Effective Thermal Conductivity Errors by Assuming Unidirectional Temperature and Heat Flux Distribution Within Heterogeneous Mixtures (Nanofluids)

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Abstract: - It is common practice to approximate temperature distribution and heat flux as unidirectional for heterogeneous mixtures if exposed to "over-all unidirectional" boundary conditions. This approach has been used to model and to arrive at the effective (or over-all average) thermal conductivity of heterogeneous mixtures (nanofluids). It is shown here, however, that due to the heterogeneity of system structure and properties the temperature distribution and heat flow will not be unidirectional (one-dimensional) and the errors due to such unrealistic (physically impossible) approximation may be much higher than anticipated.

Key-Words: - Effective thermal conductivity, unidirectional heat transfer, heterogeneous mixtures, nanofluids, cubic model, Maxwell model

1. Introduction

A unidirectional analysis and results of evaluating the effective (*e*) thermal conductivity k_e of nanofluids, a heterogeneous mixture of uniformly distributed spherical particles (*p*) in common fluid (*f*), is provided by Yu and Choi [1] for the cubical arrangement of spherical particles in base fluid, further-on referred to as the "*cubic model*" (without a liquid sublayer, thus corresponding to the Maxwell model [2], i.e., the effective media theory for dilute solutions where thermal interactions between particles are negligible). The effective thermal conductivity ratio, $k_e^* = k_e / k_f = 1.33$, based on the "cubic model," for volumetric concentration, $C_v = V_p /(V_p + V_f) = 1\%\ vol$, of copper particles in water ($k_p^* = k_p / k_f = 401/0.615 = 652$), was substantially higher than the corresponding Maxwell equation value of only 1.03. Since the difference, for the virtually the same heterogeneous concept, is surprisingly large (33% versus 3% increase), the unidirectional analysis of the cubic model is revisited again and its physical shortcomings are analyzed below, see also Fig. 1. Furthermore, the same problem (the exactly same geometry, material properties and boundary conditions) was solved using a FEM numerical method (thus solving the full, 3-dimensional heat conduction differential equation) and the results agreed with the Maxwell model (within expected numerical errors), which confirms that the unidirectional "cubic model" is unrealistic and inappropriate. The erroneous, "cubic model" over-prediction of the effective thermal conductivity (TC) is circumstantial and does not explain experimentally observed increase of TC of nanofluids due to other reasons, like different interfacial particle-fluid interactions, special particle alignments and agglomerations in force fields, particle Brownian motion, and other known and unknown phenomena. The Maxwell and "cubic model" predictions, based on continuum media theory, everything else being the same, should give the same results regardless of the spherical particle size. For example, a 1 *cm* copper sphere centered in a cube with a solid material of TC as water, or 10 *nm* copper nano-sphere centered in "stationary" water cube, should have the same effective TC if other phenomena are absent as the two models assume, but their predictions differ substantially.

2. Analysis

For the so-called uniform distribution of a small concentration of solid particles in base fluid, a uniform cubic arrangement [1] may be assumed and analysis performed for the characteristic cell of a single particle centered in a cube of fluid as presented on Fig. 1.

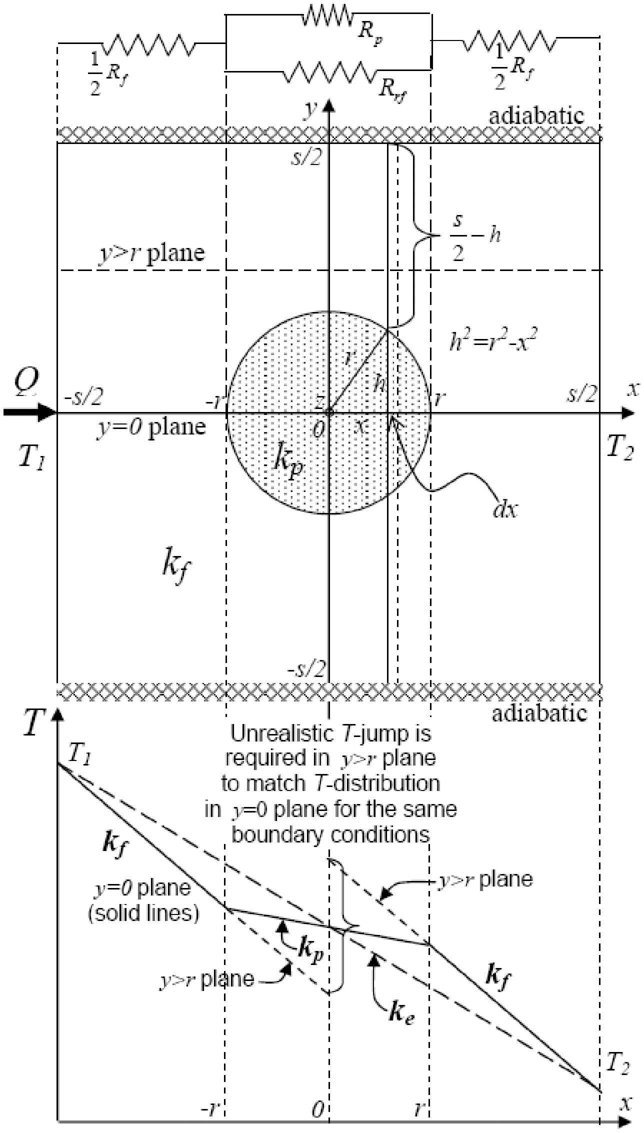

Fig. 1: Characteristic heterogeneous cell for "uniform distribution" of spherical particles (*p*) of radius, *r*, centered in a cube of side, *s*, with fluid (*f*) corresponding (thermally) to an effective (*e*) homogeneous mixture.

This also corresponds to the Maxwell model, i.e. the random distribution (equally in all directions) of spherical particles which do not interact thermally (far away from each other, i.e. for relatively small particle concentrations). Those continuous (but heterogeneous) media models produce the same results for the intensive properties (per unit of system size) and similar systems, thus the results do not depend on the absolute but relative system size. Therefore, the effective thermal conductivity (TC) for uniform particle distribution will not depend on the particle size but only the concentration in the base fluid for the same properties of the particles and the fluids.

The objective is to evaluate the so-called "effective thermal conductivity (TC)," i.e., to reduce the heterogeneous system or its representative cell to the corresponding homogeneous system with hypothetical effective TC which will provide the same conduction heat transfer under arbitrary boundary conditions (TC being a property). Constant temperature boundary condition (BC) on two opposite cube faces and adiabatic on all other cube faces, are chosen for simplicity, see Fig. 1, so that the effective (over-all average) thermal conductivity may be simply determined, using the Fourier law of heat conduction as, $k_e = \dfrac{Q}{A(T_1 - T_2)/s}$; where Q is the total heat conduction rate through the box of side *s* from one face at temperature T_1 to the opposite face at a lower temperature T_2 (in *x*-direction on Fig. 1); and $A = s \cdot s$ is the boundary face area. Since the boundary heat flux is in the *x*-direction only (the other boundary faces being adiabatic) it is tempting to assume that the heat flux, and thus temperature distribution within the heterogeneous box is unidirectional (on Fig. 1 in *x*-direction only), resulting in the following correlations for the steady state and one-dimensional heat conduction, $\dfrac{\partial(\,)}{\partial t} = \dfrac{\partial(\,)}{\partial y} = \dfrac{\partial(\,)}{\partial z} = 0;\ Q(x) = const$, i.e.:

$$Q = A \cdot k_e \frac{\overbrace{T_1 - T_2}^{\Delta T}}{s} = s^2 k_e \frac{\Delta T}{s}$$

$$\Rightarrow \frac{\Delta T}{Q} = \frac{1}{s \cdot k_e} = const \qquad (1)$$

$$Q = -A \cdot k \cdot \frac{dT}{dx} \Rightarrow -dT = \frac{Q}{A \cdot k} dx$$

$$\Rightarrow -\int_{T_1}^{T_2} dT = Q \int_{-s/2}^{s/2} \frac{dx}{A(x) \cdot k(x)} \qquad (2)$$

$$\frac{\overbrace{T_1 - T_2}^{\Delta T}}{Q} = \underbrace{\int_{-s/2}^{-r} \frac{dx}{(s^2)k_f}}_{R_f/2} + \underbrace{\int_{-r}^{0} \frac{dx}{(\pi h^2)k_p + (s^2 - \pi h^2)k_f}}_{R_{p+rf}/2} + \underbrace{\int_{0}^{r} \frac{dx}{(\pi h^2)k_p + (s^2 - \pi h^2)k_f}}_{R_{p+rf}/2} + \underbrace{\int_{r}^{s/2} \frac{dx}{(s^2)k_f}}_{R_f/2}$$

$$\frac{1}{s \cdot k_e} = 2 \cdot \left[\int_0^r \frac{dx}{(\pi h^2)k_p + (s^2 - \pi h^2)k_f} + \int_r^{s/2} \frac{dx}{(s^2)k_f} \right], \text{ where } h^2 = r^2 - x^2 \text{ (see Fig.1)} \qquad (3)$$

$$\frac{1}{k_e} = 2s \left[\int_0^r \frac{dx}{(\pi(r^2 - x^2)k_p + (s^2 - \pi \cdot r^2 + \pi x^2)k_f} + \frac{(s/2) - r}{(s^2)k_f} \right] \qquad (4)$$

Or, in dimensionless form, by introducing the following substitutions:

$$k_e^* = k_e / k_f; \; k_p^* = k_p / k_f \qquad (5)$$
$$x^* = x / r; \; s^* = s / r$$

$$k_e^* = \frac{1}{1 - \frac{2}{s^*} + 2s^* \int_0^1 \frac{dx^*}{s^{*2} + \pi(1 - x^{*2})(k_p^* - 1)}} \qquad (6)$$

$$= \frac{1}{1 - \frac{2}{s^*} + 2s^* \int_0^1 \frac{dx^*}{\underbrace{[s^{*2} + \pi(k_p^* - 1)]}_{A^2} - \underbrace{[\pi(k_p^* - 1)]}_{B^2} x^{*2}}}$$

$$= \frac{1}{1 - \frac{2}{s^*} + \frac{s^*}{A \cdot B} \cdot \ln \frac{A + B}{A - B}}, \text{ where,}$$

$$A = \sqrt{s^{*2} + \pi(k_p^* - 1)};$$

$$B = \sqrt{\pi(k_p^* - 1)} \text{ and } s^* = \sqrt{\frac{4\pi}{3C_v}}$$

For a given particle radius r and desired volumetric concentration C_v, the required cube size s is obtained from:

$$C_v = \frac{V_p}{V_f + V_p} = \frac{\frac{4\pi}{3} r^3}{s^3} = \frac{4\pi}{3 \cdot s^{*3}} \qquad (7)$$

$$\text{or } s^* = \sqrt{\frac{4\pi}{3C_v}}$$

The above correlations are derived using the same modeling as done by Yu and Choi[1] and the result (Eq. 6) is identical as their Eq. (10) [1], also presented here for reference as Eq. (8) with current nomenclature (original[1] $r^* = 1/s^*$), along with Maxwell correlation[2], Eq. (9):

As stated above, the effective thermal conductivity ratio, $k_e^* = k_e / k_f = 1.33$, based on the "cubic model," Eq. (6 or 8), for volumetric concentration, $C_v = V_p /(V_p + V_f) = 1\% \; vol$, of copper particles in water ($k_p^* = k_p / k_f = 401/0.615 = 652$), was substantially higher than the corresponding Maxwell equation value of only 1.03 using Eq. (9). The difference of the results, for the virtually the same heterogeneous concept, is surprisingly large (33% versus 3% increase). The substantial errors of the cubic model results are due to unrealistic assumptions that the heat flux within the heterogeneous particle-fluid cell, see Fig. 1, is in x-direction only, i.e. that the temperature field is function of x only. As seen on Fig. 1, for the given constant-temperature BCs, if the temperature is function of x only as is assumed, the local heat flux must be constant for the steady state conduction heat transfer process through the homogeneous liquid regions, $-s/2<x<-r$ and $r<x<s/2$. However, such constant heat flux will produce different temperature drops along different parallel paths in the non-homogeneous particle-fluid region, $-r<x<r$: for example, through the particle (in $y=0$ plane) and outside of the particle region through the fluid ($|y|>r$ plane), thus "breaking" the temperature continuity from one to the other BCs, which is physically impossible. This will always be an issue except in three special cases: (1) serial particle distribution so that heterogeneity (change of material properties are in x direction only but not in the other (y & z) directions so that integration along x will properly account for any variability; (2) parallel particle distribution so that heterogeneity is layered between the same temperature BCs and heat flux will be different to accommodate different TC of the parallel layers; and (3) serial

$$k^*_{e\,YC} = \frac{1}{1 - \frac{2}{s^*} + \frac{s^*}{\sqrt{s^{*2} + \pi(k^*_p - 1)} \cdot \sqrt{\pi(k^*_p - 1)}} \cdot \ln \frac{\sqrt{s^{*2} + \pi(k^*_p - 1)} + \sqrt{\pi(k^*_p - 1)}}{\sqrt{s^{*2} + \pi(k^*_p - 1)} - \sqrt{\pi(k^*_p - 1)}}} \qquad (8)$$

$$k^*_{e\,Mxw} = 1 + \frac{3C_v}{1 - C_v + \frac{3}{k^*_p - 1}} = \frac{2 + k^*_p + 2C_v(k^*_p - 1)}{2 + k^*_p - C_v(k^*_p - 1)}; \qquad (9)$$

where $C_v = \dfrac{4\pi}{3(s^*)^3}$

distribution of segments with parallel particle distribution but without any contact resistance between the segments to provide for equalization of temperature and redistribution of different heat fluxes in transverse direction as needed for different parallel sublayers. The last case is unrealistic since there is no ideal thermal contact case, but is widely use in electrical circuitry where different arrangements of electrical resistors are interconnected with connectors of negligible resistance. Similar concepts of thermal resistances in series and/or parallel combinations are used but errors could be much higher than anticipated as is illustrated here.

The effective TC may be derived using the related thermal resistances as depicted at the top on Fig. 1, and the effective TC will be the same as the cubic model, Eq. (6), i.e.:

$$R_e = R_f + \underbrace{\left(\frac{1}{\frac{1}{R_p} + \frac{1}{R_{rf}}} \right)}_{R_{p+rf}}; \qquad (10)$$

where, $R_e = \dfrac{s}{(s^2)k_e}$; $R_f = \dfrac{s - 2r}{(s^2)k_f}$;

$$R_p = \int_{-r}^{r} \frac{dx}{(\pi h^2)k_p}; \; R_{rf} = \int_{-r}^{r} \frac{dx}{(s^2 - \pi h^2)k_f}$$

$$Note: \; h^2 = r^2 - x^2$$

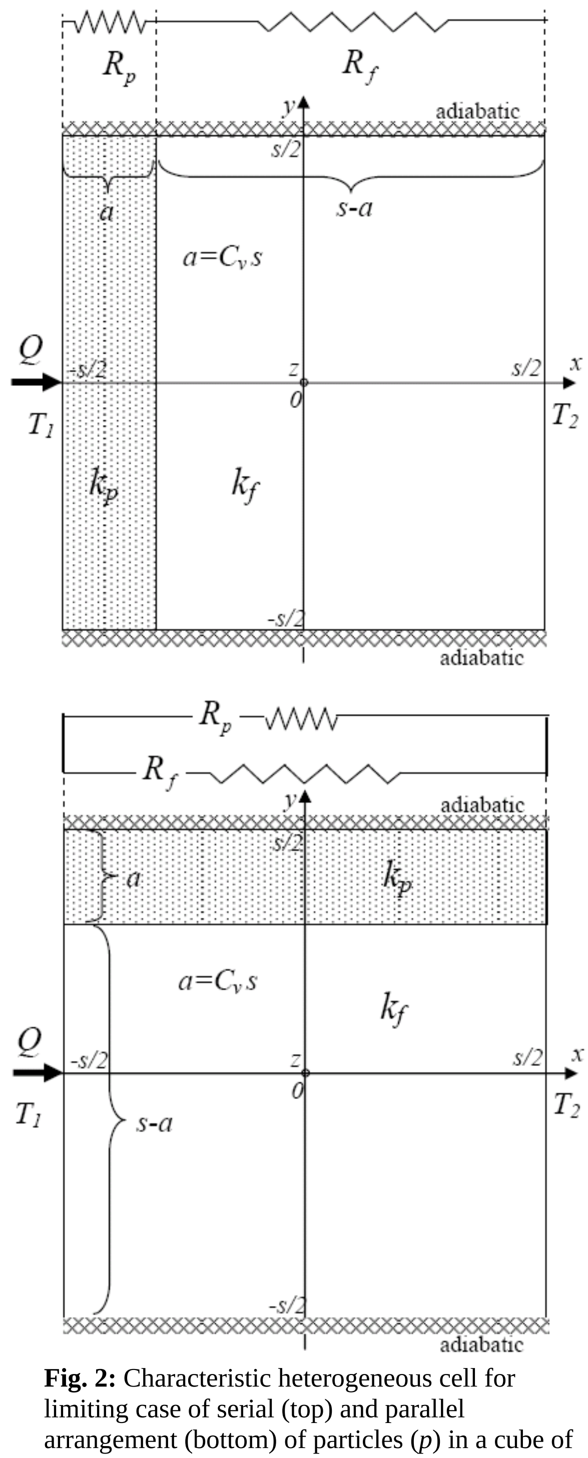

Fig. 2: Characteristic heterogeneous cell for limiting case of serial (top) and parallel arrangement (bottom) of particles (*p*) in a cube of side, *s*, with fluid (*f*) corresponding (thermally) to an effective (*e*) homogeneous mixture.

3. The Limiting Cases

The effective thermal conductivity, k_{e_S} and k_{e_P}, respectively for the limiting cases of the serial and parallel arrangement of particles in a base fluid, see Fig. 2, may be easily calculated as:

$$R_{e\_s} = R_{p\_s} + R_{f\_s} \text{ or}$$

$$\frac{s}{(s^2)k_{e\_s}} = \frac{a}{(s^2)k_p} + \frac{s-a}{(s^2)k_f} \qquad (11)$$

where $a = C_v \cdot s$

After introducing dimensionless variable (Eq. 5) and simplifying, the above equation for the serial model reduces to:

$$\frac{1}{k^*_{e\_s}} = 1 - C_v + \frac{C_v}{k^*_p} \text{ or} \qquad (12)$$

$$k^*_{e\_s} = \frac{k^*_p}{C_v + (1-C_v)k^*_p}$$

For the parallel particle arrangement in base fluid (see Fig. 2 bottom):

$$\frac{1}{R_{e\_P}} = \frac{1}{R_{p\_P}} + \frac{1}{R_{f\_P}} \text{ or} \qquad (13)$$

$$\frac{(s^2)k_{e\_P}}{s} = \frac{(s \cdot a)k_p}{s} + \frac{s(s-a)k_f}{s};$$

where $a = C_v \cdot s$

After introducing dimensionless variable (Eq. 5) and simplifying, the above equation for the parallel model reduces to:

$$k^*_{e\_P} = 1 - C_v + C_v k^*_p \qquad (14)$$

4. A Full 3-D Numerical Solution

The "cubic model" problem (the same geometry, properties and boundary conditions) was solved using a FEM numerical method [3] (the full 3-Dimensional heat conduction partial differential equation as in the Maxwell model) and the results, see Table 1, are in agreement with Maxwell results (within numerical accuracy, e.g., 2.72% ~ 3% increase for 1% *vol* copper particles in water), which is much different from the unidirectional (1-D) cubic model (the latter resulting in 33% effective TC increase for the same 1% *vol* copper particles in water). The obtained temperature distribution, see Fig. 3, was changing in all directions around the particle, thus, confirming that the cubic model, 1-Dimensional temperature and heat flow assumptions and results, are not appropriate (erroneous due to unrealistic assumptions) for the case it was supposed to model, see also Table 1.

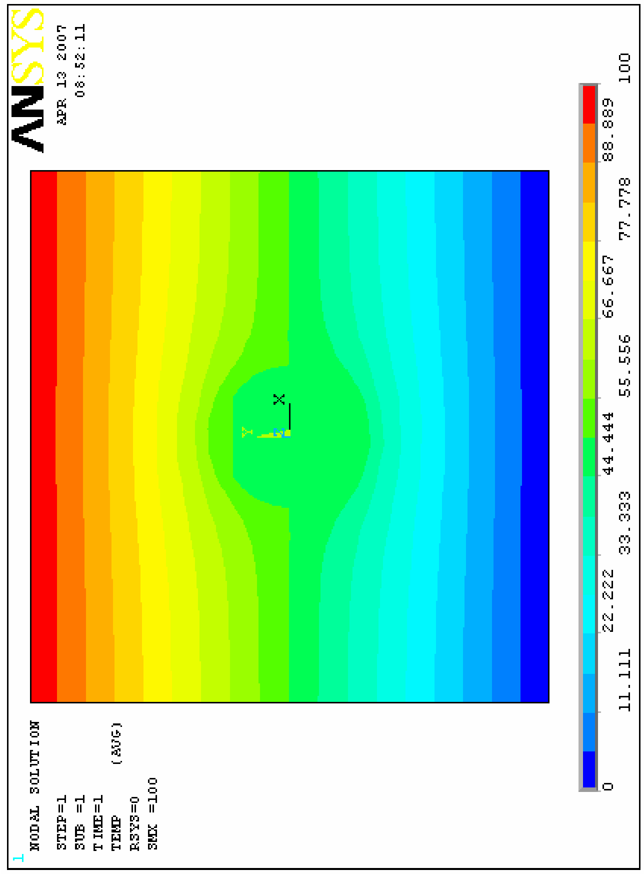

Fig. 3: Temperature distribution along the center-plane (*z=0*) for spherical copper particle (1% *vol* concentration) centered in cube of water, determined using a FEM numerical method (solving the full 3-dimensional heat conduction partial differential equation as in the Maxwell model) [2].

5. Conclusion

It should be stated that the continuum media theory accounts for the heterogeneous distribution of properties and geometry only, and the results are as good as the physical assumptions in related modeling. For example, the Maxwell model [2], Eq. (9), properly accounts for random distribution of small concentration of spherical particles in fluid (thus uniform distribution), but does not account for any other phenomena that may contribute to heat conduction, like special particle alignments and agglomerations in force-fields, different interfacial particle-fluid interactions, particle Brownian motion, and other known and unknown phenomena.

Table 1: Effective thermal conductivity ratios k_e^* for various concentrations of copper particles in water ($k_p^* = k_p / k_f = 401/0.615 = 652$)

Particle concen. $\%C_v$	Cubic model [1] $k^*_{e\_YC}$ Eq. (8)	Maxwell model [2] $k^*_{e\_Mxw}$ Eq. (9)	FEM Numerical method [3] $k^*_{e\_N}$	Serial model $k^*_{e\_S}$ Eq. (12)	Parallel model $k^*_{e\_P}$ Eq. (14)
0.1	1.109	1.003	1.003	1.001	1.650
0.5	1.237	1.015	1.014	1.005	4.255
1	**1.332**	**1.030**	**1.027**	**1.010**	**7.511**
1.5	1.407	1.045	1.041	1.015	10.766
2	1.473	1.061	1.055	1.020	14.021

The unidirectional heat flow modeling, like the "cubic model [1]" is similar to the Maxwell model, since it accounts for uniform distribution of spherical particles in a base fluid, but due to unrealistic (actually physically impossible) assumption of unidirectional heat flow and temperature distribution within the heterogeneous system (the representative mixture cell), the results may be very erroneous as demonstrated here. The erroneous, "cubic model" over-prediction of the effective thermal conductivity (TC) [1] is circumstantial and does not physically explain experimentally observed increase of TC of nanofluids due to other phenomena. The Maxwell and "cubic model" predictions, based on continuum media theory, everything else being the same, should give the same results regardless of the spherical particle size.

The serial and parallel particle distribution in base fluid, for a given particle-in-fluid mixture concentration, other phenomena being absent, represent the limiting minimum and maximum enhancement of effective thermal conductivity of the mixture, respectively, due to inclusion of higher conductive particles in lower conductive fluid. The summary of characteristic results is presented in Table 1 for comparison.

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