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## RESEARCH ARTICLE

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## Special Section:

Physical Properties of Rocks, Friction and Fracturing: The Walsh Volume

## Key Points:

- Modal mineralogy permits matrix thermal conductivity ( $\lambda$ ) calculation with  $2\sigma$ -uncertainty of  $<15\%$  using the harmonic-mean model
- Uncertainty is reduced to  $<10\%$  if rock porosity is implemented in the calculation procedure
- Method is particularly valuable for inferring  $\lambda$  of drill cuttings and enclaves, promoting heat-flow calculation and geotherm computation

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## Calculation of Thermal Conductivity of Low-Porous, Isotropic Plutonic Rocks of the Crust at Ambient Conditions From Modal Mineralogy and Porosity: A Viable Alternative for Direct Measurement?

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**Abstract** Thermal conductivity ( $\lambda$ ) is an essential physical property of minerals and rocks and fundamental in constraining the thermal field of the lithosphere. In case that adequate samples to measure  $\lambda$  are not available, it could be indirectly inferred from calculation. One of the most widely applied indirect methods for rocks involve modal mineralogy and porosity as parameters that are incorporated into mathematical mean or mixing models. Robust inferences from these approaches for crystalline rocks were impeded by a small number of studied samples or restriction to certain rock types. We employ this method and examine its applicability to low-porosity plutonic rocks by calculating bulk thermal conductivity  $\lambda_b$  for 45 samples covering the entire range from gabbro/diorite to granite. We show that the use of the harmonic-mean model for both rock matrix and porosity provided a good match between  $\lambda_{b,meas}$  and  $\lambda_{b,calc}$  of  $<10\%$  deviation ( $2\sigma$ ), with relative and absolute errors amounting to  $1.4 \pm 9.7\%$  and  $4.4 \pm 4.9\%$ , respectively. The results of our study constitute a big step forward to a robust conclusion on the overall applicability of the harmonic-mean model for inferring  $\lambda_b$  of isotropic, low-porosity, mafic to silicic plutonic and metamorphic rocks with an acceptable magnitude of error. Drill cuttings and enclaves form particularly interesting objects for application of this method, as they are poorly suited for direct  $\lambda$  measurement. Well-derived  $\lambda$  values for those rocks would permit to calculate heat flow and to model more profoundly the thermal state of the deeper lithosphere.

### 1. Introduction

Thermal conductivity ( $\lambda$ ) is, alongside with thermal diffusivity, thermal effusivity, specific heat, and volumetric heat capacity, a fundamental physical property of minerals and rocks. It is essential for the calculation of heat flow, which represents an indispensable parameter in modeling the thermal field and, thus, constraining rheological and seismic properties of a region. Understanding the thermal structure of any geological setting requires accurate knowledge of  $\lambda$  of all involved geological units. Precise  $\lambda$  data are not only inevitable for quantifying the thermal evolution of crystalline areas and sedimentary basins, but with increasing importance also in mining, geotechnical, underground, and civil engineering (Popov et al., 2016). Proper designing of nuclear-waste repository systems, the exploration for geothermal energy, or the safe underground storage of fluid and gaseous media all require accurate information of rock thermal properties.

Thermal conductivity can be inferred from various direct and indirect methods. The three most commonly applied direct methods at ambient conditions are the optical-scanning, the divided-bar, and the line-source method (Popov et al., 2016, and references therein). Indirect approaches are used, if direct measurements of  $\lambda$  cannot be performed. Those approaches infer  $\lambda$  from (I) data on mineralogical composition, porosity, and composition of saturation fluids deploying numerical mixing models or from (II) correlations of  $\lambda$  with other physical properties. Studies pertaining to group-I have addressed low-porous granitic and metamorphic rocks (Chopra et al., 2018; Drury & Jessop, 1983; Pribnow & Umsonst, 1993; Ray et al., 2015; Zhao et al., 2016). Applications to sedimentary rocks have focused on models to determine bulk (or effective) thermal conductivity ( $\lambda_b$ ) from matrix conductivity ( $\lambda_m$ ) and varying porosity (e.g., Albert et al., 2017; Fuchs et al., 2013; Merkle et al., 1976). Group-II methods mostly deployed data from sedimentary rocks measured in boreholes (e.g., Anand et al., 1973; Evans, 1977; Fuchs et al., 2015; Goss et al., 1975;

**Table 1**  
Rock Type and Location of Samples

| Sample |        | Rock type              | Location                               |
|--------|--------|------------------------|--|
| #      | #      |                        |  |
| 1      | Z5b    | granite                | Fichtelgebirge, DE                     |
| 2      | L13    | granite                | Leuchtenberg, Oberpfalz, DE            |
| 3      | M5B    | granite                | Mitterteich, Oberpfalz, DEU            |
| 4      | Hzb1   | granite                | Hauzenberg, Passauer Wald, DE          |
| 5      | ARN    | granite                | Arnbruck, Bayrischer Wald, DE          |
| 6      | IMS-1  | granite                | Ilimaussaq, Grreenland, DK             |
| 7      | Lu-1   | granite                | Lusen, Bayrischer Wald, DE             |
| 8      | L2     | granite                | Leuchtenberg, Oberpfalz, DE            |
| 9      | EHR-2  | granite                | Eberhartsrent, Bayrischer Wald, DE     |
| 10     | NE4    | granite                | Neunburg, Oberpfalz, DE                |
| 11     | TI-2   | granite                | Fürstenstein, Bayrischer Wald, DE      |
| 12     | PAG    | granodiorite           | Patersdorf, Bayrischer Wald, DE        |
| 13     | 428    | granodiorite           | Görlitz, Ostlausitzer Massiv, DE       |
| 14     | SD1    | granodiorite           | Schärding, Mühlviertel, AU             |
| 15     | TM2    | granodiorite           | Turga massif, Transbaikalia, RU        |
| 16     | PADR1  | granodiorite           | Patersdorf, Bayrischer Wald, DE        |
| 17     | 603    | granodiorite           | Kurakusik, Tian Shan, KG               |
| 18     | DP68   | granodiorite           | Hubayra, Aquaba-Araba complex, JO      |
| 19     | 599    | monzonite              | Izbairamski complex, Tian Shan, KG     |
| 20     | Cs-2   | syenite                | Jiazishan, Shidao Complex, CN          |
| 21     | Cs-3   | syenite                | Jiazishan, Shidao Complex, CN          |
| 22     | 1317   | quartz<br>monzodiorite | Meissner massif, Elbe Zone, DE         |
| 23     | DP49   | quartz<br>monzodiorite | Um Rachel, Aquaba-Araba complex,<br>JO |
| 24     | 1325   | quartz<br>monzodiorite | Meissen massif, Elbe Zone, DE          |
| 25     | WSN1   | granodiorite           | Weschnitz pluton, Odenwald, DE         |
| 26     | 594    | tonalite               | Malchen, Odenwald, DE                  |
| 27     | Fü1b   | monzodiorite           | Fürstenstein, Passauer Wald, DE        |
| 28     | GM1684 | monzonite              | Isortoq, Greenland, DK                 |
| 29     | DP71   | quartz<br>anorthosite  | Marsod, Aquaba-Araba complex, JO       |
| 30     | R4B    | diorite                | Reuth, Oberpfalz, DE                   |
| 31     | DP65   | quartz<br>monzodiorite | Taur, Aquaba-Araba complex, JO         |
| 32     | 1327   | monzodiorite           | Meissen massif, Elbe Zone, DE          |
| 33     | TMZ1   | tonalite               | Tamazeght complex, MA                  |
| 34     | 598    | quartz<br>monzodiorite | Izbairamski complex, Tian Shan, KG     |
| 35     | KH49   | nepheline<br>syenite   | Ilimaussaq, Greenland, DK              |
| 36     | 597    | monzodiorite           | Izbairamski complex, Tian Shan, KG     |
| 37     | Cs-1   | alkali gabbro          | Shidao Complex, CN                     |
| 38     | Rhu4   | gabbro                 | Isle of Rum, Scotland, UK              |
| 39     | EDB1   | alkali gabbro          | Edinburgh, Scotland, UK                |
| 40     | FTG1   | quartz<br>monzodiorite | Ochsenkopf, Fichtelgebirge, DE         |
| 41     | GM1803 | gabbro                 | Isortoq, Greenland, DK                 |
| 42     | Rhu2   | gabbro                 | Isle of Rum, Scotland, UK              |
| 43     | 1319   | gabbro                 | Meissen massif, Elbe Zone, DE          |
| 44     | SRH1   | gabbro                 | Schriesheim, Odenwald, DE              |
| 45     | FRS1   | gabbro                 | Frankenstein, Odenwald, DE             |

Note. DE = Germany; DK = Denmark; AU = Austria; RU = Russia; KG = Kirgisistan; JO = Jordan; CN = China; MA = Morocco; UK = United Kingdom.

Hartmann et al., 2005). A comprehensive list of references and a detailed discussion on the pros and cons of well-log derived  $\lambda$  estimation are provided by Fuchs and Förster (2014). In contrast to work in sedimentary settings, adequate studies in hard rocks are scarce (Gegenhuber & Kienler, 2017; Pribnow et al., 1993; Williams & Anderson, 1990).

Previous approaches to infer  $\lambda$  from quantitative data on modal mineralogy of low-porous hard rocks by applying mixing models (group I) were conflicted with one or more of the following limitations: (a) the study included only few types of rock, that is, granites, high-grade metamorphic rocks, etc.; (b) the samples represented single batholiths or geological provinces, thus were regionally limited; (c) the study involved only a limited number of samples; and (d) the study evaluated only a few of the commonly used mixing models.

Although all yet practiced indirect approaches are rated as not matching the accuracy and precision of carefully performed laboratory measurements (Popov et al., 2016), they constitute the only option to get reasonable  $\lambda$  values in case that samples appropriate for direct measurement are not at disposal. Samples unsuited or less suited for measurement include, for instance, tiny drill cuttings, mechanically weakened rocks, or small-sized enclaves and xenoliths.

This paper reports the result of seeking out the mixing model(s) providing the best match between measured ( $\lambda_{b,meas}$ ) and calculated bulk thermal conductivity ( $\lambda_{b,calc}$ ) for low-porous, igneous crustal rocks. All samples were confirmed being isotropic, that is, display identical (within limit of measurement error) of  $\lambda$  in all directions. The study encompassed 45 samples representing various geological provinces in eight countries (Table 1). In contrast to previous studies, our suite of samples covers the entire range from mafic (gabbro/diorite) to silicic rocks (granite), straddling the range 36–76 wt.% SiO<sub>2</sub> (corresponding quartz range: 0–45 vol.%), and includes both such of alkaline, peralkaline, metaluminous, and peraluminous affinity. Assessment of the quality of fit involved all frequently applied mixing models that consider quantitative data on modal mineralogy. Our evaluation clearly demonstrates that  $\lambda_b$  of low-porous igneous rocks, irrespective of being mafic or felsic, could be indirectly calculated from their mineral content with an acceptable error by employing the harmonic mean model.

## 2. Methodology and Samples

We explored the usability of the following mean models (abbreviations in parentheses) for indirect  $\lambda_b$  calculation, where  $X_i$  is the volume fraction of the  $i$ th phase relative to the total volume ( $\sum X_i = 1$ ). The physical and/or empirical backgrounds of these models have been comprehensively described by Abdulagatova et al. (2009) and Clauser (2009) in connection with computation of  $\lambda$ .

Arithmetic mean (AM; Reuss, 1929; Voigt, 1928):

$$\lambda_{AM} = \sum_{i=1}^n X_i \lambda_i \quad (1)$$

Harmonic mean (HM; Reuss, 1929; Voigt, 1928):

$$\lambda_{HM} = 1 / \sum_{i=1}^n \frac{X_i}{\lambda_i} \quad (2)$$

Voigt-Reuss-Hill average (VRH; Hill, 1952):

$$\lambda_{VRH} = \frac{1}{2} (\lambda_{AM} + \lambda_{HM}) \quad (3)$$

Geometric mean (GM; Lichtenecker, 1924):

$$\lambda_{GM} = \prod_{i=1}^n \lambda_i^{X_i} \quad (4)$$

Square-Root-Mean (SQR; Roy et al., 1981):

$$\lambda_{SQR} = \left( X_i \sqrt{\lambda_i} \right)^2 \quad (5)$$

Effective Medium Mean (Eff, Bruggeman, 1935)

$$\lambda_{Eff}^{-1} = \sum_{i=1}^n \frac{3X_i}{2\lambda_{VRH} + \lambda_i} \quad (6)$$

Hashin and Shtrikman mean (HS; Hashin & Shtrikman, 1962)

$$\lambda_{HS} = \frac{1}{2} (\lambda_{HSU} + \lambda_{HSL}) \quad (7)$$

with the upper boundary:

$$\lambda_{HSU} = \lambda_{max} + \frac{A_{max}}{1 - \alpha_{max} A_{max}} \quad (8)$$

$$A_{max} = \sum_{i=1}^n \frac{X_i}{\alpha_{max} + 1/(\lambda_i - \lambda_{max})}; \quad (9)$$

$$\alpha_{max} = \frac{1}{3\lambda_{max}}; \quad (10)$$

and with the lower boundary

$$\lambda_{HSL} = \lambda_{min} + \frac{A_{min}}{1 - \alpha_{min} A_{min}} \quad (11)$$

$$A_{min} = \sum_{i=1}^n \frac{X_i}{\alpha_{min} + 1/(\lambda_i - \lambda_{min})}; \quad (12)$$

$$\alpha_{min} = \frac{1}{3\lambda_{min}}; \quad (13)$$

Herein,  $\lambda_{min} = \min(\lambda_1, \dots, \lambda_n)$  and  $\lambda_{max} = \max(\lambda_1, \dots, \lambda_n)$ .

**Table 2**  
Whole-Rock Geochemistry (wt.%)

| #  | Sample # | SiO <sub>2</sub> | TiO <sub>2</sub> | Al <sub>2</sub> O <sub>3</sub> | Fe <sub>2</sub> O <sub>3</sub> | MnO  | MgO   | CaO   | Na <sub>2</sub> O | K <sub>2</sub> O | P <sub>2</sub> O <sub>5</sub> | H <sub>2</sub> O <sup>+</sup> | CO <sub>2</sub> | Total  |
|----|----------|------------------|------------------|--------------------------------|--------------------------------|------|-------|-------|-------------------|------------------|-------------------------------|-------------------------------|-----------------|--------|
| 1  | Z5b      | 76.10            | 0.12             | 12.60                          | 1.82                           | 0.02 | 0.09  | 0.42  | 2.66              | 4.75             | 0.21                          | 0.68                          | 0.06            | 99.53  |
| 2  | L13      | 75.40            | 0.05             | 14.10                          | 0.93                           | 0.06 | 0.07  | 0.32  | 3.76              | 4.08             | 0.16                          | 0.82                          | 0.07            | 99.82  |
| 3  | M5B      | 73.70            | 0.31             | 13.50                          | 2.10                           | 0.05 | 0.40  | 0.84  | 2.77              | 4.46             | 0.25                          | 1.10                          | 0.12            | 99.60  |
| 4  | Hzb1     | 73.30            | 0.21             | 14.40                          | 1.25                           | 0.02 | 0.26  | 0.73  | 3.11              | 5.31             | 0.25                          | 0.95                          | 0.08            | 99.86  |
| 5  | ARN      | 73.10            | 0.18             | 14.60                          | 1.43                           | 0.04 | 0.33  | 0.65  | 3.12              | 4.86             | 0.33                          | 1.07                          | 0.11            | 99.82  |
| 6  | IMS-1    | 72.95            | 0.31             | 10.41                          | 5.25                           | 0.11 | 0.05  | 0.22  | 4.73              | 4.46             | 0.02                          | 0.49                          | 0.11            | 99.11  |
| 7  | Lu-1     | 72.70            | 0.18             | 14.50                          | 1.23                           | 0.02 | 0.34  | 0.69  | 2.82              | 6.14             | 0.17                          | 0.97                          | 0.12            | 99.88  |
| 8  | L2       | 71.70            | 0.38             | 14.00                          | 2.44                           | 0.03 | 0.79  | 1.26  | 2.65              | 5.37             | 0.15                          | 0.91                          | 0.09            | 99.77  |
| 9  | EHR-2    | 71.50            | 0.25             | 15.00                          | 1.56                           | 0.03 | 0.49  | 1.98  | 3.44              | 4.51             | 0.09                          | 0.75                          | 0.14            | 99.73  |
| 10 | NE4      | 70.00            | 0.52             | 15.10                          | 2.45                           | 0.03 | 0.72  | 0.99  | 2.56              | 5.62             | 0.29                          | 1.02                          | 0.10            | 99.40  |
| 11 | Tl-2     | 69.70            | 0.43             | 15.10                          | 2.57                           | 0.05 | 0.92  | 2.44  | 3.46              | 3.80             | 0.16                          | 0.97                          | 0.11            | 99.71  |
| 12 | PAG      | 68.60            | 0.51             | 15.20                          | 3.02                           | 0.05 | 1.06  | 2.51  | 3.25              | 3.99             | 0.19                          | 1.15                          | 0.15            | 99.67  |
| 13 | 428      | 68.16            | 0.58             | 14.88                          | 3.86                           | 0.06 | 1.39  | 1.77  | 3.31              | 3.98             | 0.19                          | 1.29                          | 0.20            | 99.67  |
| 14 | SD1      | 67.90            | 0.59             | 15.30                          | 3.56                           | 0.04 | 1.35  | 1.60  | 2.71              | 4.79             | 0.29                          | 1.37                          | 0.08            | 99.58  |
| 15 | TM2      | 65.60            | 0.51             | 14.61                          | 3.49                           | 0.06 | 3.41  | 3.11  | 3.54              | 3.74             | 0.17                          | 1.28                          | 0.14            | 99.66  |
| 16 | PADR1    | 64.90            | 1.25             | 14.78                          | 5.14                           | 0.07 | 1.31  | 2.53  | 2.81              | 4.92             | 0.49                          | 1.03                          | 0.18            | 99.42  |
| 17 | 603      | 64.36            | 0.59             | 16.65                          | 4.08                           | 0.05 | 1.38  | 4.56  | 2.64              | 3.45             | 0.16                          | 1.59                          | 0.15            | 99.66  |
| 18 | DP68     | 64.14            | 0.66             | 15.62                          | 4.34                           | 0.08 | 2.22  | 4.03  | 3.60              | 3.32             | 0.20                          | 1.22                          | 0.15            | 99.58  |
| 19 | 599      | 62.85            | 0.41             | 17.60                          | 4.10                           | 0.11 | 0.42  | 1.70  | 4.35              | 7.18             | 0.10                          | 0.71                          | 0.17            | 99.69  |
| 20 | Cs-2     | 62.16            | 0.27             | 18.67                          | 2.86                           | 0.09 | 0.64  | 1.62  | 4.89              | 7.40             | 0.16                          | 0.53                          | 0.24            | 99.52  |
| 21 | Cs-3     | 61.43            | 0.37             | 18.13                          | 3.34                           | 0.10 | 0.93  | 2.22  | 3.90              | 7.68             | 0.23                          | 0.71                          | 0.25            | 99.29  |
| 22 | 1317     | 60.54            | 0.50             | 17.58                          | 4.21                           | 0.08 | 2.31  | 3.44  | 3.86              | 4.90             | 0.31                          | 1.24                          | 0.36            | 99.33  |
| 23 | DP49     | 59.04            | 0.90             | 16.85                          | 6.32                           | 0.10 | 3.55  | 5.72  | 4.10              | 2.26             | 0.25                          | 0.95                          | 0.11            | 100.15 |
| 24 | 1325     | 58.63            | 0.63             | 16.53                          | 6.05                           | 0.10 | 2.56  | 4.55  | 3.88              | 4.73             | 0.43                          | 1.02                          | 0.09            | 99.20  |
| 25 | WSN1     | 57.67            | 0.99             | 17.31                          | 5.43                           | 0.08 | 3.17  | 5.07  | 3.77              | 3.48             | 0.42                          | 1.80                          | 0.20            | 99.39  |
| 26 | 594      | 56.83            | 0.89             | 17.65                          | 8.43                           | 0.18 | 2.59  | 6.16  | 3.32              | 1.49             | 0.25                          | 1.44                          | 0.43            | 99.66  |
| 27 | Fü1b     | 56.60            | 1.48             | 16.20                          | 6.82                           | 0.11 | 3.74  | 5.84  | 3.28              | 2.91             | 0.51                          | 1.74                          | 0.16            | 99.39  |
| 28 | GM1684   | 56.34            | 1.28             | 16.87                          | 8.50                           | 0.14 | 2.35  | 4.82  | 4.75              | 3.26             | 0.33                          | n.a.                          | n.a.            | 98.64  |
| 29 | DP71     | 55.66            | 1.14             | 18.00                          | 7.36                           | 0.14 | 2.77  | 6.73  | 4.56              | 1.62             | 0.41                          | 1.33                          | 0.23            | 99.95  |
| 30 | R4b      | 55.60            | 1.49             | 17.90                          | 7.23                           | 0.11 | 4.33  | 5.93  | 2.57              | 2.19             | 0.38                          | 1.56                          | 0.15            | 99.43  |
| 31 | DP65     | 55.45            | 1.00             | 17.12                          | 7.31                           | 0.13 | 4.51  | 6.51  | 3.60              | 1.96             | 0.34                          | 1.77                          | 0.11            | 99.81  |
| 32 | 1327     | 54.51            | 0.82             | 17.13                          | 7.40                           | 0.13 | 3.59  | 5.99  | 3.49              | 4.34             | 0.54                          | 1.22                          | 0.11            | 99.27  |
| 33 | TMZ1     | 53.57            | 1.05             | 16.74                          | 7.03                           | 0.11 | 6.53  | 7.16  | 2.69              | 2.02             | 0.39                          | 1.69                          | 0.16            | 99.13  |
| 34 | 598      | 53.17            | 0.41             | 15.95                          | 7.94                           | 0.15 | 5.53  | 10.55 | 2.25              | 1.54             | 0.11                          | 1.81                          | 0.31            | 99.72  |
| 35 | KH49     | 53.07            | 0.26             | 15.26                          | 10.64                          | 0.23 | 0.21  | 2.49  | 8.61              | 4.76             | 0.02                          | 2.09                          | 0.14            | 97.79  |
| 36 | 597      | 49.95            | 0.91             | 17.90                          | 9.59                           | 0.17 | 4.17  | 8.16  | 3.22              | 3.27             | 0.38                          | 1.56                          | 0.19            | 99.47  |
| 37 | Cs-1     | 48.12            | 0.94             | 8.21                           | 7.48                           | 0.14 | 10.14 | 14.70 | 1.30              | 3.07             | 2.59                          | 1.37                          | 0.23            | 98.29  |
| 38 | Rhu4     | 48.10            | 0.25             | 16.60                          | 4.75                           | 0.08 | 12.25 | 15.79 | 0.95              | 0.03             | 0.01                          | 0.77                          | 0.12            | 99.70  |
| 39 | EDB1     | 47.52            | 1.45             | 15.89                          | 11.62                          | 0.17 | 6.30  | 7.65  | 3.99              | 0.65             | 0.18                          | 3.89                          | 0.12            | 99.44  |
| 40 | FTG1     | 46.75            | 2.88             | 14.84                          | 13.09                          | 0.20 | 6.04  | 8.69  | 2.51              | 0.93             | 0.45                          | 3.01                          | 0.11            | 99.49  |
| 41 | GM1803   | 44.57            | 2.95             | 16.79                          | 15.90                          | 0.19 | 5.08  | 7.68  | 3.69              | 1.12             | 0.48                          | n.a.                          | n.a.            | 98.45  |
| 42 | Rhu2     | 44.45            | 0.14             | 23.29                          | 4.81                           | 0.06 | 12.07 | 12.22 | 1.26              | 0.08             | 0.02                          | 1.09                          | 0.20            | 99.69  |
| 43 | 1319     | 43.69            | 1.27             | 17.89                          | 11.38                          | 0.18 | 6.39  | 11.40 | 2.43              | 1.92             | 0.95                          | 1.56                          | 0.10            | 99.16  |
| 44 | SRH1     | 43.58            | 0.53             | 5.64                           | 11.29                          | 0.18 | 23.04 | 8.44  | 0.71              | 0.64             | 0.13                          | 4.81                          | 0.26            | 99.25  |
| 45 | FRS1     | 39.20            | 0.25             | 9.70                           | 11.96                          | 0.16 | 24.14 | 5.82  | 0.52              | 0.05             | 0.03                          | 7.29                          | 0.32            | 99.44  |

Note. n.a. = not analyzed.

Since the method applied in this study is strictly applicable only to rocks characterized by values of  $\lambda$  corresponding in all directions, special care was spent to prove the isotropic nature of the samples. First,  $\lambda$  of every rock sample was measured at both air and water saturated in three directions that were at an angle of 90° to each other. Measurements yielded in each case values that were identical within the uncertainty of the method ( $\leq 3\text{--}5\%$ ). Second, two polished thin sections were manufactured from every sample that were as well oriented 90° to each other. These sections were studied by optical microscopy, which revealed no indication for a textured appearance and any preferred orientation or alignment of rock-forming minerals or micro-cracks. A potential  $\lambda$  anisotropy triggered by flow texture was also the reason for excluding volcanic rocks from this study.

**Table 3**  
Measured Bulk Thermal Conductivity ( $\lambda_{b,meas}$ ), Porosity ( $\phi$ ), and Modal Mineralogy (vol.% of Samples)

| #  | Sample # | $\lambda_{b,meas}$ W/(mK) | $\phi$ % | Qtz % | Ab % | An % | Or % | Mc % | Anl % | Ne % | Di % | Aug % | Hbl % | OI % | Prh % | Bt % | Ms/Ilm % | Chl % | Ap % | Mag % | Ilm % | Ats/Rt % | Atg % |
|----|----------|---------------------------|----------|-------|------|------|------|------|-------|------|------|-------|-------|------|-------|------|----------|-------|------|-------|-------|----------|-------|
| 1  | Z5b      | 3.20                      | 1.33     | 0.45  | 0.24 |      | 0.06 | 0.18 |       |      |      |       |       |      |       | 0.04 | 0.03     |       |      |       |       |          |       |
| 2  | L13      | 3.04                      | 1.47     | 0.38  | 0.32 |      | 0.06 | 0.12 |       |      |      |       |       |      |       | 0.02 | 0.10     |       |      |       |       |          |       |
| 3  | M5B      | 3.06                      | 1.43     | 0.41  | 0.27 | 0.03 |      | 0.18 |       |      |      |       |       |      |       | 0.03 | 0.08     |       |      |       |       |          |       |
| 4  | Hzb1     | 3.11                      | 1.25     | 0.36  | 0.22 | 0.03 | 0.03 | 0.25 |       |      |      |       |       |      |       | 0.02 | 0.08     | 0.02  |      |       |       |          |       |
| 5  | ARN      | 2.71                      | 2.17     | 0.28  | 0.29 | 0.04 | 0.31 |      |       |      |      |       |       |      |       | 0.06 | 0.02     | 0.02  |      |       |       |          |       |
| 6  | IMS-1    | 2.75                      | 1.65     | 0.30  | 0.20 | 0.06 | 0.34 |      |       |      |      |       | 0.10  |      |       | 0.03 | 0.04     | 0.01  |      |       |       |          |       |
| 7  | Lu-1     | 2.82                      | 1.65     | 0.32  | 0.21 | 0.04 | 0.04 | 0.31 |       |      |      |       |       |      |       | 0.05 | 0.03     | 0.03  |      |       |       |          |       |
| 8  | L2       | 2.72                      | 1.65     | 0.32  | 0.23 | 0.04 | 0.07 | 0.27 |       |      |      |       |       |      |       | 0.02 | 0.03     | 0.01  |      |       |       |          |       |
| 9  | EHR-2    | 2.60                      | 1.19     | 0.31  | 0.30 | 0.06 | 0.03 | 0.27 |       |      |      |       |       |      |       | 0.05 | 0.11     | 0.01  |      |       |       |          |       |
| 10 | NE4      | 2.68                      | 1.25     | 0.35  | 0.17 | 0.06 | 0.05 | 0.21 |       |      |      |       |       |      |       | 0.05 | 0.03     | 0.02  |      |       |       |          |       |
| 11 | Tl-2     | 2.56                      | 1.15     | 0.33  | 0.29 | 0.08 | 0.05 | 0.15 |       |      |      |       |       |      |       | 0.10 | 0.03     | 0.02  |      |       |       |          |       |
| 12 | PAG      | 2.70                      | 1.07     | 0.33  | 0.32 | 0.08 | 0.14 |      |       |      |      |       |       |      |       | 0.16 | 0.03     | 0.03  |      |       |       |          |       |
| 13 | 428      | 2.72                      | 1.38     | 0.28  | 0.25 | 0.08 | 0.20 |      |       |      |      |       |       |      |       | 0.06 | 0.06     | 0.03  |      |       |       |          |       |
| 14 | SD1      | 2.52                      | 1.27     | 0.36  | 0.32 | 0.10 | 0.15 |      |       |      |      | 0.03  | 0.10  |      |       | 0.07 | 0.07     | 0.02  |      |       |       |          |       |
| 15 | TM2      | 2.64                      | 1.73     | 0.18  | 0.30 | 0.10 | 0.18 |      |       |      |      |       |       |      |       | 0.16 | 0.02     | 0.02  |      |       | 0.02  |          |       |
| 16 | PADR1    | 2.38                      | 1.25     | 0.34  | 0.28 | 0.12 | 0.17 |      |       |      |      |       |       |      |       | 0.05 | 0.05     | 0.02  |      |       |       |          |       |
| 17 | 603      | 2.49                      | 1.28     | 0.20  | 0.24 | 0.10 | 0.19 |      |       |      | 0.02 | 0.03  | 0.03  |      |       | 0.02 | 0.02     | 0.01  |      |       |       |          |       |
| 18 | DP68     | 2.35                      | 1.05     | 0.25  | 0.29 | 0.17 | 0.19 |      |       |      |      |       |       |      |       | 0.07 | 0.05     | 0.02  |      |       |       |          |       |
| 19 | 599      | 2.05                      | 1.62     | 0.04  | 0.40 | 0.04 | 0.42 |      |       |      |      |       |       |      |       | 0.04 | 0.04     | 0.02  |      |       |       |          |       |
| 20 | Cs-2     | 2.07                      | 0.74     | 0.03  | 0.38 | 0.05 | 0.47 |      |       |      |      |       |       |      |       | 0.07 | 0.02     | 0.01  |      |       |       |          |       |
| 21 | Cs-3     | 2.10                      | 0.97     | 0.04  | 0.38 | 0.05 | 0.45 |      |       |      |      |       |       |      |       | 0.02 | 0.02     | 0.01  |      |       |       |          |       |
| 22 | 1317     | 2.21                      | 1.91     | 0.12  | 0.40 | 0.10 | 0.26 |      |       |      | 0.04 | 0.05  | 0.16  |      |       | 0.08 | 0.02     | 0.01  |      |       |       |          |       |
| 23 | DP49     | 2.11                      | 1.21     | 0.14  | 0.39 | 0.22 | 0.12 |      |       |      |      |       |       |      |       | 0.10 | 0.10     | 0.02  |      |       |       |          |       |
| 24 | 1325     | 2.09                      | 1.20     | 0.07  | 0.36 | 0.13 | 0.23 |      |       |      |      |       |       |      |       | 0.21 | 0.05     | 0.03  |      |       |       |          |       |
| 25 | WSN1     | 2.21                      | 1.44     | 0.21  | 0.26 | 0.16 | 0.14 |      |       |      |      |       |       |      |       | 0.05 | 0.02     | 0.01  |      |       |       |          |       |
| 26 | 594      | 2.36                      | 0.88     | 0.15  | 0.29 | 0.26 | 0.02 |      |       |      |      | 0.03  | 0.11  |      |       | 0.10 | 0.02     | 0.02  |      |       |       |          |       |
| 27 | Fu1b     | 2.28                      | 1.24     | 0.16  | 0.25 | 0.20 | 0.05 |      |       |      |      |       |       |      |       | 0.05 | 0.05     | 0.01  |      |       | 0.02  |          |       |
| 28 | GM1684   | 1.91                      | 1.16     | 0.04  | 0.20 | 0.39 | 0.17 |      |       |      | 0.08 | 0.03  | 0.03  |      |       | 0.06 | 0.03     | 0.01  |      |       | 0.01  |          |       |
| 29 | DP71     | 1.96                      | 1.00     | 0.08  | 0.07 | 0.53 | 0.07 |      |       |      | 0.14 | 0.02  | 0.02  |      |       | 0.04 | 0.02     | 0.01  |      |       | 0.01  |          |       |
| 30 | R4b      | 2.25                      | 0.74     | 0.12  | 0.10 | 0.52 | 0.02 |      |       |      |      |       |       |      |       | 0.10 | 0.04     | 0.02  |      |       |       |          |       |
| 31 | DP65     | 2.11                      | 1.09     | 0.11  | 0.04 | 0.47 | 0.07 |      |       |      |      |       |       |      |       | 0.15 | 0.04     | 0.02  |      |       |       |          |       |
| 32 | 1327     | 2.13                      | 0.28     | 0.04  | 0.20 | 0.30 | 0.21 |      |       |      | 0.05 | 0.16  | 0.16  |      |       | 0.04 | 0.04     | 0.02  |      |       |       |          |       |
| 33 | TMZ1     | 2.18                      | 1.24     | 0.08  | 0.04 | 0.44 | 0.01 |      |       |      |      |       |       |      |       | 0.02 | 0.02     | 0.02  |      |       |       |          |       |
| 34 | 598      | 2.26                      | 1.44     | 0.00  | 0.30 | 0.17 | 0.09 |      |       |      |      | 0.08  | 0.23  |      |       | 0.07 | 0.07     | 0.02  |      |       |       |          |       |
| 35 | KH49     | 2.10                      | 1.43     | 0.14  | 0.15 | 0.22 | 0.13 |      |       | 0.23 |      | 0.10  | 0.16  |      |       | 0.13 | 0.01     | 0.01  |      |       |       |          |       |
| 36 | 597      | 2.13                      | 1.45     | 0.00  | 0.05 | 0.44 | 0.13 |      |       |      |      | 0.05  | 0.19  |      |       | 0.10 | 0.06     | 0.07  |      |       |       |          |       |
| 37 | Cs-1     | 2.35                      | 2.83     | 0.05  | 0.05 | 0.05 | 0.15 |      |       |      | 0.35 | 0.17  | 0.17  |      |       | 0.10 | 0.06     | 0.07  |      |       |       |          |       |
| 38 | Rhu4     | 2.26                      | 1.34     |       | 0.10 | 0.41 |      |      |       |      | 0.39 |       |       | 0.11 |       | 0.10 | 0.06     | 0.07  |      |       |       |          |       |
| 39 | EDB1     | 2.12                      | 1.36     |       | 0.05 | 0.26 | 0.04 |      | 0.12  |      | 0.22 | 0.16  | 0.12  |      |       | 0.07 | 0.13     | 0.16  |      |       |       | 0.01     |       |
| 40 | FTG1     | 2.34                      | 1.21     | 0.03  | 0.08 | 0.29 | 0.08 |      |       |      |      |       |       |      |       | 0.06 | 0.03     | 0.03  |      |       | 0.04  |          |       |
| 41 | GM1803   | 2.05                      | 1.21     |       | 0.04 | 0.58 |      |      |       |      | 0.12 | 0.10  | 0.10  |      |       | 0.06 | 0.03     | 0.03  |      |       | 0.03  | 0.04     |       |
| 42 | Rhu2     | 2.15                      | 0.99     |       | 0.05 | 0.70 |      |      |       |      |      | 0.24  | 0.24  |      |       | 0.03 | 0.01     | 0.01  |      |       |       |          |       |
| 43 | 1319     | 2.06                      | 1.18     |       | 0.27 | 0.34 |      |      |       |      | 0.23 | 0.13  | 0.13  |      |       | 0.03 | 0.01     | 0.01  |      |       |       |          |       |
| 44 | SRH1     | 2.78                      | 1.33     | 0.01  |      | 0.02 | 0.02 |      |       |      | 0.08 | 0.04  | 0.66  | 0.06 |       | 0.03 | 0.02     | 0.02  |      |       | 0.03  |          |       |
| 45 | FRS1     | 2.41                      | 1.17     |       |      | 0.20 |      |      |       |      |      | 0.09  | 0.09  | 0.11 |       | 0.02 | 0.02     | 0.02  |      |       | 0.02  |          | 0.51  |

Note. Qtz = quartz; Ab = albite; An = anorthite; Or = orthoclase; Mc = microcline; Anl = analcime; Ne = nepheline; Di = diopside; Aug = augite; Hbl = hornblende; Ol = olivine; Prh = prehnite; Bt = biotite; Ms/Ilm = muscovite/illite; Chl = chlorite; Ap = apatite; Mag = magnetite; Ilm = ilmenite; Ats/Rt = anatase/rutile; Atg = antigorite.

To minimize analytical and measurement problems potentially associated with coarse-grained or porphyritic rocks, only fine- to medium-grained, equigranular samples were considered.

To characterize the rocks geochemically, their bulk-rock major-element compositions were determined by X-ray fluorescence analysis (PANalytical AXIOS Advanced instrument) at GFZ, Potsdam, Germany, using fused glass discs (Table 2). The quantitative modal composition was determined by X-ray powder diffraction analysis both at GFZ (PANalytical Empyrean instrument, AUTOQUAN software) and at Bureau Veritas, Wingfield, Australia (PANalytical X'Pert PRO instrument, Rietveld refinement, SIROQUANT software). Weight percentages of minerals were transferred into volume percentages using well-defined values of mineral densities (cf. Schön, 2015). Only components in excess of 1 vol.% were considered, since accessory minerals negligibly contribute to  $\lambda_b$  (Table 3).

Plagioclase solid solutions were discriminated into their end-members albite and anorthite. On the application of electron-probe microanalysis to determine the composition of other minerals forming solid solutions, such as amphiboles and pyroxenes, was consciously renounced, to keep the analytical effort for potential users of the results of this study feasible.

Archimedes method was applied to compute density and porosity ( $\varphi$ ) from the difference between dry, water-saturated, and submerged weights. Systematic error of porosity determination averaged to  $<0.1$  vol.% absolute. Mineral thermal conductivities used in this study are compiled in Figure 1.

The optical scanning technology (thermal-conductivity scanner, TCS; Popov et al., 1999, 2016) was used for measuring rock thermal conductivity under ambient conditions (20 °C, 1 atm.). In preparation for this method, rock samples were cut to pieces of  $\geq 4$  cm thickness and black painted as an optical coating that unifies the optical reflection coefficients of the rock components. The  $\lambda_b$  data compiled in Table 4 represent the arithmetic means from 3 to 5 replicate measurements on each sample under (distilled) water-saturated conditions. Reproducibility was between 2% and 3%. For reaching water saturation, samples were first dried in a vacuum oven (60 °C, 0.01 bar, 48 hr) and then evacuated and saturated in an excicator (10 mbar at 20 °C) for a minimum of two full days. After each measurement line, the sensor was recalibrated, the scanning line was moved by 1–2 mm, to gauge a representative rock conductivity value, with the samples being re-saturated prior to every measurement, to prevent systematic deviations according to near-surface dehydration. Additionally, a gabbro standard of 2.41 W/(mK) provided by the TCS manufacturer (Lippmann and Rauen GbR, Schauffling, Germany) was measured in parallel as controlling sample. Measurement runs for which the gabbro reference value was met within  $\pm 2\%$  were considered for the arithmetic-mean calculation of the samples. Absolute and relative error are reported with arithmetic mean value and  $2\sigma$  standard deviation.

### 3. Results

We scrutinized in a first step, which mean model provides the best match between measured and calculated  $\lambda$  in case that porosity is not considered, that is, we compared the correspondence between  $\lambda_{m,calc}$  and  $\lambda_{b,meas}$ . This approach was undertaken in all previous trials, which involved crystalline rocks with porosity values  $<1.5\%$  (Chopra et al., 2018; Ray et al., 2015).

All mean models shared the common feature that they overestimate  $\lambda_{m,calc}$ , but at strongly varying magnitude. From all examined models, only the harmonic-mean (HM) model provided an acceptable fit, with a relative error of  $5.8 \pm 10.0\%$  ( $2\sigma$ ) and an absolute error of  $6.4 \pm 8.3\%$  ( $2\sigma$ ; Table 4 and Figure 2). Deviations range between  $-5.5\%$  and  $13.1\%$ . The other models gave rise to considerably larger uncertainties, display corresponding relative and absolute errors, and are ranked as follows (error in parentheses): HSL ( $15 \pm 13\%$ ), GM ( $17 \pm 15\%$ ), VRH ( $20 \pm 17\%$ ), HS ( $21 \pm 17\%$ ), SQR ( $25 \pm 21\%$ ), HSU ( $27 \pm 21\%$ ), Eff ( $30 \pm 25\%$ ), and AM ( $34 \pm 28\%$ ).

In a second step, we verified the quantitative impact that consideration of porosity would have on the quality of fit between  $\lambda_{b,calc}$  and  $\lambda_{b,meas}$ . Bulk thermal conductivity was computed from  $\lambda_{m,calc}$  and porosity according to the equations from the three best-fitting matrix mean models (HM, HSL, and GM). Taking advantage of the results of step 1, we used  $\lambda_{m,calc}$  derived from the HM model as first component and  $\lambda_f$  of 0.604 W/(mK) for tap water as second component. This approach resulted in a statistically

| #  | Sample # | $\lambda_{b.meas}$<br>W/(mK) | Absolute error (%) to $\lambda_{b.meas}$ |       |       |                                   |       |       |
|----|----------|------------------------------|--|-------|-------|-----------------------------------|-------|-------|
|    |          |                              | $\lambda_{m.calc}$                       |       |       | $\lambda_{b.calc}$ with HM matrix |       |       |
|    |          |                              | HM                                       | HSL   | GM    | HM                                | HSL   | GM    |
| 1  | Z5b      | 3.20                         | 3.4%                                     | 17.7% | 22.4% | 2.4%                              | 0.6%  | 1.1%  |
| 2  | L13      | 3.04                         | 0.6%                                     | 13.5% | 17.5% | 5.1%                              | 2.2%  | 1.8%  |
| 3  | M5B      | 3.06                         | 1.7%                                     | 15.6% | 19.9% | 4.0%                              | 1.1%  | 0.7%  |
| 4  | Hzb1     | 3.11                         | 1.7%                                     | 10.9% | 14.8% | 6.4%                              | 4.0%  | 3.7%  |
| 5  | ARN      | 2.71                         | 1.3%                                     | 13.3% | 16.5% | 6.0%                              | 2.4%  | 2.0%  |
| 6  | IMS-1    | 2.75                         | 3.6%                                     | 15.5% | 18.8% | 2.4%                              | 0.7%  | 1.0%  |
| 7  | Lu-1     | 2.82                         | 3.5%                                     | 16.2% | 19.8% | 2.8%                              | 0.4%  | 0.8%  |
| 8  | L2       | 2.72                         | 8.4%                                     | 21.5% | 25.3% | 1.9%                              | 5.3%  | 5.6%  |
| 9  | EHR-2    | 2.60                         | 9.3%                                     | 23.0% | 26.7% | 4.7%                              | 7.1%  | 7.3%  |
| 10 | NE4      | 2.68                         | 10.9%                                    | 23.8% | 27.7% | 5.7%                              | 8.4%  | 8.7%  |
| 11 | TI-2     | 2.56                         | 11.5%                                    | 26.9% | 31.0% | 6.9%                              | 9.2%  | 9.5%  |
| 12 | PAG      | 2.70                         | 2.5%                                     | 15.7% | 19.3% | 1.3%                              | 0.6%  | 0.8%  |
| 13 | 428      | 2.72                         | 0.8%                                     | 11.2% | 14.3% | 5.4%                              | 3.1%  | 2.8%  |
| 14 | SD1      | 2.52                         | 12.3%                                    | 27.3% | 31.5% | 7.3%                              | 9.8%  | 10.1% |
| 15 | TM2      | 2.64                         | 1.0%                                     | 9.3%  | 11.2% | 4.7%                              | 1.9%  | 1.6%  |
| 16 | PADR1    | 2.38                         | 10.4%                                    | 25.5% | 29.2% | 6.0%                              | 8.2%  | 8.4%  |
| 17 | 603      | 2.49                         | 3.7%                                     | 13.3% | 15.4% | 0.4%                              | 1.6%  | 1.8%  |
| 18 | DP68     | 2.35                         | 7.4%                                     | 20.6% | 23.6% | 4.0%                              | 5.7%  | 5.8%  |
| 19 | 599      | 2.05                         | 11.4%                                    | 13.5% | 13.8% | 6.6%                              | 8.8%  | 9.0%  |
| 20 | Cs-2     | 2.07                         | 7.1%                                     | 9.6%  | 10.0% | 5.1%                              | 6.1%  | 6.1%  |
| 21 | Cs-3     | 2.10                         | 10.4%                                    | 10.6% | 10.7% | 7.4%                              | 8.8%  | 8.9%  |
| 22 | 1317     | 2.21                         | 9.2%                                     | 15.9% | 17.3% | 3.3%                              | 6.2%  | 6.4%  |
| 23 | DP49     | 2.11                         | 7.2%                                     | 14.6% | 15.9% | 3.7%                              | 5.4%  | 5.5%  |
| 24 | 1325     | 2.09                         | 12.1%                                    | 18.2% | 19.1% | 8.4%                              | 10.2% | 10.3% |
| 25 | WSN1     | 2.21                         | 13.1%                                    | 25.0% | 27.6% | 8.2%                              | 10.6% | 10.8% |
| 26 | 594      | 2.36                         | 0.4%                                     | 9.0%  | 10.4% | 2.1%                              | 0.9%  | 0.8%  |
| 27 | Fülb     | 2.28                         | 2.8%                                     | 10.7% | 12.1% | 0.7%                              | 1.0%  | 1.1%  |
| 28 | GM1684   | 1.91                         | 12.2%                                    | 18.6% | 19.0% | 9.0%                              | 10.5% | 10.6% |
| 29 | DP71     | 1.96                         | 8.8%                                     | 17.7% | 18.4% | 6.2%                              | 7.4%  | 7.5%  |
| 30 | R4b      | 2.25                         | 2.9%                                     | 6.3%  | 7.3%  | 4.8%                              | 3.9%  | 3.9%  |
| 31 | DP65     | 2.11                         | 1.1%                                     | 8.7%  | 9.5%  | 1.7%                              | 0.4%  | 0.3%  |
| 32 | 1327     | 2.13                         | 3.0%                                     | 8.0%  | 8.4%  | 2.2%                              | 2.6%  | 2.6%  |
| 33 | TMZ1     | 2.18                         | 4.7%                                     | 12.9% | 13.5% | 1.2%                              | 2.9%  | 3.0%  |
| 34 | 598      | 2.26                         | 2.4%                                     | 6.1%  | 6.1%  | 1.6%                              | 0.3%  | 0.5%  |
| 35 | KH49     | 2.10                         | 3.8%                                     | 6.3%  | 6.0%  | 0.1%                              | 1.9%  | 1.9%  |
| 36 | 597      | 2.13                         | 2.7%                                     | 0.0%  | 0.2%  | 6.1%                              | 4.5%  | 4.5%  |
| 37 | Cs-1     | 2.35                         | 12.9%                                    | 20.3% | 20.7% | 3.0%                              | 7.8%  | 8.2%  |
| 38 | Rhu4     | 2.26                         | 10.5%                                    | 24.2% | 25.1% | 6.0%                              | 8.2%  | 8.4%  |
| 39 | EDB1     | 2.12                         | 10.0%                                    | 23.0% | 23.2% | 5.8%                              | 7.8%  | 8.0%  |
| 40 | FTG1     | 2.34                         | 8.4%                                     | 19.1% | 20.1% | 4.3%                              | 6.3%  | 6.5%  |
| 41 | GM1803   | 2.05                         | 4.4%                                     | 13.1% | 13.3% | 1.2%                              | 2.7%  | 2.8%  |
| 42 | Rhu2     | 2.15                         | 5.5%                                     | 1.9%  | 1.9%  | 7.6%                              | 6.6%  | 6.6%  |
| 43 | 1319     | 2.06                         | 10.3%                                    | 16.7% | 16.8% | 6.8%                              | 8.5%  | 8.6%  |
| 44 | SRH1     | 2.78                         | 11.7%                                    | 16.3% | 17.1% | 5.9%                              | 8.9%  | 9.3%  |
| 45 | FRS1     | 2.41                         | 3.2%                                     | 8.6%  | 8.9%  | 0.5%                              | 1.3%  | 1.5%  |

**Figure 1.** Absolute error from mixing-model application for calculation of matrix  $\lambda$  ( $\lambda_{m.calc}$ ) from modal analysis (left) and for calculation of bulk  $\lambda$  ( $\lambda_{b.calc}$ ) from HM matrix and porosity (right). Warmer colors refer to smaller deviation, colder colors to larger deviation.

significant improvement of the goodness of fit between  $\lambda_{b.calc}$  and  $\lambda_{b.meas}$  in case that  $\lambda_m$  and  $\lambda_f$  were calculated from the HM model (Table 4 and Figure 2). Interestingly, any of the three mean model applied to treat the fluid phase gave rise to similarly good agreement. This result also holds for all other mixing models introduced in section 2 (Braune, 2016).



**Table 4**  
Mineral Thermal Conductivities

| Phases or end-members | $\lambda$ (W/[mK]) | Source |
|-----------------------|--------------------|--------|
| Quartz                | 7.64               | 1      |
| Albite                | 2.12               | 1      |
| Anorthite             | 1.69               | 1      |
| Orthoclase            | 2.33               | 1      |
| Microcline            | 2.49               | 2      |
| Analcime              | 1.27               | 3      |
| Nepheline             | 1.50               | 3      |
| Magnetite             | 4.92               | 1      |
| Apatite               | 1.49               | 1      |
| Dioside               | 4.48               | 1      |
| Olivine               | 4.57               | 3      |
| Augite                | 4.24               | 1      |
| Hornblende            | 2.81               | 1      |
| Prehnite              | 3.58               | 1      |
| Biotite               | 2.03               | 1      |
| Chlorite              | 5.17               | 1      |
| Muscovite/illite      | 2.36               | 1      |
| Antigorite            | 2.46               | 3      |
| Ilmenite              | 2.51               | 1      |
| Anatase/rutile        | 5.01               | 1      |

Note. 1 = mean value of Chopra et al. (2018); 2 = Brigaud & Vasseur (1989); 3 = Horai (1971).

The relative and absolute errors between  $\lambda_{b,meas}$  and  $\lambda_{b,calc}$  from the HM model amount to  $1.4 \pm 9.7\%$  and  $4.4 \pm 4.9\%$  ( $2\sigma$ ), respectively. For all 45 samples, the deviations are  $<10\%$  ( $-7.6$  to  $9.0\%$ ; Figure 2).

#### 4. Discussion

With respect to the mixing model and the closeness of agreement, the outcome of our study is in full harmony with those of Chopra et al. (2018), who assessed 21 granites and granitic gneisses ( $SiO_2 > 67$  wt.%) of abnormally low porosity ( $<0.3\%$ ) from the Bundelkhand craton in central India, and Ray et al. (2015), who surveyed 26 samples representing low-porosity ( $<1.5\%$ ) high-grade orthometamorphic rocks of amphibolite to granulite facies from the Indian Southern Granulite Province. The few other studies tackling this problem in crystalline rocks (Horai & Baldrige, 1972; Pribnow & Umsonst, 1993; Zhao et al., 2016) considered a smaller number of samples and came out with a poorer degree of agreement of the applied mean models, which most probably is related to the fact that the HM model was not taken into account.

Our study corroborates previous approaches not only in terms of the best-suited mean model and the magnitude of mean error (Figure 3) but also with respect to model ranking:

This study:  $\lambda_{b,meas} \sim \lambda_{HM} < \lambda_{HSL} < \lambda_{GM} < \lambda_{VRH} \leq \lambda_{HS} < \lambda_{SQR} < \lambda_{HSU} < \lambda_{Eff} < \lambda_{AM}$

Chopra et al. (2018):  $\lambda_{m,meas} \sim \lambda_{HM} < \lambda_{HSL} < \lambda_{GM} < \lambda_{VRH} < \lambda_{Eff} < \lambda_{HS} < \lambda_{HSU} < \lambda_{AM}$

Ray et al. (2015):  $\lambda_{m,meas} \sim \lambda_{HM} < \lambda_{HSL} \leq \lambda_{GM} < \lambda_{Eff} < \lambda_{HS} < \lambda_{HSU} < \lambda_{AM}$

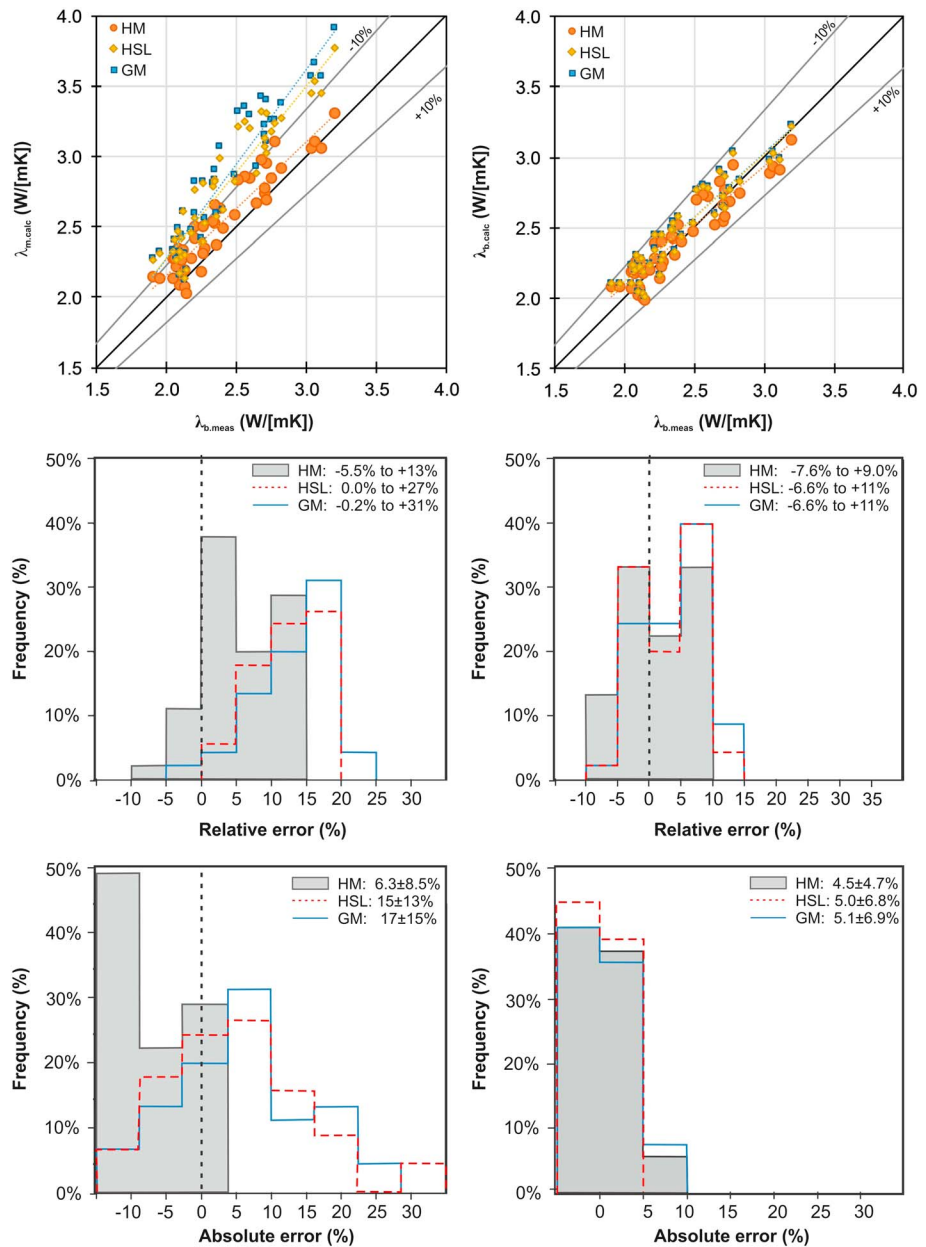
Notably, a comparable comprehensive study in sedimentary rocks yielded contrasting results, with the GM model providing by far the best fit between  $\lambda_{b,meas}$  (water-saturated conditions) and  $\lambda_{b,calc}$  (Fuchs et al., 2013).

The HM model is based on a sheet model representing a layered structure of phases, where the heat flow passes perpendicular (HM) with respect to the plane boundaries. The model is independent of the pore structure and constitute a special case (boundary) of Wiener's mixing law (Wiener, 1912), which applies to both isotropic and anisotropic mixtures. The model was introduced by Reuss (1929) to define the lower  $\lambda$  boundary. Considering the physical rationale of this model it was not necessarily foreseeable that the HM model provides the best fit for a medium where  $\lambda$  is direction independent. That this unexpected result is anyhow related to a preferred alignment of holes or cracks in the lower micrometer or nanometer scale could be excluded, since porosity accounts for only  $0.1\text{--}0.2$  mW/m<sup>2</sup> of  $\lambda_{b,calc}$  depending on the applied model. Taking into account that all models overestimate  $\lambda_{m,meas}$  we have examined whether use of mineral thermal conductivities lower than those listed in Table 4 (cf. Chopra et al., 2018), but within the range of values reported for a specific phase, would have an effect on model performance. For several samples, the use of lower mineral thermal conductivities would indeed result in a still better fit between  $\lambda_{b,meas}$  and  $\lambda_{b,calc}$ , but the relative differences between the performance of the models remained virtually unchanged.

The reason for the better performance of the HM model relative to the, for instance, direction-independent GM model is still not fully understood. One possible explanation involves the assumption that the unsystematic (chaotic) arrangement of the mineral grains provokes that the heat is transported through an isotropic rock in a fashion and in a quantity as it would do perpendicular to the plane boundaries in an anisotropic medium, that is, is considerably retarded as consequence of countless heat-refraction events.

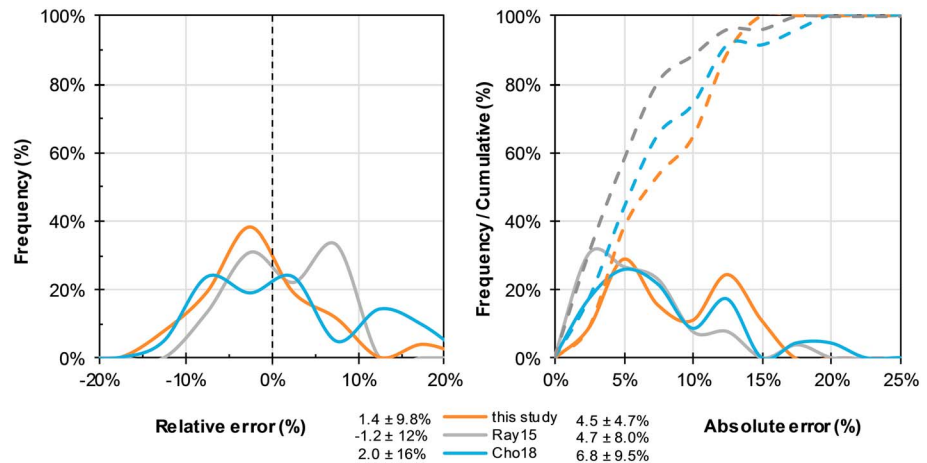
#### 5. Conclusions and Implications

Indirect calculation of  $\lambda_b$  from precisely quantified modal mineralogy and porosity is demonstrated a viable option to retrieve thermal conductivity data with an acceptable amount of error. The use in thermal modeling



**Figure 2.** Comparison of the goodness of fit of those three mixing models (HM, GM, and HSL) providing the best match between  $\lambda_{m,calc}$  from modal mineralogy and  $\lambda_{m,calc}$  from  $\lambda_{m,meas}$  (left panel) and  $\lambda_{b,calc}$  (using  $\lambda_{m,calc}$  from the HM model combined with  $\lambda_{f,calc}$  as derived from application of the HM, HSL, and GM mixing models; right panel). Top: Cross-plots of measured versus calculated  $\lambda$ . Middle and bottom: Histograms of relative and absolute errors, respectively. See text for further explanations.

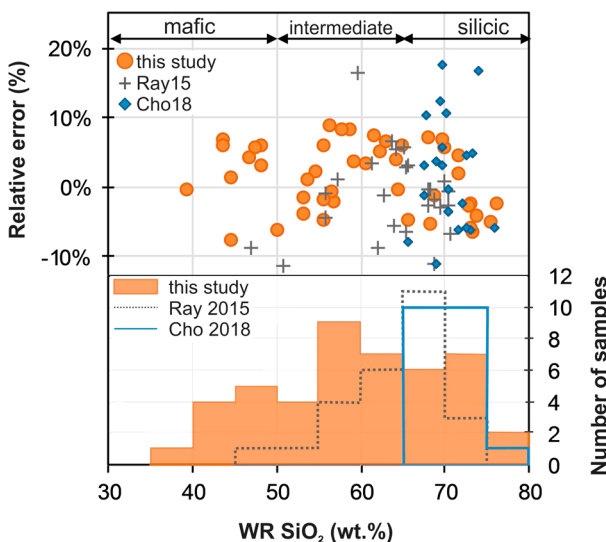
of such generated data, even being less accurate than laboratory measured  $\lambda$  values, is rated favorably relative to considering literature compilations. From the most widely examined mean models, deployment of the HM model is demonstrated giving rise to proper  $\lambda_b$  values for the entire suite of low-porosity crustal plutonic igneous rocks irrespective of being mafic or silicic (Figure 4). Since this model also properly works for high-grade orthometamorphic rocks (Ray et al., 2015), it is reasonable to conjecture that it yields acceptable results also for metamorphic equivalents of igneous rocks. This inference also holds for the extrusive (volcanic) equivalents of the here studied plutonic rocks as well as mantle rocks as long they are not anisotropic.



**Figure 3.** Comparison of relative (left) and absolute (right) errors resulting from the application of the HM model for computing  $\lambda_b$  for igneous rocks (this study, Chopra et al., 2018/Cho18) and metamorphic rocks (Ray et al., 2015/Ray15). Numbers denote to mean  $\pm 2\sigma$  standard deviation.

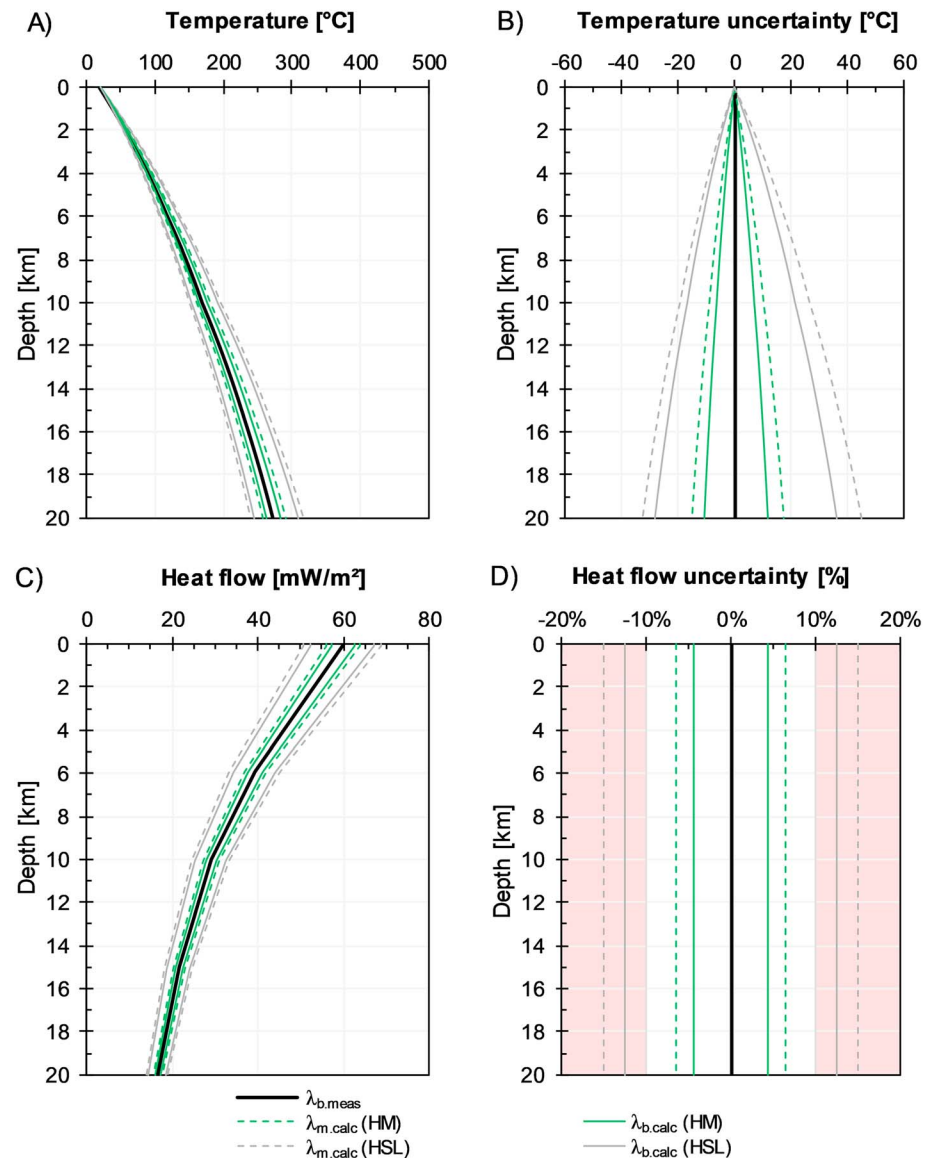
One implication of this study is that X-ray diffraction (XRD) data on modal mineralogy, if precise and accurate, could be converted into rock thermal conductivities with uncertainties of commonly  $<15\%$  ( $2\sigma$ ) by application of the HM model, even if information on porosity is missing. In case that porosity data for modal-mineralogy samples are available or could be acquired, the amount of uncertainty is further reduced by several % to values of normally  $<10\%$ . Notwithstanding, calculation of  $\lambda_b$  could never supersede its laboratory measurement, but it as well could not be judged an exercise not worth to conduct.

A significant implication of our study is that heat-flow data could be obtained from undisturbed and uncored boreholes, for which equilibrium T-logs and cuttings are available. Although direct measurement of  $\lambda_m$  is possible, this approach is time-consuming and afflicted with uncertainties on the same order as inherent in our method (Popov et al., 2018). If such drillings have exposed isotropic crystalline rocks, cuttings from all penetrated types of rock could be analyzed for quantitative modal mineralogy and eventually also porosity (for instance, from well logs or by direct measurement if size permits) and their  $\lambda$  inferred with the uncertainties discussed above.



**Figure 4.** (top) Relative errors of  $\lambda_{b,calc}$  in relation to whole-rock  $SiO_2$  contents. See Figure 3 for abbreviations of data sources. (bottom) Histogram portraying the number of studied samples.

To exemplify the quantitative uncertainties in terms of heat flow and T associated with the approach presented in this paper, we have computed a suite of geotherms for a synthetic, 20-km-thick upper-middle continental crustal section composed of typical plutonic rocks, ranging from granite in the uppermost crust to gabbro in the basal part (Figure 5). Surface heat flow was set to  $60 \text{ mW/m}^2$ , an average value for Phanerozoic-stabilized continental crust. Adopting the HM model for both calculations of  $\lambda_m$  (illustrating the case of lacking porosity data) and  $\lambda_b$  and, considering the respective mean relative model errors reported in section 3, would result in  $2\sigma$ -uncertainties in T-prediction at the middle crust-lower crust boundary of roughly  $\pm 10^\circ \text{C}$  ( $\lambda_{b,calc}$ ) resp.  $\pm 20^\circ \text{C}$  ( $\lambda_{m,calc}$ ) relative to geotherms based on  $\lambda_{b,meas}$  (Figures 5a and 5b). Use of the second best fitting model (HSL) would already significantly enlarge the prediction range to  $\sim 70^\circ \text{C}$ . In terms of heat flow, uncertainties would be on the order of  $\pm 7$  ( $\lambda_{m,calc}$ ) and  $\pm 5\%$  ( $\lambda_{b,calc}$ ), which are well within the error range accepted by the IHFC for heat-flow determination (Haenel et al., 1988; cf. Figure 5d). These percentages translate into acceptable uncertainties in heat-flow of roughly  $\pm 5$  ( $\lambda_{m,calc}$ ) and  $\pm 3 \text{ mW/m}^2$  ( $\lambda_{b,calc}$ ; Figure 5c). Heat-flow calculations based on the HSL model are afflicted with uncertainties already exceeding 10% (Figure 5d).



**Figure 5.** Uncertainties associated with the use of calculated versus measured rock thermal conductivities ( $\lambda_{b,meas}$ , bold black lines) on T-prediction (A + B) and heat-flow calculation (C + D) in the upper-middle continental crust. Geotherms were computed according to the well-established Chapman (1986) method and were performed for the two best-fitting models (HM and HSL) for calculation of matrix ( $\lambda_{m,calc}$ , stippled) and bulk thermal conductivity ( $\lambda_{b,calc}$ , full lines). The 20-km-thick synthetic crustal model consists, from top to bottom, of ( $\lambda$  in  $W/[mK]$ ; heat production in  $\mu W/m^3$ ) 6 km granite (3.0; 3.5), 4 km granodiorite (2.7; 2.5), 5 km monzodiorite (2.2; 1.5), and 5 km gabbro (2.1; 1.0). Terrestrial surface heat flow was set to  $60 \text{ mW/m}^2$ , a mean value for Phanerozoic-consolidated continental domains. (a) Geotherms computed on the basis of measured and calculated  $\lambda$ . (b) Temperature uncertainties associated with model uncertainties (cf. Figure 1; considered mean errors: 4.4% for HM, 12.5% for HSL); (c) heat-flow family calculated from geotherms in Figure 5A; and (d) relative uncertainty in heat-flow calculation; red-shaded areas is the error in heat-flow determination violating the criteria for validity by the IHFC (Haenel et al., 1988).

Another interesting area of application of the results of this study is the estimation of  $\lambda_b$  of material that was brought up to the surface from deeper parts of the crust or the upper mantle as xenoliths or enclaves. These pieces of rock are usually small in size and thermally or mechanically cracked and thus poorly suited for direct measurement. On the other hand, they are normally sufficiently big in volume that their modal mineralogy could be determined by XRD. Thus, if not re-equilibrated or otherwise

chemically altered, indirectly derived data on their thermal conductivity are essential in more properly constraining the thermal state of lithosphere domains.

Finally, Chopra et al. (2018) stated that plutonic rocks other than granites have to be studied before a substantiated statement on the overall viability of the HM model for acceptably inferring  $\lambda_b$  of crystalline rocks could be drawn. The results of this study provide a big step forward to such a robust conclusion.

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