ISSN: 1858-7658 (Online)
ISSN: 1858-7690 (Print)

Modeling thermal conductivity of carbonate rocks using image data, Subis limestone, Malaysia.

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Abstract

Thermal conductivity (TC) was modeled for carbonate rocks using a digital rock volume constructed from image data by the stacking of multiple 2D computer tomography images. The main problem with the existing models lies in that these models consider only the volume fraction of pores and don't consider the geometry of such pores. The proposed model applies finite element theory where a representative volume was taken for simulation. The model evaluated the impact of porosity on TC by comparing TC of two samples with contrasting pore network systems: connected pores, versus isolated pore network system, under both dry and saturated conditions. When modeling dry conditions by using TC of air for pore volume, the results showed extremely high matching with experimental results. Samples of relatively high porosity showed a TC value much higher compared to that computed using a mixing-law model. This is because the model considers the internal structure and not only the volume fraction of pore volume. TC simulated for saturated samples did not show that expected increase in TC value that is normally calculated when replacing the small value of air TC with that of water which is relatively high. The result obtained for saturated conductivity needs to be experimentally validated under dynamic flow to confirm dynamic modeling. In summary, the model shows that thermal conductivity is not always reduced following volume fraction of pores as computed by different mathematical models.

Keyword: thermal conductivity; porosity; modeling; carbonate rocks.

INTRODUCTION

Thermal conductivity (TC) is one of the thermal properties of rocks including heat capacity and thermal diffusivity

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[1]. TC defines how much heat flows in a rock [2],[3] and [4]. TC is crucial for the heat flow modeling required for basin thermal history and hydrocarbon generation and migration [5]. There are many different methods being used in the estimation of TC. Some methods are classified based on several criteria. Classification of methods based on whether the method is experimentally-based or modeling-based is quite common. Although experimental methods are considered to be technically acceptable, they are coasty, time wasting, and technologically limited. Modeling of TC is proposed as a low cost, easy and fast means of computing TC. The most famous and well accepted models being used are the mixing law models which consider the volume fractions of individual rock components. The main problem in these models is that they consider only volume fraction of pores. Two rocks of the same percentage of pores can show contrastingly different pore distribution based on their internal fabric. Recent studies showed that most petrophysical properties of rocks depend to a large extent on rock fabric. TC of carbonate rocks ranges between 1.2 to 5.1 w $m^{-1}k^{-1}$, and it is inversely related to porosity [6]. This might be justified knowing that carbonate minerals individually exhibit a narrower range of TC, making the influence of mineral fraction minimized. Because most earth materials are poly-mineralic, being composed of more than one phase, homogenization principles are usually applied to encounter the effect of each mineral. Several studies are based on this homogenization principle [7], most of which are based on numerical modeling. Carbonate rocks with their special pore types are expected to behave heterogeneously in terms of petrophysical properties. Pore networks in carbonate rocks are subjected to distortion by dissolution, and can show a wide range of pore types, from micropores, through vugs, to dissolution channels. Therefore, the objectives of this paper are to construct a model of thermal conductivity that considers the

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ISSN: 1858-7690 (Print)

geometry of pore network rather than considering only the pore fraction.

MATERIALS AND METHODS

Two samples of limestone from different outcrops were selected for this study. The carbonate rock are of Subis limestone, Sarawak, which is Miocene in age, and is believed to form as a result of uplift processes [8]. The samples were prepared by cutting into cuboid shape of 10 cm length and 2 cm^2 in diameter. Computer Tomography Scan (CT scan) imaging was applied to both samples to obtain information about the internal pore network system. CT scan provided vertical slices (cross sectional 2D images) for both samples at a resolution of 40 microns. Resolution of imaging was calculated based on the imaging density, where total of slices was divided by the length of the samples. Initially, samples were scanned using CT micro scan tomography of the type Inspexio @. Knowing that each sample is is 10 cm long, a number of 300 cross sectional micrographs were captured, resulting in a resolution of 30 microns. A 3D volume of the image was constructed from the CT scan micrographs after running some basic image proceeding functions such as image segmentation and thresholding. Thresholding was set by adjusting the lower and upper pixel value until the mask matches the pore.

TC was estimated experimentally using the basic Fourier's formula by using a needle probe type (HH 506 RA) with two thermocouples. The experiment was carried out under the ambient temperature.

$$k = \frac{\left(\frac{q}{dt}\right)L}{AdT} \quad (1) .$$

In which:

k = TC coefficient in $Wm^{-1}k^{-1}$.

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(q/t)=Heat flow rate in watt/hour, obtained by setting the wattage in the apparatus.

L= length of sample; obtained from the probe spacing.

A= Area across heat flow; normally computed as the contact area between the sample and apparatus.

dT= Difference in probe temperature in Kelvin degree.

In contrast, the needle probe method was the best known of the transient methods, being fast and easy, with inaccuracy limit of up to 10% [10]. The method is used at the ambient temperature, and the time required for single reading is 80 sec [9] and [11]. The wattage used was 40 watts. A 10 cm probe spacing was chosen for probe alignment at parallel equal lines (1 cm line spacing). Time required for single reading is 80 sec. [12] and [9]. Three readings for each sample were taken from a PC connected to the Needle Probe for model validation.

For model input parameters, TC of framework is considered as follows:

Assuming that composition is neglected, a value of 3.2 W m-1 k-1 is assigned for framework (grains and matrix).

TC of air =0.25 (under 25 ºC).

Boundary conditions used: boundary condition of Neumann that is used for anisotropic mixture of material (as seen from rock volume).

RESULTS

Sample 1 showed a heterogeneous distribution of pore network in the 2D view as well as in 3D, Based on the quantitative data calculated for different masks, the ratio of total pore elements to the total elements representing grains/ framework was

ISSN: 1858-7658 (Online)
ISSN: 1858-7690 (Print)

found to be 10.7 % as shown in Figure 1.

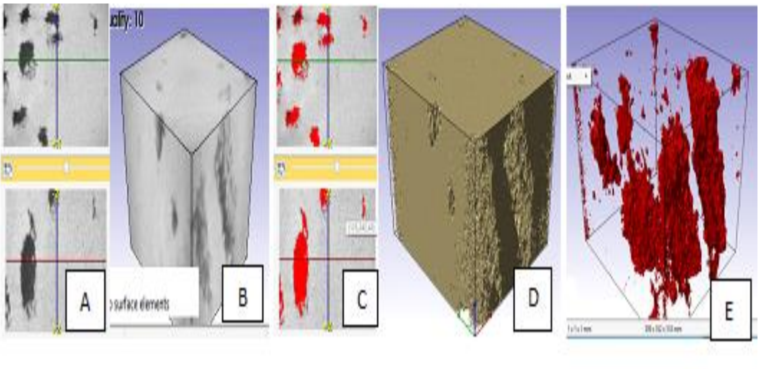

Figure 1: A : Original slices in two different direction and the B: rendered 3D volume from image stacking ; C: slices shown in Figure 1A after being segmented and mask applied; D and E rock volume after pores and framework (named background) thresholded and extracted from the 3D volume.

Statistics of rock volume are presented below (Table 1) with the software interface. Statistical data included total number of voxels (3D pixel) which is readily converted into absolute volume (mm^3) . It is clear that pore network has a ratio represents 10.7% in no matter expressed in voxels or in millimeters. Variations in mean grey scale originated when adjusting the upper and lower threshold limits that makes the mask to fit either pore network or background

Table 1: Interface showing statistics of the total 3D volume constructed. Background represents framework, and pore.

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Name	Voxel counts	Volume mm^3	Surface area (mm^2)	Mean grayscale (original)	Std Dev of grayscale (Original)
background	31273973	$31.3x10^6$	$2.18x10^6$	191	114
pores	3774643	$3.77x10^6$	$2.45x10^6$	107	41.8

Setting the model for Sample 1:

- The mask for porosity was set with lower and upper values until the mask was totally matching
- Boundary condition: Three methods for boundary conditions were selected, however, the results obtained from boundary condition of Neumann's (anisotropic material) will be considered if significantly different from other methods.
- Cube selected as representative volume is of a volume of 2556195 units, and thus representing about 7% of the total volume. Cube selected is shown in Figure.
- TC value of 5.2 for calcite, and 0.025 $Wm^{-1} k^{-1}$ for air.

Results of the model:

To save memory and time, a small cuboid was selected by cropping the 3D volume (Figure2) as part of the model setup stage. A mesh was generated, and accordingly, volume of the cuboid was calculated. Representative volume with quantification of elements representing pore networks and framework (background) was shown in Figure 2.

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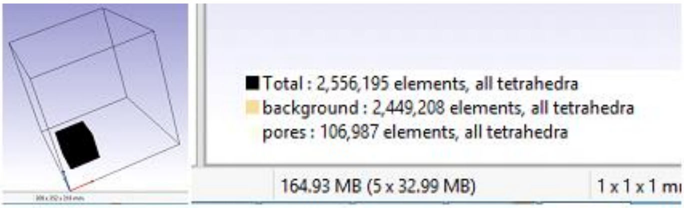
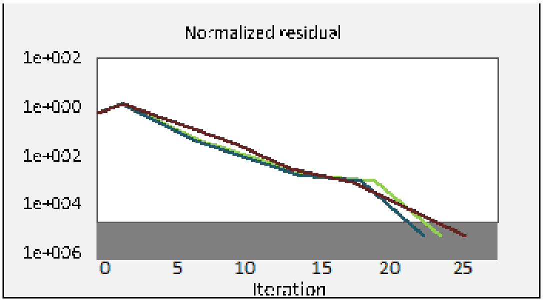


Figure 2: Representative volume (black colored), with the statistics of masks representing framework (background), and pores.

From the main menu, a physical model was selected, under which a heat transfer model was chosen.

After applying meshing function, using the boundary condition of Neumann, and running the model, a range of TC values was obtained increasing with the increase of the number of iterations. By increasing the number of iterations, residuals which is a measure of differences between actual values and predicted values, decrease, and is a measure of model or prediction accuracy. The range of TC was found to fall between 4.7609 ($Wm^{-1}k^{-1}$) and 4.7608 ($Wm^{-1}k^{-1}$). This value can be approximated to be 4.76 ($Wm^{-1}k^{-1}$). TC value was almost stable over a wide range of iterations (20 times). TC range obtained under different iterations is shown in Figure 3.



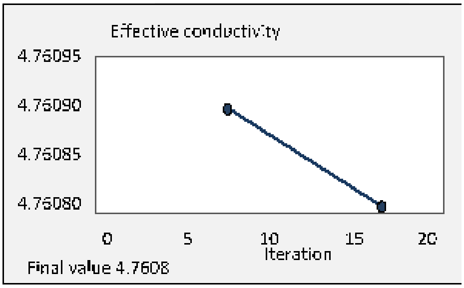


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Figure 3: Thermal conductivity range obtained under different iterations A: shows residuals trend line versus iterations (left), and B: TC range obtained under different iterations, (right).

Based on the TC obtained, the model can provide some information on the distribution of heat along each axis. Heat flow range parallel to x axis shows a range of 117-198, where as in the Y-direction the range is from 115-200, and along the Z-axis the range is from 32-103. This can show how heterogeneous is the sample, and how geothermal gradient can vary by subtracting the lowest value from the highest one, and divided by the width, length and height of the samples respectively for each axis. Variations in heat flow gradient is shown in Figure 4.

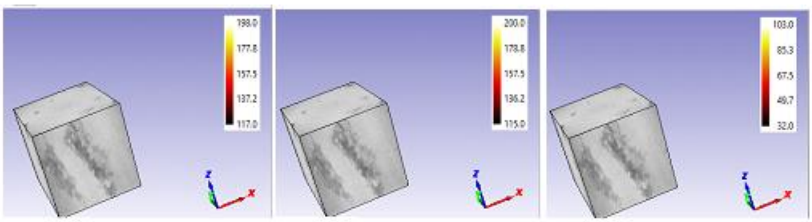

Figure 4: Variations in heat flow gradient: Heat flow gradient along X-, Y-, and Z-axis respectively.

TC model for non-connected pores:

For sample 2 which shows an internal structure of isolated pore networks, similar steps were followed. The total pores volume of this sample was computed as 33%, with pores clearly seem isolated and perfectly distributed compared to sample 1 (Figure 5).

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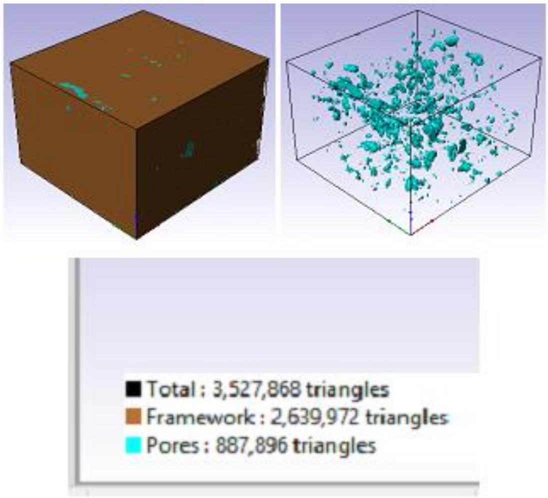

Figure 5 : Pore network of sample 2: A :Sample after applying the thresholding and masks for framework and pores (left), B Pores being extracted (middle), and C : Quantification of each component (right).

Setting the model for Sample 2:

- The mask for porosity was set with lower and upper values 40-78, while for framework is from 0-220 pixels.
- Boundary condition: Similar to sample 1.

- Cube selected as representative volume is of a volume of 250108 pixels, and thus representing about 7% of the total volume; and of a total pores of 54172, representing 21 % of cube porosity. Referring to quantitative porosity, the cube representativity can be calculated at 63% (21%/33%). Cube selected is shown in Figure 6.

  - TC value of 5.2 for calcite, and 0.025 $Wm^{-1} k^{-1}$ for air.

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ISSN: 1858-7690 (Print)

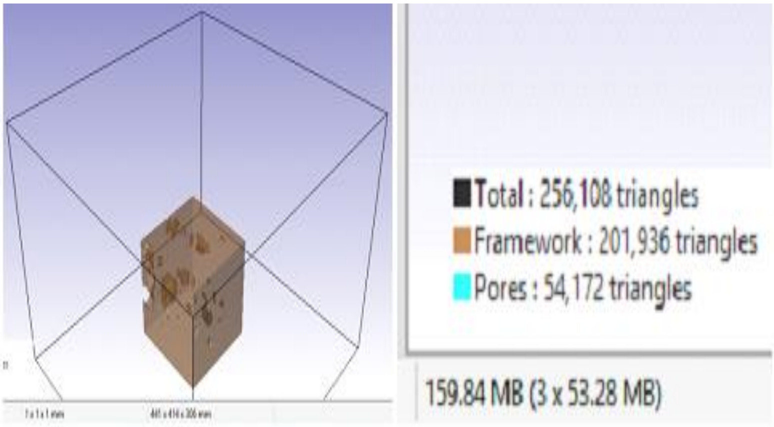

Figure 6: Cube selected: A: Representative volume (left), and B: the statistics of masks representing framework (background), and pores (right).

After the model has been run, the absolute value for TC using Neumann boundary condition configuration is found to be 5.0 W $m^{-1}k^{1}$. The model did not show a trend line for TC with different iterations, instead, a final value was obtained. Most probably because the number of iterations is too small (6 iterations). Iteration with residuals and final value of TC are shown in Figure 7.

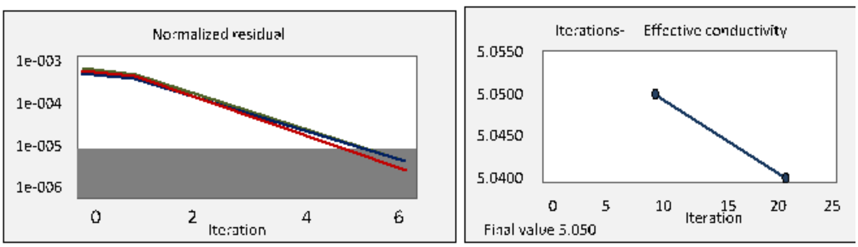

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Figure 7: A: Iterations trend line with residuals (left) and B: the final value of TC (right).

Model Validation:

Model validation is done by two means, namely; comparison of results with published data, and through experimental measurement of TC of the samples. The first step gives a quick glance on how realistic are the results. Experimental determination of the TC provides a confident judgment on actual value of TC. Experimental results for TC of both samples are shown in Table 2. An estimation of the error is given by dividing the absolute value of the TC predicted to the actual/ measured one as reference value.

Table 2 Experimental mean TC values for samples 1 and two. TC is expressed in W $m^{-1}k^{1}$.

Sample	TC1	TC2	TC3	TC mean	Accuracy % in model reading
1	4.86	4.42	4.47	4.65	97
2	4.89	4.92	5.03	4.94	98

Effect of Saturation:

After the model was validated for experimental data, it seemed appropriate to study the effect of water saturation so that one can get a value closer to reservoir or subsurface conditions. In order to do that, TC for porosity (air) was replaced with that of saturated (saline water). TC was taken as 0.59

ISSN: 1858-7658 (Online)
ISSN: 1858-7690 (Print)

W $m^{-1}k^{1}$ equivalent to sea water instead of that of air. TC value obtained is found to be 4.99, ~ 5.0 W $m^{-1}k^{1}$. Unlike that with air, the trend of TC with iteration is showing an increasing trend with the increase of number of iterations. This shows that corrected TC is in the favor of direct proportionality of TC and water, unlike the reversed case of air. Trend of TC with iterations is shown in Figure 8.

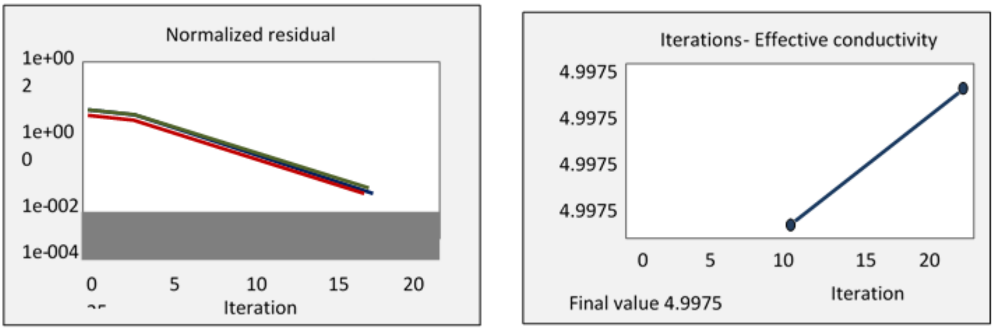

Figure 8: A: Iterations trend line with residuals (left) and B: the final value of TC (right).

Discussion:

The relationship of TC versus porosity, all trends show that TC decreases as porosity increases. All models take the quantitative value of porosity, regardless of pore size, shape and distribution. Sample 2 has a higher porosity value (33%) compared to sample 1 (10%). However, TC of the former is shown to be higher compared to the later. Referring to the internal structure of sample 2, it can be easily interpreted in that the isolated nature of the pore systems has no effect on TC. The overall value of TC is 5 W $m^{-1}k^{1}$. which is almost the same as that of massive limestone. Applying the arithmetic mean for TC, this samples

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should have a TC value of 3.43 W $m^{-1}k^{1}$ (5.2 *0.66 + 0.025*0.33) instead. This value found by the arithmetic mean model is far below the actual value that has been estimated experimentally. This can give a clue that it is erroneous to model TC based on volume fraction of porosity as isolated pores can behave as massive rock. This is also clear when replacing TC of air with that of water; almost the same result is obtained, indicating that these pores are not effective.

Regarding the value obtained for saturated samples, TC was expected to show a significant increase as air conductivity was replaced by waster conductivity. The value obtained did not show that much of increase; an instead, almost the same value was obtained. We are not sure if the model calculated this value with permeability considered or not. If this assumption is correct, it would be acceptable to assume that the expected increase in TC value is reduced by the effect of permeability where fluids redistribute heat flow. In such case, the model can be said to be applicable for measuring dynamic TC. The authors do not support this assumption because for each model, parameters needs to be set before running, which is not done for permeability model. However, there is no available equipment that measures dynamic TC in order to validate these results.

Conclusion and Recommendation:

Estimation of TC model for carbonate rocks extracted from rock volume was simulated for both dry and wet samples. The model for dry situation proved experimentally valid, with accuracy much higher compared to that computed using volume fraction-models. This is mainly because this models

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ISSN: 1858-7690 (Print)

considers the geometry and internal structure and not only the absolute value of porosity as in the cased of isolated pore which is proven that it has no significant effect on TC despite of the high volume fraction. The model simulated under saturated condition, didn't show the expected results, therefore, an experimental estimation under dynamic conditions is recommended in order to check the validity of the model under conditions closer to the subsurface conditions.

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