

Generalized Fourier law for heat flow in a fluid with a strong, nonuniform strain rate

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We derive the leading terms of a generalized Fourier law for heat conduction in fluids under strong, nonuniform shear by expanding the heat flux vector as a Taylor series about the equilibrium state in powers of the temperature gradient, the velocity gradient (the first spatial derivative of the streaming velocity or the strain rate tensor), and, in an extension of previous work, the second spatial derivative of the streaming velocity (a third rank tensor). This results in a general macroscopic constitutive equation, independent of any microscopic model, and valid for all flow geometries. Assuming that the fluid is isotropic at equilibrium, we find a term representing heat flow due to a gradient in the square of the strain rate. This shows that it is possible for a nonuniform velocity gradient to generate a heat flow in the absence of a temperature gradient. We also find terms corresponding to heat flow parallel to the streamlines that are not present in uniform shear flow.

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I. INTRODUCTION

Coupled transport processes in fluids are well understood in the context of linear nonequilibrium thermodynamics. A classic example is the Dufour effect, in which heat flow can be caused by a concentration gradient in the absence of a temperature gradient [1]. Coupled linear transport processes for isotropic fluids are governed by a set of rules that result from the symmetry of the fluid and the parities of the relevant thermodynamic forces and fluxes. These considerations together are known as Curie's principle [1,2], and can be stated briefly as follows: In an isotropic fluid under the influence of small thermodynamic forces, the expression for a thermodynamic flux only contains terms that are directly proportional to the thermodynamic forces having the same tensor rank and parity as the flux itself. This allows a heat flux (first rank polar tensor) to be caused by a concentration gradient (first rank polar tensor), but prohibits a strain rate tensor (second rank polar tensor) from causing a heat flux.

Couplings between fluxes and forces of different tensor rank and/or parity become possible when we allow nonlinear relationships between thermodynamic fluxes and forces. Investigation of these nonlinear couplings has been the subject of several recent publications dealing with isotropic fluids [3–9]. Note that coupling between thermodynamic fluxes and forces of different tensor rank or parity is possible even in the linear regime, for anisotropic fluids such as liquid crystals [10].

Baranyai, Evans, and Daivis [4] have previously reported the results of nonequilibrium molecular dynamics simulations of a simple fluid subjected to a spatially sinusoidal transverse force. The force resulted in sinusoidal streaming velocity, shear stress, temperature gradient and heat flux fields. By applying a position-dependent constraint force thermostat that homogeneously removed the viscous heat, they eliminated all temperature gradients in the system. Surprisingly, a heat flux that was proportional to the gradient of

the square of the strain rate was found in the absence of any temperature gradient. This strain rate dependent heat flux was also observed in independent investigations of Poiseuille flow in narrow channels [11,12], but a detailed understanding of its origin was not achieved. In this paper, we show by macroscopic arguments that this term can be found by inclusion of the gradient of the strain rate as a thermodynamic force.

II. THEORY

We begin by assuming that the heat flux vector in a strongly shearing fluid can be written as a Taylor series expansion about the equilibrium state, in powers of the thermodynamic forces [2,5]. For example, with three vector forces, we would have

$$\begin{aligned} \mathbf{J}(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3) = & \mathbf{J}(0) + \sum_{i=1}^3 \mathbf{X}_i \cdot \left. \frac{\partial \mathbf{J}}{\partial \mathbf{X}_i} \right|_{X=0} \\ & + \frac{1}{2!} \sum_{i=1}^3 \sum_{j=1}^3 \mathbf{X}_i \mathbf{X}_j : \left. \frac{\partial^2 \mathbf{J}}{\partial \mathbf{X}_i \partial \mathbf{X}_j} \right|_{X=0} \\ & + \frac{1}{3!} \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^3 \mathbf{X}_i \mathbf{X}_j \mathbf{X}_k (\cdot)^{[3]} \\ & \times \left. \frac{\partial^3 \mathbf{J}}{\partial \mathbf{X}_i \partial \mathbf{X}_j \partial \mathbf{X}_k} \right|_{X=0} + \dots, \end{aligned} \quad (1)$$

where the partial derivatives are evaluated at equilibrium, and $\mathbf{J}(0)$, the equilibrium flux, is equal to zero. The symbol $(\cdot)^{[3]}$ represents a third order contraction between the third rank tensor $\mathbf{X}_i \mathbf{X}_j \mathbf{X}_k$ representing the thermodynamic force and the fourth rank phenomenological coefficient tensor given by the partial derivative. This is easily generalized to thermodynamic forces of higher rank.

A crucial step in applying this method to the current problem is the identification of the relevant thermodynamic forces. We explicitly consider the non-linear regime, so higher order tensor forces must be included. The temperature

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gradient ∇T is obviously important, and the magnitude of the strain rate is assumed to be large, so we also include higher order products involving the strain rate tensor $\nabla \mathbf{u}$ and ∇T . The second derivative of the streaming velocity, $\nabla \nabla \mathbf{u}$ will also be included, because we will allow the strain rate to be spatially inhomogeneous. The expression that results is complicated, so it will be developed in parts. The first order terms are:

$$\nabla T \cdot \left. \frac{\partial \mathbf{J}}{\partial \nabla T} \right|_0 + \nabla \mathbf{u} \cdot \left. \frac{\partial \mathbf{J}}{\partial \nabla \mathbf{u}} \right|_0 + \nabla \nabla \mathbf{u} \cdot \left. \frac{\partial \mathbf{J}}{\partial \nabla \nabla \mathbf{u}} \right|_0. \quad (2)$$

The partial derivatives are phenomenological coefficient tensors and are material properties. They are evaluated at equilibrium, and if we assume that the equilibrium fluid is isotropic, some simplification results. The heat flux vector is a polar vector, and the thermodynamic forces are polar tensors, so the first phenomenological coefficient tensor must be a second rank isotropic polar tensor. There is only one such tensor—the unit tensor, which we will write as $\mathbf{1}$ or $\delta_{\alpha\beta}$. Thus, the first term can be written as a constant multiplied by the second rank isotropic tensor:

$$A_{\alpha\beta} = \lambda \delta_{\alpha\beta}. \quad (3)$$

The constant in this equation is the usual thermal conductivity. There are no isotropic polar third rank tensors, so the second term is zero due to symmetry, and the phenomenological coefficient tensor in the third term must be a linear combination of the three isotropic fourth rank polar tensors:[2,13]

$$B_{\alpha\beta\gamma\delta} = b_1 \delta_{\alpha\beta} \delta_{\gamma\delta} + b_2 \delta_{\alpha\gamma} \delta_{\beta\delta} + b_3 \delta_{\alpha\delta} \delta_{\gamma\beta}. \quad (4)$$

Further simplification of this tensor is made possible by using the additional symmetry [14] implied by $\nabla_{\alpha} \nabla_{\beta} \mu_{\gamma} = \nabla_{\beta} \nabla_{\alpha} \mu_{\gamma}$. This results in the relationship $b_2 = b_3$. When these expressions for the phenomenological coefficient tensors are inserted into the constitutive equation and the contractions performed, we obtain an equation for the heat flux vector that is correct to linear order in the chosen thermodynamic forces, i.e.,

$$\mathbf{J}(\nabla T, \nabla \mathbf{u}, \nabla \nabla \mathbf{u}) = \lambda \nabla T + b_1 \nabla \nabla \cdot \mathbf{u} + b_2 \nabla \cdot (\nabla \mathbf{u})^T + b_2 \nabla \cdot \nabla \mathbf{u}, \quad (5)$$

where the superscript T denotes the transpose. Although this equation results from the first order terms of the expansion, it contains terms that are second derivatives of the streaming velocity. Terms of this type are not usually included in linear constitutive equations, and they would only become important for strongly nonuniform flow profiles.

Next, we consider the second order terms in the expansion. Only the isotropic polar tensors of even rank will contribute, so we can simplify the second order terms to obtain the following equation for the heat flux vector to second order:

$$\begin{aligned} \mathbf{J}(\nabla T, \nabla \mathbf{u}, \nabla \nabla \mathbf{u}) = & \mathbf{J}(\mathbf{X}^1) + \nabla T \nabla \mathbf{u}(\cdot)^{[3]} \mathbf{C} + \nabla \mathbf{u} \nabla T(\cdot)^{[3]} \mathbf{D} \\ & + \nabla \mathbf{u} \nabla \nabla \mathbf{u}(\cdot)^{[5]} \mathbf{E} + \nabla \nabla \mathbf{u} \nabla \mathbf{u}(\cdot)^{[5]} \mathbf{F}, \end{aligned} \quad (6)$$

where $\mathbf{J}(\mathbf{X}^1)$ represents the first order terms. The fourth rank tensors \mathbf{C} and \mathbf{D} again possess additional symmetry due to the equality of the mixed second order partial derivatives that appear in their definitions [see Eq. (1)], giving $C_{\alpha\beta\gamma\delta} = C_{\gamma\alpha\beta\delta} = D_{\alpha\beta\gamma\delta}$. This results in relationships similar to the one between the coefficients appearing in Eq. (4). The sixth rank tensors \mathbf{E} and \mathbf{F} can be written as linear combinations of the 15 isotropic sixth rank tensors, e.g.,

$$\begin{aligned} E_{\alpha\beta\gamma\delta\epsilon\zeta} = & e_1 \delta_{\alpha\beta} \delta_{\gamma\epsilon} \delta_{\delta\zeta} + e_2 \delta_{\alpha\beta} \delta_{\gamma\delta} \delta_{\epsilon\zeta} + e_3 \delta_{\alpha\beta} \delta_{\gamma\zeta} \delta_{\delta\epsilon} \\ & + e_4 \delta_{\alpha\gamma} \delta_{\beta\delta} \delta_{\epsilon\zeta} + e_5 \delta_{\alpha\gamma} \delta_{\beta\epsilon} \delta_{\delta\zeta} + e_6 \delta_{\alpha\gamma} \delta_{\beta\zeta} \delta_{\delta\epsilon} \\ & + e_7 \delta_{\alpha\delta} \delta_{\beta\gamma} \delta_{\epsilon\zeta} + e_8 \delta_{\alpha\delta} \delta_{\beta\epsilon} \delta_{\gamma\zeta} + e_9 \delta_{\alpha\delta} \delta_{\beta\zeta} \delta_{\gamma\epsilon} \\ & + e_{10} \delta_{\alpha\epsilon} \delta_{\gamma\delta} \delta_{\beta\zeta} + e_{11} \delta_{\alpha\epsilon} \delta_{\beta\gamma} \delta_{\delta\zeta} + e_{12} \delta_{\alpha\epsilon} \delta_{\gamma\zeta} \delta_{\beta\delta} \\ & + e_{13} \delta_{\alpha\zeta} \delta_{\gamma\delta} \delta_{\epsilon\beta} + e_{14} \delta_{\alpha\zeta} \delta_{\beta\gamma} \delta_{\delta\epsilon} + e_{15} \delta_{\alpha\zeta} \delta_{\gamma\epsilon} \delta_{\beta\delta}. \end{aligned} \quad (7)$$

Again, the equality of mixed second order partial derivatives and the symmetry implied by the relationship $\nabla_{\alpha} \nabla_{\beta} \mu_{\gamma} = \nabla_{\beta} \nabla_{\alpha} \mu_{\gamma}$ lead to considerable simplification, with the result that $\mathbf{E} = \mathbf{F}$ and all of the e_i are found to be equal. After substituting Eqs. (7) into (6) and evaluating the contractions, the complete expression for the heat flux vector to second order in the chosen thermodynamic forces becomes:

$$\begin{aligned} \mathbf{J}(\nabla T, \nabla \mathbf{u}, \nabla \nabla \mathbf{u}) = & \mathbf{J}(\mathbf{X}^1) + c [\nabla \mathbf{u} + (\nabla \mathbf{u})^T + \nabla \cdot \mathbf{u} \mathbf{1}] \cdot \nabla T \\ & + e \{ [\nabla \mathbf{u} + (\nabla \mathbf{u})^T \\ & + \nabla \cdot \mathbf{u} \mathbf{1}] \cdot [\nabla \nabla + (\nabla \nabla)^T + \nabla \cdot \nabla \mathbf{1}] \cdot \mathbf{u} \\ & + [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] : [\nabla (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] \\ & + \nabla \nabla \mathbf{u} : [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] \}. \end{aligned} \quad (8)$$

The third-order terms can be treated in a similar way. We are only interested in the weak temperature gradient, strong shear case, so we restrict our attention to those terms that are of linear or lower order in the temperature gradient. Considering the combinations of thermodynamic forces that give rise to phenomenological coefficient tensors of even rank (as the odd rank tensors will not contribute), the remaining combinations of thermodynamic forces are $\nabla \mathbf{u} \nabla \mathbf{u} \nabla T$, $\nabla \nabla \mathbf{u} \nabla \nabla \mathbf{u} \nabla T$, $\nabla \mathbf{u} \nabla \mathbf{u} \nabla \nabla \mathbf{u}$, $\nabla \nabla \mathbf{u} \nabla \nabla \mathbf{u} \nabla \nabla \mathbf{u}$. We will only consider the first, as the others result in phenomenological coefficient tensors of rank greater than 6. They also involve high-order products of the second derivative of the streaming velocity, and may thus be considered to be negligible compared with the first term.

Making use of similar symmetry arguments as before, we obtain our final form for the heat flux vector

$$\begin{aligned} \mathbf{J}(\nabla T, \nabla \mathbf{u}, \nabla \nabla \mathbf{u}) = & \mathbf{J}(\mathbf{X}^1) + \mathbf{J}(\mathbf{X}^2) + f \{ [\nabla \mathbf{u} + (\nabla \mathbf{u})^T \\ & + \nabla \cdot \mathbf{u} \mathbf{1}] \cdot [\nabla \mathbf{u} + (\nabla \mathbf{u})^T + \nabla \cdot \mathbf{u} \mathbf{1}] \\ & + [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] : [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] \\ & + [\nabla \mathbf{u} : \nabla \mathbf{u} + \nabla \mathbf{u} : (\nabla \mathbf{u})^T] \mathbf{1} \} \cdot \nabla T, \end{aligned} \quad (9)$$

where the first- and second-order terms are given by Eqs. (5) and (8).

These equations might be simplified by using the irreducible representations [13] of the tensors, but it is difficult to express the general sixth-rank isotropic tensors in irreducible form, so the approach taken here is probably the simplest.

III. DISCUSSION

The results given in the previous section are far simpler when specific flow geometries are considered. We now consider some specific examples.

The first simplification is to consider a general velocity field of the form $\mathbf{u} = \mathbf{i}u_x(y)$, which we will call general planar shear. This results in the strain rate tensor given by

$$\nabla \mathbf{u} = \begin{bmatrix} 0 & 0 & 0 \\ \dot{\gamma}(y) & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (10)$$

where $\dot{\gamma}(y) = \partial u_x(y)/\partial y$. It is immediately apparent that in this case, $\nabla \cdot \mathbf{u} = 0$, which eliminates many of the terms in Eqs. (5), (8), and (9). The constitutive equation for the heat flux that results is made more compact by combining the terms that contain the temperature gradient into an effective, strain rate-dependent thermal conductivity tensor for the shearing fluid, as was done in previous work [5]. This allows us to write the expression for the heat flux vector in the relatively simple form

$$\mathbf{J} = \boldsymbol{\lambda}_{\text{eff}} \cdot \nabla T + b_2 \frac{\partial \dot{\gamma}(y)}{\partial y} \mathbf{i} + 3d \dot{\gamma}(y) \frac{\partial \dot{\gamma}(y)}{\partial y} \mathbf{j}, \quad (11)$$

where

$$\boldsymbol{\lambda}_{\text{eff}} = \begin{bmatrix} \lambda + 3f\dot{\gamma}^2 & c\dot{\gamma} & 0 \\ c\dot{\gamma} & \lambda + 3f\dot{\gamma}^2 & 0 \\ 0 & 0 & \lambda + f\dot{\gamma}^2 \end{bmatrix}. \quad (12)$$

In the case of simple planar shear (linear velocity gradient), only the first term of Eq. (11) survives. This is in agreement with the conclusions reached in previous work [5,6]. The additional two terms correspond to longitudinal and transverse heat fluxes that are caused by a transverse gradient in the strain rate. The transverse heat flux term could also be written as

$$\xi \partial \dot{\gamma}^2(y)/\partial y = 2\xi \dot{\gamma}(y) \partial \dot{\gamma}(y)/\partial y, \quad (13)$$

which is the form of the shear induced heat flux that was postulated by Baranyai *et al.* to explain their sinusoidal transverse force molecular dynamics simulation results [4], and has been found essential to properly describe heat flow in narrow pores containing fluids undergoing Poiseuille flow by Todd and Evans and Ayton *et al.* [11,12]. It was also found by Cordero and Risso in their investigations of Poiseuille flow of dilute gases using the Boltzmann equation [9].

Another flow geometry that is of particular interest is that of simple planar elongational flow, in which the strain rate tensor is given by

$$\nabla \mathbf{u} = \begin{bmatrix} \dot{\epsilon} & 0 & 0 \\ 0 & -\dot{\epsilon} & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (14)$$

and the elongation rate is assumed to be constant. The result in this case is a constitutive equation of the form

$$\mathbf{J} = \boldsymbol{\lambda}_{\text{eff}} \cdot \nabla T, \quad (15)$$

where the effective thermal conductivity tensor, given by

$$\boldsymbol{\lambda}_{\text{eff}} = \begin{bmatrix} \lambda + 2c\dot{\epsilon} + 12f\dot{\epsilon}^2 & 0 & 0 \\ 0 & \lambda - 2c\dot{\epsilon} + 12f\dot{\epsilon}^2 & 0 \\ 0 & 0 & \lambda + 4f\dot{\epsilon}^2 \end{bmatrix} \quad (16)$$

contains terms of both first and second order in the elongation rate in the diagonal elements.

An obvious question that arises is whether the new terms are physically significant. The answer, based on the evidence currently available, is that they are. In the analysis of non-equilibrium molecular-dynamics computer simulations, erroneous values of the thermal conductivity will be obtained if the correct constitutive equation including the heat—shear coupling term is not used [4,11]. A dimensional analysis, similar to that given by Baranyai [4], but more general, will now be discussed.

The heat equation for the case where $\mathbf{u} = \mathbf{i}u_x(y)$ (and consequently $\nabla \cdot \mathbf{u} = 0$) can be written as

$$\frac{dT}{dt} = -\frac{1}{\rho c_v} \nabla \cdot \mathbf{J} - \frac{1}{\rho c_v} \boldsymbol{\Pi}^T \cdot \nabla \mathbf{u}, \quad (17)$$

where T is the temperature, ρ is the density, c_v is the specific heat capacity and $\boldsymbol{\Pi}^T$ is the transpose of the nonequilibrium part of the pressure tensor [2]. If we assume a generalized Newtonian constitutive equation for the nonequilibrium stress, the viscous heat production is given by

$$\boldsymbol{\Pi}^T \cdot \nabla \mathbf{u} = \Pi_{yx}(y) \dot{\gamma}(y) = -\eta(y) \dot{\gamma}^2(y). \quad (18)$$

Substituting Eq. (11) for the heat flux vector converting the whole equation to dimensionless form, we obtain

$$\frac{dT^*}{dt^*} = -\nabla^* \cdot \left(\frac{1}{\text{Re Pr}} \boldsymbol{\lambda}_{\text{eff}}^* \right) \cdot \nabla^* T^* - \frac{\xi}{\rho L^3 u_0} \frac{\text{Br}}{\text{Pr}} \frac{\partial}{\partial y^*} \left(\frac{\partial \dot{\gamma}^{*2}}{\partial y^*} \right) + \frac{\text{Br}}{\text{Re Pr}} \eta^* \dot{\gamma}^{*2}. \quad (19)$$

In this equation, we have used a characteristic velocity u_0 length L and temperature difference $T_1 - T_0$ as the reduction parameters, following Bird, Stewart, and Lightfoot [15]. This gives the reduced time as $t^* = tu_0/L$ and the reduced temperature as $T^* = (T - T_0)/(T_1 - T_0)$. The dimensionless effective thermal conductivity tensor and viscosity appearing in eq. (19) are formed by dividing $\boldsymbol{\lambda}_{\text{eff}}$ and $\eta(y)$ by their linear values, λ and η_0 and the standard dimensionless groups in the equation are the Reynolds number $\text{Re} = Lu_0\rho/\eta_0$, the Prandtl number $\text{Pr} = c_v\eta_0/\lambda$, and the Brinkman number $\text{Br} = \eta_0 u_0^2/\lambda(T_1 - T_0)$. The dimensionless num-

ber related to the heat-shear coupling term, $\xi Br/\rho L^3 u_0 Pr = \xi u_0/\rho L^3 c_v(T_1 - T_0)$ shows that this term will be significant in relation to the other terms for a given fluid when the characteristic length L is small, the maximum temperature difference is small and the maximum velocity is large. This corresponds to fast flow in a very narrow pore or channel with very efficient removal of viscous heat. However, it should be noted that the theory described here assumes that the fluid is isotropic at equilibrium. This is not the case for a fluid confined to a pore that is so narrow that it induces a layered structure in the fluid.

Note that Eq. (19) does not contain the constant b_2 (corresponding to the longitudinal heat flow), because it occurs in a term of the heat flux vector with zero divergence. Thus, it has no effect on the temperature profile, but it should be accessible by direct computation of the heat flux vector.

IV. CONCLUSION

We have derived the leading terms of a general macroscopic constitutive equation for heat flow in a fluid undergo-

ing strong, nonuniform shear from a Taylor series expansion of the heat flux vector in terms of the temperature gradient, the strain rate tensor, and the spatial derivative of the strain rate tensor. We find a term due to the coupling of heat flow to the strain rate and the gradient of the strain rate that is identical to the one postulated by Baranyai, Evans, and Daivis [4] to explain their nonequilibrium molecular dynamics simulations of a nonuniformly sheared simple fluid. Our results are consistent with theoretical results from kinetic theory studies of heat flow in dilute gases undergoing simple shear and Poiseuille flow [9], but they are independent of any microscopic fluid model and they apply to any flow geometry. The new constitutive equation should be particularly useful in studies of non-Newtonian fluids under strong, non-uniform shear.

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