Particulate thermal conduction

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Contents

0.0.1 History

First version 2009feb09, modified 2010mar15
2010jul16 Add dependence on Knudsen Number and revise the numerical intergration section

1 Introduction

This is an unsolicited attempt to look at the form of the variation of thermal conductivity of unconsolidated and consolidated "soils" (spherical grains in a lattice network) as a function of cement volume. It was instigated by a review of the manuscripts by Sylvain Piqueux, [2] [Paper 1] and particularly [3] [Paper 2], and was done largely in 2008nov-2009feb.

Many of the relations developed are coded in: **idl/themis/partcond.pro**. Reference to '@n' is to part n of the large case statement therein.

The equation numbers are the normal LaTeX dynamic way of doing things; the "eq:xxx" to the right of some equations are additional static labels I use for convenience and keying to the code.

§2 develops the form for radiative conductivity, including fractional emissivity

§3 relates the volume of cement disk (cylindrical walls) to the central angle between the host sphere contact point and the edge of the cement disk

§5 Is a simple model of the cement as a flat plate of uniform thickness, but same volume as a meniscus

§6 Is the analytic solution [?] for a meniscus model. Although §6.1 show a solution, the corresponding calculation has wild results, so there must be an error someplace. There are a couple changes of variables, which complicates things a bit. §6.2 shows the form I used for numerical integration, which is the basis for most of the Figures. §6.3 shows small-angle-approximations (SMX) used for some testing (comparisons of full versus the much simpler SMX integrations); it is not used in the results shown.

§7 Has a few random comments related to the IDL code.

§8 Has some results for input values similar to those of [3]

2010jul14 Separate gas conductivity into two parts: between spheres $_g$ and across open cell $_G$, and each is dependant upon Knudsen number.

2 Radiative conductivity in uniform particulate medium

Model as consistent heat flow across stack of radiative intervals.

For packed spheres, the normalized density F ranges roughly from $\pi/6 = 0.5236$ to $\frac{\pi}{3\sqrt{2}} = .7405$. A 1-m cube packed with spheres will contain $F/(\frac{4}{3}\pi r^3)$ spheres, so the number of "layers" along one axis is $N = \sqrt[3]{F/(\frac{4}{3}\pi)}\ \frac{1}{r}$

For each interval

$$H/A = \epsilon\sigma_B T_1^4 - \epsilon\sigma_B T_2^4 = \epsilon\sigma_B \left(T_1^4 - (T_1+\delta)^4\right) \sim -\epsilon\sigma_B 4\delta T^3$$

where A is the radiating area, σ_B the Stephan-Boltzmann constant, and ϵ the emissivity (assumed to be near unity). Basic definition of k is $-H = Ak\frac{dT}{dz}$. Without loss of generality, assume a bulk volume of 1 m cube, with ΔT between upper and lower surface. Across the stack, $\Delta T = N\delta$.

$$k = -\frac{H/A}{\Delta T} = \epsilon\sigma_B 4\delta T^3 \ / \ \Delta T = 4\sqrt[3]{(\frac{4}{3}\pi)/F)}\ r\epsilon\sigma_B T^3 \qquad \text{thus} \qquad k = [3.564:4.0]D\frac{\epsilon}{2-\epsilon}\sigma_B T^3 \tag{1}$$

Where the values in brackets is f_P, the packing factor, D is the grain diameter in meters and the values with brackets represent the range for various packed spheres, the result for non-unit emissivity from the next section is included.

2.1 Non-unit emissivity

Between two plane surfaces of the same emissivity, heat transfer is $H/A = F_\downarrow - F_\uparrow$ where

$$F_\downarrow = \epsilon\sigma T_2^4 + (1-\epsilon)F_\uparrow \qquad \text{and} \qquad F_\uparrow = \epsilon\sigma T_1^4 + (1-\epsilon)F_\downarrow$$

Solve:

$$F_\downarrow = \epsilon\sigma T_2^4 + (1-\epsilon)\left(\epsilon\sigma T_1^4 + (1-\epsilon)F_\downarrow\right) = \frac{(1-\epsilon)\epsilon\sigma T_1^4 + \epsilon\sigma T_2^4}{1. - (1-\epsilon)^2}$$

similarly

$$F_{\uparrow} = \frac{(1-\epsilon)\epsilon\sigma T_2^4 + \epsilon\sigma T_1^4}{1. - (1-\epsilon)^2}$$

$$H/A = \frac{\epsilon\sigma}{2\epsilon - \epsilon^2}\left[(1-\epsilon)T_1^4 + T_2^4 - \left((1-\epsilon)T_2^4 + T_1^4\right)\right] = \frac{\epsilon}{2-\epsilon}\sigma\left[T_2^4 - T_1^4\right] \simeq \frac{\epsilon}{2-\epsilon}4\sigma T^3 \Delta T$$

3 Volume of cement versus contact angle

Symbols

R = radius of conductive sphere
x = central angle from contact point. Unit cell has side of $2R$.
B = central angle to edge of cement cylinder
V_1 = volume of one cement ring between two spheres
V_c = volume of 3 orthogonal cylinders as fraction of unit cell = $\frac{3V_1}{(2R)^3}$
V_s = volume of 3 orthogonal cylinders as fraction of host sphere = $\frac{3V_1}{\frac{4}{3}\pi R^3}$

Model a face-centered lattice, wherein spheres are stacked directly on top of each other. Initial pore proportion is $1 - \frac{4}{3*8}\pi = 0.4764$

$$V_1 = \int_0^B 2\pi R \sin x \cdot 2R(1-\cos x) \cdot d\left(R\sin x\right) \tag{2}$$

for B=90°, this formulation should yield $V_1 = \pi R^2 \cdot 2R - \frac{4}{3}\pi R^3 \equiv \frac{2}{3}\pi R^3$, although at 45°, cylinders begin to intersect and the formula is no longer correct.

$$V_1 = 4\pi R^3 \int_0^B \sin x \cdot (1-\cos x) \cdot d\sin x \qquad \text{eq : V}_1 \tag{3}$$

$$Q \equiv \frac{V_1}{4\pi R^3} = \left(\int_0^B \sin x \cos x \, dx - \int_0^B \sin x \cos^2 x \, dx\right) \tag{4}$$

$$Q = \left[{}_0^B - \frac{\cos^2 x}{2}\right] - \left[{}_0^B - \frac{\cos^3 x}{3}\right] \tag{5}$$

$$Q = \left(-\frac{1}{2}(\cos^2 B - 1)\right) - \left(-\frac{1}{3}(\cos^3 B - 1)\right) \equiv \frac{1}{2}(1-\cos^2 B) - \frac{1}{3}(1-\cos^3 B) \qquad \text{eq : B} \tag{6}$$

For $B = \pi/2$, this yields $Q = 1/2 - 1/3 = 1/6$, as expected. Volume of 3-rings of cement, relative to the volume of sphere, is $V_s \equiv 3V_1/\frac{4}{3}\pi R^3 = 9Q$ is only valid for $B < 45°$

3.1 Small angle approximation

For small angles, these involve small differences of large numbers, so use small-angle approximations:
$\cos x \simeq 1 - \frac{x^2}{2} + \frac{x^4}{4!}$ and $(1. - \delta)^n \sim 1 - n\delta$.
Then $\cos^2 x \sim 1. - x^2$ and $\cos^3 x \sim 1. - \frac{3}{2}x^2$ so $1 - \cos^2 x =\sim x^2$ and $1 - \cos^3 x \sim \frac{3}{2}x^2$. Eq. 6 becomes:

$$Q =\sim \left(\frac{B^2}{2} - \frac{B^2}{2}\right) \equiv 0 \tag{7}$$

Thus, need to include higher-order terms. Including higher-order terms in the trig. functions after integration generates a lot of terms. Rather, try small-angle approximations before integration, and Eq. 3 becomes:

$$Q \simeq \int_0^B x \cdot \frac{x^2}{2} \cdot dx \equiv \left[{}_0^B \frac{x^4}{8}\right] \qquad \text{or} \qquad V_1 \simeq \frac{\pi}{2} R^3 B^4 \qquad \text{eq : Vb} \tag{8}$$

where the ignored terms are two or more degrees higher than those included.

With this approximation, $V_c \simeq \frac{3\pi}{16} B^4$ and $V_s \simeq \frac{9}{8} B^4$; cement volume as fraction of solids is $V_s/(1+V_s)$

4 Gas conductivity

Follow the development of [2], where the conductivity of a gas in a pore k_{gas} is a function of the bulk gas conductivity at the appropriate temperature, k_0 and the Knudsen number Kn.

k_0 is assumed to be known; Paper 1 Eq. 14 gives an emperical relation for CO_2. Paper 1 Equations 30 to 32 give

$$k_{\text{gas}} = \frac{k_0}{1 + e^{\frac{2.15 - \text{Log}_{10}(Kn^{-1})}{0.55}}}$$

The Knudsen number is the ratio of the mean free path to the pore size L, or (Paper 1, Eq. 7)

$$Kn = \frac{k_B}{\sqrt{2}\pi d_m^2} \cdot \frac{T}{LP} \tag{9}$$

where k_B is the Boltzmann constant, and d_m is the molecule collisional diameter; the first term is a constant for a given molecule.

Here, L is taken to be $2R$ in the open corner region and the average separation of the spheres, L_S, in the region between the outer edge of the cement and the projected edge of the grain.

$$L_S = \text{Volume/Area} = \int_B^{\pi/2} 2R\,(1-\cos\theta)\, 2\pi R \sin\theta\; R\cos\theta\; d\theta \;\; / \;\; \int_B^{\pi/2} 2\pi R \sin\theta\; R\cos\theta\; d\theta$$

$$= 2R \left(\int_B^{\pi/2} \left(\sin\theta\cos\theta - \sin\theta\cos^2\theta \right) d\theta \;\; / \;\; \int_B^{\pi/2} \sin\theta\cos\theta d\theta \right)$$

$$= 2R \left(\left[_B^{\pi/2} \frac{\sin^2\theta}{2} + \frac{\cos^3\theta}{3} \right] \; / \; \left[_B^{\pi/2} \frac{\sin^2\theta}{2} \right] \right)$$

$$L_S = 2R \left(1 - \sin^2 B - \frac{2\cos^3 B}{3} \right) \;\; / \;\; \left(1 - \sin^2 B \right) \tag{10}$$

Check limits: $B \to \frac{\pi}{2}, L_S \to 2R$, correct; $B \to 0, L_S \to \frac{2}{3}R$, correct.

To avoid complications in attempt at analytic solutions, the $B \to 0$ limit has been used for all B . This is within 10% for $B < 0.3$ radian. However, the full L_S will be used in the numerical integrations.

5 Crude estimate of net effect of small amounts of cement

Model is a stack of "cement" plate of radius r_c that is Y thick, in series with a cylinder of the sphere material of cross-section σ_h that is $2R - Y$ thick. Treat heat flow as strictly parallel to axis, except for "magic" lateral dispersal at the cement-host interface.

For this crude approximation, include only conduction through the solids, ignoring the effect of gas conduction and radiation.

Let r_c be the radius of the cement cylinder ($\sim BR$ above). Let Y be the average thickness of the cement in the heat-flow direction: $Y \equiv V_1/\sigma_c$.

Let the thermal conductivity of the sphere (the "host" material) be k_h and that of the cement be k_c.

Because of the relatively larger physical cross-sections of the host sphere than the cement ring, assume the effective cross-section of the host sphere σ_h to be $G\sigma_c$; the minimum for G would be unity. One possibility for σ_h would be the geometric mean between the cross-section of the cement ring and central cross-section of the sphere, $G\sigma_c = \sqrt{\sigma_c \cdot \pi R^2}$ or $G = 1/B$. An alternate would be to assume the average: $G\sigma_c = \frac{\sigma_c + \pi R^2}{2}$ or $G = \frac{1/B^2+1}{2}$.

Because cement and host are in series, heat-flow is the same in the cement and host portions.

$$H = \Delta T_c k_c \sigma_c / Y = \Delta T_h k_h \sigma_h / (2R - Y) \tag{11}$$

where $\Delta T = \Delta T_c + \Delta T_h$. Effective net conductivity is $k = H/(2R\Delta T)$

$$k = \frac{H/\,2R}{\frac{YH}{k_c\sigma_c} + \frac{(2R-Y)H}{k_h G\sigma_c}} \tag{12}$$

With some manipulation; get effective thermal conductivity of the cell:

$$\frac{k}{k_h} = \frac{\sigma_c/(2RY)}{\frac{k_h}{k_c} + \frac{2R/Y\ -1}{G}} \tag{13}$$

Using Eq. 8 and with the small-angle approximation: $Y = \frac{1}{2}B^2 R$ and $\sigma_c = \pi(BR)^2$ and $\frac{\sigma_c}{2RY} = \pi$.

$$\frac{k}{k_h} = \frac{\pi}{\frac{k_h}{k_c} + \frac{1}{G}\left(\frac{4}{B^2} - 1\right)} \qquad \text{and} \qquad B = \sqrt[4]{\frac{16}{3\pi}V_c} \qquad \text{eq : kkh} \tag{14}$$

Implemented @2. The results for several options for G are shown in Figure 1. For very small cement fractions, the gas conductivity, and possibly radiation, would be important.

6 Attempt at analytic model for both non-cemented and cemented

Try for face-centered (Paper 1, Fig. 5 left). Start with assumption that all heat flow is parallel to vertical axis. Thus, for any radial distance from contact point, up to end of cylindrical cement, B', which may be zero, heat flow in host is equal to that in cement. Outside this and up to particle radius R, heat flow in solid is equal to sum of gas and radiation heat flow; for an infinitesimal area

$$H_s = H_g + H_r \qquad \text{eq : H} \tag{15}$$

Outside R, there is only gas and radiation heat flow across the full unit cell.

Let temperature of lower side of cell (through center of particle) be T_1 and that of upper side be T_4, temperature at upper surface of lower particle is T_2, temperature at mid-line is T_m, by symmetry (ignoring the small change in T^3, $T_m = (T_1 + T_2)/2$. For notation convenience, define $U \equiv T_m - T_1$ and temperature change across 1/2 the gap is $\delta \equiv T_m - T_2$. R is the sphere radius (and 1/2 the unit cell side), $r = R \sin x$ is the radial coordinate, and y is the vertical distance between the sphere surface and the mid-line; $y = R(1 - \cos x)$; for small angles $y \simeq Rx^2/2$.

General form for heat flow: $\frac{dH}{dA} = k \bigtriangledown T$. For notation simplicity, represent $\frac{dH}{dA}$ by H for each component of heat flow.

Total heat flow across the unit cell is $\mathbf{H_t} = \int_0^R H_{(r)} 2\pi r dr + \mathbf{H_o}$ where $\mathbf{H_o}$ is the heat flow across the open corners of the cell where there is no particle. Beware: $H_{(r)}$ is total heat flow for infinitesimal area and H_r is only the radiative portion.

Effective net conductivity:

$$k_t = \frac{\mathbf{H_t}}{A}\frac{\Delta z}{\Delta T} = \frac{\mathbf{H_t}}{4R^2}\frac{2R}{2U} = \frac{\mathbf{H_t}}{U 2\pi R^2} \cdot \frac{\pi R}{2} \tag{16}$$

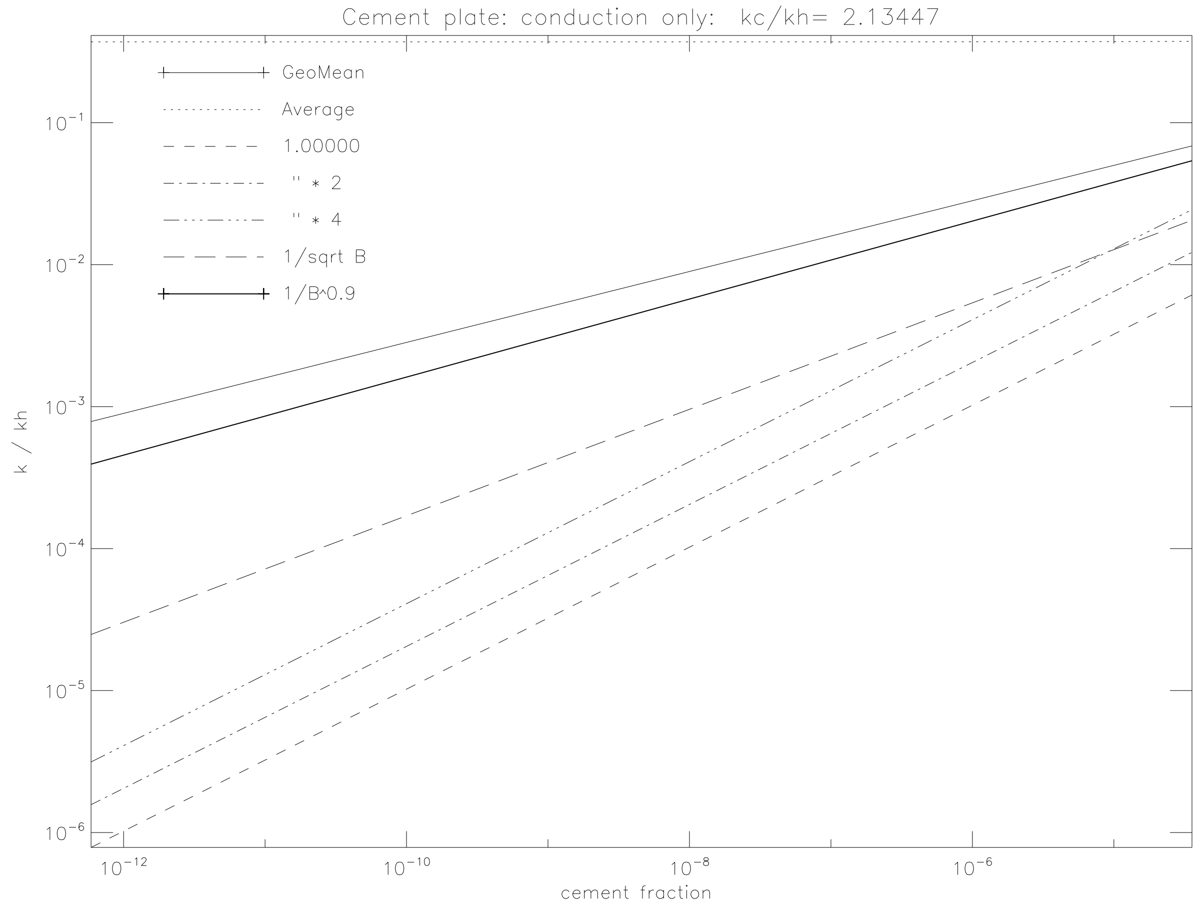

Figure 1: Normalized conduction through circular flat plate of cement between cylinders of host material for several options of $G = \sigma_h/\sigma_c$. Largest B is 40°.

Total heat flow:

$$\mathbf{H_t} = \int_0^{B'} H_c 2\pi r dr + \int_{B'}^{R} (H_g + H_r) 2\pi r dr + \int_R^{\text{corner}} (H_G + H_r) dA \tag{17}$$

Sticking with r as the independent variable leads to forms such as $\int \frac{r}{b+\sqrt{a^2-r^2}} dr$, for which I could not find a solution. Hence the formulation in terms of the central angle x where $r = R \sin x$.

$$\int_A^B F_{(r)} r dr = R^2 \int_{\arcsin \frac{A}{R}}^{\arcsin \frac{B}{R}} F_{(r \to x)} \sin x d \sin x \qquad \text{And} \qquad d \sin x = \cos x \ dx$$

Change coordinates from radial distance from the contact point to angle from the contact point:
$\mathbf{H_t} - \mathbf{H_o} = 2\pi R^2 \int_0^{\pi/2} H_{(x)} \sin x \ d \ \sin x$. Central angle of the edge of cement is B.

For a possible cemented section, allow the effective cross-section in the host to be larger than strictly parallel heat flow by a factor $G_{(B)}$; if this causes significant complications, will drop this option.

$$\mathbf{H_t} = \int_0^{B} H_c 2\pi R \sin x dx + \int_{B}^{\pi/2} (H_g + H_r) 2\pi R \sin x dx + \int_R^{\text{corner}} (H_G + H_r) dA \tag{18}$$

$H_c = k_c \frac{\delta_c}{y}$ and $H_g = k_g \frac{\delta_c}{y}$ and $H_r = \frac{\epsilon}{2-\epsilon} 4 \sigma_B T^3 \cdot 2\delta \equiv C\delta$. Units of C are W m^{-2} K^{-1}.

For $0 \le x \le B$, heat flow in the host is same as in the cement

$$k_h G \frac{U-\delta_c}{R-y} = k_c \frac{\delta_c}{y} \qquad \text{and} \qquad \delta_c/U = \frac{Gk_h}{R-y} / \left[\frac{Gk_h}{R-y} + \frac{k_c}{y}\right] = \frac{1}{1+\frac{k_c}{k_h}\frac{R-y}{Gy}} = \frac{1}{1+\frac{k_c}{Gk_h}\frac{\cos x}{1-\cos x}} \qquad \text{eq : delcu} \tag{19}$$

$$\frac{\delta_c}{Uy} = \frac{1}{y+\frac{k_c}{k_h}\frac{R-y}{G}} = \frac{1}{R(1-\cos x)+\frac{k_c}{Gk_h}R\cos x} = \frac{1/R}{1+\left(\frac{k_c}{Gk_h}-1\right)\cos x} \qquad \text{eq : delc} \tag{20}$$

For $B < x \le \pi/2$, expand terms in Eq. 15 (all units are W m^{-2}).

$$k_h \frac{U-\delta}{R-y} = k_g \frac{\delta}{y} + C\delta \qquad \text{and} \qquad \delta/U = \frac{k_h}{R-y} / \left[\frac{k_h}{R-y} + \frac{k_g}{y} + C\right] \qquad \text{eq : del} \tag{21}$$

$$\delta/U = \frac{1}{1+\frac{k_g}{y}\frac{R-y}{k_h}+C\frac{R-y}{k_h}} = \frac{1}{1+\frac{k_g}{k_h}\frac{\cos x}{1.-\cos x}+\frac{CR}{k_h}\cos x} = \frac{1-\cos x}{1-\cos x+\frac{k_g}{k_h}\cos x+(1-\cos x)\frac{CR}{k_h}\cos x}$$

$$= \frac{1-\cos x}{1+\left(\frac{k_g+CR}{k_h}-1\right)\cos x-\frac{CR}{k_h}\cos^2 x} \qquad \text{eq : delU} \tag{22}$$

$$\frac{\delta}{yU} = \frac{\delta}{U}\frac{1}{R\,(1-\cos x)} = \frac{1/R}{1+\left(\frac{k_g+CR}{k_h}-1\right)\cos x-\frac{CR}{k_h}\cos^2 x} \qquad \text{eq : yU} \tag{23}$$

6.1 Solved integrals

$$\mathbf{H_t} = 2\pi R^2 \int_0^B k_c \frac{\delta_c}{y} \sin x \;\; d\sin x + 2\pi R^2 \int_B^{\frac{\pi}{2}} \left(k_g \frac{\delta}{y} + C\delta\right) \sin x \; d\sin x + (4-\pi) R^2 \left[k_G \frac{U}{R} + CU\right] \qquad \text{eq : Ht} \tag{24}$$

Note that $k_g\frac{\delta}{y} + C\delta = (k_g + CR)\,\frac{\delta}{y} - CR\frac{\delta}{y}\cos x$ in order to separate integrals of similar form.

$$\frac{\mathbf{H_t}}{U 2\pi R^2} = k_c \int_0^B \frac{\delta_c}{Uy} \sin x \; d\sin x + (k_g + CR) \int_B^{\frac{\pi}{2}} \frac{\delta}{Uy} \sin x \; d\sin x - CR \int_B^{\frac{\pi}{2}} \frac{\delta \cos x}{Uy} \sin x \; d\sin x + \frac{4-\pi}{2\pi}\left[\frac{k_G}{R} + C\right]$$

$$= \underbrace{\frac{k_c}{R}\int_0^B \frac{1}{1+\left(\frac{k_c}{Gk_h}-1\right)\cos x} \sin x \; d\sin x}_{I1} + \left(\frac{k_g}{R} + C\right) \underbrace{\int_B^{\frac{\pi}{2}} \frac{1}{1+\left(\frac{k_g+CR}{k_h}-1\right)\cos x - \frac{CR}{k_h}\cos^2 x} \sin x \; d\sin x}_{I2}$$

$$\underbrace{-C\int_B^{\frac{\pi}{2}} \frac{\cos x}{1+\left(\frac{k_g+CR}{k_h}-1\right)\cos x - \frac{CR}{k_h}\cos^2 x} \sin x \; d\sin x}_{I3} + \left[\frac{k_G}{R} + C\right] \underbrace{\frac{4-\pi}{2\pi}}_{I4} \qquad \text{eq : HU} \tag{25}$$

Integral I1 has the form: $\int \frac{\cos x \sin x}{a+b\cos x} dx$. Use variable transform $z = \cos x$ to get $\int -\frac{z}{a+bz} dz$, and the integration limits become 1. to $\cos B$. Then use [1] 91.1 for $X \equiv a + bx$ to get

$$\int \frac{x\; dx}{X} = \frac{1}{b^2}\left[X - a \ln |X|\,\right] \qquad \text{eq : i1} \tag{26}$$

Integral I2 has the form: $\int \frac{\cos x \sin x}{1+b\cos x + a\cos^2 x} dx$. Use variable transform $z = \cos x$ to get $\int -\frac{z}{1+bz+az^2} dz$, and the integration limits become $\cos B$ to 0. Then use [1] 160.11 for $X \equiv ax^2 + bx + c$ to get

$$\int \frac{x\; dx}{X} = \frac{1}{2a} \ln \mid X \mid - \frac{b}{2a} \int \frac{dx}{X} \qquad \text{eq : i2} \tag{27}$$

The RHS integral has solution that depends upon sign of $b^2 - 4ac$, see [1] 160.01. This looks promising, so get rough order of terms using typical values. Using $\epsilon = 0.9$ and $T = 240.$ yields $C = 5.13$; using R =100.E-6 and $k_h = 2$, yields $a = -\frac{CR}{k_h}$=- 2.6E-4; using $k_g = 0.012$, get $b = \frac{CR+k_g}{k_h} - 1$ =-.988 . $c = 1$ and $b^2 - 4ac$=+.979

For $b^2 > 4ac$, roots of $X = 0$ are real; $p, q = \frac{-b\pm\sqrt{b^2-4ac}}{2a}$ and use [1] 160.01;

$$\int \frac{dx}{X} = \frac{1}{a\,(p-q)} \ln \left| \frac{x-p}{x-q} \right| \qquad \text{eq : dxox} \tag{28}$$

Integral I3; can be written:

$$I3 = \int_{\cos B}^{0} \frac{z^2}{az^2+bz+c} dz, \qquad \text{eq : i3} \tag{29}$$

where the three constants have the same values as in Integral I2; use [1] 160.21

$$\int \frac{x^2 dx}{X} = \frac{x}{a} - \frac{b}{2a^2} \ln |X| + \frac{b^2-2ac}{2a^2} \int \frac{dx}{X} \qquad \text{eq : i32} \tag{30}$$

The last integral has the same form as Eq. 28.

Implemented @4.

6.2 Numerical Integration

The forms in Eq. 25 can be integrated by any of several means. Because this simple model does not have lateral heat flow, the cement part can be integrated outward once (for any set of fixed parameters excluding B) saving the results for increasing B and the non-cement parts integrated inward once, also saving the results as a function of B. Then the results for any B found by simply adding the results.

Numerical integration alternate to I2 and I3 is to retain form in Eq. 24 and compute $\int_B^{\frac{\pi}{2}} \left(k_g \frac{\delta}{Uy} + C\delta/U\right) \sin x \; d\sin x$ where the () term is $\frac{\left(\frac{k_g}{y}+C\right)\cdot\frac{k_h}{R-y}}{\left(\frac{k_g}{y}+C\right)+\frac{k_h}{R-y}}$. This is a check against some algebra or coding errors, and was found to yield the identical result.

Expand Eq. 24 in the fashion of Eq. 25, but keeping gas and radiation separate:

$$\frac{\mathbf{H_t}}{U2\pi R^2} = k_c \int_0^B \frac{\delta_c}{Uy} \sin x \; d\sin x + \int_B^{\frac{\pi}{2}} \frac{k_g \delta}{Uy} \sin x \; d\sin x + C \int_B^{\frac{\pi}{2}} \frac{\delta}{U} \sin x \; d\sin x + \frac{4-\pi}{2\pi} \left[\frac{k_G}{R} + C \right]$$

$$= \frac{k_c \Delta x}{R} \sum_0^B \underbrace{\frac{1}{1+\left(\frac{k_c}{Gk_h}-1\right)\cos x} \sin x \cos x}_{J1} + \frac{\Delta x}{R} \sum_B^{\frac{\pi}{2}} \underbrace{\frac{k_g}{1+\left(\frac{k_g+CR}{k_h}-1\right)\cos x - \frac{CR}{k_h}\cos^2 x} \sin x \cos x}_{J2}$$

$$+ C\Delta x \sum_B^{\frac{\pi}{2}} \underbrace{\frac{1-\cos x}{1+\left(\frac{k_g+CR}{k_h}-1\right)\cos x - \frac{CR}{k_h}\cos^2 x} \sin x \cos x}_{Jr} + \left[\frac{k_G}{R}+C\right] \underbrace{\frac{4-\pi}{2\pi}}_{I4} \qquad \text{eq : HN} \tag{31}$$

Implemented @43, with Small-angle-approximation (SMX) for $1 - \cos x$ if single precision and $x < 0.001$.

6.3 Small-angle-approximation integrals

For each of the integrals in Eq. 25, evaluate for $x \ll 1$: then $\sin x \simeq x$ and $\cos x \simeq 1 - x^2/2$

Make B small and replace $\pi/2$ with $q = 2B$ as a test of coding the solved integrals.

I1, using $b = \frac{k_c}{Gk_h} - 1$ and $X = g^2 \pm x^2$, [1] 121.1 and 141.1 :

$$\int \frac{x}{1+b(1-x^2/2)} dx = \int \frac{x\ dx}{1+b-\frac{b}{2}x^2}$$

$$\text{I1} \xrightarrow{b>0} \frac{2}{b}\int \frac{x\ dx}{g^2-x^2} \xrightarrow{141.1} \frac{2}{b}\left[\frac{-1}{2}\ln \mid g^2-x^2 \mid\right] \Longrightarrow \frac{-1}{b}\left[\ln(\mid g^2-\epsilon^2) \mid -\ln g^2\right] \qquad \text{eq : S1} \tag{32}$$

where $g^2 = 2\frac{1+b}{b}$. If $b < -1$ then:

$$\text{I1} \xrightarrow{b<-1} \frac{2}{b}\int \frac{x\ dx}{g^2+x^2} \xrightarrow{121.1} \frac{2}{b}\left[\frac{-1}{2}\ln(g^2+x^2)\right] \Longrightarrow \frac{-1}{b}\left[\ln(g^2+\epsilon^2)-\ln g^2\right] \tag{33}$$

If $-1 < b < 0$ need to define $g^2 = -2\frac{1+b}{b}$, then:

$$\xrightarrow{-1<b<0} \frac{-2}{b}\int \frac{x\ dx}{g^2+x^2} \xrightarrow{121.1} \frac{-2}{b}\left[\frac{-1}{2}\ln g^2+x^2\right] \Longrightarrow \frac{1}{b}\left[\ln(g^2+\epsilon^2)-\ln g^2\right] \tag{34}$$

6.3.1 Treating cos x as 1.

I1 becomes $\int_0^B \frac{\sin x}{1+\left(\frac{k_c}{Gk_h}-1\right)\cos x}\ d\sin x \to \int_0^B \frac{\sin x}{c_1} d\sin x$ where $c_1 = \frac{k_c}{Gk_h}$ yielding $= \left[{}^B_0\ \frac{\sin^2 x}{2c_1}\right] = \frac{\sin^2 B}{2c_1}$.

I2 becomes $\int_B^p \frac{1}{1+\left(\frac{k_g+CR}{k_h}-1\right)\cos x - \frac{CR}{k_h}\cos^2 x} \sin x\ d\sin x \to \int_B^p \frac{\sin x}{1+\left(\frac{k_g+CR}{k_h}-1\right)-\frac{CR}{k_h}}\ d\sin x$ where the denominator is now constant $c_2 = \frac{k_g+CR}{k_h} - \frac{CR}{k_h} = \frac{k_g}{k_h}$ yielding $= \left[{}^p_B\ \frac{\sin^2 x}{2c_2}\right] = \frac{\sin^2 p - \sin^2 B}{2c_2}$.

Similarly, I3 becomes $\int_B^p \frac{\cos x \sin x}{c_2}\ d\sin x = \frac{1}{c_2}\int_B^p \cos^2 x \sin x dx = \frac{-1}{c_2}\left[{}^p_B\ \frac{\cos^3 x}{3}\right]$ and $\cos^3 \epsilon \simeq 1. - \frac{3}{2}\epsilon^2$.
Thus I3 $= \frac{\cos^3 p - Cos^3 B}{3c_2} \simeq \frac{3(p^2-B^2)/2}{3c_2} = \frac{p^2-B^2}{2c_2}$

7 Comments on the IDL code

Code model in **partcond.pro**. Include both analytic and numerical integration. Also include test section with small-angle-approximation where replace $\pi/2$ limit with $2B$. Coded as a large case statement (as is my habit) so it is not very easy to follow.

7.1 Arguments

7.1.1 Parameters

Default values for input parameters:

```
@16: Inputs: Float values
       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  k0: bulk gas cond.  J/m.s.K
       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       500.000  P: Pressure in Pascal
       9     0.0100000  B: Cement contact angle, radian
      10   4.65000e-10  Dm: molecule collision diameter, m
      11       77.7700  vvvv:--numerical parameters
```

```
12      0.00000  flag: test integrals
13     0.100000  beta: SMX limit radian
14      30.0000  nLo: steps along cement [Int]
15      100.000  nHi: steps along gap [Int]
16      0.00000  DP: Flag, double precision
17   0.00100000  B1: Initial B
18      1.10000  Brat: ratio for loop
```

For these values, the contributions to thermal conductivity from the corner areas are: gas = 0.000643805, radiation = 0.000146148, and their sum = 0.000789953.

7.1.2 Actions

Targets in the large case statement:

@-4... return 43 [nB,2] 0]=volume fraction cement 1]=net conductivity
@-2... 2: return,knet
@0.... Stop
@123.. start auto-script
@125.. kons=[20,4,42,44,126,-3] Loop over set of Bval
@126.. loop sequence
@127.. kons=[20,43,128,-3] Loop kc REQ 43
@128.. loop sequence
@131.. kons=[20,2,43,-1,431,-1,432,-1,433,-1,434,-1,435,-1,436] std
@132.. kons=[4,42,44,51,-1,57,-1,577] Details for one Bval
@16... Modify parr
@20... Set limits and constants. Auto after 16
@2.... Crude cement only
@4.... Solved integrals
@42... Simplest numerical integration
@425.. Simplest numerical integration 2010jul
@43... Numerical integration for all B
@4302. Test of 42 & 43
@431.. CHART: vvv
@4312. vrs vol.
@432.. CHART www
@4322. vrs vol.
@433.. Plot k_t
@434.. vrs vol.
@435.. Plot 5A1
@436.. 5B1
@437.. Plot 5A
@4372. 2nd set
@438.. 5B
@44... Sum parts REQ 4,42
@51... Plot del/U vrs B
@52... CHART,qqq
@53... CLOT,qqq
@54... CHART knet
@56... CHART qab
@561.. " qb/qa
@562.. " qb*qa
@57... CLOT qab
@577.. " Log10
@58... Add parr 12:14 Subtitle
@77... oldstuff:

Standard actions of **kon91**:

```
0=Stop  121=kons=-3  122=Edit Kons      801/803 output to LP/.jpg
Plots : 8=new  80=restart  85[x]=SETCOLOR  87=close  88=subtitle  9=plot
MAKE99: 991=Expand current kons   992/995=1-line each   994=expand all
```

7.1.3 Arrays

Contents of the `vvv` [*,8] array (Figure 2):
- 0] B as independent variable
- 1] G, the Grain conductivity factor
- 2] Knudsen number
- 3] gas conductivity
- 4] denominator in I2 and Ir
- 5] J1 function; Normalized heat flow through cement
- 6] J2 function; Normalized gas heat flow
- 7] Jr function; Normalized radiative heat flow

Contents of the `www` [*,4] array (Figure 3):
- 0] outward summation of J1 $= q\frac{k_c}{R} \cdot \sum$ vvv[*,5]
- 1] inward summation of J2 $= q\frac{1}{R} \cdot \sum$ vvv[*,6]
- 2] inward summation of Jr $= qC \cdot \sum$ vvv[*,7]
- 3] total of above 3, plus the open corner conduction
  where $q = \frac{\Delta x}{\frac{\pi}{2}R}$

7.1.4 Common Sequences

Input for $G =$ parr[7].
- if ≤ -2, uses $G = 1/B$
- else if ≤ -1, uses $G = \frac{1/B^2+1}{2}$.
- else if < 1 uses $G = 1/B^x$
- else if ≥ 1 uses that fixed value

@42 does one B in detail

@43 does a larger range of B values at once.

To generate results for 6 values of k_c for 130 values of B takes 8 millisec.

Make Fig 4 by defaults, 127,437, 16,: 7=G=.5, 127, 4372, 16: 7=G=.9, 127, 4372
Make Fig 5 as above; change only 437 to 438, leave 4372

8 Results

NOTE: All in this sub-section used $k_g = k_G =$ constant. The routine is archived as partcond.2010may16

The small value of a in the analytic integrals leads to large values for some terms in I2 and I3, and I have not been able to get realistic results; must be an error in the algebra or code someplace.

Analytic solution to integrals involves small differences of large numbers, but single versus double precision yields virtually same result, so numerical precision is not the source of the unrealistic results.

Numerical integration of alternate form (last sentence of §6.1) had initially been run in double precision to avoid zero divide, so I added a small-angle approximation, single precision now agrees with numerical integration of Eq. 25 to six decimal places. The ratio of $\frac{\left(\frac{k_g}{y}+C\right)}{\frac{k_h}{R-y}}$ ranges over 6 orders of magnitude, whereas their product ranges over 3.5 orders of magnitude.

Coded test cases for small-angle approximation and numeric integrations agree well.

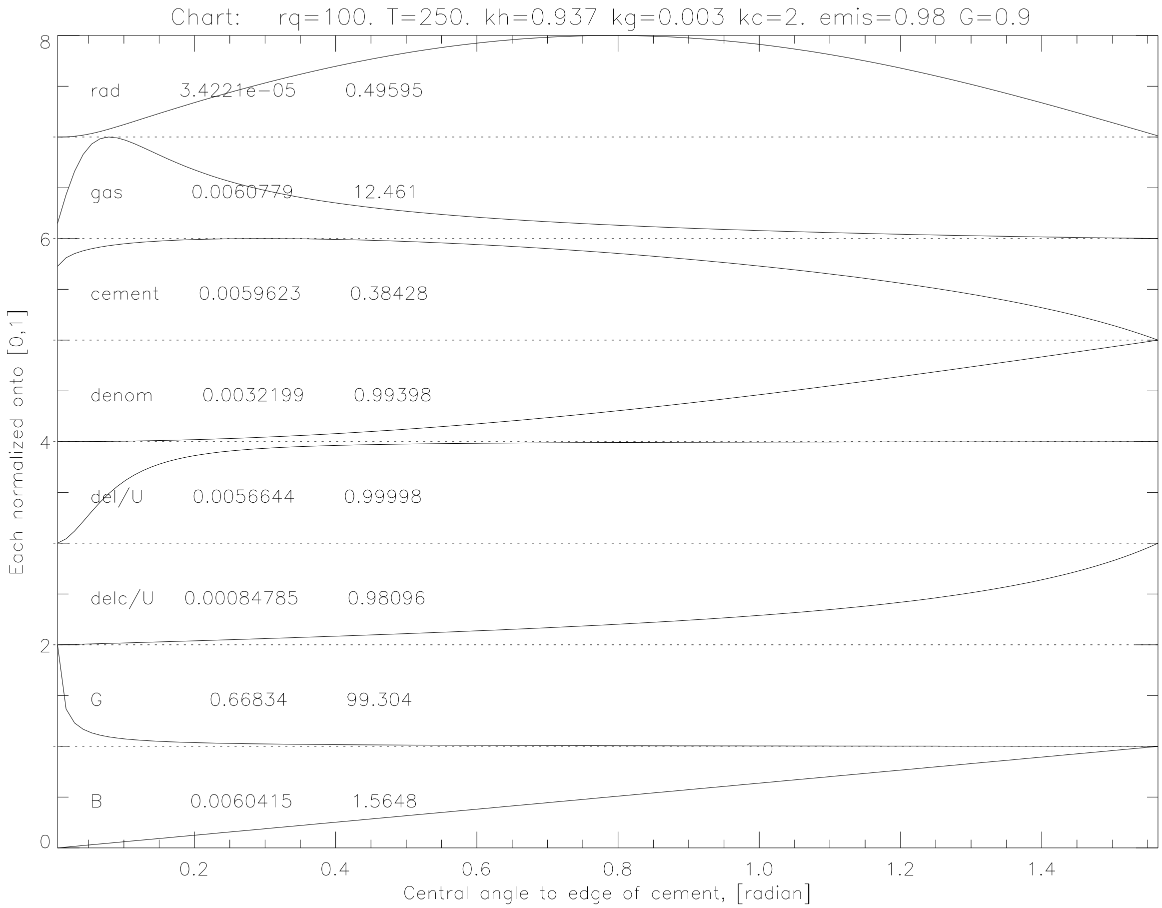

Figure 2: Chart of radial behavior, each scaled to the ranges listed, for the independent heat-flow elements; conditions are shown in the upper label. The top three curves are the heat flow due to cement conduction, gas conduction, and radiation, as a function of radius. del/U is the fractional temperature jump across the open gap; delc/U the corresponding temperature difference with cement in place; there would be a substantial lateral temperature discontinuity at the edge of the host sphere with this model when B is 0.2 radian.

The ratio of Gas/radiation conduction ranges from 150 for small B to 20 for large. The cement has greater conduction than gas for $B > 0.085$ radian, or cement volume $> 5{\times}10^{-5}$, for the parameters shown in Figures 2 and 3.

The differences between the results here and in [3] are probably from two main differences in the models:

1. Lateral expansion of heat flow away from the contact point. Crudely estimated here by the G factor
2. Heat flow through the four cement disks around the axes perpendicular to the main heat flow. Omitted entirely here. This should be significant only for large cement volume fractions.

```
generate Fig 5A       to generate 5B, change only 437 to 438
43  127  8  437   16,7 -2   127 4372  16,7 -1  127  4372  88 9

@42 produces the numeric integration for one B value ggg =[I1,I2,I3]
IDL>  print,ggg
   0.00238796      2.24765      1.80089
```

8.1 Using variable k_g: 2010jul14

Figures 6 and 7 are the revised versions of Figs. 2 and 3 respectively.

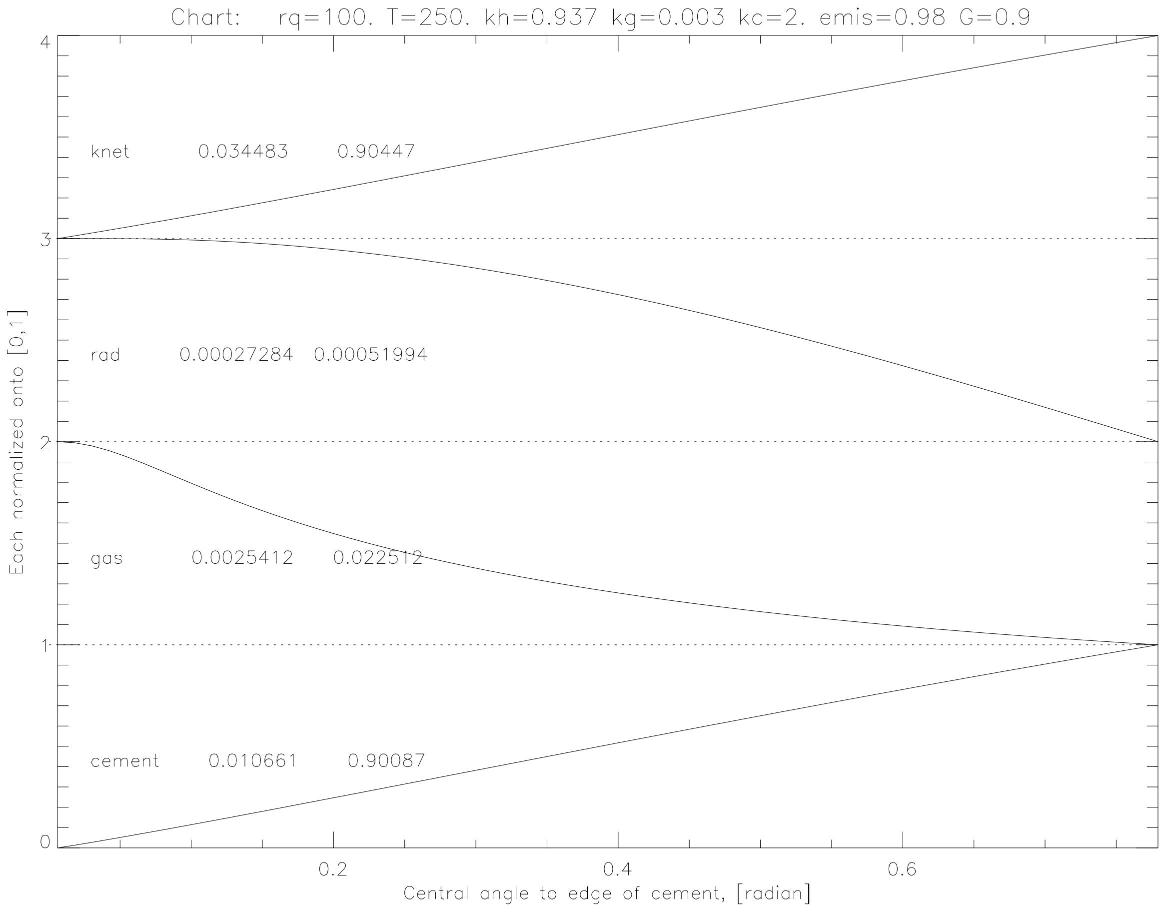

Figure 3: Chart of heat-flow magnitudes and net conductivity as a function of central angle to the edge of cement, same conditions as Figure 2. See §7 for full list of curves for www

References

[1] H. B. Dwight. *Tables of Integrals and other Mathematical Data.* MacMillan, New York, 1961. 4th ed., 336 pp.

[2] S. Piqueux and P. Christensen. A model of thermal conductivity in planetary soils: 1. Theory for unconsolidated soils. *J. Geophys. Res. (Planets)*, 114(E13):9005–+, September 2009.

[3] S. Piqueux and P. Christensen. A model of thermal conductivity in planetary soils: 2. Theory for cemented soils. *J. Geophys. Res. (Planets)*, 114(E13):9006–+, 2009.

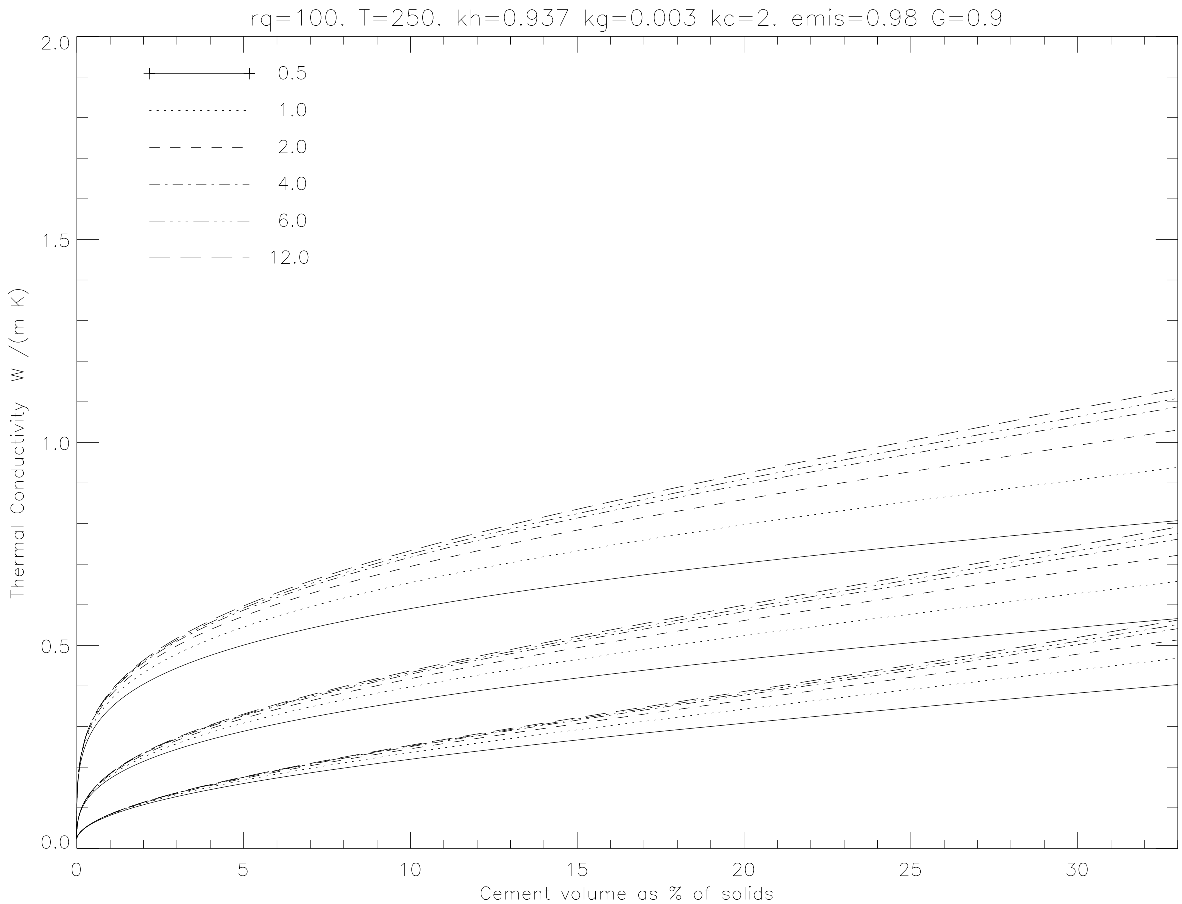

Figure 4: Net thermal conductivity as function of cement fraction for several cement thermal conductivities and 3 options for $G = \sigma_h/\sigma_C$; similar to Fig 5A in Paper 2. Values of k_c shown in the legend. The lower set of 6 curves is for $G = 1$, then middle set for $G = 1/\sqrt{B}$ and the upper set for $G = 1/B^{0.9}$.

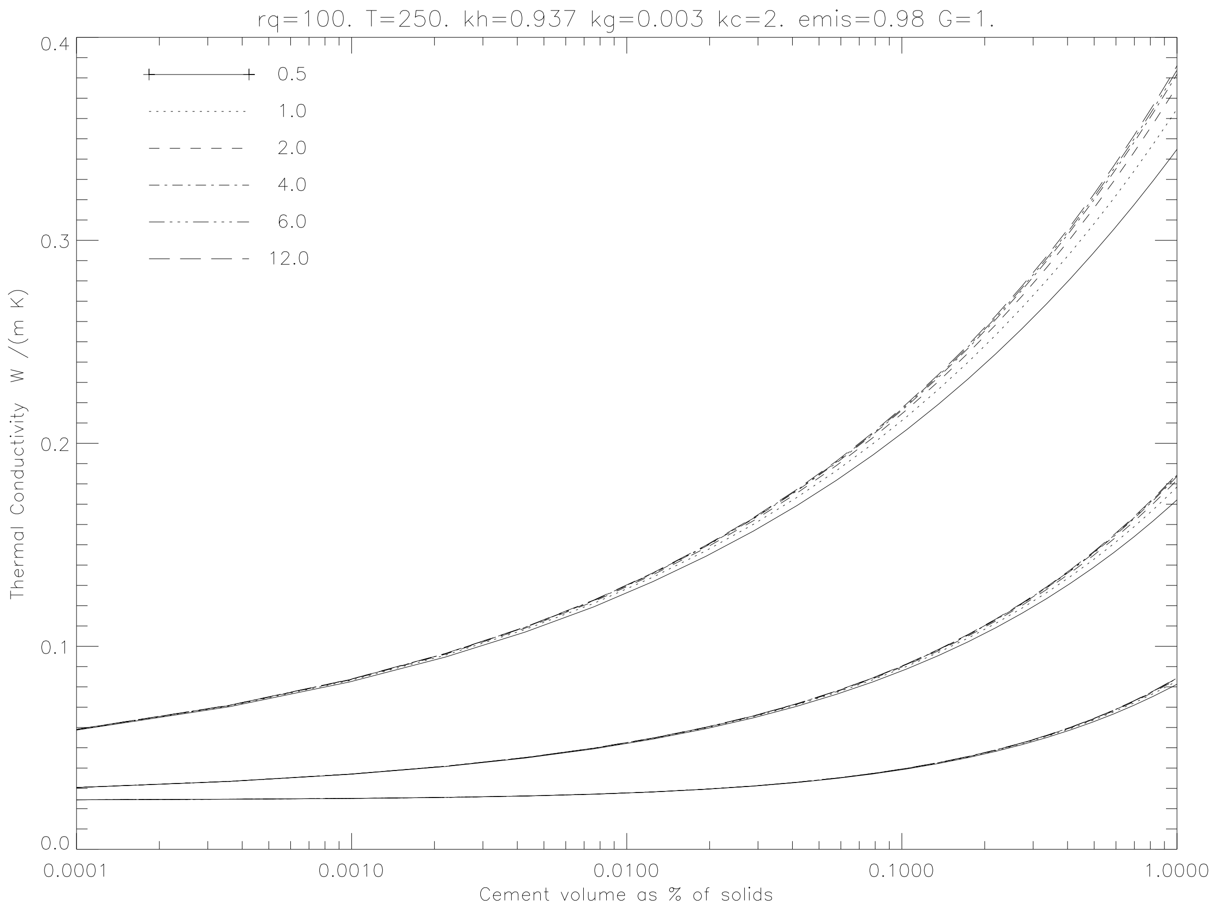

Figure 5: Same data as Figure 4, with logarithmic abscissa; similar to Fig 5B in Paper 2.

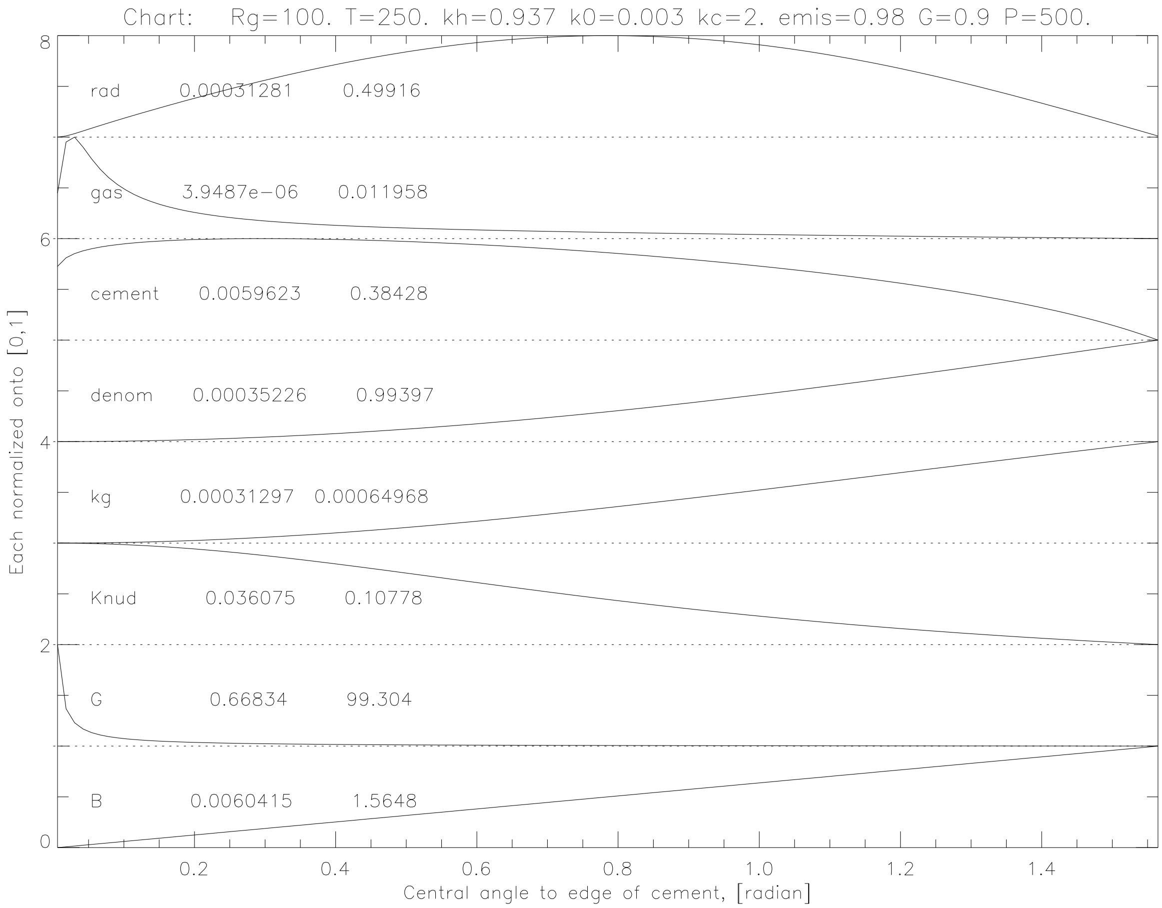

Figure 6: Chart of radial behavior, each scaled to the ranges listed, for the independent heat-flow elements; conditions are shown in the upper label. The top three curves are the heat flow due to cement conduction, gas conduction, and radiation, as a function of radius. Third and 4th curve show the Knudsen Number and the resulting gas conductivity. See §7 for full list of curves for vvv.

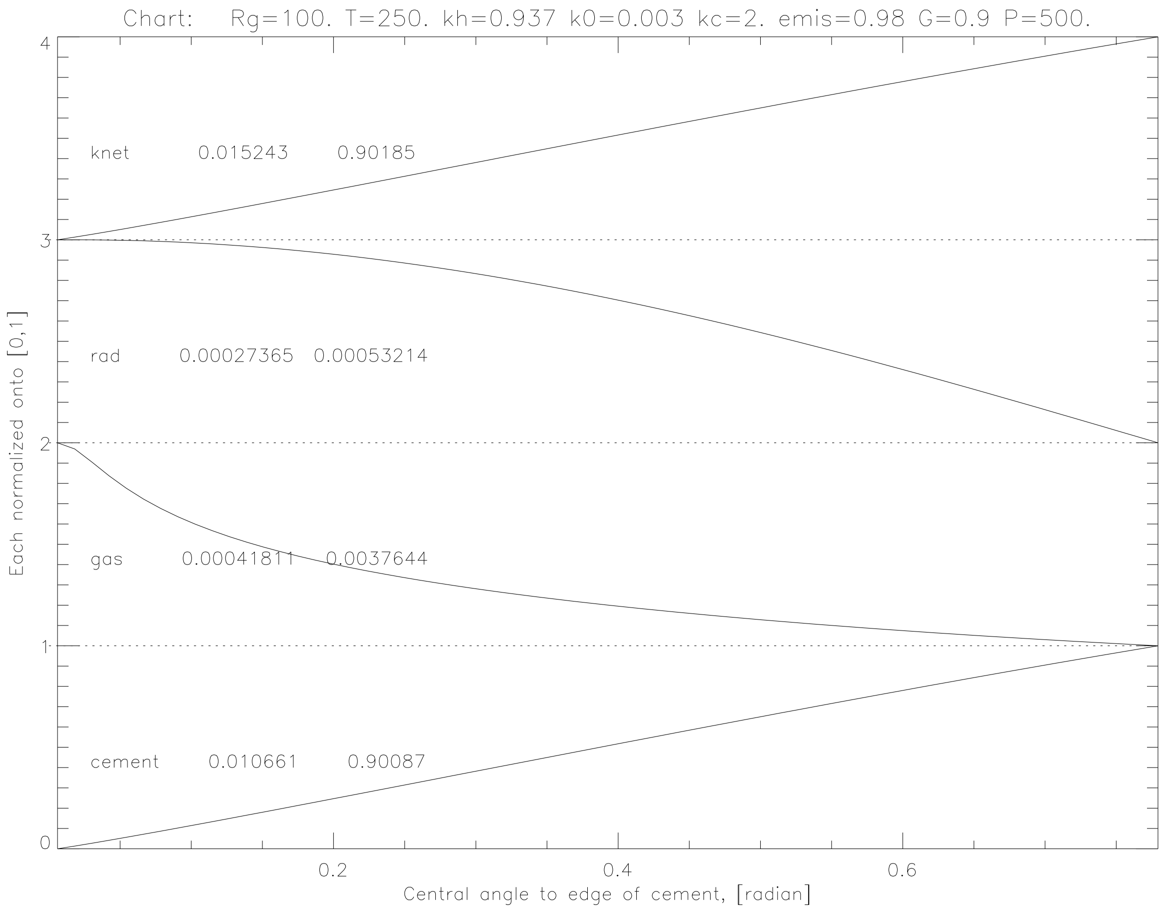

Figure 7: Chart of heat-flow magnitudes and net conductivity as a function of central angle to the edge of cement, same conditions as Figure 2. See §7 for full list of curves for www