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Numerical study of radiative properties of nanoporous silica aerogel

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ABSTRACT

Silica aerogel as a super-insulating material has a large application potential in many engineering fields. This article aims at studying the radiative properties of silica aerogel in three aspects including nanoscale effect, radiative thermal conductivity and optimal temperature-dependent density. Firstly, radiative properties of three-dimensional silica aerogel made up of chain-like equal-sized nanospheres are investigated by considering the dependent scattering. The results indicate that the effect of nanostructure is limited on radiation insulating performance of silica aerogel. Secondly, we simulate the radiative transfer in bulk silica aerogel, and the parameter errors of extinction coefficient and mean temperature in Rosseland equation are discussed. The modified extinction coefficient is given and more accurate radiative thermal conductivity is observed. Finally, by evaluating the effective thermal conductivity from the total contributions of solid phase, gas phase and radiation as a function of temperature and density, we obtain the optimal temperature-dependent density at which the heat transfer in silica aerogel can be mostly suppressed.

1. Introduction

Silica aerogel is a type of super-insulating material with ultra-low thermal conductivity (~0.005 W/m K at ambient temperature under vacuum) which is made of nanoporous (80–99.8% of porosity) network of silicon dioxide nanoparticles (around 7 nm of diameter) and has low density (~0.003 g/cm^3), low index of refraction (~1.05) and high specific surface area (500–1200 m^2/g) [1–6]. Generally, the solid phase conduction, gas phase conduction and radiation contribute to the total thermal conductivity of silica aerogel [7]. However, in the applications of high temperature, the drastically increased radiative heat transfer is much harmful to the insulating performance of the silica aerogel. It is therefore crucial to figure out the radiative transfer mechanism, to understand the radiative heat transfer phenomena better and optimize such materials.

Studies have been carried out to characterize the radiative properties of silica aerogel. Earlier researches on silica aerogel concentrated on coupling effect between the conduction and radiative heat transfer. Kamiuto [8] analyzed combined conduction and radiative heat transfer through the evacuated silica aerogel and discussed the effects of the porosity, layer thickness and wall emissivity on heat transfer characteristics. Heinemann et al. [9] considered silica aerogel as non-gray media and then studied the interaction of radiation with conduction theoretically and experimentally, and the radiative properties were computed from Mie theory or determined experimentally. As the nanotechnology has been developing, researchers tend to uncouple the conduction and the radiation in silica aerogel. Enguehard [10] developed a model that could be used to quantify the level of radiation heat transfer by relating with the compositions (size, volume fraction, and physical nature of different populations of constituents) of the nanoporous material based on Rosseland approximation and Mie theory. Lallich et al. [11] wrote a code based on Discrete Dipole Approximation (DDA) to compute the radiative properties of silica nanoparticle aggregates whose structure was generated by the diffusion-limited cluster–cluster aggregation algorithm. Wei et al. [12] used a combined experimental and theoretical method to investigate the radiative heat transfer in silica aerogel and its composite insulation materials. Yu et al. [13,14] applied the multi-sphere T-matrix method and diffusion-limited aggregation (DLA) aggregates to study the radiative properties of opacified aerogel containing silica nanoparticles and micro-sized opacifier grains. Zhao et al. [15] investigated the radiative properties of opacified silica aerogel by the Mie theory and the improved Kramers–Kronig (KK) relation.

The present research on radiative properties of silica aerogel is based on three aspects: the nanoscale effect in the form of absorption and scattering, the radiative thermal conductivity of bulk

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Nomenclature

A, B	coefficient matrix of energy conservation equations
e_b	blackbody emissive power [J]
$e_{b\lambda}$	spectral blackbody emissive power [J]
$e(T)$	temperature-dependent specific extinction coefficient [m^{-1}]
C_{abs}	absorption cross section [m^2]
C_{ext}	extinction cross section [m^2]
C_{sca}	scattering cross section [m^2]
D	plate–plate spacing [m]
d	particle diameter [nm]
g	anisotropy factor
k_a	optical thickness
k_c	conductive thermal conductivity [W m^{-1} K^{-1}]
k_{bulk}	solid thermal conductivity of bulk silicon dioxide [W m^{-1} K^{-1}]
k_e	effective thermal conductivity [W m^{-1} K^{-1}]
k_g	gas phase thermal conductivity [W m^{-1} K^{-1}]
k_s	solid phase thermal conductivity [W m^{-1} K^{-1}]
k_r	radiative thermal conductivity [W m^{-1} K^{-1}]
k_{unit}	conductive thermal conductivity of basic unit cell [W m^{-1} K^{-1}]
L	thickness [m]
l	phonon mean free path [nm]
m	complex refractive index
n	refractive index
P_{HG}	Henyey–Greenstein phase function superscript
p	pressure [Pa]
Q_e	extinction efficiency
Q_s	scattering efficiency
$R_d(i \rightarrow j)$	radiative transfer factor
R_s, R_θ, R_ϕ, R_φ	random number [0,1]
r	particle radius [nm]
r^*	non-dimensional particle radius
s	distance [m]
S_{ae}	specific surface area [m^2 g^{-1}]
t_a	temperature matrix of volume elements
t_b	temperature matrix of area elements
T_m	mean temperature [K]
V	volume [m^3]

Greek symbols

β	extinction coefficient [m^{-1}]
β_λ	spectral extinction coefficient [m^{-1}]
γ	side ratio
ΔS	area element [m^2]
ΔV	volume element [m^3]
ε	emissivity
θ, ϕ	zenith and azimuth angle [rad]
λ	wavelength [μm]
φ_{ae}	porosity
ρ_{ae}	density of aerogel [kg m^{-3}]
ρ_{bulk}	bulk density [kg m^{-3}]
σ	Stefan–Boltzmann constant
τ	transmittance
χ	size parameter

Superscript

in	incident directions
sc	scattering directions
′	modified value

Subscript

p	particle coordinates
s	system coordinates

silica aerogel and optimal temperature-dependent density for silica aerogel insulation. Since the radiative heat transfer in nanostructure is much complicated, most of the existing works concentrate on the transfer problem itself and assume mathematically simplistic scattering behavior for the individual particle. This simplification is known as the independent scattering which can be defined as a condition whereby the scattering from a single particle in a cloud is not affected by the proximity of its neighbors [16]. On the contrary, the dependent scattering occurs when the scattering from a single particle is affected by the presence of its neighbors. This dependent scattering pertains to many engineering heat transfer applications including fluidized and packed beds, conglomerated soot particles, packed-sphere regenerators, etc [16]. The typical structure of silica aerogel is made up of chain-like packed-nanoparticles and the particles are close to each other. The radiative heat transfer in such a structure needs to consider the dependent scattering effect. Thus, an elaborate numerical simulation considering dependent scattering effect is required to determine the radiative properties of such materials. The Generalized Multiparticle Mie-solution (GMM) is a practical approach to calculate the radiative properties of clusters of spheres [17], by which the size effect of radiation in nanostructure can be evaluated. The GMM is based on an explicit solution of the Maxwell equations and is numerically accurate and much more efficient than the traditional methods.

For the bulk silica aerogel, if the study is still based on the electromagnetic wave theory, the tremendous computing workload would make it nearly impossible, because the scale of bulk silica aerogel is much larger than its wavelength of thermal radiation. The Monte Carlo method is of advantages in calculating radiation in three-dimensional participating medium, by which the scattering and absorption in the material can be captured. In view of this, we resort to the Monte Carlo method to model the radiative heat transfer in bulk silica aerogel. The Monte Carlo method has already been employed to simulate the radiative transfer in porous media [18–23]. The major restriction of the Monte Carlo method in porous media is that it requires the characteristic scale to be large enough compared to the wavelength of the incoming radiation, so that the rules of geometric optics can be applied [18]. In the present algorithm, the ray directions are altered only by the scattering, and its occurrence probability is determined by the albedo. The altered directions are computed by the phase function. Indeed, the propagation of rays undergoes a series of refracting, reflecting, diffracting and transmitting through the medium, but all alteration of the directions of rays belongs to the category of scattering [24]. The general procedure in the Monte Carlo method is to emit enormous energy bundles from random locations and directions on a given surface, and then trace their propagation through the nanoporous media until they are exited from the domain, or are exhausted owing to the absorption. The detailed flowchart can be referred to Fig. 1.

The nanoscale effect is discussed in Section 2. Section 3 shows parametric studies for computing the radiative thermal conductivity. The optimization of silica aerogel density to minimize heat transfer is obtained in Section 4, followed by a brief conclusion in Section 5.