RADWASTE

ESTIMATION OF THE THERMAL CONDUCTIVITY OF SOME CRYSTALLINE ROCKS FROM THEIR MINERAL COMPOSITION

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The thermal conductivity of a rock is a function of the conductivities, amount and distribution of its several constituents. Various expressions have been reported in the literature for modelling multicomponent systems. The data file of thermal conductivity, porosity, density and mineralogy of rocks, maintained by the Geothermal Service, provides an excellent source for evaluating the several models. This report concerns the data available on crystalline rocks from the Superior Province and on samples from Radwaste boreholes at Chalk River and Whiteshell. In general more detailed mineralogical analyses exist for the latter.

Three distinct models of the "solid" conductivity, k_s, are used, and each of these is refined by three further models that take into account the presence of fluid, of conductivity k_f, in pores and cracks. Minerals were assigned conductivities based on published data. These are listed in Table 1. Two of the solid models have previously been discussed by Jessop et al. (1979): one based on quartz content, and the second a similar model that considers the conductivity and content of each mineral. The expressions for calculated conductivity, k_c, for these models respectively are:

Model S1: $$k_c = 7.7^{\phi} \times 2.0^{(1-\phi)} \qquad (1)$$

Model S2: $$k_c = \prod_{r=1}^{n} k_r^{\phi_r} \qquad (2)$$

where ϕ is the volume fraction of quartz, ϕ_r is the volume fraction of the r'th mineral in the aggregate and k_r its conductivity, and n is the number of minerals. In equation (1), quartz is assigned a conductivity of 7.7 W/mK and all other minerals 2.0 W/mK. Hashin and Shtrickman (1962) derived xpressions for the upper and lower bound conductivities, k_u and k_l, of a multicomponent system in terms of component conductivities:

$$k_u = k_{max} + A_{max} / (1 - x_{max} A_{max})$$

$$k_l = k_{min} + A_{min} / (1 - x_{min} A_{min})$$

Where $k_{max} = \max (k_1, k_2, - - - -, k_r)$

$$x_{max} = 1/3 \, k_{max}$$

$$A_{max} = \sum_{k_r \neq k_{max}}^{n} ((k_r - k_{max})^{-1} + x_{max})^{-1} \phi_r$$

(with similar expressions for k_{min}, x_{min}, A_{min}).

The thermal conductivity of a multicomponent aggregate could then reasonably be estimated as

Model S3: $k_c = 1/2 \, (k_u + k_l)$ (3)

The conductivity of water and air is much less than that of most minerals, so that the conductivity calculated from the mineral content may be too high for a porous rock. Most crystalline rocks have low porosity, typically less than 1%, and the effect of fluid content on conductivity should be small. There are several ways of modelling the effect of porosity. For a two-phase ystem (i.e. solid and fluid) the simplest expressions are for a planar arrangement of the phases with the conductances either in series or parallel.

Such expressions would only be relevant if a homogeneous rock contained oriented cracks, and so are not considered here. Hashin and Shtrickman's (1962) analysis can also be applied to a two-phase system. If the fluid has a lower conductivity than the solid, the Hashin-Shtrickman upper bound to the aggregate conductivity corresponds to the case of fluid-filled vesicles in a solid matrix. The lower bound corresponds to the case of spherical spheres in a continuous fluid matrix. Model P1 is the mean of the upper and lower bounds. Brailsford and Major (1964) give an expression for a random mixing of the two phases: -

Never that is round!!!

$$k_m = 1/4 \left(A + (A^2 + 8k_s k_f)^{1/2}\right) \qquad (4)$$

$$\text{where } A = (3\phi_s - 1)\, k_s + (3\phi_f - 1)\, k_f$$

Here ϕ_s, ϕ_f, k_s and k_f are the volume fractions and conductivities of the two phases and k_m the model conductivity. This is model P2. Waff (1974) derived a mathematically analogous expression for the electrical conductivity of a system of solid cubic grains in a continuous fluid matrix. For thermal conductivity this becomes: (model P3):

$$k = \frac{k_s k_f \phi_s^{2/3}}{k_s \phi_s^{1/3} + k_f (1 - \phi_s^{1/3})} + k_f (1 - \phi_s^{2/3}) \qquad (5)$$

in which k_s and k_f are the solid and liquid conductivities and ϕ_s, ϕ_f the volume fractions.

For the purposes of modelling the effect of porosity, the solid phase conductivity is taken as k_c from equations 1-3 and the fluid conductivity is 0.59 W/mK for water. Least squares regression analyses of observed conductivity k_o against model conductivity k_m were performed to find best fits to the functions:

$$k_o = a\ k_m + b \qquad (6a)$$

$$k_o = c\ k_m^{\ d} \qquad (6b)$$

Results for the linear regression are given in Tables 2-7. The Superior Province results are for samples for which mineral content was simply estimated, whereas for the Radwaste borehole samples (Chalk River gneisses and Whiteshell granites) mineral content was more accurately determined by the point count technique. In Tables 2-7 only the two-phase model that yields the highest correlation, R, between calculated and observed conductivity is listed. Differences in N, the number of samples, within each data set arise if some samples do not contain quartz (when model S1 cannot be calculated) or if porosity data are missing (when no two-phase conductivity can be calculated). In Figures 1 and 2 are plotted k_o against k_m for the Radwaste data, with the best-fitting functions defined by equation 6 included.

A number of points can be seen from the results.

1. The mean conductivity calculated from the quartz model (S1) is lower than the mean observed conductivity, for all sample sets.
2. The mean conductivity calculated from model S2 is higher than the mean observed conductivity for all sample sets except the Whiteshell granites.

3. The conductivity calculated from the Hashin-Shtrikman multicomponent model (S3) is always higher than that from the other solid models.
4. There seems to be a difference between massive and foliated or banded rocks in terms of the slope (a) and intercept (b) of the linear fit of k_o on k_m. For the massive rocks studied - granites and norites - a is less than 1 and b greater than 1. For Chalk River gneisses and Superior Province biotite schists a is a greater than 1 and b less than zero. The Superior Province gneisses (for which mineral content is only estimated) do not fit this observation.
5. It is clear from Figs 1 and 2 that expressing k_o as a power function of k_m does not yield any significant improvement over the linear relationship. Indeed, for the Whiteshell granites the portions of the curves about which the data points cluster are virtually indistinguishable.
6. It is clear from Table 2 that a reasonable estimate of conductivity, k_e, can be obtained for the Chalk River gneisses solely from knowledge of the quartz content, by combining equation 1 with the relevant entry in Table 2:

$$k_e \simeq 1.13\,(7.7^{\phi} \times 2.0^{(1-\phi)}) - 0.08$$

This gives the sample conductivity to an accuracy of approximately 10%.
7. For the Whiteshell granites the best empirical equation is less simple. No model correlates well with the observed conductivities. The highest correlation coefficient (0.555) is for model S2P3, although the correlation coefficient is 0.481 for model S1. The sample conductivity can be estimated, generally to better than 5%, by using model S1 modified by the linear regression parameters of Table 4. Only a slight improvement is afforded by the use of model S2P3, modified by the linear regression

parameters, from which conductivity can be predicted to an accuracy of about 4%.

8. The Hashin-Shtrickman multicomponent model appears to be of little use for predicting the conductivity of the samples studied, except for the Whiteshell granites. The observed Whiteshell granite conductivities can be estimated, usually to better than 7%, by the parameters for model S3 in Table 4. For these samples use of model S3 is facilitated by their relatively uniform and simple mineralogy (Drury 1980).

The limitations of the models are obvious. The conductivity assigned to a specific mineral remains fixed at an average value derived from the literature, whereas wide variations are possible. Quartz, for example, is anisotropic with respect to thermal conductivity. The solid models do not include any term that describes the effect of anisotropy within the samples. Further work is clearly necessary, in particular, the effects of grain size, grain boundary thermal resistances, and of conductivity anisotropy must be considered. However, for the purposes of the Radwaste programme, useful expressions can be given for estimating the thermal conductivity of rock from its mineral content. For both Chalk River gneisses and Whiteshell granites conductivity can be estimated to better than 10% solely from measurement of sample quartz content.

References

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TABLE 1: CONDUCTIVITY VALUES ASSIGNED TO MINERALS

MINERAL	CONDUCTIVITY, W/mK
Actinolite	3.5
Apatite	1.4
Biotite	2.0
Calcite	3.6
Chlorite	5.0
Epidote	2.8
Feldspar	2.0
Garnet	3.5
Hornblende	2.8
Potass. Feldspar	2.4
Mafics	4.5
Olivine	4.3
Phlogopite	2.1
Quartz	7.7
Sphene	4.0
Serpentine	3.5
Zircon	4.0
Carbonate	3.3
Cummingtonite	3.6
Hypersthene	4.4
Microcline	2.4
Opaques	4.7
Plagioclase	2.0
Sillimanite	9.0
Allanite	2.8
Clinopyroxene	4.5
Pyroxene	4.5
Muscovite	2.3
Pyrite	19.2
Sulphide	13.4

TABLE 2

ROCK TYPE: GNEISS (Point count analysis)

SOURCE: Chalk River

MEAN CONDUCTIVITY: 2.71 ± 0.47 W/mK

MEAN POROSITY: 0.004 ± 0.003

MEAN QUARTZ CONTENT: 15 ± 10%

MODEL	MEAN CONDUCTIVITY (CALCULATED) W/mK	a	b	R	N
S1	2.47 ± 0.34	1.13 ± 0.03	-0.08 ± 0.07	0.806	73
S2	2.99 ± 0.29	1.33 ± 0.03	-1.25 ± 0.09	0.816	73
S3	3.11 ± 0.32	1.24 ± 0.02	-1.12 ± 0.08	0.835	73
S3 P3	3.08 ± 0.32	1.26 ± 0.02	-1.16 ± 0.07	0.844	73

TABLE 3

ROCK TYPE: GNEISS (Mineralogy esimated)

SOURCE: SUPERIOR PROVINCE

MEAN CONDUCTIVITY: 3.04 ± 0.57 (only samples) (with quartz): 3.02 ± 0.57 (all samples) W/mK

MEAN POROSITY: 0.003 ± 0.002

MEAN QUARTZ CONTENT: 27 ± 10%

MODEL	MEAN CONDUCTIVITY (CALCULATED) W/mK	a	b	R	N
S1	2.90 ± 0.41	0.67 ± 0.04	1.09 ± 0.13	0.493	184
S2	3.46 ± 0.42	0.58 ± 0.05	1.04 ± 0.16	0.416	189
S3	3.66 ± 0.46	0.52 ± 0.04	1.11 ± 0.16	0.424	189
S2 P2	3.39 ± 0.41	0.72 ± 0.05	0.66 ± 0.18	0.499	149

TABLE 4

ROCK TYPE: GRANITE (Point count analysis)

SOURCE: WHITESHELL

MEAN CONDUCTIVITY: 3.34 ± 0.16W/mK

MEAN POROSITY: 0.004 ± 0.002

MEAN QUARTZ CONTENT: 28 ± 5%

MODEL	MEAN CONDUCTIVITY (CALCULATED) W/mK	a	b	R	N
S1	2.92 ± 0.18	0.43 ± 0.02	2.09 ± 0.06	0.481	31
S2	3.15 ± 0.17	0.51 ± 0.02	1.74 ± 0.06	0.536	31
S3	3.33 ± 0.19	0.45 ± 0.02	1.86 ± 0.06	0.530	31
S2 P3	3.13 ± 0.17	0.53 ± 0.02	1.68 ± 0.06	0.555	31

TABLE 5

ROCK TYPE: GRANITE (Mineralogy estimated)

SOURCE: SUPERIOR PROVINCE

MEAN CONDUCTIVITY: 3.37 ± 0.37 W/mK

MEAN POROSITY: 0.006 ± 0.013

MEAN QUARTZ CONTENT: 30 ± 7%

MODEL	MEAN CONDUCTIVITY (CALCULATED) W/mK	a	b	R	N
S1	3.01 ± 0.32	0.81 ± 0.02	0.92 ± 0.07	0.686	109
S2	3.48 ± 0.34	0.60 ± 0.03	1.30 ± 0.10	0.547	109
S3	3.66 ± 0.35	0.60 ± 0.03	1.18 ± 0.10	0.563	109
S1 P3	2.94 ± 0.23	0.38 ± 0.01	2.25 ± 0.04	0.486	65

TABLE 6

ROCK TYPE: BIOTITE SCHIST (Mineralogy estimated)

SOURCE: SUPERIOR PROVINCE

MEAN CONDUCTIVITY: 2.70 ± 0.63 W/mK

MEAN POROSITY: 0.004 ± 0.003

MEAN QUARTZ CONTENT: 21 ± 6%

MODEL	MEAN CONDUCTIVITY (CALCULATED) W/mK	a	b	R	N
S1	2.66 ± 0.23	2.06 ± 0.08	-2.78 ± 0.21	0.753	87
S2	3.57 ± 0.37	1.10 ± 0.07	-1.22 ± 0.24	0.634	87
S3	3.76 ± 0.33	1.35 ± 0.06	-2.37 ± 0.25	0.703	87
S1 P3	2.67 ± 0.30	2.19 ± 0.18	-2.66 ± 0.48	0.803	19

TABLE ,

ROCK TYPE: NORITE (Mineralogy Estimated)

SOURCE: SUPERIOR PROVINCE (SUDBURY)

MEAN CONDUCTIVITY: 2.83 ± 0.28 (quartz present); 2.72 ± 0.30 (all) W/mK

MEAN POROSITY: no porosity data

MEAN QUARTZ CONTENT: 7 ± 4%

MODEL	MEAN CONDUCTIVITY (CALCULATED) W/mK	a	b	R	N
S1	2.19 ± 0.11	1.04 ± 0.07	0.55 ± 0.15	0.428	61
S2	3.92 ± 0.19	0.46 ± 0.05	1.34 ± 0.15	0.281	86
S3	3.12 ± 0.20	0.52 ± 0.04	1.08 ± 0.13	0.346	86

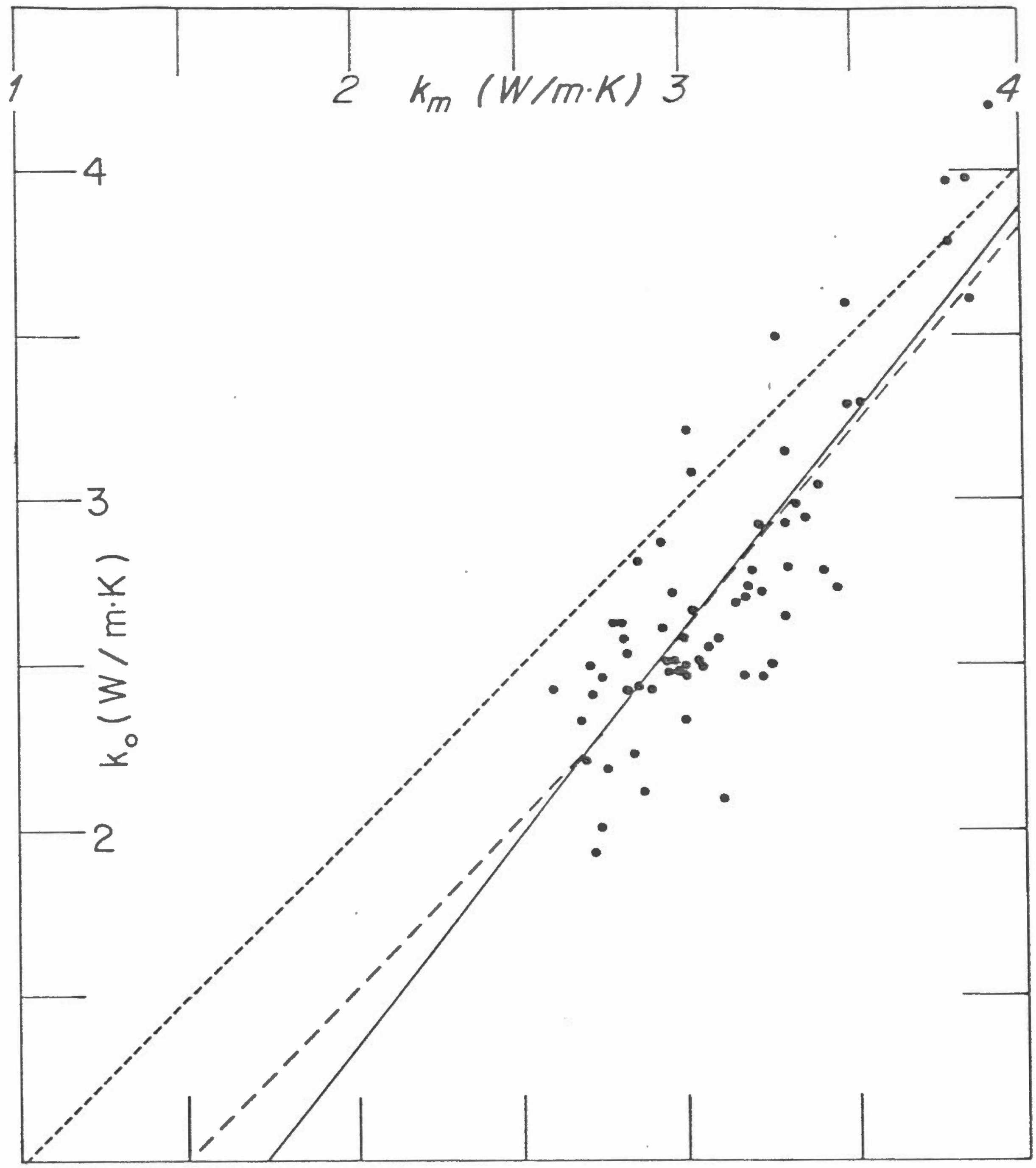

Fig. 1 Observed conductivity k_o plotted against modelled conductivity k_m for Chalk River gneisses.

Solid line: linear regression (eqn. 6a). Parameters are: $a = 1.26$, $b = -1.16$, $R = 0.844$. Long-dashed line: regression for eqn. 6b. Parameters are: $c = 0.59$, $d = 1.35$, $R = 0.830$. Short-dashed line: plot of $k_o = k_m$.

k_m is calculated from model S3P3.

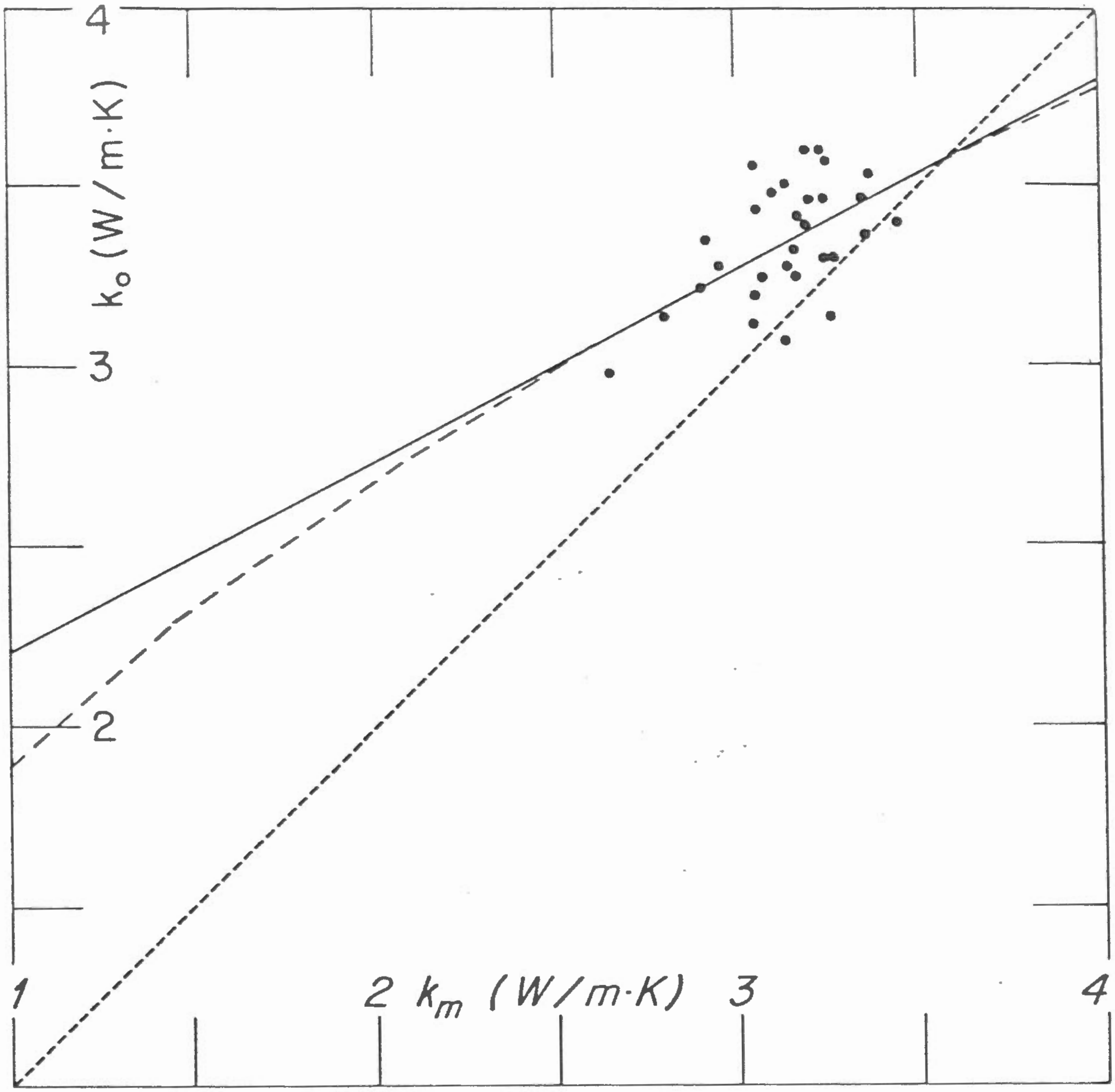

Fig. 2 Observed conductivity k_o plotted against modelled conductivity k_m for Whiteshell granites. Legend as for Fig. 1.

Parameters are: a = 0.53, b = 1.68, R = 0.555.

c = 1.88, d = 0.50, R = 0.569.

k_m is calculated from model S2P3

Note that with the two lowest values of k_m omitted, the parameters are a = 0.39, b = 2.14, R = 0.345.