LIMITED VALUES OF THERMAL CONDUCTIVITY BY VARIATIONAL PRINCIPLE OF MINIMUM

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Abstract

It is shown in which way the variational principle limits values of thermal conductivity of the three-phase system. The inequality (11) shows such limits.

Thermal conductivity of a three-phase system

In this article we are looking for limits of thermal conductivity of a three-phase system which are setting by the variational principle of minimum on it. It is assumed that λ(**r**) - the molecular thermal conductivity - is determined by (1) and (2), where λ_i of each phase being constants. $i = 0,\ 1,\ 2$.

$$\lambda(\mathbf{r}) = \delta_1(\mathbf{r})\lambda_1 + \delta_2(\mathbf{r})\lambda_2, \quad í = 0,1,2 \text{ , assuming } \lambda_0 = 0,\ \lambda_1 \neq \lambda_2 \tag{1}$$

where

$$\delta_1(\mathbf{r}) = \begin{matrix} 1 & \mathbf{r} \in \textit{in phase } 1 \\ 0 & \mathbf{r} \in \textit{in phases } 0 \textit{ and } 2 \end{matrix} \qquad \delta_2(\mathbf{r}) = \begin{matrix} 1 & \mathbf{r} \in \textit{in phase } 2 \\ 0 & \mathbf{r} \in \textit{in phases } 0 \textit{ and } 1 \end{matrix} \tag{2}$$

T is temperature and V is the volume of the system. We see that λ(**r**) is the discontinuous function. Functional L closely connected to stationary ($\partial T/\partial t \equiv 0$) differential equation of thermal conductivity

$$\nabla \cdot (\lambda(\mathbf{r})\nabla T) = 0 \tag{3a}$$

is determined as follows (see Appendix1)

$$L = \int_V \Gamma\, dV = \int_V \lambda(\mathbf{r})(\nabla T)^2\, dV \tag{3b}$$

If, the solution T_0(**r**) of the eq. (3a) is known then value of $L\{T_0\}$ = const. If the solution of the eq. (3a) is unknown searching for this solution means to solve variational problem

$$\delta L = 0 \tag{3}$$

We introduce the mean temperature gradient **G** and density of the thermal flow **q** as follows

$$\mathbf{G} = \frac{1}{V}\int_V \nabla T \, dV \tag{4a}$$

$$\mathbf{q} = -\lambda_{\text{eff}}\mathbf{G} = -\int_V \lambda(\mathbf{r})\nabla T \, dV \tag{4b}$$

Let us actual temperature gradient be $\nabla T = \mathbf{G} + \nabla T'$, where T' is so called geometrical fluctuation of temperature, then the functional L takes the form

$$L = \int_V \lambda(\mathbf{r})(\mathbf{G} + \nabla T')^2 dV = VG^2(\lambda_1\eta_1 + \lambda_2\eta_2) + 2\mathbf{G}\cdot\int_\mathrm{V} \lambda(\mathbf{r})\nabla T' dV + \int_\mathrm{V} \lambda(\mathbf{r})\nabla T'\cdot\nabla T' dV \tag{5}$$

where

$$\eta_i = \frac{1}{V}\int_V \delta_i(\mathbf{r})\, dV, \qquad i = 1 \text{ or } 2 \tag{6}$$

are the correlation functions of the medium.

If the minimum of the functional L is realized by the fluctuation T'' and $T'' = \varepsilon T'$ where ε is nothing else but variation parameter, then the substitution of this last assumption leads to the condition for minimum of L (5)

$$\frac{\partial L}{\partial \varepsilon} = L_\varepsilon = 0 \tag{7}$$

which is fulfilled by the value of

$$\varepsilon = -\left[\int_V \lambda(\mathbf{r})\mathbf{G}\cdot\nabla T'' dV\right]\left[\int_V \lambda(\mathbf{r})\nabla T''\cdot\nabla T'' dV\right]^{-1} \tag{8}$$

(see Appendix 2).

The value of L is minimum at $\varepsilon = 1$ (in accordance with upper assumption, and $T'' = T'$ in this case). The condition (8) gives us

$$L(\varepsilon = 1) = -\mathbf{G}\cdot\mathbf{q} = \lambda_{\text{eff}}G^2 = \min \tag{9}$$

However, the actual value of temperature fluctuation T'' which minimized the funtional L is unknown, for this reason the optimal value of the parameter ε differs from one ($\varepsilon \neq 1$). In this sense the best value of the parameter ε is given by the relation (8).

With respect to the condition for minimum of L

$$L(\varepsilon = 1) \le L(\varepsilon \neq 1) \tag{10}$$

we finally obtain the inequality for thermal conductivity of the three-phase system

$$\lambda_{eff} \le V(\lambda_1\eta_1 + \lambda_2\eta_2) - \frac{\left\{\mathbf{G}\cdot\int\limits_V \lambda(\mathbf{r})\nabla T' dV\right\}^2}{\mathbf{G}\cdot\mathbf{G}\int\limits_V \lambda(\mathbf{r})\nabla T'\cdot\nabla T' dV} \le V(\lambda_1\eta_1 + \lambda_2\eta_2) \qquad (11)$$

because the term behind the minus sign (obtaining integrals) is positive.

Conclusion

We have obtained the limits for thermal conductivity of a three – phase system as a consequence of variational principle. The method we have used resembles to that one used by Prager S. [1] for effective diffusion coefficient.

Porous building materials (bricks. concrete – and others – can be considered as two – phase system ; pores being the phase number 0 and building material free of pores can be taken for phase 1. The phase number 2 can be for example a liquid. Then one can imagine the three-phase system as being a certain porous building material with absorbed liquid (water). Possible chemical reaction as well as phase transition are not considered.

The question arises if the functional L of the form (3b) can be identified with total entropy production P in the system? It cannot: at least for the reason that physical dimensions of both quantities are different. Dim $L \neq$ Dim P. This problem is discussed in work (e.g. [2]). There, the case under consideration is based on the assumption for the function $\lambda(\mathbf{r}) = \lambda\{T(\mathbf{r})\}$ which is quite different from our assumption (1) and (2).

References

[1] Prager S., Physica 1963, Vol. 29, p. 129-140
[2] Kiss E., Periodica Polytechnica, Ser. Chem. Eng. Vol.41, No 2. 1997, pp. 205 - 211

Appendix 1

Multiplication of the expression $\nabla\cdot(\lambda(\mathbf{r})\nabla T)$ from the left hand side by T and subsequent integration gives

$-L' = \int\limits_V T\nabla\cdot(\lambda(\mathbf{r})\nabla T)dV$ and we see that $-L'(T_0) = \int\limits_V T_0\nabla\cdot(\lambda(\mathbf{r})\nabla T_0)dV = 0$

Accounting the relation $\nabla\cdot\{T\lambda(\mathbf{r})\nabla T\} = \nabla T\cdot(\lambda(\mathbf{r})\nabla T) + T\nabla\cdot(\lambda(\mathbf{r})\nabla T)$ one can write

$$-L' = \int_V \operatorname{div}\{T\lambda(\mathbf{r})\nabla T\}\,dV - \int_V \nabla T \cdot (\lambda(\mathbf{r})\nabla T)\,dV$$

Applying Gaussian theorem

$$\int_V \operatorname{div}\{T\lambda(\mathbf{r})\nabla T\}\,dV = \oint_\Sigma T\lambda(\mathbf{r})\nabla T \cdot d\,\mathbf{\Sigma} = \oint_\Sigma (T\lambda(\mathbf{r})\nabla T)_n\,d\,\Sigma$$

If on the surface Σ of the system boundary conditions are fixed $\oint_\Sigma (T\lambda(\mathbf{r})\nabla T)_n\,d\,\Sigma = const$ then

$-L' = const - L$ where $L = \int_V \Gamma dV = \int_V \lambda(\mathbf{r})(\nabla T)^2\,dV$ and so

$\delta L = \delta\int_V \lambda(\mathbf{r})(\nabla T)^2\,dV = \delta L'$.

Now, to solve the problem $\delta L = 0$ this enables us to apply the methods of variation in problem with fixed boundaries. The problem is reduced to solution of Euler`s – Ostogradsky equation

$$\frac{\partial \Gamma}{\partial T} - \sum_{\alpha=1}^{3}\frac{\partial}{\partial x_\alpha}\frac{\partial \Gamma}{\partial T_{x_\alpha}} = 0\,.$$

We have $\Gamma(\mathbf{r},\nabla T) = \lambda(\mathbf{r})\left(T_{x_1}^2 + T_{x_2}^2 + T_{x_3}^2\right)$.

Substitution into Euler`s equation gives

$2\sum_{\alpha=1}^{3}\frac{\partial}{\partial x_\alpha}\lambda(\mathbf{r})\frac{\partial T}{\partial x_\alpha} = 0$ which is the equivalent of the initial eq. $\nabla \cdot (\lambda(\mathbf{r})\nabla T) = 0$.

This way it was indicated that the upper mentioned principle of variation works
One advantage of variational method is that the functional L obtains derivatives of T with respect to coordinates one order lower than the derivatives occurring in the stationary differential equation of heat conduction.

Appendix 2:

At this value of ε the function $L(\varepsilon)$ achieves a minimum because $L_{\varepsilon\varepsilon}(\varepsilon) > 0$.