mentioned that not only thermal insulation of buildings has been considered but also aerospace applications including cryogenic fluid containers, thermal barriers, fire retardation, amongst other thermal applications are also a topic of study [11,12].
In the present paper a mathematical model is developed to describe the thermal behavior of a silica aerogel wall coating subjected to a certain ambient temperature. Variables such as thermal conductivity and the microstructure of the material were considered on the algorithmic implementation of the model which was built in Matlab to analyze different conditions of the thermal flow within the porous material. The objective of this research is to visualize the heat flow behavior on the inside of the microstructure (SiO$_2$ aerogel) to determine the efficiency of the material that can be used in construction applications.

2. Mathematical modeling and computational implementation

2.1. Mathematical description

The heat transfer equation in steady-state regime was established to model the thermo-conductive behavior inside of the porous microstructure of the material. The mathematical representation defined for the model was:

$$k_c \nabla^2 T = -\rho h \in \Omega^2$$  \hspace{1cm} (1)

Where $T$ corresponds to the temperature of the material on a specific point, $k_c$ is the thermal conductivity of the aerogel SiO$_2$ which takes values between 13–14 mW/(mK) and $\rho h$ is the rate of heat generation or accumulation of internal energy within the material.

And the heat flow conditions or temperature that is applied over the external surface can be described through:

$$k_a \frac{\partial T}{\partial x} = h_c (T - T_\infty) \in \Omega^2$$  \hspace{1cm} (2)

$$T = \beta \in \partial \Omega$$  \hspace{1cm} (3)

Where $\partial T/\partial x$ is the heat flow due to convection through the boundaries, $h_c$ is the convective coefficient of the fluid to which the surface is exposed, $k_a$ is the thermal conductivity of air in W/mK, $T$ is the temperature along the boundary and $T_\infty$ is the ambient temperature.

2.2. Microstructure of the material and implemented boundary conditions

A sample of the material was determined by capturing a micrograph image [12]. An image processing was made on the sample to improve sharpness, shapes and microstructural definitions. Following, it is described by the flow chart the treatment made on the sample, figure 1.

![Figure 1. Scheme for the microstructure sample treatment.](image-url)
A fraction of the microstructure sample was selected according to the degree of porosity and monolithic material content to subsequently numerically fragment the sample through a uniform lattice by squared elements, see figure 2.

![Figure 2. SEM micrograph of the porous medium sample [12], where the dashed lines indicate the selected fraction (a), and uniform 6192 node lattice for the numerical development (b).](image)

2.3. Numerical-computational description

A computational algorithm was built to develop the differential equations system using Taylor series approximations:

\[ T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} = 4T_{i,j} + h_x^2 T_{x}^{''}_{i,j} + h_y^2 T_{y}^{''}_{i,j} \]  

That after truncation lead to an F.D.M model [13], which was applied to the mathematical model as follows:

\[ -2 \left( \frac{1}{h_x^2} + \frac{1}{h_y^2} \right) T_{i,j} + \frac{T_{i+1,j}}{h_x^2} + \frac{T_{i-1,j}}{h_x^2} + \frac{T_{i,j+1}}{h_y^2} + \frac{T_{i,j-1}}{h_y^2} = -\rho h \frac{\partial T}{\partial x} \]  

Where \( h_x \) and \( h_y \) are the determined partitions to numerically fragment the microstructure.

In the computational implementation, the porous surfaces were defined with lattice nodes to represent energy absorbent voids, and for the monolithic material, lattice nodes were defined to represent thermal energy conductive surfaces.

3. Results and discussion

In figures 3a, 3b and 3c; temperature distribution can be seen through the porous microstructure for three thermal circumstances. The implementation of the material was considered for structures located in cold, tropical and hot regions. At considerably low ambient temperatures the porous material had a thermal conservation of -73.15 °C, at tropical temperatures the material had a thermal conservation-dissipation of 7 °C and at high ambient temperatures the material had a thermal dissipation of 27 °C.

Temperature conservation can be seen in the inside as the thermal flow spreads between the micropores, avoiding energy losses due to constraints in the microsystem. In high-temperature ambient regions, the porous material allows maintaining a conservative state of steady temperature as the pore generates a thermal balance that keeps the system refrigerated.

In general, the simulations performed on the aerogel SiO₂ coating show the ability of the material in retaining heat and therefore the conservation of a certain temperature, generating a comfort ambient inside the architecture in which it was implemented. Also, in the three cases developed by simulations
it can be seen that the pores act as a kind of absorbent medium, that is, as the heat flow approaches the pore, the temperature gradient decreases drastically. It is essential to develop the analysis in different locations of the micrograph sample due to high heterogeneity and amorphism of the porous microstructure.

![Temperature in °K](image1)

(a)

![Temperature in °K](image2)

(b)

![Temperature in °K](image3)

(c)

**Figure 3.** Numerical solutions at an ambient temperature of -74 °C (a), 25 °C (b) and 56 °C (c).

4. **Conclusions**

The drastic environmental changes that are happening globally have demanded architectural designs to be built with special materials that guarantee adequate control of temperature in enclosed spaces. Silica aerogel then becomes an appropriate alternative to achieve stable temperature environments. Achieving that the same material meets different performance features is quite complex, nevertheless, the type of material here implemented could become an alternative to commercial use. A versatile computational algorithm was built, which allows evaluating different environmental thermal flows, it is even possible to vary the properties of the material. Porous materials have the benefit of being lighter than conventional monolithic materials. This research offers clarifications about the benefits that the silica aerogel material can provide with the possibility of being implemented in other applications such as aeronautics/aerospace and military industry.
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