Modeling of Effective Thermal Conductivity of Dunite Rocks as a Function of Temperature

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Received: 3 February 2008 / Accepted: 21 July 2008 / Published online: 15 August 2008 © Springer Science+Business Media, LLC 2008

Abstract The thermal conductivity, thermal diffusivity, and heat capacity per unit volume of dunite rocks taken from Chillas near Gilgit, Pakistan, have been measured simultaneously using the transient plane source technique. The temperature dependence of the thermal transport properties was studied in the temperature range from 303 K to 483 K. Different relations for the estimation of the thermal conductivity are applied. A proposed model for the prediction of the thermal conductivity as a function of temperature is also given. It is observed that the values of the effective thermal conductivity predicted by the proposed model are in agreement with the experimental thermal conductivity data within 9%.

Keywords Density \cdot Dunite \cdot Porosity \cdot Thermal conductivity \cdot Transient plane source (TPS) technique

1 Introduction

A knowledge of thermal transport properties of rocks as a function of temperature has become important with the widespread interest in thermal processes. For example, underground storage of nuclear waste generally involves the use of long-life containers that are stored in underground chambers in a variety of rock types. Heat released from the nuclear waste is dissipated through the surrounding rocks. The relatively low

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A. Maqsood (⊠) School of Chemical and Materials Engineering, National University of Science and Technology, Islamabad, Pakistan e-mail: tpl.qau@usa.net e-mail: asgharimaqsood@yahoo.com thermal diffusivity of most of the rocks could lead to excessive temperature build-up in the containers and the surrounding rocks, resulting in possible damage to the containers and leakage of radioactive waste material. Calculation of heat dissipation from underground nuclear explosions and the rate of heat loss from earth due to geothermal gradients depend upon the thermal characteristics of the rock involved. The determination of heat losses from underground steam and hot-water pipes requires a knowledge of the thermal conductivities of soils and rocks. Some of these processes include thermal methods of enhanced oil recovery and management of geothermal reservoirs [1]. The design of thermal-insulating materials also depends upon the heat transfer characteristics of porous media. The most relevant thermal parameters of rocks are thermal conductivity, heat capacity per unit volume, and thermal diffusivity. The first two parameters give the capability of a material to conduct and accumulate heat, respectively, and the last one represents how fast heat diffuses through a material.

The samples studied here belong to a group of igneous rocks, which are further subdivided into four groups on the basis of silica content [2]. These subgroups are granite (SiO₂ > 65%), diorite (65% > SiO₂ > 52%), basalt (52% > SiO₂ > 40%), and dunite (SiO₂ < 40%). The samples studied in this paper belong to the dunite group. The thermal conductivity, thermal diffusivity, and heat capacity per unit volume of eleven porous consolidated dunite rock samples have been measured using the transient plane source (TPS) technique [3,4] in the temperature range from 303K to 483K and at atmospheric pressure using air as a saturant in the pore spaces. American Society of Testing and Materials (ASTM) Standards test methods have been used to measure the porosity, specific gravity, and density under ambient conditions.

The objective of this work is to develop an empirical model for the determination of the thermal conductivity of consolidated porous media as a function of temperature and in terms of parameters (which we have to measure once at a reference temperature) such as the porosity, the thermal conductivity of fluid (air) in pores, and the thermal conductivity of the constituent solid phase.

2 Existing Models for Thermal-Conductivity Prediction

Precise values of the thermal conductivity of rocks are difficult to measure and are very time-consuming. Consequently, a lot of effort has been made to develop models relating the thermal conductivity with easily measurable parameters such as porosity, density, chemical composition, grain size, temperature, and pressure, rather than going into tedious experimentation.

According to Kingery [5], Clark [6], Schatz and Simmons [7], Seipold [8], and others, the high-temperature thermal conductivity of many electrically non-conducting solids, including rocks, is given by

$$\lambda = \lambda_{\rm L} + \lambda_{\rm R},\tag{1}$$

or

$$\lambda = \frac{1}{A + BT} + CT^3,\tag{2}$$

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where λ_L is the lattice conductivity and λ_R is the radiative conductivity. The radiative conductivity, which obeys the T^3 - law, becomes relevant at about 1000 K [9]. So, at temperatures less than 1000 K, only the first term of the right-hand side of Eq. 1 or 2 is used. Thus,

$$\lambda = \lambda_{\rm L} = \frac{1}{A + BT},\tag{3}$$

where $A(W^{-1} \cdot m \cdot K)$ and $B(W^{-1} \cdot m)$ are coefficients/parameters related to the scattering properties of phonons. According to Schatz and Simmons [10], A is related to scattering of phonons by impurities and imperfections, and B is related to phonon-phonon scattering and is approximately proportional to an inverse power of sound velocity [11].

Instead of using parameters A and B, we can use two other parameters, namely, the thermal conductivity at a reference temperature λ_0 and a single temperature coefficient of thermal conductivity b (K⁻¹). Thus, the following relation is used [9,12]:

$$\lambda(T) = \lambda_0 (1 + bT_0)/(1 + bT), \tag{4}$$

where b is a parameter controlling the temperature dependence of the thermal conductivity and is related to parameters A and B of Eq. 3, as

$$b = B/A \tag{5}$$

The reference value of the thermal conductivity (λ_0) is simply derived from Eq.3, using $T = T_0$ (reference or room temperature).

Zoth and Hänel [13] give a relation to predict the lattice thermal conductivity as a function of temperature, as given below:

$$\{\lambda(T)\} = \{A'\} + \frac{\{B'\}}{350 + \{T'\}} \tag{6}$$

where T is in °C, and the empirical constants A' and B' are determined from a least-squares fit to measured data for different types of rocks [14].

3 Measurement Techniques and Sample Characterization

The samples were collected in collaboration with the Geological Survey of Pakistan (GSP), Islamabad, and were cut in rectangular shapes having approximate dimensions of $4.5 \text{ cm} \times 4.5 \text{ cm} \times 2.5 \text{ cm}$. There were eleven specimens with four samples of each type. The average values of the measurements are presented here.

The samples were dried at (105 ± 5) °C in a furnace for 24 h. After drying, the samples were cooled at room temperature for 30 min and then kept in desiccators. For mass measurements, a digital balance with 0.001 g tolerance was used. The density-related properties are explained in detail by Maqsood et al. [15]. In this present paper,

Table 1 Percentage porosity (Φ) , bulk density (ρ_0) , and specific gravity (a_0) of the specimens at room temperature and atmospheric pressure	Specimen	Φ (%)	$ \rho_0 (10^3 \text{kg} \cdot \text{m}^{-3}) $ $ \pm 0.002 $	<i>a</i> ₀
	Dn1	0.130	3.408	3.413
	Dn2	0.153	3.393	3.398
	Dn3	0.155	3.243	2.967
	Dn4	0.184	3.388	3.394
	Dn5	0.239	3.342	3.450
	Dn6	0.285	3.367	3.376
	Dn7	0.426	3.392	3.406
	Dn8	0.429	3.354	3.368
	Dn9	0.455	3.472	3.487
	Dn10	0.520	3.388	3.406
	Dn11	0.665	3.347	2.649

only the measured data for the porosity, bulk density, and specific gravity are presented (Table 1).

The transient plane source (TPS) technique [4] was utilized to measure the thermal conductivity because it allows measurements without any disturbance from the interfaces between the sensor and the bulk samples. Also, simultaneous measurements of the thermal conductivity and thermal diffusivity are possible [4]. In this technique, a TPS element is used both as a constant heat source and a sensor of temperature. For data collection the TPS element (20 mm in diameter), sandwiched between two halves of the sample in a bridge circuit [16,17], was used. When a sufficiently large direct current is passed through the TPS element, its temperature changes and there is a voltage drop across the TPS element. By recording this voltage drop for a particular time interval, detailed information about the thermal conductivity (λ) and thermal diffusivity (a) of the test specimen is obtained. The heat capacity per unit volume (ρc_P) is then calculated from the relation

$$\rho c_P = \frac{\lambda}{a},\tag{7}$$

where ρ is the mass density of the samples.

For thermal conductivity measurements, each sample consisted of two identical rectangular slabs of the same specimen. The surfaces of the samples were made smooth to have good thermal contact with the TPS element and to minimize the thermal contact resistance. The thickness of the samples was chosen so as to satisfy the probing depth criteria [3]. The results of the thermophysical measurements on the samples at different temperatures and atmospheric pressure are shown in Figs. 1–3.

Taking into consideration the errors of the technique [17,18], standard deviations of the measurements, and the sampling errors, the estimated uncertainties of the thermal conductivity and thermal diffusivity data are 5% and 7%, respectively. The estimated uncertainty in the volumetric heat capacity is around 10%.

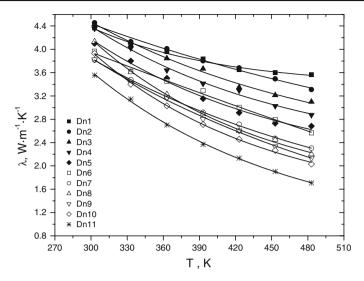


Fig. 1 Experimental values of the thermal conductivity as a function of temperature for samples Dn1 to Dn11

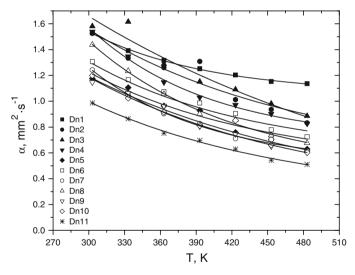


Fig. 2 Experimental values of the thermal diffusivity as a function of temperature for samples Dn1 to Dn11

4 Results and Discussion

Thermal transport properties of porous rocks depend upon their structure, mineral composition, porosity, density, the ability of their constituent minerals to conduct heat, temperature, pressure, etc.

The density-related properties such as porosity, bulk density, and specific gravity are given in Table 1. The porosity of these samples varies from 0.130% to 0.665%,

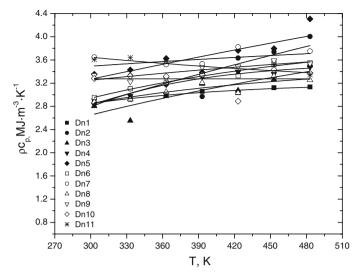


Fig. 3 Experimental values of the heat capacity per unit volume as a function of temperature for samples Dn1 to Dn11

the bulk density from $3.243 \text{ g} \cdot \text{cm}^{-3}$ to $3.472 \text{ g} \cdot \text{cm}^{-3}$, and the specific gravity from 2.649 to 3.487. These values are in excellent agreement with those in an earlier report [19].

The temperature dependence of the thermal conductivity, thermal diffusivity, and heat capacity per unit volume is measured from room/reference temperature (303 K) to 583 K at 30 K intervals, and the results are averaged. These results are shown in Figs. 1–3. It is observed that the thermal conductivity decreases by about 18 % to 52 % in the measured temperature range. This is in agreement with results in earlier reports [19]. The thermal diffusivity shows a decreasing trend whereas the heat capacity per unit volume shows an increasing trend, again in agreement with theory.

4.1 Prediction of Thermal Conductivity at Elevated Temperatures

Before providing a proposed model for thermal conductivity predictions as a function of temperature, some of the already existing models, Eqs. 4 and 6, were tested. For dunite samples, using Eq. 4, the empirical coefficient *b* is taken to be equal to 2891 K⁻¹ and λ_0 to be 4.758 W · m⁻¹ · K⁻¹ at 303 K [9], whereas in Eq. 6, *A'* and *B'* are taken to be 0.73 W · m⁻¹ · K⁻¹ and 1293 W · m⁻¹, respectively [14].

Using the above values of the adjustable parameters, thermal conductivity values are predicted and are plotted along with the experimental measurements in Fig. 5. It is to be noted that, in both equations, all the parameters affecting the thermal conductivity (such as porosity, density, thermal conductivity values of constituent minerals and the fluid inside the pores) are fitted by adjustable parameters and the errors in predicting the thermal conductivity are also high (up to 75 % and 78 % for Eqs. 4 and 6, respectively).

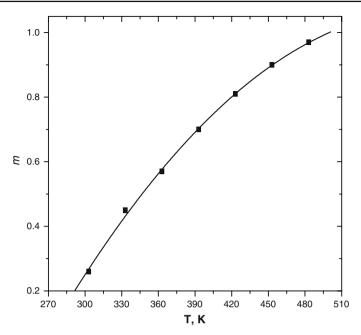


Fig. 4 Fit parameter m versus T (K)

So, keeping in mind the limitations of the above models, in the following, we use our proposed empirical model [20] to fit the experimental data.

4.2 Proposed Model

The proposed model for the prediction of the thermal conductivity of porous consolidated media as a function of temperature is expressed as

$$\frac{1}{\lambda_{\rm e}} = \frac{1}{\lambda_{\rm s}} + \frac{m\Phi}{\lambda_{\rm f}} \left(\frac{T}{T_{\rm o}}\right) \tag{8}$$

where T_0 (reference or room temperature) and T are measured in K, λ_s is the thermal conductivity of the solid phase at room temperature and is set equal to $4.695 \,\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$ [21], $\lambda_f = 0.026 \,\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$ for air in pore spaces [22], Φ is the fractional porosity, and m is an empirical coefficient. The value of m can be determined using experimental data of the thermal conductivity and corresponding values of Φ and λ_s as

$$m = \lambda_{\rm f} T_{\rm o} \left[\frac{\sum \left(1/\lambda_{\rm exp} - 1/\lambda_{\rm s} \right)}{\sum \left(T \Phi \right)} \right] \tag{9}$$

In the present case the calculated values of *m* are 0.26, 0.45, 0.57, 0.70, 0.81, 0.90, and 0.97 at (303, 333, 363, 393, 423, 453, and 483) K, respectively. A graph for *m*



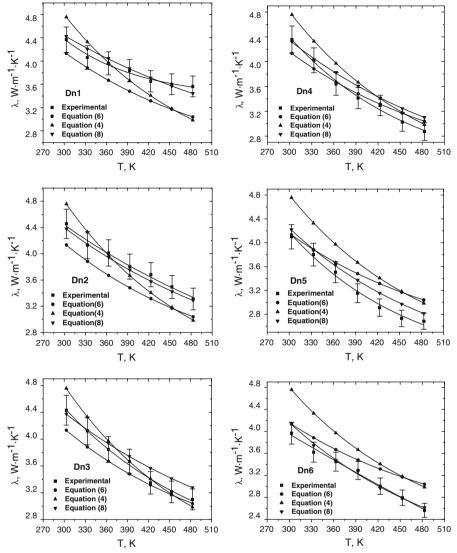


Fig. 5 Comparisons of experimental and predicted thermal conductivity values as a function of temperature for samples Dn1 to Dn11

versus *T* is plotted in Fig. 4. To get the values of *m* other than these, the process of interpolation may be used. From Eq. 8, it is obvious that when $T = T_0$, this formula resembles our proposed equation at room temperature [21].

The thermal conductivities of all the samples are also predicted by the proposed model (Eq. 8) and are plotted in Fig. 5. A maximum deviation of 9% is observed between predicted and experimental thermal conductivities. Our proposed model predicts effective thermal conductivities as a function of temperature, which are in close agreement with experimental values.

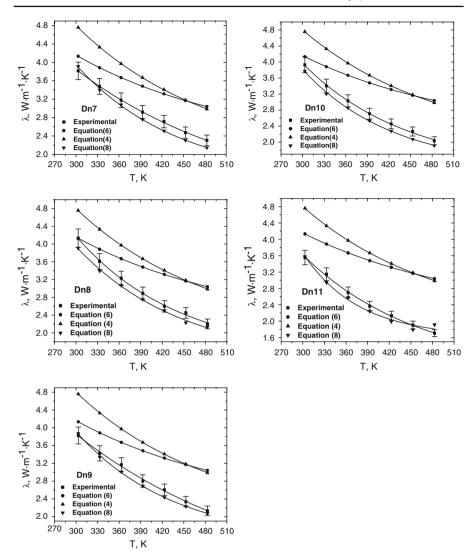


Fig. 5 continued

5 Conclusions

The thermophysical properties of rock samples are measured using Gustafsson's probe in the temperature range from 303 K to 483 K, at atmospheric pressure, and with air in the pore spaces of the samples.

To predict the thermal conductivity of dunite samples as a function of temperature, existing empirical models are tested. In this study, a new empirical model has been proposed. It is noted that experimental thermal conductivities and values predicted by the proposed empirical model are in agreement within 9%. To check the application of this proposed model, further work is in progress.

Acknowledgments The authors wish to thank Dr. M. Anis-ur-Rehman, Kashif Kamran, Dr. Iftikhar Hussain Gul, Liaqat Ali Khan, Mr. Matloob Hussain (Earth Science Department, QAU), and Mr. Muhammad Saleem Mughal (Statistics Department, QAU) for their helpful discussion. The author (Aurangzeb) is grateful to Higher Education Commission, Pakistan, for supporting the doctoral studies.

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