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Research paper

An inverse analysis to estimate the endothermic reaction parameters and physical properties of aerogel insulating material

Tao Xie [a], Ya-Ling He [a, *], Zi-Xiang Tong [a], Wei-Xu Yan [b], Xiang-Qian Xie [b]

[a] *Key Laboratory of Thermo-Fluid Science and Engineering of MOE, School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi, 710049, PR China*

[b] *Beijing Institute of Nearspace Vehicle's Systems Engineering, Beijing, 100076, PR China*

HIGHLIGHTS

- Enthalpy model was used to study transient heat transfer of material.
- Inverse method was applied to determine some crucial parameters.
- The variation of thermal properties would greatly affect the heat transfer process.
- The most probably reaction was the evaporation of adsorbed water inside aerogel.

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ABSTRACT

Silica aerogel is a kind of highly nano-porous material with excellent performance in heat insulation. Some researches showed that during the heating process, some kind of reactions happened inside the material accompanying with endothermic/exothermic phenomenon, such as evaporation of water or residual solvent. These reactions will greatly change the properties of the material as well as affect its insulation performance at high temperatures. Therefore, it is crucial for silica aerogel insulating material to understand its transient heat transfer characteristics and to identify the thermal properties as well as some other key parameters. In this study, a numerical heat transfer model is constructed to study the transient heat transfer characteristics of the aerogel material in which the reaction effect is taken into account. Finite volume method combined with Enthalpy method are used to numerically solve the heat transfer problem. In order to determine the key parameters of the heat transfer model, an inverse analysis is conducted based on the Levenberg–Marquardt method. Through the inverse analysis technique, parameters such as thermal conductivities before and after the reaction, $\lambda_{\mathrm{virgin}}$ and $\lambda_{\mathrm{reacted}}$, reaction temperature T_{reaction} and reaction heat L, can be estimated by using a group of experimentally measured temperature history curves. Besides, sensitivity analysis as well as the influence of measurement errors are also discussed. The results show that (1) The optimum values for these parameters which are consistent with the actual situation are $X_{\mathrm{u}}^{0} = (\lambda_{\mathrm{virgin}}, \lambda_{\mathrm{reacted}}, T_{\mathrm{reaction}}, L) = (0.1380\ \mathrm{W/(m \cdot K)}, 0.0535\ \mathrm{W/(m \cdot K)}, 355.45\ \mathrm{K}, 230{,}670\ \mathrm{(J/kg)})$; (2) The accompanying thermal effect of the reaction heat is small and can be neglected. The main effect of reaction on the heat transfer characteristics is due to the change of the component of the material. The component change of material will then lead to the variation of thermal properties which greatly affect the heat transfer process.

1. Introduction

Silica aerogel has attracted more and more attentions to be a candidate with great potential in the industrial application of super insulating material. It is a sort of highly nano-porous and open cell structure material. Due to its special nano-sized matrix and highly nano-porous structure, the thermal conductivity of silica aerogel is very low.

Silica aerogel is always used under high temperature and high heat flux environment, so its heat transfer characteristics under high temperature has attracted more and more attention. Recently, a few studies pointed out that when silica aerogel was used under high temperature and high heat flux environment, some reactions

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[*] Corresponding author. Tel.: +86 29 8266 5930, 86 29 8266 3300; fax: +86 29 8266 5445.

E-mail address: yalinghe@mail.xjtu.edu.cn (Y.-L. He).

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happened inside aerogel. Mah and Chung [1] measured the thermogravimetric curve of a kind of dried gels and divided the curve into three regions, which correspond to the desorption of physically adsorbed water (Region 1, ~150 °C), the removal of organics accompanied by polymerization and structural relaxation (Region 2, 150–550 °C), and the shrinkage (Region 3, above 550 °C) respectively. Rao and Kulkarni [2] used thermogravimetric analysis (TGA) and differential thermal analysis (DTA) to study the thermal stability of TMOS-based silica aerogels experimentally. The results showed that hydrophobic aerogels were thermally stable up to a temperature of 300 °C. Above this temperature, the (CH_3) groups and other residual organic groups of aerogels oxidized and the aerogels became hydrophilic. Nayak and Bera [3] studied the nature of thermal stability of the aerogel by FTIR (Fourier Transform Infrared Spectroscopy) and DSC (Differential Scanning Calorimetry)/TG respectively. They demonstrated that there was a sharp weight loss up to a temperature of 150 °C due to the evaporation of residual water from the aerogel and further a significant weight loss in the temperature range of 300–700 °C which attributed to the progressive poly-condensation and dehydration of aerogel. Gao [4] experimentally studied the infrared spectral characteristics of nano-porous SiO_2 aerogel under different temperature conditions. The infrared spectrogram showed that when heat treated from 300 °C to 600 °C, some of the remained Si–OH and adsorbed water inside aerogel disappeared gradually and SiO_2 aerogel completely formed the Si–O–Si network structure. Cui et al. [5] analyzed the thermal stability of hydrophobic silica aerogels by simultaneous TG–DSC analysis and the chemical composition as well as the hydrophobicity/hydrophilicity of the aerogels were investigated by FTIR. Their results also showed that while aerogel was treated under high temperature, its composition and structure were altered with accompanying exothermal effect.

Through the above literature review [1–5], it can be seen that the reactions which happened inside aerogel will lead to the variation of its component. The variation of component could further greatly influence the thermal properties of the material as well as its insulating performance. Most of the current heat-transfer-in-aerogel-related studies focused on establishing effective thermal conductivity model of aerogel insulating materials. For example, Zeng et al. [6] used three kinds of cubic arrays to represent the structure of silica aerogel and derived their thermal conductivity models by using equivalent circuit method. Zhao et al. [7] developed an improved analytical model for the total thermal conductivity of fiber-loaded silica aerogels. Their model included numerous influence factors of fibers and silica aerogel such as the complex refractive index, size, orientation, volume fraction and morphology. A fractal-intersecting sphere model for the nano-porous silica aerogel was proposed by Xie et al. [8] in which the complex microstructure as well as the scale effect on gas conduction and solid-matrix conduction were both considered. In the paper, a complete computing procedure was also showed for calculating the thermal conductivities of silica aerogel composite insulating materials. Zhao et al. [9] developed a pressure-dependent model for gaseous thermal conductivity of aerogels which took into account the effects of solid–gas coupling effect as well as the pore and particle microstructures. Recently, He and Xie [10] have analyzed the heat transfer characteristics inside aerogel material in detail and summarized almost all of the current effective thermal conductivity models for the nanoporous silica aerogel insulating material in their review paper. So readers who are interested in the heat transfer of the aerogel material can refer to this review.

It can be seen that few of current heat-transfer-in-aerogel-related studies have considered the endothermic/exothermic reaction effects on the transient heat transfer characteristics of silica aerogel insulating materials. And almost none of them focused on how to determine the reaction parameters of endothermic reaction as well as the thermal properties of aerogel material.

In heat transfer area, direct heat transfer problem is to obtain the temperature field under conditions that the governing equation, initial and boundary condition as well as thermal properties are all known. In contrast, the inverse problem is always to determine the unknown input parameters by utilizing the known temperature information. Presently, applying the inverse heat transfer technique to get thermal properties of material has attracted wide attentions. Kinds of optimization algorithms have been used to solve the inverse heat transfer problem, such as genetic algorithm [11,12] and Levenberg–Marquardt method [13–15] etc. Levenberg–Marquardt method was proposed by Levenberg [16] and Marquardt [17] in 1944 and 1963 respectively. It is used to minimize the least square norm problems. Because of its robustness in solving the ill-posed nonlinear problems, this method has been used extensively in solving the inverse heat transfer problems. Zhao et al. [15] solved a one-dimensional coupled radiation-conduction heat transfer problem and used Levenberg–Marquardt method to determine the effective thermal conductivity of fibrous insulating material. Ukrainczyk [18] applied the Levenberg–Marquardt method on inverse one-dimensional diffusion problem and estimated the thermal diffusivity.

In one of the previous study [19], an experimental research has been made to reveal the endothermic mechanism under heating condition of aerogel insulating material. Then based on the experimental results, a numerical model was constructed to consider its internal endothermic reaction and investigated the transient heat transfer characteristic of silica aerogel insulating material. The purpose of the present study is to make an inverse analysis to estimate the thermal properties and reaction parameters of aerogel based on the constructed heat transfer model. To our knowledge, this has not been studied by any others. The heat transfer model will be showed in part 2 (Direct problem). Enthalpy method is adopted to solve the direct problem. An inverse analysis will then be conducted to identify the key parameters of heat transfer problem based on the Levenberg–Marquardt method. The sensitivity analysis is also applied to study the effect of each parameters on thermal performance of aerogel insulating material.

2. Direct problem

One dimensional unsteady energy equation in which reaction is involved can be written as [20]

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + g \tag{1}$$

In Eq. (1), the source term g represents the absorbed heat when "reaction" happened. Source term g can be represented by Ref. [20]

$$g = -\rho \frac{\partial f}{\partial t} L \tag{2}$$

where L is the heat of reaction of the material, ρ is the density, f is the fraction of reacted material and minus symbol indicates that the reaction is endothermic. Assume that the reaction happens at a specified temperature, f can be determined as [20]

$$\begin{cases} f = 0 & T < T_{\text{reaction}} \\ 0 < f < 1 & T = T_{\text{reaction}} \\ f = 1 & T > T_{\text{reaction}} \end{cases} \tag{3}$$