# Temperature dependence of rock thermal properties

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## Contents

# List of Figures

**Abstract**

The temperature dependence of the specific heat $C_p$ and thermal conductivity $\lambda$ for geologic materials are extracted from the literature. Measurements below 0°C are rare, especially for $\lambda$. These data and methods to extend them to cover the temperature range for Mars have been coded into IDL routines. Models of unconsolidated [51] and cemented [39] particulates are used to generate the effective thermal conductivity of these materials and hence the thermal inertia as a function of temperature. For all materials, the coefficents ready for inclusion in the KRC thermal model, a third-degree polynomial in scaled temperature, can be generated. Apart from mm and larger uncemented grains, the intrinsic thermal variation of the bulk properites has a signficantly larger effect on the temperature dependance of thermal inertia of particulates than does grain size.

# 1 Introduction

I did not set out for this to become so involved:

> Life is what happens while you are busy making other plans.
> *John Lennon*
>
> In theory there is no difference between theory and practice. In practice there is.
> *Yogi Berra*
>
> If we knew what it was we were doing, it would not be called research, would it?
> *Albert Einstein*
>
> It doesn't make a difference what temperature a room is, it's always room temperature.
> *Steven Wright*

This document covers the background for inclusion of temperature-dependent thermal properties capability of the KRC thermal model.

To aid in choosing the form for incorporating temperature dependence, I searched the literature for information on the variation of both thermal conductivity ($k$ or $\lambda$) and specific heat ($C_P$) with temperature. Any variation of density ($\rho$) with temperature, which is commonly characterized through the linear thermal expansion coefficient, was ignored as this coefficient of order 1.E-5 per Kelvin ; e.g., [25, Fig.8].

Whereas there is quite a bit of information on $C_P(T)$ at temperatures appropriate for the martian surface, most work on $\lambda(T)$ of geologic materials has been directed toward study of the Earth's crust and mantle, and hence is at room temperature and above. I had little success finding conductivity measurements in the 100-273 K range.

A number of suggested analytic forms for $C_P(T)$ and $\lambda(T)$ were coded, along with the listed coefficients for a number of materials. In addition, for a few materials, original measurement data were found, and these are also included.

For each material or relation, the temperature range of measurements and an estimated range of applicability is assigned; the latter is subjective and only a guide. These values are returned by the thermal-properties routines.

The KRC thermal model is in Fortran. All the code for generating the coefficients is in IDL.

Major IDL routines are effectively large case statements; the coding style is described in *-xtex/idlstyle.tex*. The **@** here refers to specific elments of a case statement identified by its case control index, **kon**

The thermal properties are covered by two routines;
**koft.pro** for thermal conductivity, see §3
**specheat.pro** for specific heat, see §4
This routine also include $k(T)$ for $H_2O$ ice because of source table structure.

These two routines are accessed by the main program **koftop.pro**, see §5, which can fit the returned values to the standard form chosen for KRC, a cubic polynomial to scaled temperature, and print the coefficients in a form ready for cut-and-paste into a KRC input file.

Unfortunately, $C_p$ and $\lambda$ are not both available for many materials, and for none of the expected Martian materials. Thus, the defaults listed in §2.2 may seem strange; thay are chosen to hopefully be close to likely Martian surface materials.

A user could incorporate additional relations or materials by adding a section to the appropriate thermal properties routine, and running **koftop** for the desired temperature range.

Although virtually all the literature research and coding of thermal properties is for materials of higher thermal inertia (TI) than common on Mars, §6 uses these to derive the temperature-dependent properties for particulates, covering the common TI range for Mars.

§10 is an unstructured set of notes, and will be of little interest to most readers.

Many of the figures are more usefully viewed in color; change the extension on the file name that ends the caption to .jpg. They are also listed in the List of Figures.

# 2 Running koft.pro

## 2.1 Overview

Typical sequence of actions using **koftop.pro**

A temperature range is chosen, and a spacing within this range adequate to support representative polynomial fits of order 3 (or more).

For either $C_P$ or $\lambda$, a source index and sub-index is selected. The appropriate routine, specheat or koft, respectively, is called to supply the values V at these temperatures.

These values are fit with a functional form that matches KRC; currently a cubic polynomial for both properties.
Fit uses scaled (or unscaled) temperature
Could choose any order of 2 or larger
Also available are forms $1/(A+BT)$, useful for conductivity, and $c_0+c_1/\sqrt{T}+c_2/T^2+c_3/T^3$, only for unscaled temperature.

The polynomial representation is tested uniformly across the desired temperature range and a RMS residual reported.

Sample applications that are coded:

- The conductivity values for two materials can be used for the grains and cement of a particulate conduction model and the resulting effective conductivity fit with a cubic.
- The cubic coefficients for a conductivity and a specific heat can be used to compute a thermal inertial table versus temperature.

## 2.2 Sequence to prepare coefficents for KRC

in IDL: **.rnew koftop**. This will automatically do several initialization steps
**@**71... Defaults for Particulates
Sets the parameter groups: `park, parp`, to their firm-code defaults, shown in §5.2
Set the default materials for the grains and the particulate cement
Conductivity: `matk` BasicRocks:Zoth88, limestone
Specific heat: `matp` Sphene, clinochlore:Fe=0.89
**@**25... Setup T
Set the temperature range `parr[11:13]` to the defaults shown in §5.2
Set the temperature scaling to defaults. DO NOT CHANGE
**@**260.. Empty XYY storage. This will store data for materials used
**@**60... Initiate bbb. This will store interpolated points
**@**5.... x=scaled T. Use scaled (versus absolute) temperature as the independent variable
**@**856.. Set colors to a nice set of six.

Option: Change temperature range and resolution: **@**16 Modify [11:13]. Then **@**25, **@**5

Option: Change properties of the Grains: Do **C** and **K** below. Then do **@**710 to store as grain properties

**C:** Option: change material for specific heat. You may need to look at **SPECHEAT** for details.
**@**15 parc: Change any of the following

[1:2] Set material index and sub-index, as listed in §4
If Material =1, then set [3]= Debye temperature in K and [5]=$C_P$ at 0° C
**@41** Transfer parameters and call SPECHEAT
**@33** Compute cubic fit coefficents
**@57**: Save coef as: Cp

**K:** Option: change material for conductivity. You may need to look at **KOFT** for details.
**@12** pari: Change any of the following
[1:2] Set material index and sub-index, as listed in §3
If more than one material listed, the sub-index is the 0-based count in the order listed.
[7:8] Cold extension method and number of points. Change not recommended
**@31** Transfer parameters and call KOFT
**@32** Extend to lower temperatures. Will do nothing if not needed.
**@33** Compute cubic fit coefficents
**@56**: Save coef as: $\lambda$

Choice 1: treat as pure solid:
For both $C_P$ and k=$\lambda$, Cut and paste the coefficients printed @33
between the > and < into KRC input for upper or lower material
**@59** Will print thermal inertia table

Choice 2: treat as uncemented: [do not need cement properties at all]
[ **@36** Will print SP90A parameters for a default set of inputs]
**@16** parr: Change any of the following
0: Grain radius, micrometer
1: Pressure in Pascal
2: Porosity fraction. Routine is based on 0.259 to 0.476
4: Density of a grain
8: Point-contact conductivity.
**@37** Run Piqueux unconsolidated model
**@377** Prepare results for fit

Choice 3: treat as cemented:
Option: Change properties of the cement: Do **C** and **K** above.
Then do **@711** to store as cement properties
**@16** parr: Change any of the following
4: Density of a grain
5: Cement volume fraction
7: Density of cement
**@701** Modify PARTCOND parameters
1: grain radius, micrometer
Do not change items 2:5, these will be replaced for each temperature
The rest can generally be left at their defaults.
**@717** Run Kieffer cemented model

After choice 2 or 3:
**@74** Cubic fit to conductivity
Cut and paste the values for $C_P$ and k=$\lambda$ into KRC input for upper or lower material
**@75** Print thermal inertia table

# 3 Thermal conductivity $\lambda(T)$: koft.pro

At very low temperatures, typically below about 20K and not of interest here, expect a $T^3$ relation. Above this and over most of the range below the Debye temperature, expect for crystals a $1/T$ relation according to the 3-phonon scattering Umklapp effect Kittel76=[42]. The temperature dependence for glasses is quite different, usually increasing with temperature, e.g. Birch40=[10] Figure 4, crystalline rocks, versus, Fig. 6, glasses.

Measurements of probable Mars materials under Mars-appropriate conditions are rare.

A relation $1/\lambda = A + BT$ has been found to be a rough fit for minerals Petrunin95=[50]. A linear fit to $1/\lambda$ for several published data are shown in Figure 1 and 2 of Petrunin95=[50]; I estimated the values at 200 and 800 K in these figures, from which A and B are derived and which allows extension over the range of Martian temperatures.

Relations coded, only 2 and 5 are algebraically different from $1/(A + BT)$.

1: Horai70b $1/\left[A + B(T - 300)\right]$
   Dunite, Pyroxenite, Diabase, Gabbro, Anorthosite, Albitite, Granite
2: Zoth88 $A + B/(350 + T_c)$
   RockSalt, Limestones, Metamorphics, AcidRocks, BasicRocks, Ultra-basics, Aveof5types
3: Sass92 elaborate form of $1/(A + BT)$
4: Clauser95 $1/(A + BT)$
   gneiss, metabasite
5: Seipold98 $1/(A + BT_c) + CT_c^3$
   paragneiss, amphibolite
      $T_c^3$ term is clearly inappropriate below 0°C.
6: Vosteen03 $1/\left[0.99 + T_c(A - B/k_0)\right]$
   crystalline, sedimentary
7: Petrunin95 $1/(A + BT)$
   Fig 1: labradorite, microcline, garnet, pyroxenite, SynGalGarnet, garnet, SynOlivine, olivine, alpha-SiO2
   Fig 2: Granite, Diorite, Diabase, Dunite, Gabbro, Serpentenite, Eclogite, mica
8: Hobbs74
   Ice Ih

For 1 through 7, the lower limit of applicability was arbitrarily set at 123K.

Data points

11: Kanamori 1968
   quartz001, quartz001, olivine, periclase
12: Yang 1981, NaCl
13: Birch 1940, silica glass
14: Glassbrenner 1964, pure Si and Ge
   These ideal materials, measured over wide range, are instructive for typical behaviour.
15: Abdulagatov 2006
   Sandstone, Limestone, Amphibolite, Granulite, Pyroxene-Granulite
16: Slack 1971, Grossularite
17: Slack 1980, Ice Ih

Some of these are shown in Figure 1

## 3.1 Extending measurements to lower temperatures

Conductivity measurements of geologic materials commonly do not extend below laboratory ambient. Where analytic relations are given, here they are simply used for low temperatures. Materials 1:10 are analytic, no need to extend; materials 11:20 are based on data points. For data-point sets, a cubic spline is used to interpolate between data points; a "natural spline" is specified for extrapolation. For extension of data points to lower temperatures; **koft** can be called a second time with the material index set to:

21: a linear extension of the coldest two measured points
   Mathematically robust, but amplifies errors.
22: a $1/\lambda = A + BT$ exact fit to the coldest two measured points
   Tends to generate a pole and wild extensions
23: a $1/\lambda = A + BT$ fit to the coldest N=`pari[8]` measured points (uses linear fit)
   If pole within 50 to 800K, displays plot and fits $1/\lambda = BT$
24: a $\lambda = 1/(A + BT)$ fit to the coldest N=`pari[8]` measured points (uses Simplex method)
   Both coefficients limited to $>10^{-8}$ to avoid poles, and these limits are commonly hit!

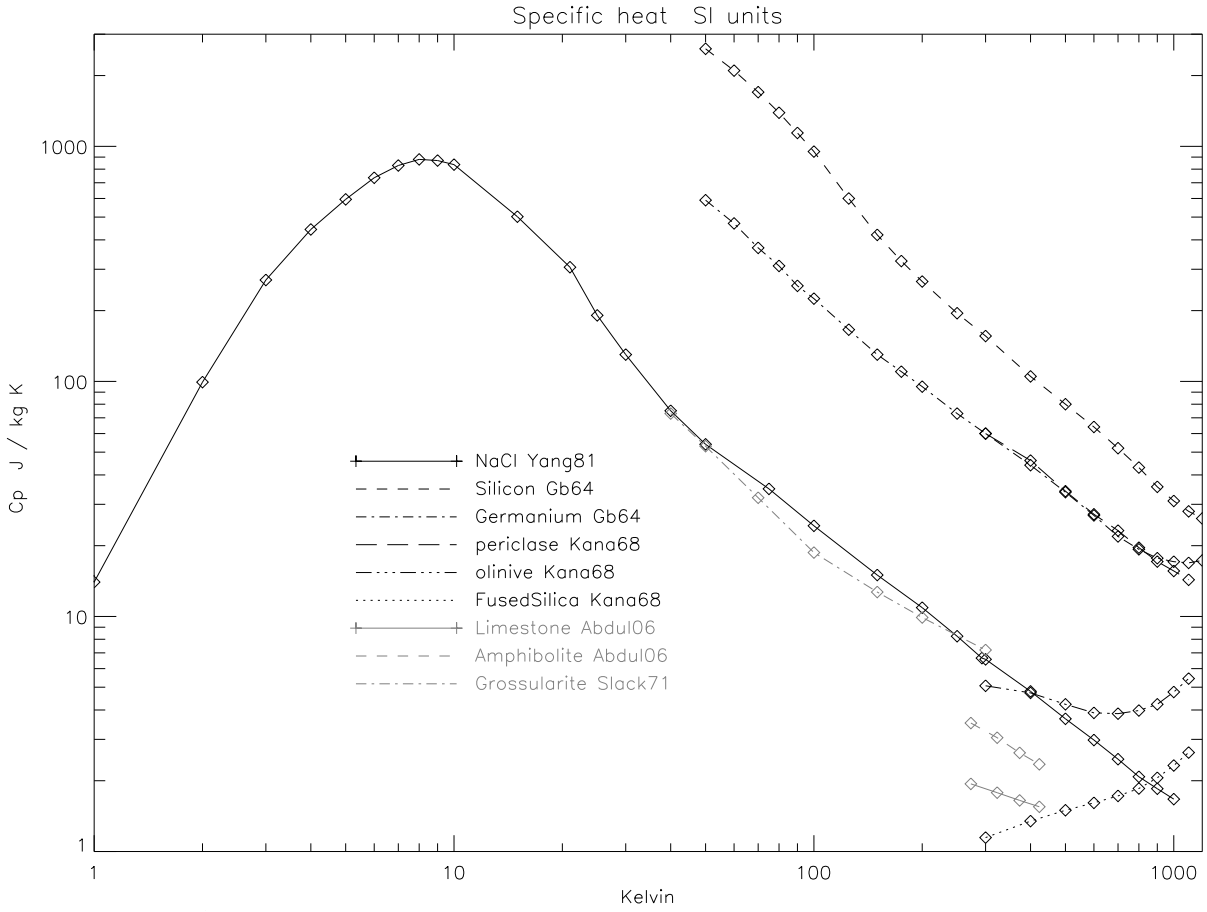


Figure 1: Measured values of thermal conductivity versus temperature. NaCl displays the transition from $T^3$ at very low temperatures to $1/T$ over planetary surface temperature range. $\lambda$ begins to increase near the Debye temperature, as shown for Olivine and Germainium (which is otherwise indistinguishable from Periclase). The rocks Limestone and Amphibolite, measured over 273-423 K, are lower than all minerals. The garnet Grossularite is similar to NaCl. kex.eps

## 3.2 $\lambda$ of Ice

Note, $\lambda(T)$ for $H_2O$ ice returned by **specheat** with `arg2`=9 and `arg3`=6

Theoretical expectation is for a 1/T relation; as discussed by Slack80=[65]. The relation used of this form is taken from Figure 5.7 in Hobbs; $k = 0.4685 + 488.19/T$. Because ice Ih is anisotropic, one can't really expect different lab measurements of polycrystalline ice to agree within a few percent. Action sequence: 138, which sets T range to 120:280 by 10 and sets the sequence:

```
25... Setup T
48... H2O k from 3 sources, find A+B/T, fit cubic to that
5.... x=scaled T
33... Cubic coefficents for KRC
56... Save coef as: k
Gives results:
0.00861 >    2.766722   -1.298966   0.6292242  -0.5272908 <Cond H2O:ice3sources
RMS fit residual represents 0.8% of the value at 220K.
```

Several published relations are shown in Figure 3.2

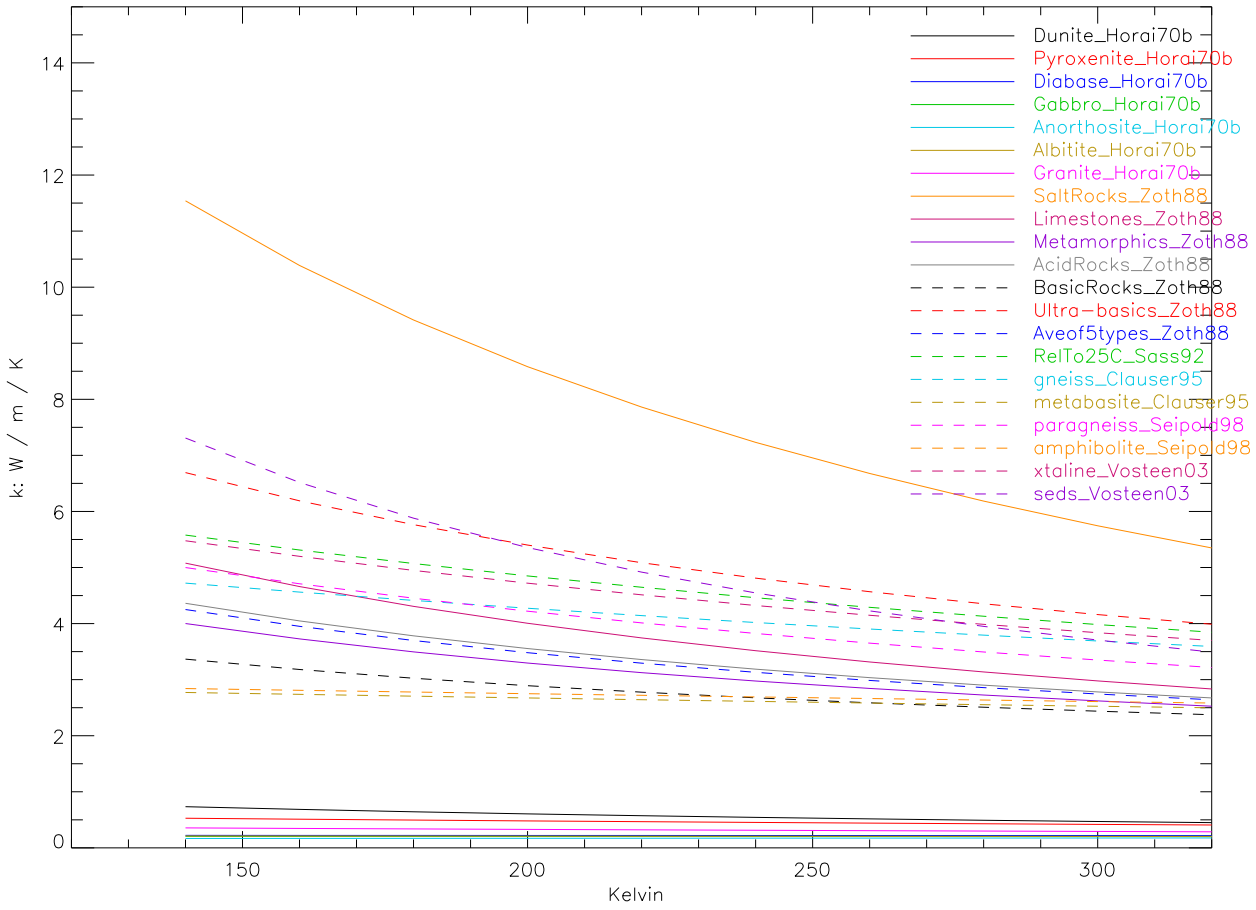


Figure 2: Thermal conductivity versus temperature for several of the pre-coded materials. 34ac

### 3.3 Other materials

To include additional materials, add a section to the case statement in **koft.pro**

## 4 Specific heat $C_P(T)$: specheat.pro

Specific heat increases with temperature across the temperature range of our interest. Representations range from linear with T (for $H_2O$) to the Debye form:

$C_v = 9Nk\left[\frac{T}{T_D}\right]^3 \int_0^{T_D/T} \frac{x^4 e^x}{(e^x-1)^2} dx$ where $T_D$ is the Debye temperature for a material.

Berman85=[5] explicitly address extension below 298.15K=25C but their interest is focused on Earth-interior temperatures. They use the form $C_p = k_0 + k_1 T^{-0.5} + k_2 T^{-2} + k_3 T^{-3}$ T in Kelvin, and provide in Table 3 these coefficient for an extensive set of minerals based on prior reported measurements. This form is widely used.

Waples04=[72] shows in Fig 2 typical $C_P(T)$ for 0-800C. Table 1 list $C_P$ for about 250 minerals, mostly at 20C or "room temperature". Based on an empirical fit to many minerals and non-porous rocks over 0-1200C, they propose a normalized temperature relations: $C_{Pn}(T) = 8.95E-10T^3 - 2.13E-6T^2 + 0.00172T + 0.716$ . However, they do not discuss the range below 0C, so that at most the slope of this relation at 0C is relevant for martian temperatures.

Index [and sub-index] and Materials:

1: Debye theory Debye12=[17], presented in Chapter 5 of Kittel76=[42]
Debye temperature, and arg4 is $C_p$ at 0C

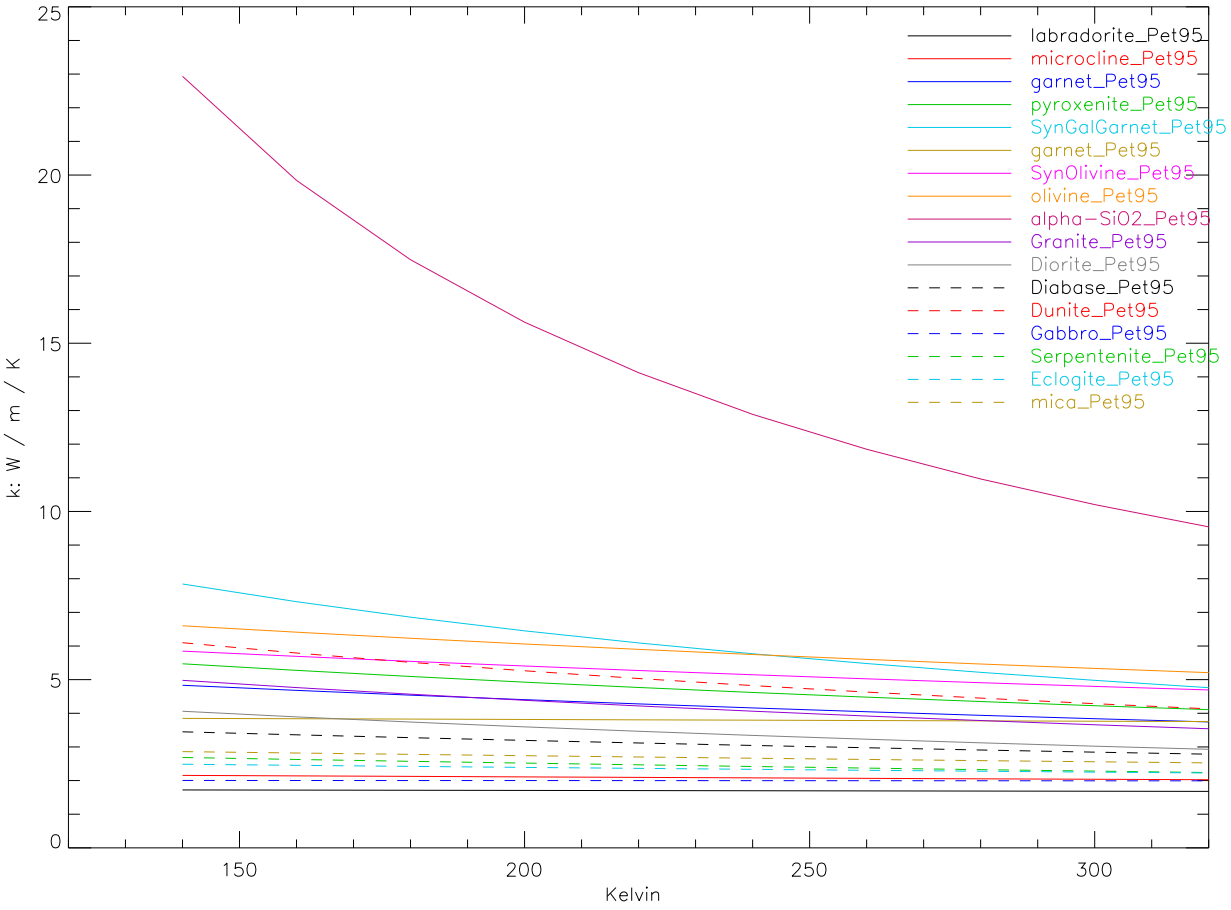


Figure 3: Thermal conductivity versus temperature relations from Petrunin95=[50]  34bc.eps

Romberg intergration of Debye function in **debyefunc.pro**

2: Normalized relation for solid rocks, Waples04=[72] . Analytic
Reference temperature in C

3: Apollo lunar samples, Horai70=[34] Analytic
0: sample 10020; fine-grained vesicular crystalline igneous
else: sample 10046; breccia
Both also output $\lambda$

4: Lunar material to high T, Ledlow92=[45] . Analytic

5: Sphene, King54=[41] Points

6: Chlorites: clinochlore - chamosite. Analytic
0,1,2,3 are index of four specific Fe abundances, listed below. 4.x is x fraction FE
Four Fe/(Fe+Mg) ratios: 0, 0.116, 0.889, 1.0 . 143-623K Bertoldi01=[6]
Analytic function tends to derivative=0 at 120K
Mg and Fe end-members measured over 5:500K Bertoldi07=[7]
Data table at 10K interval up to 300K

9: $H_2O$ ice, including some $\lambda$ values. Points. arg3=:
0: Spline interpolation ofGiauque36=[21]
1: Hobbs Figure 5.7, straight line
2: Table of $C_P$ [and k, and $\rho$] from http://www.engineeringtoolbox.com/
3: Giauque36=[21] 16:267 K
4: Haida74=[24] 119:230 K
5: Yamamuro87=[74] 13:164 K
6: k from web table

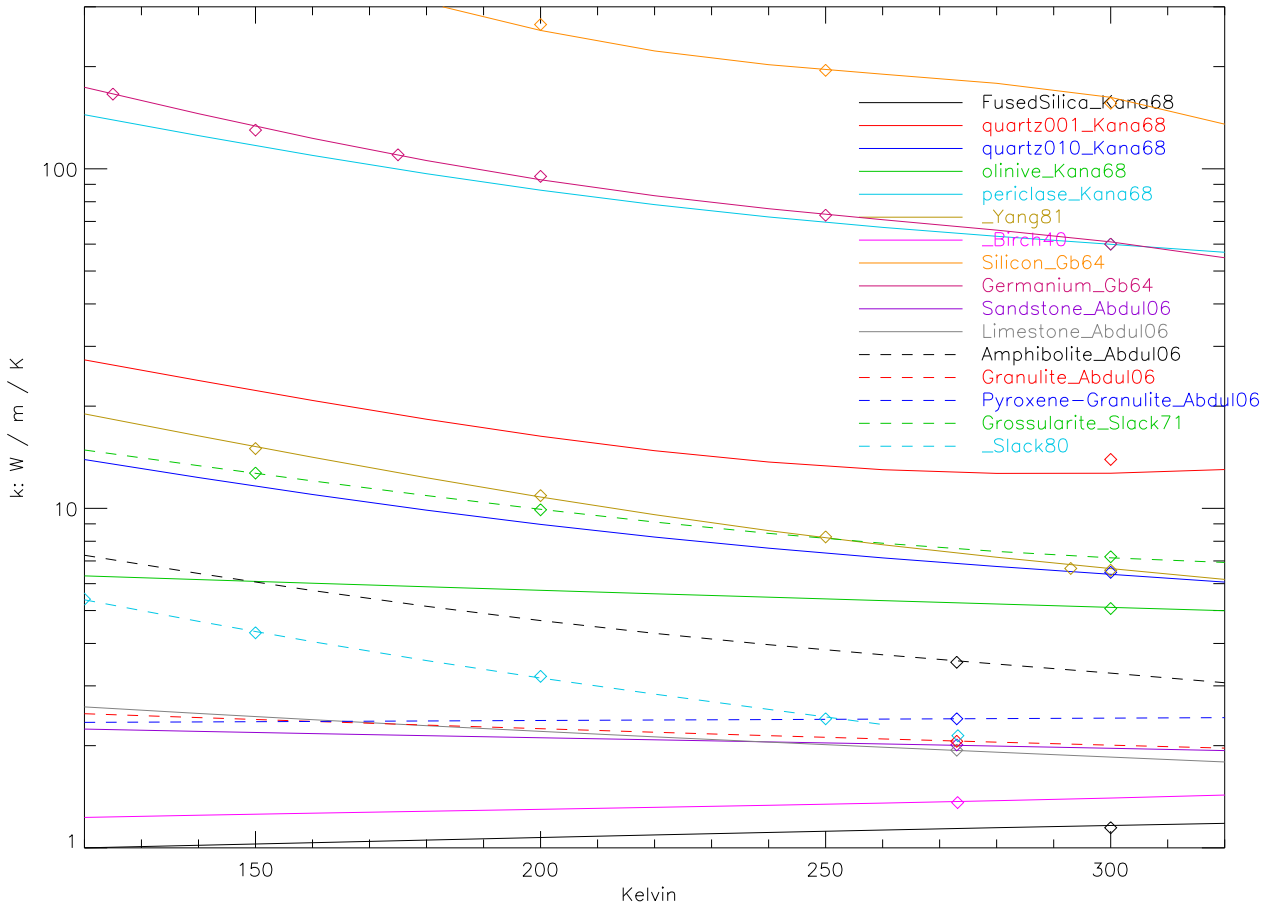


Figure 4: Thermal conductivity versus temperature for data-points (diamonds) for several materials. Where less than 2 data points fell at or below 320 K, then fit method 23 above was used to generate points at 20 K intervals below the coldest data point. The lines represent cubic fit to data and generated points within 120:320 K. 35c.eps

7: Concatenation of those in 3:5 that are within range of request T.
8: Plot of 1:5 above

Temperature curves for a number of materials are generated by @44, the results are shown in Figure 4 and in color image CP9.jpg. Measurements of probable Mars materials under Mars-appropriate conditions are rare.

## 4.1 $C_P$ of $H_2O$ Ice

**specheat** includes tables of measurements for ice Ih taken by Giauque36=[21], Haida74=[24], and Yamamuro87=[74]. These data are shown in Figure 4.1. A cubic fit was done to the aggregate of their data over 120K to 273K, with an RMS residual of 0.23%

Running to get $H_2O$ ice Cp, using all data sources, Do 139, which creates:

```
49... Cp H2O data points       Will all be below 0C
491.. move T points into ttt
315.. Plot one material
5.... x=scaled T
33... Cubic coefficents for KRC
25... Setup T
5.... x=scaled T
482.. Make points on uniform T
```

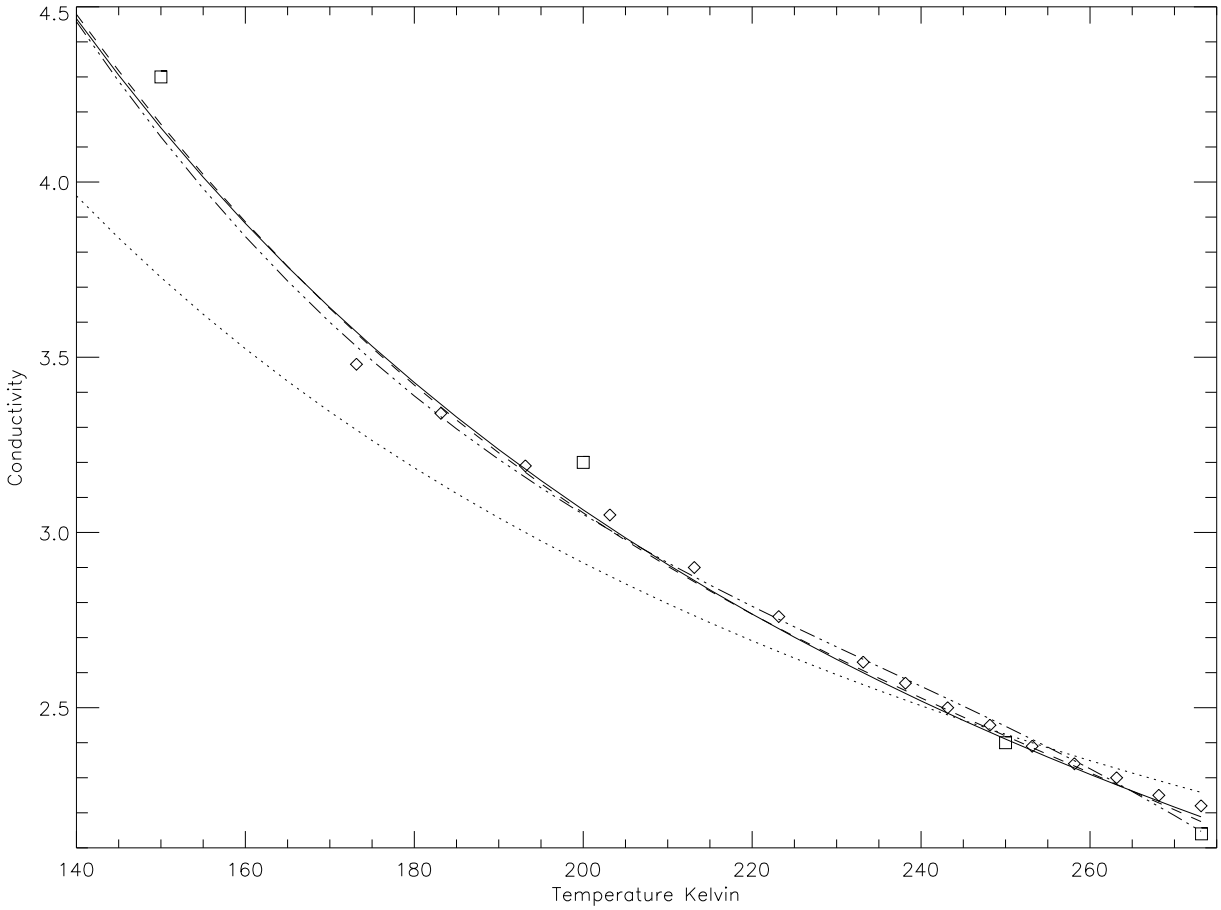


Figure 5: Thermal conductivity versus temperature for ice Ih. Data-points from the website http://www.engineeringtoolbox.com/ice-thermal-properties-d_576.html0 (diamonds), the measurements of Slack80=[65] are shown (squares) and the relation given by Hobbs74=[27] (dotted line). The website point were weighted 1 [total weight 15, the Slack points by 4 [total 20] and the every-5-degrees points of the Hobbs relation by 1/4 [total 8]. Also shown are the fit to A+B/T (solid line), the cubic fit to the data points (dot-dot-dot-dash) and the cubic fit to the A+B/T fit (dashed) kH2Ob.eps

```
335.. Oplot fit
57... Save coef as: Cp
3.95779 >      1710.648      721.8740      57.44873      24.37532 <  H2O:Ice 3sources
```

## 4.2 Other materials

To include additional materials, add a section to the case statement in **specheat.pro**

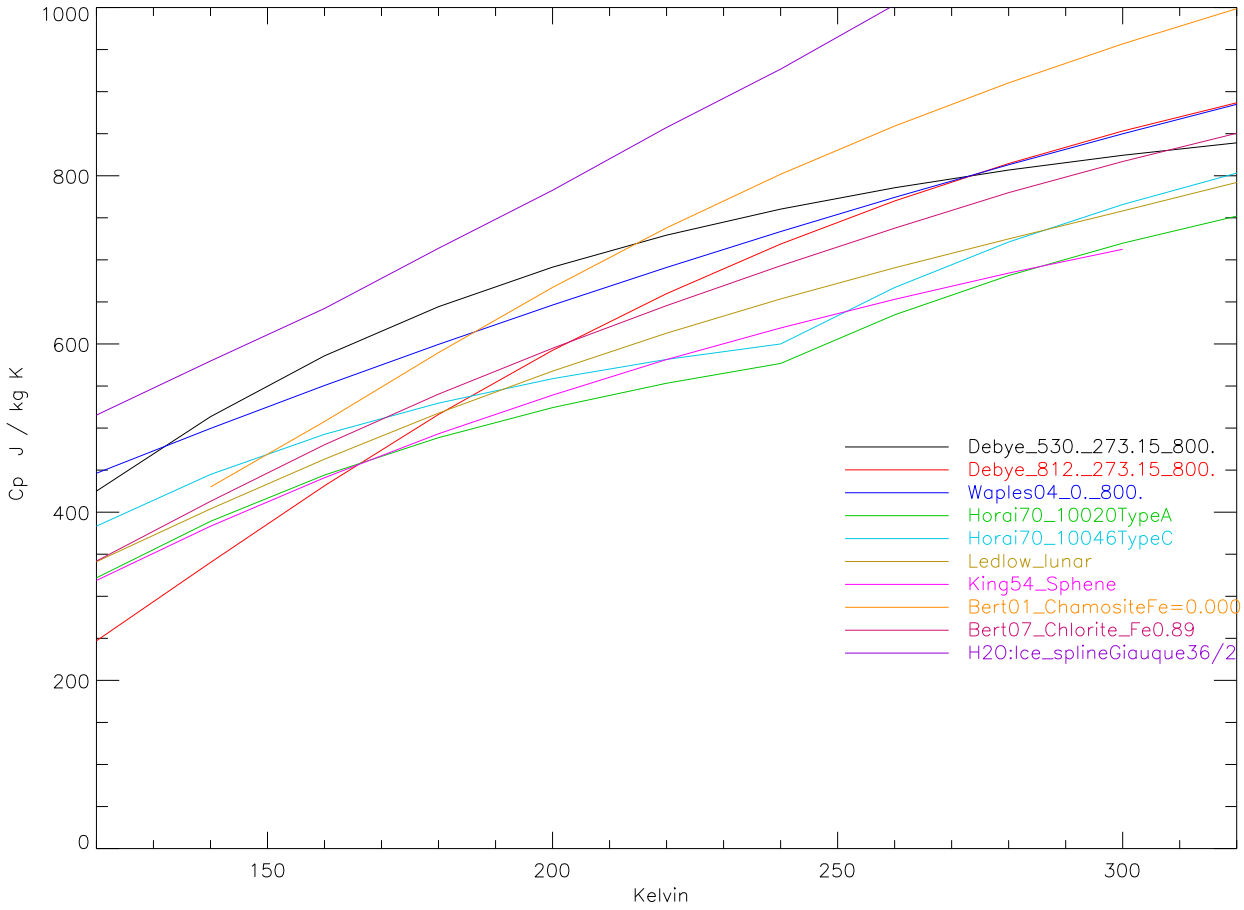


Figure 6: Specific heat versus temperature for several of the pre-coded materials. The inflection for the Horai Apollo sample comes from his recommendation to use the Debye relation below 240K. $H_2O$ ice would be off the top of this plot; it is shown at half scale. Cp9c

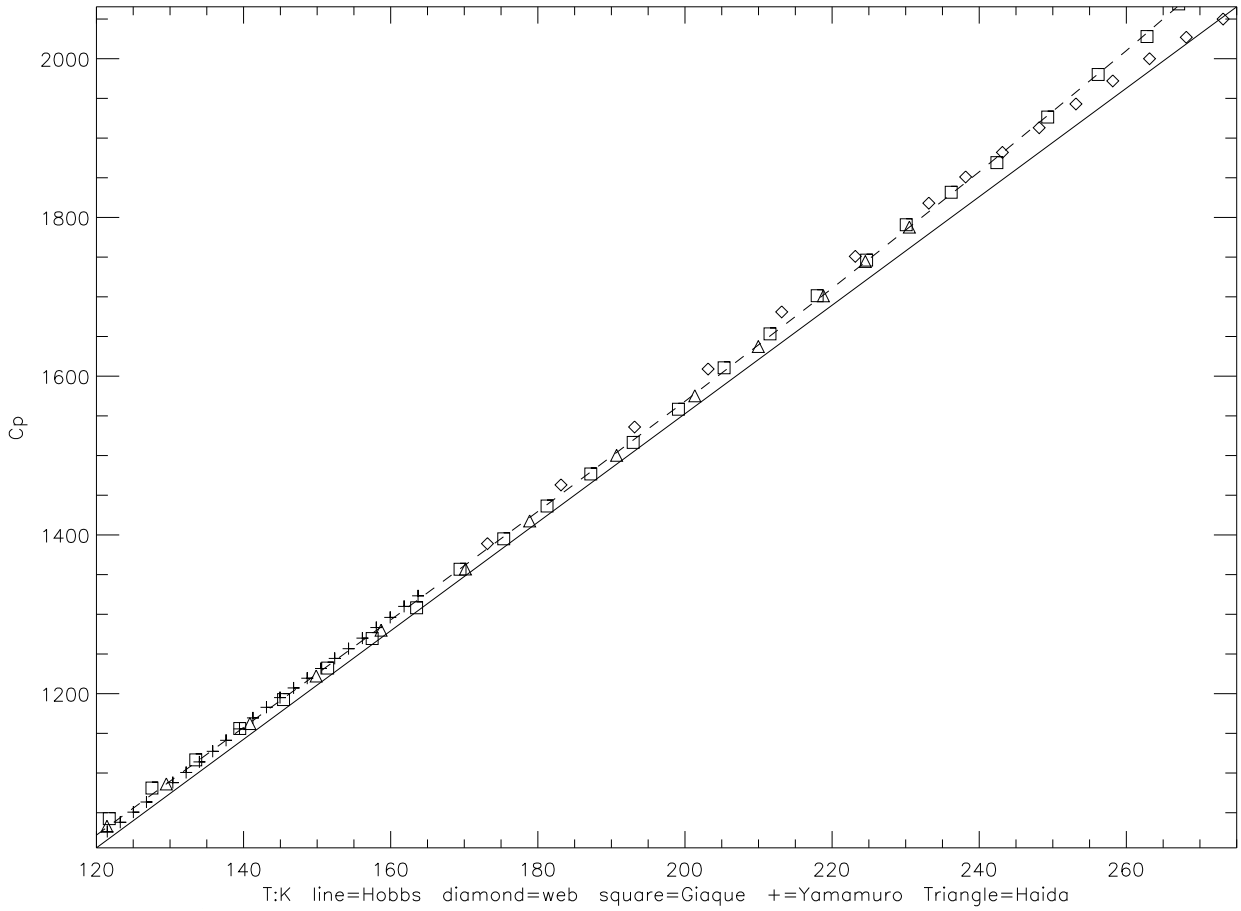


Figure 7: Specific heat versus temperature data from Giauque36=[21]=square, Haida74=[24]=triangle, Yamamuro87=[74]=plus sign, and http://www.engineeringtoolbox.com/ice-thermal-properties-d_576.html0 =diamond, along with the relation of Hobbs74=[27]=line. The dashed line is a cubic fit to first 3 sources listed. CpH2O

# 5 Thermal properties main program: koftop.pro

All data are firm-coded into subroutines, so the **koftop** uses no files.

New routines: **KOFTOP, KOFT, SPECHEAT, FIT_ABX, PARTCOND, SPSPREAD**

**XYY5** is a package that allows storage of un-equal length arrays, in this case temperature-values data points for $C_P$ or $\lambda$. It has a plot function for displaying these data.

## 5.1 Functional fit for KRC use

A set of uniformly-spaced points over the request temperature range is generated, and these are fit with a 3rd order polynomial.

## 5.2 Modifiable parameters

```
12: Cond. Ints: pari
  Limits=      -1     999
       0       6  Last @34
       1       5  Material index
       2       2  Secondary index
       3       3  Fit kode @51
       4       0  bbb index, -=auto
       5       8  Size of bbb.
       6       0  Ylog flag @73
       7      24  Cold extension: KofT action
       8       4   " Max points to use
       9       1  Flag: full material list

13: PARTCOND: parm
       0      0.00000  edit: flag -=stop >1=help
       1      100.000  Rg: grain radius, mu m
       2      250.000  T: temperature, K
       3     0.937000  kh: grain thermal conductivity
       4   0.00300000  kg: gas cond.  J m^-1 s^-1 k^-1
       5      2.00000  kc: cement cond.  =SI
       6     0.980000  emis: grain emissivity
       7     0.900000  G: host grain cond. factor -1=ave -2=geomean
       8    0.0100000  B: Cement contact angle, radian
       9      77.7700  vvvv:--numerical parameters
      10      0.00000  flag: test integrals
      11     0.100000  beta: SMX limit radian
      12      30.0000  nLo: steps along cement [Int]
      13      100.000  nHi: steps along gap [Int]
      14      0.00000  DP: Flag, double precision
      15   0.00100000  B1: Initial B
      16      1.10000  Brat: ratio for loop

14: FitPlot: parg
       0    0.0100000  Fit toler  \ FIT_ABX
       1    0.0500000  Frac.Scale / > Amoeba
       2     -7.00000  ----spare
       3     -7.00000  ----spare
       4      20.0000  Plot Ymax for k
       5      1000.00   " "  for Cp
       6      220.000  @76 X left \ Normaliz | middle Xval
```

```
       7     0.800000  Y of first | locations| offset units of char height
       8      1.00000  Delta Y    | for      | c.size LABEL_CURVE
       9      1.00000  Line Lenght/ Guide    | c.thick
      10      1.00000                        |leave: 0=clear

15: Cp values: parc
       0      2500.00  Density, SI
       1      5.00000  Material index
       2      5.00000  Secondary index
       3      850.000  Debye Temp. K
       4      20.0000  Reference temperature C
       5      700.000  Reference Cp
       6     0.670000  X of left   \ Normalized
       7     0.930000  Y of first  | locations
       8   -0.0240000  Delta Y     | for
       9    0.0800000  Line Lenght / Guide

16: Cond. values: parr
       0     -1.00000  Rg: Grain radius, micron -=table
       1      600.000  P: pressure Pascal
       2     0.350000  phi: Porosity fraction
       3     0.937000  host grain conductivity
       4      2400.00   " "  density
       5  -0.00100000  Cement fraction  -=table
       6      2.00000   "  conductitity
       7      1400.00   "  density
       8   0.00100000  Point-contact conduct.
       9      4.00000  k @25C for Sass92
      10     0.700000  @632 YplotMax
      11      120.000  T min, Kelvin
      12      320.000   " max
      13      20.0000   " delta
      14     -7.77000  vvv-Beware-vvv
      15      220.000  T scaling offset
      16    0.0100000  " " multiplier

17 GrainCemK: park
       0      2.77401  Grain K ConCof
       1    -0.535400  Grain K LinCof
       2     0.204288  Grain K ^2 Cof
       3   -0.0710305  Grain K ^3 Cof
       4      3.79146  Cement K ConCof
       5     -1.29785  Cement K LinCof
       6     0.345378  Cement K ^2 Cof
       7   -0.0386713  Cement K ^3 Cof


177 GrainCemCp: parp
       0      581.378  Grain Cp ConCof
       1      198.189  Grain Cp LinCof
       2     -52.2628  Grain Cp ^2 Cof
       3      12.0520  Grain Cp ^3 Cof
       4      636.157  Cement Cp ConCof
       5      272.547  Cement Cp LinCof
       6     -28.1283  Cement Cp ^2 Cof
       7     -39.3450  Cement Cp ^3 Cof
```

## 5.3 Action guide

Actions:

@0.... Stop
@112.. kons=[25,5,34,64] Do conductivity: Group 1
@113.. kons=[34,64] Group 2
@114.. kons=[35,64,-1, 64,655] data points
@115.. kons=[12,15,16, 25,60,41,5,51,55,61,62] Do one specific heat fit
@116.. kons=[25,50,44,64] Do specific heat family
@117.. kons=[717,74,75,76,-1,73,-1] k(T) solids in partcond,
@118.. kons=[260,60, 31,261,32,33,61,62,1182, 651,88] loop for big picture
@1182. increment
@131.. kons=[15,25,41,315, 5, 33,335,57] Cp for one material
@132.. kons=[12,25,31,315,5,33,335,56,710] k for one material
@138.. kons=[48,33,335,56,25,5] Use H2O k
@139.. kons=[49,491,5,33,57,25,5] Use H2O Cp
@123.. Start auto-script
@12... Integers: pari
@13... PARTCOND: parm
@14... Fit,plot: parg
@15... Cp values: parc
@16... Cond. values: parr
@166.. Mix control and values
@17... Partic K of T: park
@177.. Partic Cp of T: parp
@18... Guides and help
@25... Setup T
@260.. Empty XYY storage
@261.. Add material data to XYY
@31... Thermal conductivity of 1 mineral
@315.. Plot one material
@32... Extend data sets to lower T REQ 31
@33... Cubic coefficents for KRC
@335.. Oplot fit
@34... Test all analytic K for all their materials
@35... Test all data-set materials
@36... SP09a parameters
@37... Particulates using SP09A
@377.. Convert to use 73+ OVERRIDES 717
@38... Presley conductivity REQ 37
@41... Specific heat capacity of 1 mineral
@44... Test many SPECHEAT options
@48... fit H2O k RESETS ttt
@482.. Make points on uniform T
@49... Cp H2O data points
@491.. Move T points into ttt
@50... x=Kelvin
@5.... x=scaled T
@51... Fit to Tk
@52... Use DoublePrec.
@55... Print fit results
@56... Save coef as: k
@57... Save coef as: Cp

@59... Print Inertia(T) of solids
@60... Initiate bbb
@61... Plot data
@62... Plot fit
@631.. CHART cement k
@632.. Plot rrr,ggg UPDATE
@64... Plot of bbb
@65... Data plot
@651.. Big picture
@655.. Overplot
@70... Constant solid conductivity
@701.. PARTCOND: Modify params only
@702.. Full access
@71... Defaults for Particulates
@710.. Set Grain coefs.
@711.. Set Cement coefs
@717.. Compute particulate k for 1 or set cement volumes
@721.. kons=[166,722, 31,33,56, 41,33,57,710 ,48,33,56, 49,491,5,33,57,25,711, 725] Full mix sequence
@722.. transfer Mix
@725.. Linear mix for grain, ice=cement and void
@73... CLOT partCond
@735.. oCLOT
@738.. Plot gas conds
@74... Calc and Print coefficients for particulates
@75... Print thermal inertia table
@76... CLOT inertia
@-3... ——— KON91 null
@-1... Wait
@-9... Stop in KON91 ———
@122.. Modify kons sequence
@121.. + Reset to null
@801.. Write positive .eps file Expect color on white
@802.. Write .png
@803.. Write .jpg
@804.. Reverse Black and white image to 1-bit .eps file
@8.... Start Graph to file and printer
@80... Reset plot output device
@85... Set Color,line,symbol scheme
@87... Close plot device, no spawn of plot
@88... Add subtitle to plot
@9.... End a plot, save and print the file

Details

**@31**

@49 gets the points, non-monotonic
@491 moves data-point T into normal uniform T vector
@51 does the fit to T
kfit=pari[3] 2:n are polynomial, -4=Berman form for Cp, -2=1/(A+BT) for k.
@25 restores normal T vector
@482 generates uniform points
@5 Specifies normalized T'
@33 does cubic fit to T'

**@33**

Call SPSPREAD to get kgas
call PARTCOND to get cement volume fraction
For each grain size

Call SPSPREAD results into ddd
Call PRESLEY results into ggg
Call PARTCOND results into ppp

## 5.4 Typical use

Control sequences for doing one material conductivity or specific Heat are preset.
@131 for specific heat . Default is, Bertoldi clinclore Fe fraction 0.89.
@132 for conductivity. Default is: BasicRocks Zoth88

After doing these two, the results can be for either the grain material **@**710 or the cement material **@**711.

For the Kieffer09=[39] particulate model then do the sequence ??

## 5.5 Fitting Cp of T for Mars temperature range

Below are examples of some cubic fits to scaled temperature martian temperatures; done at **@**44. The fits were restricted to the valid temperature range specified in the **specheat** routine.

```
T range and delta=      120.000      320.000      20.0000
Values between > < are the coefficents
Value before > is the Standard Deviation of fit
```

| Std.Dev | constant | Linear | T'^2 | T'^3 | Material |
|---|---|---|---|---|---|
| 0.85597 > | 730.3778 | 171.1534 | -97.36093 | 35.92560 < | Debye 530. 273.15 800. |
| 1.67749 > | 658.1685 | 318.4424 | -93.07760 | 1.813520 < | Debye 812. 273.15 800. |
| 8.68950 > | 559.6317 | 178.1158 | -15.88013 | 39.01124 < | Horai 1970 10020 |
| 11.85039 > | 590.3480 | 166.5212 | 12.34777 | 46.07032 < | Horai 1970 10046 |
| 0.18631 > | 581.3780 | 198.1888 | -52.26276 | 12.05196 < | King et al Sphene |
| 1.82517 > | 719.6918 | 319.2454 | -62.06202 | -8.264219 < | clinclore Bert01 Fe=0.116 |
| 1.81581 > | 639.2908 | 261.6666 | -44.44849 | -12.14468 < | clinclore Bert01 Fe=0.889 |
| 1.75006 > | 642.4306 | 245.8746 | -37.44404 | -13.46644 < | clinclore Bert01 Fe=1.000 |
| 0.92818 > | 646.6275 | 246.6678 | -49.82160 | 7.951969 < | Chlorite Bert07 Fe=0.89 |
| 0.99128 > | 611.7469 | 214.1993 | -46.28867 | 11.27204 < | Ledlow |
| 0.00000 > | 690.9838 | 218.3245 | -25.39334 | 0.9999385 < | Waples^2 2004 0. 800. |
| 2.96565 > | 1711.052 | 728.0281 | 26.30519 | -22.12386 < | H2O:Ice Giauque36 |
| 3.95779 > | 1710.648 | 721.8740 | 57.44873 | 24.37532 < | H2O:Ice_3sources |

## 5.6 Fitting $\lambda$ of T for Mars temperature range

Results of **@**34

```
T range and delta=      120.000      320.000      20.0000
```

| Std.Dev | constant | Linear | T'^2 | T'^3 | Material |
|---|---|---|---|---|---|
| 0.00038 > | 0.5727402 | -0.1567263 | 0.04650183 | -0.01300548 < | Dunite Horai70b |
| 0.00002 > | 0.4669398 | -0.06774209 | 0.01004124 | -0.001465128 < | Pyroxenite Horai70b |
| 0.00000 > | 0.2209081 | -0.002332719 | 2.464336e-05 | -2.588600e-07 < | Diabase Horai70b |
| 0.00000 > | 0.2053396 | -0.0003023222 | 4.537213e-07 | 1.835347e-09 < | Gabbro Horai70b |
| 0.00000 > | 0.1717570 | 0.004935535 | 0.0001419527 | 4.088490e-06 < | Anorthosite Horai70b |
| 0.00000 > | 0.2071287 | -0.005126931 | 0.0001269907 | -3.158598e-06 < | Albitite Horai70b |
| 0.00001 > | 0.3213432 | -0.03948743 | 0.004927245 | -0.0006079461 < | Granite Horai70b |
| 0.01602 > | 7.844152 | -3.343426 | 1.275726 | -0.4435667 < | SaltRocks Zoth88 |
| 0.00581 > | 3.738380 | -1.211992 | 0.4624507 | -0.1607930 < | Limestones Zoth88 |
| 0.00382 > | 3.120837 | -0.7963225 | 0.3038468 | -0.1056470 < | Metamorphics Zoth88 |

```
 0.00437 >      3.353852    -0.9115353     0.3478075    -0.1209317 <  AcidRocks Zoth88
 0.00257 >      2.774009    -0.5354000     0.2042885   -0.07103046 <  BasicRocks Zoth88
 0.00700 >      5.078216     -1.460490     0.5572681    -0.1937604 <  Ultra-basics Zoth88
 0.00417 >      3.289425    -0.8697424     0.3318611    -0.1153873 <  Aveof5types Zoth88
 0.00097 >      4.646508    -0.9689192     0.2114329   -0.04462963 <  Sass92
 0.00024 >      4.142231    -0.6348214    0.09965667   -0.01537151 <  gneiss Clauser95
 0.00000 >      2.642703    -0.1536450   0.008963052 -0.0005217241 <  metabasite Clauser95
 0.00172 >      4.010569    -0.9906328     0.2589533   -0.06405231 <  paragneiss Seipold98
 0.00000 >      2.720438    -0.1448558   0.007374227 -0.0001738053 <  amphibolite Seipold98
 0.00118 >      4.511555    -0.9920732     0.2295133   -0.05116162 <  xtaline Vosteen03
 0.01894 >      4.898468     -1.988685     0.9858879    -0.4227412 <  seds Vosteen03

 0.00000 >      1.701741   -0.02365008  0.0003287113 -4.536606e-06 <  labradorite Pet95
 0.00000 >      2.095118   -0.07242709   0.002506750 -8.661032e-05 <  microcline Pet95
 0.00019 >      4.278776    -0.6132959    0.08976835   -0.01293881 <  garnet Pet95
 0.00034 >      4.767582    -0.7651988     0.1261028   -0.02038259 <  pyroxenite Pet95
 0.00433 >      6.086648     -1.697102     0.5148059    -0.1468391 <  SynGalGarnet Pet95
 0.00000 >      3.806140   -0.05311756  0.0007416263 -1.065313e-05 <  garnet Pet95
 0.00013 >      5.272266    -0.6485804    0.08102152   -0.01000797 <  SynOlivine Pet95
 0.00019 >      5.899489    -0.7830707     0.1058212   -0.01411335 <  olivine Pet95
 0.11737 >      14.00425     -6.624243      4.223161     -2.169872 <  alpha-SiO2 Pet95
 0.00062 >      4.217541    -0.8062869     0.1600958   -0.03091895 <  Granite Pet95
 0.00042 >      3.464935    -0.6342483     0.1201894   -0.02220582 <  Diorite Pet95
 0.00007 >      3.118103    -0.3743126    0.04559595  -0.005495317 <  Diabase Pet95
 0.00127 >      5.032161     -1.097111     0.2514201   -0.05555261 <  Dunite Pet95
 0.00000 >      1.998668  -0.006657808  2.226491e-05 -8.915301e-08 <  Gabbro Pet95
 0.00003 >      2.467480    -0.2516543    0.02593687  -0.002652605 <  Serpentenite Pet95
 0.00000 >      2.362759    -0.1460787   0.009066172 -0.0005610733 <  Eclogite Pet95
 0.00001 >      2.701478    -0.1885311    0.01322170 -0.0009237803 <  mica Pet95

 0.00872 >      2.800166     -1.346557     0.3501616     0.1681532 <  Cond H2O:Ice_k_Web
```

## 5.7 Extension of $\lambda$ for Mars temperature range

Used method 24 as described in §3.1 Fit to data points. FIT_ABX preceding a material line are the values used for the cold extension based on a fit to the lowest 4 measured points; reports: A, B, # iterations, and $\sum (y_f - y_m)^2$. With unrestricted coefficients, can get some wild results.

Using 120 to 320 K with 10° interval, and with both coefficients restricted to be >1.e-8, get:

```
<a means A coeff set to 1.E-8 in method 24, <b ditto for B.
 NP   StdDev           c0           c1           c2           c3      Note  MaterialSource
  9  0.03898 >      1.412375    0.02452806    -0.1340093    -0.1581136 <b  FusedSilica Kana68
  9  0.30994 >      16.41876     -7.531681      5.085024     -1.124730 <a  quartz001 Kana68
  9  0.12127 >      9.264705     -4.216154      2.689451    -0.8292275 <a  quartz010 Kana68
  9  0.00834 >      5.561930    -0.6203964    0.06161419  -0.008579915 <  olinive Kana68
  9  0.56404 >      80.26309     -36.46237      21.45405     -8.871257 <a  periclase Kana68
  9  0.13921 >      9.597675     -5.494487      2.905688    -0.8641065 <  NaCl Yang81
 11  0.01750 >      1.448836   -0.03569783   -0.02221565    0.01746422 <b  SilicaGlass Birch40
 11  9.19763 >      223.8652     -129.5840      159.1353     -120.5962 <  Silicon Gb64
 11  1.79470 >      83.58900     -41.13925      29.67271     -17.77364 <  Germanium Gb64
  4  0.00097 >      2.081675    -0.1465059   0.005840617  -0.007324098 <  Sandstone Abdul06
  4  0.00095 >      2.126523    -0.3922069    0.07423300   -0.01850849 <  Limestone Abdul06
  4  0.01386 >      4.262733     -1.704368     0.8369164    -0.3302984 <  Amphibolite Abdul06
```

```
  4  0.00069 >      2.190314    -0.2586301    0.03525489  0.0006817337 <  Granulite Abdul06
  4  0.00572 >      2.428892   -0.01149608  -0.009635572   0.003171192 <b  Pyroxene-Granulite Abdul0
  p means pole found in method 23
Pnts  StdDev      constant      Linear       T'^2       T'^3 ImatIndx  FracError  MaterialSource
  9  0.00665 >    1.091483    0.093408   -0.001069   -0.002900 <11 0   0.02881 FusedSilica_Kana68
  9  0.52537 >   14.783381   -6.529418    5.406845   -0.651217 <11 1 p 0.10486 quartz001_Kana68
  9  0.05237 >    8.229383   -3.315201    1.762486   -0.612077 <11 2   0.02422 quartz010_Kana68
  9  0.01472 >    5.602027   -0.655032    0.057136   -0.010448 <11 3   0.00910 olinive_Kana68
  9  0.65126 >   78.440620  -35.572323   22.115486   -8.210652 <11 4 p 0.04364 periclase_Kana68
  9  0.15363 >    9.578611   -5.463079    2.998692   -0.937991 <12 0   0.00000 _Yang81
 11  0.00218 >    1.316066    0.088869    0.013780    0.011769 <13 0   0.00590 _Birch40
 11 10.46090 >  222.443665 -127.432655  166.026962 -125.695374 <14 0   0.00000 Silicon_Gb64
 11  2.03035 >   83.329773  -40.659798   30.927271  -18.896624 <14 1   0.00000 Germanium_Gb64
  4  0.00128 >    2.080575   -0.144384    0.005582   -0.007667 <15 0   0.00229 Sandstone_Abdul06
  4  0.00148 >    2.122916   -0.386039    0.072786   -0.019517 <15 1   0.00310 Limestone_Abdul06
  4  0.01762 >    4.283615   -1.745720    0.885490   -0.358901 <15 2   0.00462 Amphibolite_Abdul06
  4  0.00075 >    2.190432   -0.258238    0.034715    0.000095 <15 3   0.00218 Granulite_Abdul06
  4  0.00003 >    2.379631    0.038286    0.000698    0.000166 <15 4   0.00007 Pyroxene-Granulite_Ab
  4  0.07660 >    9.114331   -3.728876    1.776449   -0.235030 <16 0   0.00000 Grossularite_Slack71
  4  0.02355 >    2.836758   -1.497172    0.612160   -0.431729 <17 0   0.00000 _Slack80
```

# 6 Particulate materials

Use the relations from Piqueux09a=[51] for Knudsen number and its influence on effective gas conductivity.

Their relation for $k_0$, the large-volume conductivity of $CO_2$ gas, differs by only a few percent from the fit to Johnston46=[37]. The effective gas conductivity in pores is $k_{gas} = \frac{k_0}{1+e^{xi(Kn^{-1})}}$ where $\xi\left(Kn^{-1}\right) = \frac{\log_{10}\left(Kn^{-1}\right)-2.15}{0.55}$ is derived from their numerical model.

The Knudsen number is the ratio of mean free path to the pore size; $Kn = \frac{k_B T}{\sqrt{2}\pi\theta^2 LP}$ where $k_B$ is the gas Boltzmann's constant, $\theta$ is the molecule collision diameter, $L \approx \sqrt[3]{\frac{\phi}{1-\phi}} \cdot r$ is the pore size ($\phi$ is the porosity) and $P$ is the pressure [all in SI units].

Piqueux09b=[52] does not provide a simple algorithmic approximation to his finite element model of cemented soils, so I will use my simple analytic model Kieffer09=[39], which displays the same general behavior.

Overview of sequence:

select grain size, cement fraction, environment conditions
Call **PP_CO2** to get gas conductivity
Call PARTCOND once to get relation between indices for various cement volumes.
Compute effective gas conductivity
Loop over grain size calling SPSPREAD and PRESLEY for a set of temperatures
loop over temperature calling PARTCOND to get net conductivity
For each grain size and cement fraction, fit particulate K to cubic in T'

## 6.1 SP09A: Piqueux unconsolidated model

Summary of Piqueux09a=[51]

Contact conductivity is expected to be <.001, assumed to be zero [27.5]
Radiative conductivity goes as $T^3$ described by Eqs 2,3,4
While mentioned at [5.8], never explicitly added into k ???
Unconfined gas conductivity $k_0$ follows fit to experimental data, Eq. 14
Effective gas conductivity $k_{gas}$ expected to depend on Knundsen number. Eq. 12
Major numerical model to relate net conductivity to gas conductivity
Model run for simple cubic(SC) and close cubic(CC)cells

Results shown in Fig 8.
Results fit with rational functions, Eq. 26 coefficents in Table 1, rows 2 and 3
For other pore fractions, linear interpolation between SC and CC results, Eq. 28

I did a fit to $CO_2$ gas measurements of Johnston46=[37] with form $\ln \lambda = a + b \ln T$; get $\lambda = 5.46772e-06 T^{1.407266}$ This agrees closely with http://encyclopedia.airliquide.com/Encyclopedia.asp?GasID=26 . Thermal conductivity (1.013 bar and 0 C ) : 14.65 mW/(m.K)

Can call **sp09a** for any set of:

| | |
|---|---|
| Temperature: | negative yields default set [150.,230.,315] |
| Grain radius in micrometer: | negative yields default set [10.,50.,200.] |
| Pressure in torr: | negative yields default set [0.5,5,10.] |
| Optional Pore fraction: | negative yields default set [0.30,0.35,0.4,0.45] |
| | absence yields 0.35 |

16 output items for each set of input conditions:

| i | name | value | Description |
|---|---|---|---|
| -2 | kcontact | 0.0000 | Contact conductivity; assumed |
| -1 | kgrain | 0.93700 | Solid grain conductivity; assumed |
| 0 | R um | 100.00 | Grain radius, micrometer. Input |
| 1 | Phi | 0.35000 | Porosity. Input |
| 2 | T | 240.00 | Temperature, K. Input |
| 3 | Pa | 500.00 | Pressure, Pa. Input |
| 4 | MFP | 7.0493e-06 | Mean Free path, m. Eq 7 |
| 5 | K0 | 0.012183 | Bulk gas conductivity. Eq 14 |
| 6 | Pore | 8.1523e-05 | Typical length of Pore. Eq 11 |
| 7 | Kn | 0.086470 | Knudsen Number, Eq 7 |
| 8 | xi | -1.9761 | Exponent in kgas. Eq 29,30,31 |
| 9 | Kgas | 0.0014831 | Gas thermal conductitivy, Eq. 32 |
| 10 | KeffCC | 0.015480 | Effective gas conductivity, close cubic Eq 25 |
| 11 | KeffSC | 0.049761 | Effective gas conductivity, simple cubic |
| 12 | keff | 0.029856 | Effective gas conductivity, interpolated to porosity Eq 27 |
| 13 | krad | 0.00036468 | Radiative part of conductivity |
| 14 | knet | 0.030221 | Total conductivity |
| 15 | kVasa | 0.0013620 | Vasavada 99 relation for radiative term |

Sample results, default radii set: 10 $\mu$m to 50 mm

```
Tmin,Tmax, Tdel=      120.000      320.000      20.0000
   Grain Cp >  581.3780  198.1888  -52.2628   12.0520 <Sphene
```

| | 1000\|err\| | c0 | c1 | c2 | c3 | Ind.Param |
|---|---|---|---|---|---|---|
| 0 | 0.02347 > | 0.008292 | 0.001725 | -0.000119 | 0.000019 < | 10.0 |
| 1 | 0.03971 > | 0.012572 | 0.002880 | -0.000214 | 0.000038 < | 20.0 |
| 2 | 0.07774 > | 0.021995 | 0.005493 | -0.000459 | 0.000096 < | 50.0 |
| 3 | 0.11164 > | 0.032834 | 0.008660 | -0.000788 | 0.000183 < | 100. |
| 4 | 0.12810 > | 0.047054 | 0.013195 | -0.001242 | 0.000320 < | 200. |
| 5 | 0.10286 > | 0.069647 | 0.021717 | -0.001770 | 0.000553 < | 500. |
| 6 | 0.06743 > | 0.087617 | 0.030218 | -0.001627 | 0.000740 < | 1.00e+03 |
| 7 | 0.03380 > | 0.104917 | 0.040653 | -0.000353 | 0.000983 < | 2.00e+03 |
| 8 | 0.04042 > | 0.127544 | 0.059495 | 0.004676 | 0.001686 < | 5.00e+03 |
| 9 | 0.05149 > | 0.148618 | 0.082637 | 0.013420 | 0.002938 < | 1.00e+04 |
| 10 | 0.05040 > | 0.181254 | 0.123653 | 0.030915 | 0.005528 < | 2.00e+04 |
| 11 | 0.03781 > | 0.268984 | 0.240701 | 0.083247 | 0.013403 < | 5.00e+04 |

| T | 120.0 | 140.0 | 160.0 | 180.0 | 200.0 | 220.0 | 240.0 | 260.0 | 280.0 | 300.0 | 320.0 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| GasK*1000 | 4.8 | 5.9 | 7.0 | 8.2 | 9.5 | 10.8 | 12.2 | 13.6 | 15.1 | 16.6 | 18.1 |
| Grain k | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 |

```
 Grain  Cp 318.9 383.2 441.0 493.0 539.6 581.4 619.0 653.1 684.1 712.7 739.4
Ind.Param  ____________ Thermal inertia _______________
      10.0  56.6  63.9  70.4  76.4  81.8  86.7  91.3  95.6  99.6 103.3 106.9
      20.0  68.5  77.7  86.0  93.6 100.4 106.8 112.6 118.1 123.2 128.1 132.7
      50.0  89.1 101.6 112.9 123.1 132.6 141.2 149.3 156.8 163.8 170.5 176.9
      100. 107.4 123.0 137.1 149.9 161.7 172.6 182.6 192.0 200.8 209.2 217.2
      200. 126.8 145.8 163.0 178.8 193.2 206.6 219.0 230.5 241.4 251.7 261.6
      500. 150.6 174.4 196.0 216.0 234.3 251.3 267.2 282.0 296.1 309.5 322.5
  1.00e+03 165.5 192.6 217.5 240.5 261.9 281.9 300.6 318.4 335.3 351.5 367.3
  2.00e+03 176.9 207.0 234.9 260.9 285.4 308.5 330.4 351.4 371.6 391.3 410.6
  5.00e+03 188.0 221.5 253.2 283.3 312.2 340.1 367.2 393.8 420.0 446.1 472.3
  1.00e+04 195.0 231.4 266.5 300.6 334.1 367.1 400.0 433.0 466.2 499.9 534.4
  2.00e+04 203.2 243.6 283.7 323.9 364.3 405.4 447.4 490.4 534.6 580.2 627.5
  5.00e+04 220.9 271.0 323.0 377.4 434.3 493.9 556.4 621.7 690.1 761.6 836.3
```

### 6.1.1 SPSPREAD: Piqueux Spreadsheet for cemented particles. OBSOLETE

Reverse engineer Sylvain Piqueux thermal conductivity spreadsheet emailed 2008nov11 and described in a two-page 2008nov16 email from him, into IDL. Also coding of his two-page equations explicitly.

Can call with same flexability of inputs as **sp09a**. Output array(row,19) of all the spreadsheet columns in order. Rows are formed by looping over the above four parameters, pore fraction fastest, temperature slowest. Internally:

`ddd` are values based on reverse engineering of spreadsheet
Then reformatted for `gg`
`www` are values based on 2-page writeup.

If dbug is set, will print all results for the first row. Then prints a comparison of spreadsheet versus writeup: starting at -1, columns of

i: Row count
labw[i]: Piqueux ID of computed parameter
www[0,i]: values for first row
qq[i]: gg[0,select], based on 2-page writeup
labp[ii[i]]: Brief ID of item
ii[i]: Location in `gg`

Some disagreements between spreadsheet and writeup:

$k_0$: Eq 1. versus Column E in 2nd version

$k_{gas}$: Eq. 5 versus column O of first version. (not in 2nd)

### 6.1.2 Calling from koftop

Parr 1 through 8 set inputs to particulate models.
parr[0] sets grain radius, or negative invokes a large set
parr[5] sets cement volume, or negative invokes a large set

An inner loop runs through a range of temperatures, replacing the bulk materials $C_P$ and $\lambda$ with values derived above, and outer loop run over a range of grain sizes.

Results for a wide range of grain sizes are shown in Figure 6.1.2; these are at porosity=.35 and pressure of 500 Pa.

## 6.2 PARTCOND: Kieffer analytic model for cemented particles

The IDL routine **partcond.pro** implements the model of cemented particles described in Kieffer09=[39] [available upon request]. This routine requires a gas conductivity, which is obtained by calling **PP_CO2** and selecting the Hilsenrath60=[26] relation given by Piqueux09a=[51].

Input parameters are defined under 13: PARTCOND in §5.2. Lacking good $C_P$ values for carbonates, I choose to use the values for clinclore:Fe=0.89 based upon its similarity with limestone near 300K.

**partcond** is written as a large case statement

```
konc=[16,43 ,-4]              ; return [vol,knet]
16: modify values
```

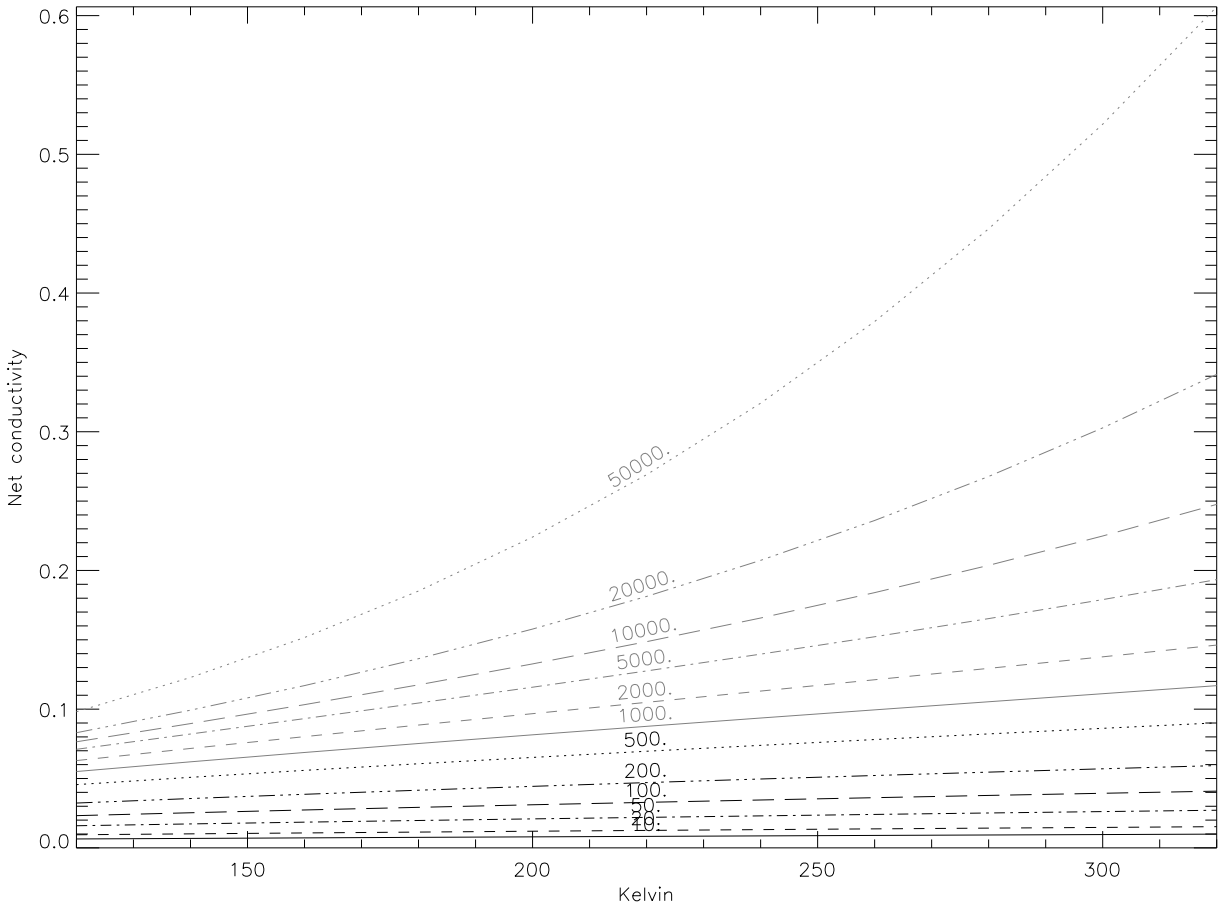


Figure 8: Results for the Piqueux un-cemented particulate model. Grain size ranges from 10 $\mu$m to 50 mm. The grain conductivity is a constant

```
20: [auto] begin; Set limits and constants
43:  Numerical integration for all B
; first evaluate the parts: cement, gas, radiation, for all radii
; Then integrate the cement outward and the others inward
; Sum to get the results for all values of B

Returns [nB,2] where 0]=volume fraction cement,  1]=net conductivity,
and nB is the total number of cement contact angles =parm[12]+parm[13].
```

Sample results; 10 ppb to 10% cement volume

```
Tmin,Tmax, Tdel=      120.000      320.000      20.0000
  Grain k  >  2.774009 -0.535400  0.204288 -0.071030 < BasicRocks:Zoth88
 Cement k  >  3.791455 -1.297852  0.345378 -0.038671 < limestone
  Grain Cp >  581.3780  198.1888  -52.2628   12.0520 < Sphene
 Cement Cp >  636.1573  272.5468  -28.1283  -39.3450 < clinclore:Fe=0.89
  1000|err|       c0        c1        c2        c3       Ind.Param
 0  0.12972 >  0.114758  0.030359  0.002328 -0.001066 <    1.00e-08
 1  0.07328 >  0.183835  0.016928  0.007453 -0.002852 <    1.00e-06
 2  0.04431 >  0.256925  0.002279  0.013186 -0.004888 <    1.00e-05
 3  0.05256 >  0.388408 -0.026003  0.024181 -0.008647 <    0.000100
 4  0.02827 >  0.636632 -0.082858  0.044519 -0.015196 <     0.00100
 5  0.03033 >  1.098480 -0.189480  0.080076 -0.026705 <      0.0100
```

```
 6  0.03544 >  1.305149 -0.236999  0.095629 -0.031734 <      0.0200
 7  0.04390 >  1.650960 -0.316747  0.121512 -0.039990 <      0.0500
 8  0.05213 >  1.989642 -0.395644  0.146817 -0.047868 <       0.100
Doing ---------------->      75
         T 120.0 140.0 160.0 180.0 200.0 220.0 240.0 260.0 280.0 300.0 320.0
 GasK*1000   4.8   5.9   7.0   8.2   9.5  10.8  12.2  13.6  15.1  16.6  18.1
  Grain  k   3.6   3.4   3.2   3.0   2.9   2.8   2.7   2.6   2.5   2.4   2.4
  Cement k   5.5   5.1   4.7   4.4   4.1   3.8   3.5   3.3   3.1   3.0   2.8
 Grain  Cp 318.9 383.2 441.0 493.0 539.6 581.4 619.0 653.1 684.1 712.7 739.4
 Cement Cp 374.8 420.3 471.0 525.2 580.8 636.2 689.2 738.2 781.1 816.0 841.2
Ind.Param  ____________ Thermal inertia _______________
  1.00e-08 187.6 211.1 232.7 252.8 271.7 289.7 306.8 323.2 339.0 354.2 368.9
  1.00e-06 266.6 291.7 313.3 332.6 350.2 366.6 382.1 396.7 410.7 424.1 437.0
  1.00e-05 330.7 358.1 380.7 400.3 417.6 433.4 448.1 461.8 474.7 487.1 498.7
  0.000100 423.5 454.8 479.6 500.0 517.5 532.9 546.9 559.7 571.5 582.6 592.8
   0.00100 559.4 597.2 626.0 648.7 667.1 682.7 696.2 708.1 718.8 728.3 736.8
    0.0100 753.3 801.2 836.7 863.8 884.9 902.0 916.0 927.7 937.6 945.8 952.4
    0.0200 830.0 881.6 919.9 948.9 971.4 989.41004.01016.01025.91033.91039.9
    0.0500 956.61013.61056.01088.41113.51133.51149.51162.51172.81180.61185.9
     0.1001087.31148.31194.61230.41258.51281.01299.11313.61324.71332.71337.2
```

### 6.2.1 Calling from koftop

The program **koftop** can call **partcond** with temperature-dependent (cubic in T) conductivity for the solids (grains and cement). Using the relations for BasicRocks for grains and Limestone for cement yields the results in Figure 6.2.1. The cubic coefficient values for the solids and cemented mix are:

```
Grain and cement materials=  BasicRocks   limestone
Tmin,Tmax, Tdel=      120.000      320.000      20.0000

    sigResid          c0           c1           c2          c3         cem.Vol
 BasicRocks >      2.797455    -0.5733288     0.1525714   -0.01708314 <
  limestone >      3.791455     -1.297852     0.3453778   -0.03867132 <
 0  0.00002 >     0.3911251   -0.03036693    0.01817816  -0.002487207 < 0.000100
 1  0.00001 >     0.6414463   -0.09064570    0.03389244  -0.004121674 < 0.001000
 2  0.00001 >      1.107040    -0.2033801    0.06119198  -0.006863785 < 0.010000
 3  0.00001 >      2.004835    -0.4204147     0.1133001   -0.01237263 < 0.100000
```

Results for a wide range of cement volumes are shown in Figure 6.2.1; the corresponding thermal inertias are in Figure 6.2.1. The opposing slopes in these two figures is the result of the temperature dependence of specific heat being the larger effect.

Setting the solid temperature dependence to zero yields nearly T-independent behavior:

```
    sigResid          c0           c1           c2          c3         cem.Vol
 BasicRocks >      2.797455     0.000000     0.000000     0.000000 <
  limestone >      3.791455     0.000000     0.000000     0.000000 <
 0  0.00001 >     0.3911375    0.03798161   0.001679920 -0.0004527534 < 0.000100
 1  0.00001 >     0.6414520    0.03236581   0.002237705 -0.0004111509 < 0.001000
 2  0.00000 >      1.107043    0.02312554   0.002075447 -0.0002425569 < 0.010000
 3  0.00000 >      2.004842    0.01198547   0.001259117 -9.197257e-05 < 0.100000
```

# 7 Papers on hand

Articles that I could find and access through the ASU system. and a few articles on lunar surface materials for which I had hard-copy.

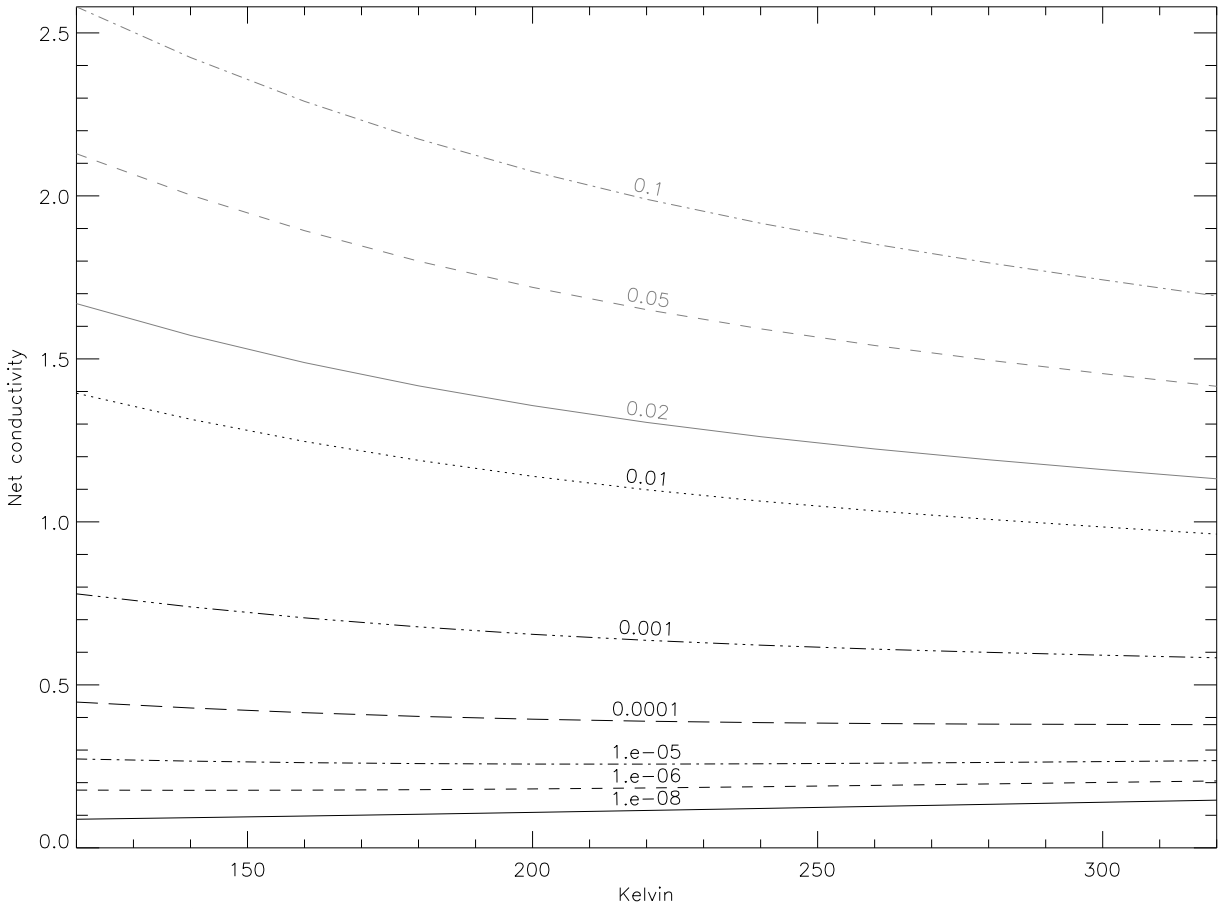


Figure 9: Thermal conductivity results using temperature-dependent solids in the Kieffer cemented particulate model. Cement volume fraction ranges from 10 ppb to 10%. If the temperature dependance of the solids conductivity, but not the gas, is set to zero, net conductivity increases slightly with temperature; 10% for 0.1% cement[Dashed lines on color version only.] cemk.eps

## 7.1 Rocks and minerals

Abdul06=[1], Andersson94=[2], Aurangzeb07=[4], vdBerg01=[69], Berman85=[5], Bertoldi01=[6], Bertoldi05=[8] Bertoldi07=[7], Birch40=[10], Birch40b=[9], Clauser95=[15], Cahill89=[11], Cahill92=[12], Carruthers92=[13], Cermak82=[16],Fountain70=[19], Ghormley68=[20], Giauque36=[21], Giesting02=[22], Glassbrenner64=[23], Haida74=[24], Heuze83=[25], Hofmeister01=[29], Hofmeister04=[32], Hofmeister06=[30], Hofmeister07=[31] Horai69=[35], Horai70b=[36], Kanamori68=[38], SWKieffer79=[40], Klug91=[43], Ledlow92=[45], McGaughey04=[47], Mottaghy08=[48], Petrunin95=[50], Popov03=[53], Presley97=[54], Presley97b=[55],Pribnow93=[56], Sass71=[59], Sass84=[60], Seipold98=[64], Seipold98g=[63], Slack80=[65], Sugasaki68=[67], Vosteen03=[71], Waples04=[72], Whittington09=[73], Yamamuro87=[74]

These files are in /work2/Reprints/rock/; the file names are typically first author name followed by the last two digits of the year.

I found no access to, or only abstracts for: Cermak82=[16], Chai96=[14], Diment88=[18], Jessop 2008, Linvill84=[46], Robie68=[57], Yang94=[75]

## 7.2 Carbon dioxide gas

Articles on gas conductivity:

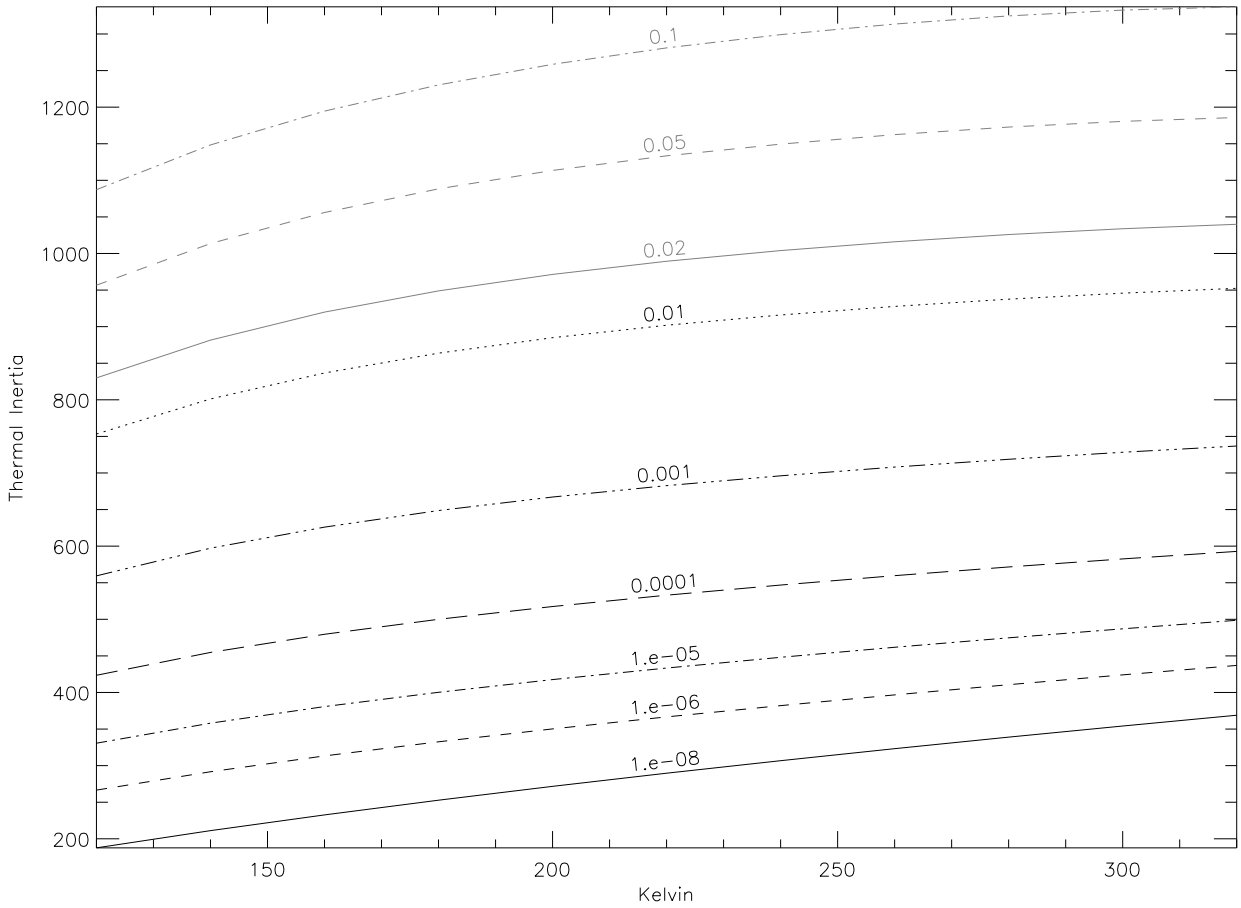


Figure 10: Thermal inertia results using temperature-dependent solids in the Kieffer cemented particulate model. Cement volume fraction ranges from 10 ppb to 10%. cemi.eps

Johnston46=[37] has original measurements. I have used these in IDL routine **pp_co2.pro**

Vesovic90=[70] is synthesis addressing high pressures.

Seiferlin96=[62] Used crushed commercial dry ice; results in Fig. 15 suggest $\lambda$ 0.03 to 0.06 W/m-K at 140K . Sumarokov03=[68] Measurements 1.5 to 35K. They show points up to 100 K from L. A. Koloskova, I. N. Krupskii, V. G. Manzhelii, B. Ya. Gorodilov, and Yu. G. Kravchenko, Fiz. Tverd. Tela Leningrad 16,3089 1974 Sov. Phys. Solid State 16, 1993 1975 (Amer. Inst. Phys indicates available, but I can't locate)

Scalabrin06=[61] Develop 30-term (6 are zero) function to fit massive set of observations from the literature. Eq. 7 with coefficents in Table 3 ; validity range 216.59-1000K, up to 200 Mpa. Table 11 has three low pressure (0.01MPa) points at 225,250,275K; 11.037 12.849, 14.727 mW m-1 K-1. Figure 5 indicates that Johnston and Grilly have quadratic deviation from this new relation, +3.2% at 186K, 0 at about 280, +1.9% at 380. This is similar form, but about twice the magnitude, of deviation from my fit using $\ln \lambda = a + b * \ln T$

Konstan06=[44] shows large decrease in $\lambda$ of solid $CO_2$ with a few percent inert gas as solid solution. Although their work at 140Mpa, the physical explanation seems relevent for $CO_2$/ Ar on Mars.

# 8 Example of use to generate KRC input

Here, the possible different materials for KRC upper and lower layers are completely separate; **KOFTOP** does only one material or intimate-mix composite at a time. Thus, the following sequence is done separately for upper and lower layers.

Set all to defaults

Decide on bulk minerals, use of any cement, and if dirty ice will be involved.

## 8.1 Bulk material

Conductivity: @34 and 35 will list and plot conductivity for all materials:
The two integers to the right of the < are the material and secondary indices
Set these by @12, items 1 and 2
@34: Materials with analytic relations
Then do @31
@35: Materials with data point input,
Then do @32 and 33

Specific heat: @44 will list and plot specific for all materials
The integer and real to the right of the < are the material and secondary value
Set these @15, `parc`: items 1 `=imat` and 2 `=arg3`
item 2 exceptions: If imat =1, set item 3; if imat=8, set item 4.
Item 5 `=arg4` is required for imat= 1 or 8
Then run @41 to get specific heat coeffs

For $H_2O$ ice, special sequences:
Conductivity: @138 =[48,33,335,56,25], 123
Specific heat: @139 =[49,491,5,33,57,25], 123

@710 to set Grain coefs into `park`(k) and `parp`($C_p$) [*,0].

@711 to set Cement coefs into `park`(k) and `parp`($C_p$) [*,1].

## 8.2 Un-cemented Particulates

Using grains with T-independent conductivity; Piqueux unconsolidated model:
@16 set items [0,1,2,8] for Grain radius, pressure, Porosity, Point-contact conductivity
@37 SP09A
This produces `dd4`[temperature, radii,item]
item 0 is grain radius in $\mu$m
item 2 is temperature
item 14 is total conductivity
@377 Extract and transfer items to fit
@74 Produce table of cubic coefficients for k and Cp. Right column is grain radius in $\mu$m
Cp will be same for each radius

### 8.2.1 Cement

Using the values in `park` for cubic fit to variation of k with temperature. . @16, parr[5] sets the cement volume fraction; a negative value will compute a table based on the firm-code `vvset`, which covers each decade from 1.E-8 to 1%, plus 2,5 and 10%.

Use PARTCOND model as function of cement volume; grain, cement and gas have T-dependent conductivity
@13 to set parameters. 2,3,4,5 will be overridden in temperature loop
@717 Calls PARTCOND in T loop. Produces `pp4`[T,cemVol] total conductivity
@74 Produces table of cubic coefficients for k and Cp. Right column is cement volume fraction
Cp will be same for each volume.

## 8.3 Dirty Ice

Presume dirt grains are embedded in ice with good thermal contact. Allow a small fraction of voids. Model this as a linear mix of bulk properties, ignoring conductivity across the voids. @721 will setup a 20-step sequence which

compute this model: Set the bulk rock and ice coefficients as in the §8.1. Put selected rock material into "grain". Put ice properties into "cement". Using the values in `park` and `parp`: compute and print the mix conductivity, specific heat and density.

**@**166: Set the desired values in `pars`

**@**725: Will transfer the material indicies

# 9 Cookbook for generation of KRC T-dependent input values

Peruse Ref 1, particularly Figures 2 and 3

@16,parr [11:13] set the desired temperature range and spacing
defaults are 120,320,20 K
[15:16] set the temperature scaling. they MUST not be changed if generating
coeff. for KRC, where they are firm-coded in **tday.f** .

@25 to create the T points

@20 will list available references; if @12 [9] is set, also all materials

@12: set 1= material index
listed in §3
If set to 3 (Sass) , then @16 set 9= to conductivity at 25C
If planning more than one material, set 4=-1 to auto-index storage
@21 will list all available materials for this ref
set @12:2= secondary index

@31 Extract one material
Will print name and four temperature limits:
1: Low limit for appliability; my estimate
1: Low limit for measured data
1: High limit for measured data
1: High limit for appliability; my estimate

@315 Plot data points

@32 Optional extend to lower temperatures, for data-point materials only
Must be done before any other calls to **koft**. See §3.1
first must have set @12 pari[7]: Cold extension: KofT action
Will print 'no-action' if request was inappropriate
21= extend lowest 2 points linearly
22= extend lowest 2 points using 1/(A+BT)
24= fit data to 1/(A+BT) to extend points
First set @12 pari[8] to the number of lowest T data points to use

@33 Generate cubic-fit coefficients.

@335 will over plot cubic fit on @315

@56 Save coef as conduct.

Specific Heat @40 will list available references; if @15[0] is set, also all materials

@15 set [1] material, and [2] secondary index

@43 get one material

@315 Plot data points

@33 Generate cubic-fit coefficients.

@335 will over plot cubic fit on @315

@57 Save coef as Cp

After the 56 and 57 steps, then can do @59 to print table of k,Cp,I

@710 store current k and Cp as particulate grain properties

@711 store current k and Cp as particulate inter-grain cement properties

Now, primary parameters are grain size and cement fraction.

Particulate Conductivity in vacuum, ratio of total k for P=0/P=500 Pa less than 1.
by 10% for cement volumn of 1.e-5 at 200K

by 1% for cvol of 0.001. at 200K
Effect about 1/2 this at 80K, about 1.5 this at 400K

@13[1] set grain radius [8] set pressure
@717 runs PARTCOND and yield pp4[T,cemVol] net thermal conductivity
@74 prints table of cubic-fit coeffs for k and Cp for each cemVol
@75 print table of I

```
2013 Jan 21 22:25:45 run to compute partially cemented soil to serve as upper
material in sample file

Upper material: weakly cemented particulates:
Grain:  k: BasicRocks_Zoth88    2:4
       Cp: Chlorite_Bert07_Fe=0.89  6:4.89
Cement: k: Limestone Zoth88 2:1
       Cp: Sphene, which has relatively strong T dependence  5:0


  0.00257 >      2.774009    -0.5354000     0.2042885   -0.07103046 <Cond BasicRocks_Zoth88
  0.92818 >      646.6275      246.6678     -49.82160      7.951969 <Sph Bert07_Chlorite_Fe0.89
BasicRocks_Zoth88 Bert07_Chlorite_Fe0.89 Dens=      2400.00
 i    T         k     Cp         I      dif*E6
  0  120.0    3.58  342.19   1715.8     4.365
  1  140.0    3.37  413.34   1828.3     3.397
  2  160.0    3.18  478.97   1913.2     2.770
  3  180.0    3.03  539.48   1979.2     2.337
  4  200.0    2.89  595.24   2031.8     2.023
  5  220.0    2.77  646.63   2074.8     1.787
  6  240.0    2.67  694.03   2110.7     1.606
  7  260.0    2.59  737.83   2140.7     1.461
  8  280.0    2.51  778.41   2165.9     1.344
  9  300.0    2.44  816.15   2186.2     1.246
 10  320.0    2.37  851.43   2201.5     1.161

  0.00581 >      3.738380     -1.211992     0.4624507    -0.1607930 <Cond Limestones_Zoth88
  2.25813 >      580.0737      193.6600     -45.46967      23.37377 <Sph King54_Sphene
Limestones_Zoth88 King54_Sphene Dens=      2400.00
 i    T         k     Cp         I      dif*E6
  0  120.0    5.57  317.57   2061.1     7.313
  1  140.0    5.09  384.08   2165.3     5.518
  2  160.0    4.67  442.46   2226.1     4.395
  3  180.0    4.31  493.84   2259.5     3.634
  4  200.0    4.00  539.34   2275.6     3.091
  5  220.0    3.74  580.07   2281.3     2.685
  6  240.0    3.51  617.17   2281.2     2.372
  7  260.0    3.32  651.76   2277.9     2.121
  8  280.0    3.14  684.95   2273.0     1.912
  9  300.0    2.98  717.87   2266.8     1.731
 10  320.0    2.83  751.64   2258.7     1.568

@13 set parm[8]=546. for pressure in Pa

koftop Enter selection: 99=help 0=stop 123=auto> 74
Tmin,Tmax, Tdel=      120.000      320.000      20.0000
  Grain k  >  2.774009 -0.535400  0.204289 -0.071030 < BasicRocks_Zoth88
 Cement k  >  3.738380 -1.211992  0.462451 -0.160793 < Limestones_Zoth88
  Grain Cp >  646.6275  246.6678  -49.8216    7.9520 < Bert07_Chlorite_Fe0.89
```

```
 Cement Cp >  580.0737  193.6600  -45.4697   23.3738 < King54_Sphene
  1000|err|        c0        c1        c2        c3       Ind.Param
    0.08397 >  0.050087 -0.002145  0.002347 -0.000750 <Con    1.00e-08
 0          >  646.6275  246.6678  -49.8216    7.9520 <Sph    1.00e-08
    0.02715 >  0.119390 -0.015679  0.007531 -0.002559 <Con    1.00e-06
 1          >  646.6273  246.6677  -49.8216    7.9520 <Sph    1.00e-06
    0.01136 >  0.194131 -0.030683  0.013256 -0.004548 <Con    1.00e-05
 2          >  646.6262  246.6667  -49.8215    7.9523 <Sph    1.00e-05
    0.00765 >  0.331213 -0.058424  0.023697 -0.008162 <Con    0.000100
 3          >  646.6148  246.6576  -49.8208    7.9549 <Sph    0.000100
    0.00959 >  0.590457 -0.111003  0.043376 -0.014991 <Con     0.00100
 4          >  646.5007  246.5668  -49.8133    7.9813 <Sph     0.00100
    0.01582 >  1.066522 -0.208885  0.079828 -0.027659 <Con      0.0100
 5          >  645.3812  245.6751  -49.7401    8.2408 <Sph      0.0100
    0.01875 >  1.277624 -0.253056  0.096192 -0.033347 <Con      0.0200
 6          >  644.1807  244.7190  -49.6616    8.5189 <Sph      0.0200
    0.02349 >  1.629155 -0.327826  0.123769 -0.042934 <Con      0.0500
 7          >  640.8301  242.0504  -49.4425    9.2953 <Sph      0.0500
    0.02823 >  1.971912 -0.402363  0.151111 -0.052437 <Con       0.100
 8          >  635.9618  238.1729  -49.1242   10.4234 <Sph       0.100

koftop Enter selection: 99=help 0=stop 123=auto> 75
         T  120.0 140.0 160.0 180.0 200.0 220.0 240.0 260.0 280.0 300.0 320.0
 GasK*1000    4.8   5.9   7.0   8.2   9.5  10.8  12.2  13.6  15.1  16.6  18.1
  Grain  k    3.6   3.4   3.2   3.0   2.9   2.8   2.7   2.6   2.5   2.4   2.4
  Cement k    5.6   5.1   4.7   4.3   4.0   3.7   3.5   3.3   3.1   3.0   2.8
 Grain  Cp  342.2 413.3 479.0 539.5 595.2 646.6 694.0 737.8 778.4 816.1 851.4
 Cement Cp  317.6 384.1 442.5 493.8 539.3 580.1 617.2 651.8 684.9 717.9 751.6
Ind.Param  ____________ Thermal inertia _______________
  1.00e-08  154.3 167.1 177.6 186.7 194.7 201.8 208.4 214.4 220.1 225.4 230.3
  1.00e-06  249.9 267.9 282.0 293.6 303.2 311.6 318.9 325.5 331.3 336.6 341.1
  1.00e-05  323.1 345.4 362.6 376.4 387.7 397.3 405.6 412.8 419.2 424.7 429.3
  0.000100  425.9 454.5 476.3 493.5 507.4 519.0 528.9 537.3 544.6 550.7 555.7
   0.00100  572.1 609.8 638.4 660.7 678.6 693.3 705.6 716.0 724.8 732.1 737.7
    0.0100  775.2 825.7 863.7 893.1 916.5 935.6 951.4 964.6 975.7 984.7 991.4
    0.0200  853.5 908.9 950.5 982.61008.01028.61045.71060.01071.91081.51088.6
    0.0500  979.11042.41089.61125.81154.31177.31196.21212.01225.11235.71243.5
     0.100 1103.91175.01227.61267.61298.81323.91344.41361.51375.61387.11395.6

Select  1.00e-08 cement fraction to yield I~200 at 220K

lower material: H2O Ice
k: koftop: 48
fit to A+B/T fit      2.766722 -1.298966  0.629224 -0.527291 <k H2O:ice3sources
Cp: koftop:,49,491,5,33 yields:
   3.95779 >     1710.648      721.8740      57.44873      24.37532 <SpH H2O:Ice_3sources
```

# 10 Random notes during literature search

Aurangzeb07=[4] present $\rho C_P$ for limestone over 293:443K, but the figure is difficult to follow and the errors are stated to be 10%. The average value of $C_P$ at 293K is about 880.

Slack71=[66] Fig. 2 shows conductivity for 5 natural garnets, Table V lists the measured values for Grossularite, which had the highest values In Waples, neither Fig 13 or 14 seems to agree with equation 18

Pribnow93=[56] has short table of conductivities, uses linear and harmonic means, weighting by volume fraction, as

upper and lower limits for mixtures.

$$\lambda_u = \sum_{i=1}^{n} \phi_i \lambda_i \qquad \text{and} \qquad \frac{1}{\lambda_L} = \sum_{i=1}^{n} \frac{\phi_i}{\lambda_i} \qquad \text{and} \qquad \lambda_G = \sqrt{\lambda_U \lambda_L}$$

Following Sass71, for a two phase system (cuttings in water), uses

$$\lambda_r = \lambda_w \left( \frac{\lambda_m}{\lambda_w} \right)^{\frac{1}{1-\phi}}$$

where $\lambda_w$ is thermal conductivity of water, $\lambda_m$ thermal conductivity of the mixture, $\phi$ the volume fraction of water in the mixture, and $\lambda_r$ the thermal conductivity of the dry rock. And then the square-root of their product as a general representation

```
Title   CRC handbook of physical properties of rocks. Volume III
Creator/Author  Carmichael, R.S.
Publication Date 1984 Jan 01  No access

The estimation of rock thermal conductivity from mineral content: an ...
MJ Drury, AM Jessop - Zentralbl. Geol. Palaeontol, 1983  No access

   99577  Bertoldi01.pdf   http://www.springerlink.com/content/mea9vg4j4363vmx8/
 1957679  ClauserHuenges95.pdf  http://www.geophysik.rwth-aachen.de/html/publikationen.htm
  882459  vasavada99merc.pdf
  370463  Vosteen03.pdf     0-500C conductivity \lambda  Eq 4,5
```

Yang94=[75] no access. Thermal expansion properties of synthetic orthopyroxenes (Fe0.20Mg0.80)SiO3, (Fe0.40Mg0.60)Si (Fe0.50Mg0.50)SiO3, (Fe0.75Mg0.25)SiO3 and (Fe0.83Mg0.17)SiO3 from 296 to 1300K. ... The thermal Debye temperatures are composition-dependent, decreasing linearly from 812 (MgSiO3) to 561 K (FeSiO3), and are systematically higher than the corresponding acoustic Debye temperatures.

Eventually located Birch40=[10]. Figs 2,3,4 show approximate 1/T for several minerals and rocks. Fig 5 shows Anorthosite and gabbro nearly independent of T, Fig 6 shows k of silica glass, increasing nearly linear over 50-300C

For the first time this notion was introduced by the German physicist Paul Debye to express the connection between heat capacity of poly-atomic solid and its elastic coefficient.

$(C_v)_{T\to 0} = 77.938 \cdot 3R \left(\frac{T}{\theta}\right)^3$

where: $C_v$- substance heat capacity,$R$ gas constant, $T$ absolute temperature.

The Debye temperature is constant for a given (present) substance, and defines the maximum frequency in the spectrum of particle vibration of the solid. $\theta = \frac{h\nu_{max}}{k}$

$h$ Planck's constant, $k$ Boltzmann's constant, $\nu_{max}$ maximal frequency of vibration of solid.

```
http://journals.lww.com/soilsci/Citation/1962/12000/
Specific_Heat_Capacity_of_Soils_and_Minerals_As.7.aspx

Specific Heat Capacity of Soils and Minerals As Determined With A Radiation Calorimeter
BOWERS, S. A.; HANKS, R. J.
Soil Science:   December 1962 - Volume 94 - Issue 6 - ppg 392-396

http://ccm.geoscienceworld.org/cgi/content/abstract/53/4/380
```

Bertoldi05=[8]

$C_p = 610.72 - 5140.0xT^{-0.5} - 5.88486x10e6T^{-2} + 9.5444x10e8T^{-3}$ is recommended for thermodynamic calculations above 298 K involving berthierine.

Bertoldi07=[7] 40 to 40 temperature points from 5 to 300K with logarithmic spacing, smoothed into Table 2 covering 5-900K

Determination of specific heat capacity on rock fragments
Ueli Schrli and Ladislaus Rybach
Geothermics Volume 30, Issue 1, February 2001, Pages 93-110

Cermk, V., Rybach, L., 1982. Thermal properties. In: Angenheister, G. (Ed.), Landolt-Brnstein, Numerical Data and Functional Relationships in Science and Technology, Vol. 1a: Physical Properties of Rocks, Springer-Verlag, Berlin, pp. 305-343.

Touloukian, Y.S., Roy, R.F., Beck, A.E., 1981. Thermophysical properties of rocks. In: Touloukian, Y.S., Ho, C.Y. (Eds.), Physical Properties of Rocks and Minerals. Cindas data series on material properties, Vol. II-2, pp. 409-502.

Thermodynamic properties of minerals and related substances at 298.15 K and 1 bar (10/sup 5/ pascals) pressure and at higher temperatures
Robie, R.A. ; Hemingway, B.S. ; Fisher, J.R. 1978
USGS-BULL-1452

Heat capacity, relative enthalpy, and calorimetric entropy of silicate minerals; an empirical method of prediction
Gilpin R. Robinson, and John L. Haas
American Mineralogist; June 1983; v. 68; no. 5-6; p. 541-553

SUPCRT92: a software package for calculating the standard molal thermodynamic properties of minerals, gases, aqueous species, and reactions from 1 to 5000 bar and 0 to 1000 degree C.

Johnson, James W | Oelkers, Eric H | Helgeson, Harold C
Computers & Geosciences. Vol. 18, no. 7, pp. 899-947. 1992
in Fortran, SPRONS92.DAT, database

followup: http://www.geology.wisc.edu/flincs/fi/disc/supcrt.html

JAMES W. JOHNSON, ERIC H. OELKERS, and HAROLD C. HELGESON
Earth Sciences Department, L-219, Lawrence Livermore National Laboratory, Livermore, CA 94550 and Laboratory of Theoretical Geochemistry, Department of Geology and Geophysics, University of California, Berkeley, CA 94720, U.S.A.

Need to login: Soil Science

Christian.Bertholdi@sbg.ac.at Universitat Salzburg
bottom page 381

standard entropy:$S_o = \int_0^{298.15} \frac{C_p}{T} dT$
bottom page 381 ... low-T Cp-T data into three parts fitting each to a $C_p$ polynomial of the form: $Cp = ko + k1T^{-0.5} + k2T^{-2} + k3T^{-3}(+k4T + k5T^2 + k6T^3)$

http://hyperphysics.phy-astr.gsu.edu/Hbase/solids/phonon.html#c2

Derived Debye specific heat (also in Kittel Eq.31)

$U = \frac{9NkT^4}{T_D^3} \int_0^{T_D/T} \frac{x^3}{e^x - 1} dx$

$C_v = 9Nk \left[\frac{T}{T_D}\right]^3 \int_0^{T_D/T} \frac{x^4 e^x}{(e^x-1)^2} dx$ where$T_D$ is the Debye temperature for a material.

Law of Dulong and Petit: Upper limit is: $C_v = 3kN_A = 24.94$ / mole K

## 10.1 SWK

SWKieffer79=[40]

$C_v = C_p - TV\epsilon^2 B$ 3 Eq 29 where: $\epsilon$ is the volume coefficient of thermal expansion. $B$ is the bulk modulus and $V$ is the specific volume. Many in Clark[1966]

$(C_P - C_V)/C_V$ generally <1% at 100K and about 4% at 700K. Exception is halite, about 5% at 300K (page 43.8b)

## 10.2 Palankovski Dissertation

Palankovski00=[49]

Simulation of Heterojunction Bipolar Transistors
Vassil Palankovski Dec. 2002
http://www.iue.tuwien.ac.at/phd/palankovski/node34.html

### 10.2.1 3.2.4 Thermal Conductivity

The temperature dependence of the basic materials and insulators is modeled by a simple power law

$$\kappa_{\mathrm{L}}(T_{\mathrm{L}}) = \kappa_{300} \cdot \left(\frac{T_{\mathrm{L}}}{300\mathrm{K}}\right)^{\alpha}$$

Table 3.5: Parameter values for thermal conductivity

Material $\kappa_{300}$ [W/K m] $\alpha$ Reported $\kappa_{300}$ [W/K m] References

$SiO_2$ 1.38 0.33 1.4 [85,86]

### 10.2.2 3.2.4 Specific heat

The specific heat capacity $c_{\mathrm{L}}$ is modeled by:

$$c_{\mathrm{L}}(T_{\mathrm{L}}) = c_{300} + c_1 \cdot \frac{X - 1}{X + \frac{c_1}{c_{300}}}$$

where $X = \left(\frac{T_L}{300\mathrm{K}}\right)^{\beta}$

Parameter values for the specific heat

Material $c_{300}$ [J/K kg] $c_1$ [J/K kg] $\beta$ Reported $c_{300}$ [J/K kg] References

$SiO_2$ 709 696 1.5 1000

## 10.3 From Vosteen 2003 Section 4:

in abstract, T in C., k in W / m / K

$$\lambda(T) = \frac{\lambda(0)}{0.99 + T(a - b/\lambda(0))} \qquad \text{eq : V3} \tag{1}$$

0-500C for crystalline a=0.0030±0.0015, b=0.0042±0.0006
0-300C for sedimentary: a=0.0043±0.0006, b=0.0039±0.0014

Vosteen03=[71] Section 4: cite Zoth88=[76] who suggest form $k(T) = \frac{A}{350+T} + B$

Zoth88=[76] Manage to display using Google books.

### 10.3.1 Mottaghy08

Mottaghy08.pdf Mottaghy08=[48]

They cite for Vosteen 03: using $Kx$ for $\lambda(x)$

for crystalline, alpine rocks: $K0 = 0.53K25 + \frac{1}{2}\sqrt{1.13K25^2 - 0.42K25}$, using Eq. 1

For Kola samples: $K0 = 0.52K25 + \frac{1}{2}\sqrt{1.09K25^2 - 0.36K25}$, and Eq. 1 is modified slightly in that the constant is 0.99.

Table 2 has k, $\rho$, and $C_P$ for 7 rocks, presumably at 25C.

Cite Seipold98=[64] for: $\kappa(T) = 1/(A + BT) + CT^3$; $10^{-6}$ $m^2$ $s^{-1}$
A=1.25, B=2.13E-3 C=1.25E-10 for amphibolite MUST BE WRONG
A=0.779, B=2.55E-3, C=1.15E-10 for paragneiss

However, in Seipold98=[64] have: thermal diffusivity of amphibolites result in (0.8 0.2) E-6 $m^2$ $s^{-1}$ under ambient conditions.

Form: $\lambda = 1/(A + BT) + CT^3$, T in C.

Fig 5: shows steeper Tc dependence for paragneiss A=0.282 B=6.17E-4 C=1.91E-9 . values at 200C about 2.4 , checked relation

Fig 6: Amphibolite A=0.378 B=1.96E-4 C=0.24E-9 values at 200C about 2.4

—

Seipold98g=[63] tries several simple modifications of the Eucken law
WLF1: $K \equiv \lambda = 1/(A + BT)$
WLF2: $K = 1/(A' + B'T) + C'T^3$
WLF3: $K = D'/T^n$
WLF4: $K = T/(E + FT)$

Table 1 has A and B for 8 rock types. They state extrapolation better with WLF4 than WLF1. Form WLF1 is better for thermal diffusivity

Makes an error in treating $T^3$ as a radiation term when T is in °C

## 10.4 Clauser & Huenges 1995

Clauser95=[15]

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http://www.geophysik.rwth-aachen.de/html/publikationen.htm
 has Clauser pubs
```

page 110: Zoth & Hanel (1988) $\lambda(T) = A + \frac{B}{350+Tk}$ Eq. 3a
Zoth88 derived, using form $K = X/(Tc + 77) + Y$, with X,Y, High T=
474., 1.18, 1100 for basic rocks Fig 10.5
807 0.64, 1300 for acid rocks Fig 10.4
705,0.75, 1200 for metamorphic Fig 10.3
1073,0.13, 500 for limestones Fig 10.2
2960 ,-2.11, 350 salt rocks Fig 10.1
1293,0.73, 1380 Ultra basics Fig 10.6

```
page 112: Values of A and B for Eq 3a nearly all 0C and higher

Buntebarth(1991) 1/k = D+ET   Eq 3b

metamorphics: D=0.16+- 0.03  m K W   E=0.37+-0.03 mK/W
```

Sass et al(1992) propose empirical relation:

$\lambda \equiv k(T) = \frac{\lambda(0)}{1.007+T\left(0.0036-\frac{0.0072}{\lambda(0)}\right)}$

where $\lambda(0) = \lambda(25)\left[1.007 + 25\left(0.0037 - \frac{0.0074}{\lambda(25)}\right)\right]$

## 10.5 Other papers

Although some papers propose models by which k can be derived from vibration spectra, e.g. Giesting02=[22], I did not code up these models.

Aurang08=[3] aurangzebbabar@yahoo.com

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

Several papers by Anne Hofmeister, Hofmeister99=[28], Hofmeister06=[30], Hofmeister07=[31]

Hofmeister01=[29]; Eq. 19 indicates k proportional to Cv

Hofmeister04pre. high-temperature partial derivative of k. Separates lattice from radiation.

Hofmeister06 Fig 7 has k(t) for Grossular derived from diffusivity, density and specific heat 0-1500K. k for Grossular peaks near 100, Pyrope 250K uses form $D = A + B/T + C/T^2$, but says later that at moderate temperatures $1/D = A + BT + CT^2$ is best representation.

Hofmeister07 Concentrates on diffusivity

Hofmeister, A.; Whittington, A. G.; Nabelek, P. I. Not obtained

Horai70b=[36] cites Birch40 for thermal resistivity linear with temperature, and gives coefficients for 7 rocks in Table 2. $R \equiv 1/K = a + b(T - 300)$, R in cm sec deg /cal, T in K

Horai71=[33] Has table of many minerals, but no discussion of T-dependence.

Roufosse74=[58] Theory only; says lattice component (versus radiative component) of minerals should follow $\lambda \propto 1/T$

Models of thermal conductivity of crystalline rocks. Alan M. Jessop
International Journal of Earth Sciences Volume 97, Number 2 / April, 2008
Terrestrial heat flow: Recent advances in modeling and interpretation
% ASU not registered

Abdul06=[1] measures thermal conductivity of sandstone, limestone, amphibolite, granulite, and pyroxene-granulite over 273-473K and up to 1500MPa. Data at every 100C in Table 1. However, values for granulite, and pyroxene-granulite are identical at all T and P, where as Figs 3 4 shows pyroxene-granulite with much higher k and consistent; I use the latter.

Giesting02=[22]k calculated from spectra, modified Debye. No figures nor tables of k versus T. Table III of k does not list temperature

vdBerg01=[69] Eq 1 is from: Hofmeister99=[28]

$k\,(T,P) = k_0\,(298/T)^a \exp\left[-\,(4\gamma + 1/3)\,\alpha\,(T - 298)\right]\left(1 + \frac{K_0' P}{K_0}\right) + \sum_{i=0}^{3} b_i T^i$

where $k_0 = 4.7$ W K$^{-1}$m$^{-1}$, $T$ is in Kelvin, Grueneisen parameter $\gamma = 1.2$, thermal expansivity $\alpha = 2.0$E-5 K$^{-1}$, the bulk modulus $K_0 = 261$ GPa, pressure derivative of bulk modulus $K_0' = 5$. Radiative contribution given by coeff. $b_i$ from least squares fit to spectra of overtones. The fitting parameter $a$ is 0.9 for oxides and 0.3 to 0.4 for silicates.

Cahill89=[11] Zr-, Hf, Y-doped and $Y_{66}$ boron crystals measured from 30K to 1000K

Cahill92=[12] Measures from 30K to ambient using $3\omega$ method[19]. Mostly non-geologic materials, but has several feldspars, data from Linvill. Largest conductivity for nearly pure Albite, $Ab_{99}An_1$

M.L. Linvill 1987, unpublished PhD thesis, Cornell University

I could not find in Cornell Library search

Also: M.L. Linvill R.O. Pohl, in Thermal conductivity 18 (Ed. T.Ashworth and D.R. Smith) 1985, p653

Also: M.L. Linvill and J.W. Vandersande and R.O. Pohl,
Thermal conductivity of feldspars.
Bulletin de Mineralogie. 107,p521-527, 1984

The thermal conductivity of several alkali and plagioclase feldspars was measured over the range 0.3-500 K. Between 10 and 100 K the conductivity decreases by over one order of magnitude from albite to bytownite. In some of the feldspars, the conductivity above 100 K approaches that of glass of composition Ab50An50, indicating very strong phonon scattering. It is tentatively suggested that this scattering occurs at lamellar structures with a spacing of tens of A found within intergrowths in feldspars.-R.A.H.

The Bulletin de Minralogie ceased publication in 1989. Along with the S.F.M.C., the D.M.G. (Deutsche Mineralogische Gesellschaft) and the S.I.M.P. (Societ Italiana di Mineralogia e Petrologia) renounced to their national publications and launched the European Journal of Mineralogy.

Cited by: Abdulagatov, I.M. , Emirov, S.N. , Abdulagatova, Z.Z.
Effect of pressure and temperature on the thermal conductivity of rocks
(2006) Journal of Chemical and Engineering Data
and: Ray, L. , Forster, H.-J. , Schilling, F.R.
Thermal diffusivity of felsic to mafic granulites at elevated temperatures
(2006) Earth and Planetary Science Letters

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Degiovanni, A. and Andre, S. and Maillet, D. in Thermal Conductivity 22 (ed. Tong, T. W.) 623-633 (Technomic, 1994). Could not find

Richard B. Stephens
Intrinsic low-temperature thermal properties of glasses
Phys. Rev. B 13, 852-865 1976
All near 1K

Joseph Callaway
Model for Lattice Thermal Conductivity at Low Temperatures
Phys. Rev. 113, 1046-1051 , 1959
Germanium. predict roughly proportinal to T^-(3/2) for normal material
but T^-2 for single isotope material in the range 50-100K

M. G. Holland
Analysis of Lattice Thermal Conductivity
Phys. Rev. 132, 2461-2471, 1963
Fit silicon and Germanium,2-1000K
use G.A.Slack & C. Glassbrenner Phys Rev, 120 782,1960 and TBPub
M.G.Holland and Neuringer ? Bull. Am. Phys Soc. 8,15,1963
T.T.Geballe & G.W.Hull Phys Rev 110 773 1958

GEORGE S. DIXON and VALENTINA A. STEPHEN and SURINDER K. SAHAI

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A pulse method for studying thermal transport properties of sedimentary rocks
Tectonophysics, 148 (1988) 317-322
limestone diffusivity linear between  20C,11.5 and 130C,7.5 x1.e-3 cm^2/s

Popov03.pdf
Include materials from Ries impact structure.

http://www.osti.gov/energycitations/product.biblio.jsp?osti_id=5659536
Creator/Author    Lagedrost, J.F. ; Capps, W.
Publication Date 1983 Dec 01
Thermal expansions ...  Associated rocks were from 0.6 to 1.6 percent.
Basalts were close to 0.3 percent at 500 C.

http://www.britannica.com/EBchecked/topic/505970/rock/80194/Thermal-expansion
rock type linear-expansion coefficient (in 1.E-6 per degree Celsius)
granite and rhyolite       8 +- 3
andesite and diorite       7 +- 2
basalt, gabbro, diabase  5.4 +- 1
sandstone                 10 +- 2
limestone                  8 +- 4
marble                     7 +- 2
slate                      9 +- 1

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Lindroth, D.P. ; Krawza, W.G.
Heat content and specific heat of six rock types at temperatures to 1000 C
Rep. Invest. - U.S., Bur. Mines; (United States); Journal Volume: 7503
1971 Apr 01
26 pages
```

Bertoldi01=[6] ; Measured 143 to 623 K units= J / mol-K

; fit to Berman and Brown's (1985) form for heat capacities.

Bertoldi07=[7] measured five chlorites of different Fe-Mg composition over 5-303K (data in file Bertoldi07Ap.doc) and presents in Table 2 the smoothed values for $C_P$ from 5 to 900K for the two end-members.

Stolen, S., Glockner, R., Gronvold, F., Atake, T. and Izumisawa, S. (1996) Heat capacity and nearly stoichiometric wustite from 13 to 450 K. American Mineralogist, 81, 973-981.

Major peak in Cp near 190K

# 11 Acknowledgments

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Sylvain Piequeux and Ashwin Vasavada provided incentive and helpful comments along the way.

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