

Maxwell and Cattaneo's Time-Delay Ideas Applied to Shockwaves and the Rayleigh-Bénard Problem

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Abstract: We apply Maxwell and Cattaneo's relaxation approaches to the analysis of strong shockwaves in a two-dimensional viscous heat-conducting fluid. Good agreement results for reasonable values of Maxwell's relaxation times. Instability results if the viscous relaxation time is too large. These relaxation terms have negligible effects on slower-paced subsonic problems, as is shown here for two-roll and four-roll Rayleigh-Bénard flow.

Key words: shockwaves, Maxwell-Cattaneo, temperature tensor, time delay, Rayleigh-Bénard flow

I. INTRODUCTION

In 1867 James Clerk Maxwell [1] noted that an initial shear stress in a dilute gas, (like air) when unsupported by an underlying shear motion, will decay with a relaxation time $\tau = (\eta/P)$ (about 200 picoseconds for air), where η is the shear viscosity and P the pressure. His governing relaxation equation for the shear stress modifies Newton's $\sigma = \eta\dot{\epsilon}$ to read

$$\sigma + \tau\dot{\sigma} = \eta\dot{\epsilon}.$$

Here σ is the stress, η the viscosity, and $\dot{\epsilon}$ the strain rate. The superior dots represent comoving time derivatives.

Nearly a century later Carlo Cattaneo [2] argued that Fourier's law for heat conduction should be similarly modified, in order to avoid the supersonic heat flow implied by a parabolic (diffusion equation) transport law. One could equally well argue that a heat flux, when unsupported by a temperature gradient, would decay with a microscopic relaxation time τ like Maxwell's. Cattaneo's approach can be written in a form like Maxwell's, but with a partial (fixed in space) rather than a comoving time derivative:

$$Q + \tau(\partial Q/\partial t) = -\kappa\nabla T.$$

Cattaneo's rationale for using a partial time derivative rather than one fixed in the material is unclear. Here Q is the heat flux, T the temperature, and κ the heat conductivity. With Cattaneo's relaxation assumption, "heat waves" can propagate at about the speed of sound [3]. On physical grounds Maxwell's approach, with the comoving time derivative, seems more "realistic" than Cattaneo's. Cattaneo's form for the relaxation time makes no contribution at all in stationary steady-state problems such as the structure of a steady fluid shockwave.

Oddly enough, modern treatments of time delay [3, 4] often use Cattaneo's partial-derivative formulation rather than Maxwell's comoving time derivative. The purpose of the present work is to elucidate the usefulness of the relaxation concept and to explore its limits in applications of fluid mechanics. In the following Sections we consider the relatively fast-paced steady shockwave problem as well as the slower-paced steady convective Rayleigh-Bénard flow. A final Section summarizes our findings. For simplicity we use units in which the Boltzmann constant and atomic mass are both equal to one.

II. STRONG DENSE-FLUID SHOCKWAVES

The structure of strong shockwaves has long served as a testing ground for continuum models like the Navier-Stokes-Fourier equations (here given for a two-dimensional fluid with vanishing bulk viscosity, $\eta_V = 0$):

$$\begin{aligned} \dot{\rho} &= -\rho \nabla \cdot v; \quad \rho \dot{v} = -\nabla \cdot P; \quad \rho \dot{e} = -\nabla v : P - \nabla \cdot Q; \\ P &= I[P_{\text{eq}} + \eta \nabla \cdot v] - \eta[\nabla v + \nabla v^t]; \quad Q = -\kappa \nabla T. \end{aligned}$$

The time derivatives, here as before indicated by the superior dot, are all *comoving* derivatives, like Maxwell's, time rates of change in a coordinate frame moving with the fluid velocity v . Solving the three differential equations for the density ρ , velocity v , and energy e requires a knowledge of the pressure tensor P and heat flux vector Q . The simplest models are shown here, with two transport coefficients, the Newtonian shear viscosity η and the Fourier heat conductivity κ defined in the usual way. I is the unit tensor, with $I_{xx} = I_{yy} = 1$ and $I_{xy} = I_{yx} = 0$.

Landau and Lifshitz' analytic solution of the shockwave structure for a gas with constant transport coefficients and a shockwidth λ provides a useful initial condition for both macroscopic continuum and microscopic molecular dynamics simulations [5]:

$$\begin{aligned} \rho(x) &= \frac{\rho_C e^{-x/\lambda} + \rho_H e^{+x/\lambda}}{e^{-x/\lambda} + e^{+x/\lambda}} \longrightarrow \\ \longrightarrow &\{v(x), P_{xx}(x), Q_x(x)\}. \end{aligned}$$

Their solution smoothly interpolates the density between cold fluid, with density ρ_C , and hot fluid, with ρ_H .

Molecular dynamics shockwave simulations [6–15] have been carried out in the two different ways shown in Figure 1: (1) by following the two moving waves generated by the inelastic collision of two blocks of material; (2) by studying the single stationary wave formed with two boundary “treadmills” – on the left boundary cold fluid is introduced at the “shock speed” v_s while at the right boundary hot fluid is extracted at the slower speed $v_s - v_p$, where v_p is the “particle speed”. In either case, in a coordinate frame centered on the shockwave the mass, momentum, and energy fluxes are all constant:

$$\{\rho v, P_{xx} + \rho v^2, \rho v[e + (P_{xx}/\rho) + (v^2/2)] + Q_x\}$$

constant for all x .

For “weak” shocks the Navier-Stokes-Fourier description is “good” [16]. For “stronger” shocks (twofold compression) several contradictions to this simple description arise [8–15]. To illustrate these points typical mechanical and thermal shockwave profiles are shown in Figure 2.

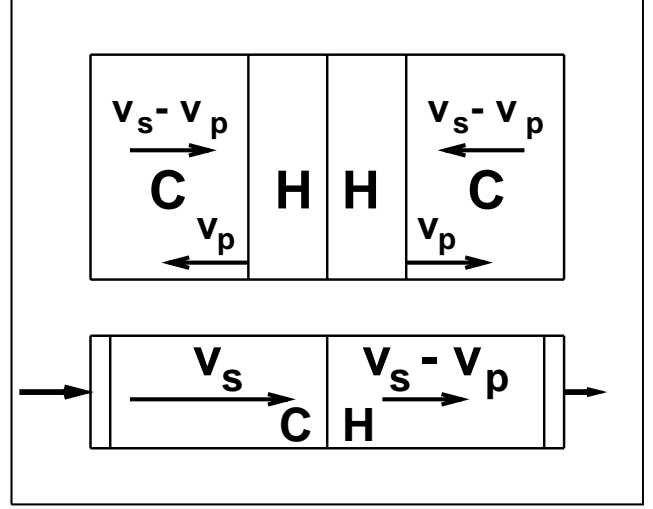


Fig. 1. Two colliding fluid blocks generate symmetric shockwaves (velocities $\pm v_p$) as the blocks, moving at $\pm[v_s - v_p]$ collide and come to a stop (shown above). Two treadmill boundaries, one fast (velocity v_s) and one slow (velocity $v_s - v_p$), maintain a single stationary shockwave in the center of the system (shown below)

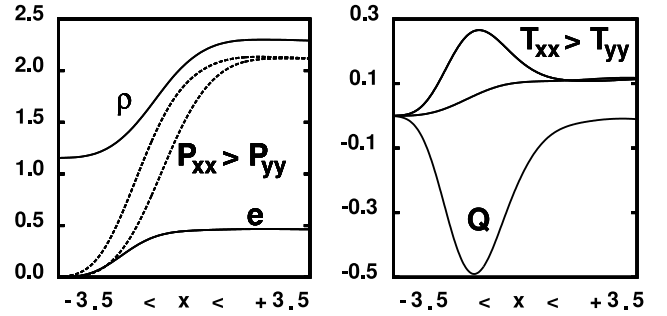


Fig. 2. Density, pressure, internal energy, temperature tensor, and heat flux in a strong shockwave simulation using molecular dynamics. In the cold unshocked material the nearest-neighbor spacing is unity. The hot shocked fluid has a density exactly twice that of the cold material. Figure based on data described in reference [14]

First, the local longitudinal and transverse temperatures differ, often by more than a factor of two (see Figure 2). Second, as is also shown in Figure 2, the shear stress $(P_{yy} - P_{xx})/2$ and the heat flux Q_x both lag behind the velocity gradient (dv_x/dx) and the temperature gradients (dT_{xx}/dx) and (dT_{yy}/dx) , suggesting the presence of Maxwell-type relaxation times [12, 15]. Third, the fact that temperature is so very anisotropic makes it necessary to consider separate xx and yy contributions to the heat flux [8–15]:

$$Q_x = -\kappa_{xx} \nabla_x T_{xx} - \kappa_{yy} \nabla_x T_{yy}.$$

Fourth, the same anisotropy also suggests including asymmetric divisions of the work and heat contributions (indicated by \triangleright) to the thermal energy change:

$$(\rho C_V/2) \dot{T}_{xx} \supset [-\alpha \nabla v : P_{\text{Thermal}} - \beta \nabla \cdot Q];$$

$$(\rho C_V/2) \dot{T}_{yy} \supset [-(1-\alpha) \nabla v : P_{\text{Thermal}} - (1-\beta) \nabla \cdot Q].$$

Fifth, a mechanism for the decay of temperature anisotropy must also be included:

$$[\dot{T}_{xx} - \dot{T}_{yy}] \supset 2[T_{yy} - T_{xx}]/\tau.$$

Last, the molecular dynamics results imply that a bulk viscosity η_V , approximately equal to the shear viscosity, must be included [12]. Though a continuum model incorporating all of these ideas is necessarily relatively complex, a successful implementation of all six of these additions to the Navier-Stokes-Fourier model is described in References [11], [13], and [14].

In those works all of the continuum field variables were derived from molecular dynamics simulations using a short-ranged repulsive pair potential,

$$\phi(r < 1) = (10/\pi)(1-r)^3.$$

The prefactor $(10/\pi)$ was chosen to give a potential energy integral of unity for a random particle distribution at unit density:

$$\int_0^1 2\pi r \phi(r) \equiv 1.$$

The initial zero-pressure zero-temperature state was compressed twofold to obtain a hot dense fluid state. Lucy's normalized weighting function [17, 18] was used to compute spatial averages of the various field variables:

$$w(r < h) = (5/\pi h^2)[1 - (r/h)]^3[1 + 3(r/h)] \rightarrow \int_0^h 2\pi r w(r) \equiv 1.$$

The *smooth-particle* average of the particle quantity f_j is given by a weighted sum,

$$\langle \rho(r) f(r) \rangle = \sum_j m_j f_j w(r-r_j); \quad \rho(r) \equiv \sum_j m_j w(r-r_j).$$

This smooth-particle definition has two advantages: (1) all of the field variables defined in this way have two continuous space derivatives; (2) the continuity equation (with f_j equal to the particle velocity v_j) is satisfied exactly:

$$\left\{ \rho = \sum_j m_j w(r-r_j); \quad \rho v = \sum_j m_j v_j w(r-r_j) \right\} \rightarrow \dot{\rho} \equiv -\rho \nabla \cdot v.$$

Here ρ and ρv are defined *everywhere* in this way, not just at the particle locations. The range h of the "weighting function" $w(r < h)$ is typically chosen so that about 20 particles contribute to field-point averages. With this approach the microscopic pressure tensor and heat flux vector at any point

in space are expressed in terms of nearby individual particle contributions to these nonequilibrium fluxes [19, 20].

To appreciate the effect of the various modifications of the Navier-Stokes-Fourier model we next study the stability of solutions using a continuum model which is a rough representative of the molecular dynamics results [10–12].

III. STABILITY STUDIES WITH AN IDEALIZED GRÜNEISEN MODEL

For stability studies we choose an equilibrium equation of state based on Grüneisen's separation of the energy and pressure into cold and thermal parts:

$$P_{\text{eq}} = \rho e = (\rho^2/2) + 2\rho T; \quad e = (\rho/2) + 2T.$$

A shockwave satisfying all the conservation laws results when a cold fluid is compressed to twice its initial density by a shockwave moving toward that fluid at twice the particle velocity ($v_s = 2v_p = 2$). In this case the constant mass, momentum, and energy fluxes are respectively

$$\left\{ \rho v = 2; \quad P_{xx} + \rho v^2 = (9/2); \quad \rho v [e + (P_{xx}/\rho) + (v^2/2)] + Q_x = 6 \right\}.$$

The various hydrodynamic variables then cover the following ranges within the shockwave:

$$\begin{aligned} & [2 > v(x) > 1]; \quad [1 < \rho(x) < 2]; \\ & [(1/2) < e(x) < (5/4)]; \\ & [(1/2) < P_{\text{eq}} < (5/2)]; \quad [0 < T_{\text{eq}} < (1/8)]. \end{aligned}$$

(Note that T_{xx} can exceed the "hot" value of $(1/8)$ within the shockwave.) The details of the shockwave structure depend upon the nonequilibrium constitutive relations for the shear stress and the heat flux. Next, we summarize two separate situations, (1) vanishing conductivity with a scalar temperature; (2) tensor conductivity, with separate longitudinal and transverse temperatures, with different contributions from work and heat. Both these models lead to the conclusion that the mechanical relaxation time cannot be too large. By contrast, the thermal relaxation time can be either "small" or "large".

III. 1. Relaxation without heat conduction

The simplest case results when both heat conductivity and thermal anisotropy are omitted. Then the density and energy can both be eliminated from the three flux equations,

$$\begin{aligned} \rho v = 2; \quad (\rho e) - \sigma + 2v = (9/2); \\ 2[e + e - (v/2)\sigma + (v^2/2)] = 6, \end{aligned}$$

giving the shear stress,

$$\sigma = (P_{yy} - P_{xx})/2 = \rho e - P_{xx},$$

as a function of velocity:

$$\sigma = (3/v)(v-1)(v-2) < 0.$$

Evidently the viscous stress is everywhere negative (compressive). If we introduce Maxwell's idea of comoving stress relaxation,

$$\begin{aligned} \sigma + \tau \dot{\sigma} &= \sigma + \tau v(d\sigma/dx) = \sigma + \tau v(d\sigma/dv)(dv/dx) \\ &= \eta(dv/dx), \end{aligned}$$

we find that the velocity gradient (dv/dx) diverges unless the ratio (τ/η) is sufficiently small:

$$\tau_\sigma < (\eta/3).$$

It is physically reasonable that too long a memory can lead to instability in fast-paced complex flows like shockwaves. On the other hand the relaxation equation by itself, with a smooth strain increment localized near zero time ($t = 0$),

$$\sigma + \tau \dot{\sigma} = \frac{1}{[e^{-t} + e^{+t}]},$$

provides smooth solutions even for large τ [13, 14]. The present analytic shockwave limit on $\tau_\sigma < (\eta/3)$ is in full accord with two kinds of numerical simulations. First, the stationary flux equations can be solved for the temperature and stress fields, just as was indicated above for the case of vanishing conductivity. Second, it is possible to solve the dynamical equations for

$$\begin{aligned} &\{ (\partial\rho/\partial t), (\partial v/\partial t), (\partial e/\partial t) \} \\ &\quad \text{or} \\ &\{ (\partial\rho/\partial x), (\partial v/\partial x), (\partial e/\partial x) \} \end{aligned}$$

starting with the Landau-Lifshitz profile. The two methods agree. They show that the stress relaxation time in shockwaves must be sufficiently small, $\tau_\sigma < (\eta/3)$ for stability.

We next extend the thermal constitutive model to include tensor temperature with anisotropic heat conduction. We also include separate relaxation times for the longitudinal and transverse heat fluxes, and the separation of work and heat into longitudinal and transverse parts [11, 13].

III. 2. Lack of relaxation without viscosity

Viscosity, as opposed to heat conduction, is essential to the shock process. To appreciate this need, consider the conservation equations for our simple model *without* viscosity and with the heat conductivity equal to unity:

$$\begin{aligned} e &= (\rho/2) + 2T; \quad \rho v = 2; \quad \rho e + \rho v^2 = (9/2); \\ \rho v[2e + (v^2/2)] - (dT/dx) &= 6. \end{aligned}$$

According to the first three equations the temperature has its maximum value of ($T_{\max} = 0.238 > T_{\text{hot}} = 0.125$) within the shock:

$$\{\rho, v, T\} = \{1.4436, 1.38545, 0.23800\} \text{ for } T = T_{\max}.$$

But the fourth (energy-flux) equation gives (dT/dx) = 0.7106 for that thermodynamic state, contradicting the presence of a maximum. Thus this model, lacking viscosity, cannot sustain a stationary shockwave.

Exactly this same conclusion follows also for the inviscid ideal gas, with twofold compression from unit density, pressure, and temperature, with $v_s = \sqrt{8}$ and the wholly thermal pressure $P = \rho e = \rho T$. Because heat conductivity in the absence of viscosity is not enough to provide a shockwave, the relaxation effects are quite different for conductivity and viscosity, as we show next.

III. 3. Relaxation with tensor temperature, apportioned work and heat

The analysis becomes more complicated when heat flow is included, along with relaxation and separated contributions of the heat and work to the longitudinal and transverse temperatures. Here the heat flux evolves following the tensor relaxation equation:

$$Q_x + \tau_Q \dot{Q}_x = -\kappa_{xx}(dT_{xx}/dx) - \kappa_{yy}(dT_{yy}/dx).$$

The divergence of the heat flux provides net heating and is apportioned between the longitudinal and transverse temperatures:

$$\rho \dot{T}_{xx} \supset -\beta(dQ_x/dx); \quad \rho \dot{T}_{yy} \supset -(1-\beta)(dQ_x/dx).$$

The contributions of the heat flux divergence $\nabla \cdot Q$ to heating are indicated by the inclusion symbol, " \supset ". We include also an analogous separation of the thermodynamic work into longitudinal and transverse parts:

$$\rho \dot{T}_{xx} \supset -\alpha P_{\text{Thermal}} : \nabla v; \quad \rho \dot{T}_{yy} \supset -(1-\alpha) P_{\text{Thermal}} : \nabla v.$$

Finally, the two temperatures necessarily relax toward one another:

$$\dot{T}_{xx} \supset (T_{yy} - T_{xx})/\tau_Q; \quad \dot{T}_{yy} \supset (T_{xx} - T_{yy})/\tau_Q.$$

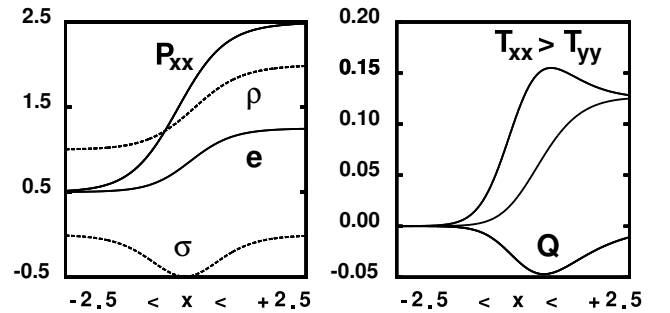


Fig. 3. Solution of the continuum model for twofold compression with the Grüneisen equation of state using $\tau_\eta = (1/10)$ and $\tau_Q = \tau_R = 1$. The mass, momentum, and energy fluxes are $\{2, (9/2), 6\}$. Compare with Figure 4 noting particularly the differences between T_{xx} and T_{yy}

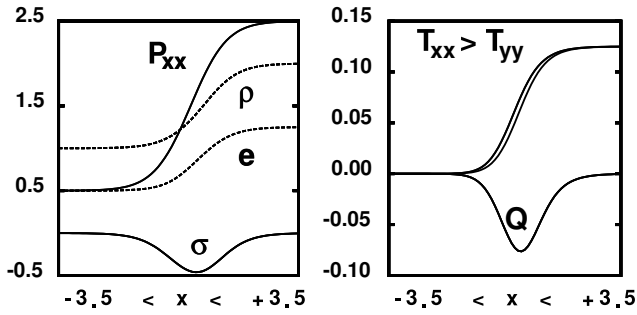


Fig. 4. Solution of the continuum model for twofold compression with the Grüneisen equation of state using $\tau_\eta = \tau_Q = \tau_R = (1/10)$. The mass, momentum, and energy fluxes are $\{2, (9/2), 6\}$. Compare with Figure 3

For simplicity we choose the two thermal relaxation times [for the heat flux Q and the temperature anisotropy ($T_{xx} - T_{yy}$)] to have a common value, τ_Q . For illustrative purposes we emphasize the difference between the two temperatures by choosing the apportionment parameters α_x and β_x both equal to unity, so that both the work and the heat provide longitudinal heating, with the transverse temperature lagging behind.

Then straightforward (at least for a computer) algebra provides solutions of the shockwave problem and reveals not one, but *two* restrictions on τ_Q . For stable solutions to exist we found in this way that the thermal relaxation time must be either sufficiently small or sufficiently large. Setting the distance scale of the shockwave with the constant transport coefficients

$$\eta = 2\kappa_{xx} = 2\kappa_{yy} = 1,$$

computer algebra gives the following restrictions on the relaxation times:

$$0 < \tau_\eta < (1/3); \tau_Q < (1/8) \text{ or } \tau_Q > (1/4).$$

Figures 3 and 4 show typical continuum profiles using these constitutive relations. The continuum profiles were generated in two quite different ways: (1) solving the time-dependent equations for $\{\rho, v, e, \sigma, Q\}$ starting with the Landau-Lifshitz approximation; (2) solving the stationary flow equations for the mass, momentum, and energy fluxes using a computer algebra program (we used “Maple”). The latter approach provides page-long formulæ for (du/dx) , (dT_{xx}/dx) , and (dT_{yy}/dx) as well as numerical solutions. The stationary equations for the shockwave profile have no solution if the relaxation time for the shear stress τ_σ is greater than $(\eta/3)$ or if the relaxation time for the heat flux lies between $(\kappa/8)$ and $(\kappa/4)$.

To summarize, our findings for shockwaves establish that momentum-flux relaxation has to be “fast” for stability. Thermal relaxation can either be likewise fast or quite slow, with a window of instability separating these two regimes. Where the thermal relaxation is slow the shockwave structure is dominated by viscosity rather than conductivity. It is natural to

speculate on the effect of relaxation in ordinary hydrodynamic situations. In order to see what consequences arise from these effects in subsonic fluid mechanics we next introduce delay into the hydrodynamic equations describing a compressible, conducting, viscous flow, the Rayleigh-Bénard problem.

IV. RAYLEIGH-BÉNARD FLOW

To investigate the stability of moderate flows to the presence of viscous and thermal relaxation we revisit some finite-difference Rayleigh-Bénard simulations of two-roll, four-roll, and six-roll flows [21, 22]. The simulations picture a viscous conducting fluid, heated from below in the presence of a vertical gravitational field. Sufficiently strong heating causes a transition from static heat conduction to one of a number of nonequilibrium steady states with stationary convection rolls. Stationary and transient sample flows are shown in Figures 5 and 6.

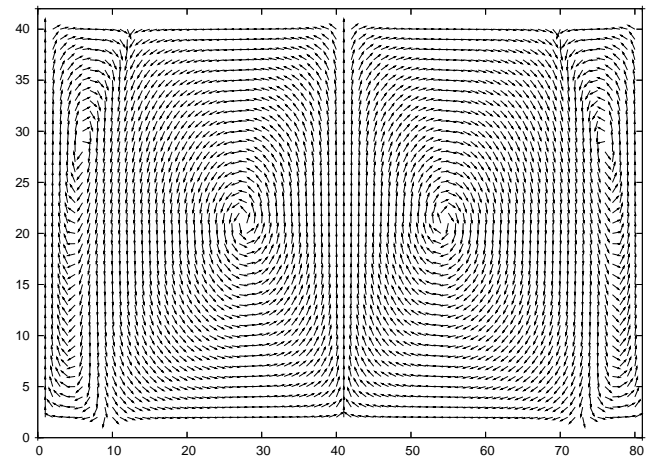


Fig. 5. Transient flow field for the Rayleigh-Bénard problem at time $t = 1000$. The initial state was two weakly-rotating rolls. The viscous, heat-conducting, compressible fluid is heated at the bottom and cooled at the top with a gravitational field directed downward. The vertical boundaries at the sides are periodic. The number of computational cells shown here is $80 \times 40 = 3200$. The transport coefficients, $\eta = \kappa = (1/5)$ were selected to give a Rayleigh number of 40,000. The relaxation times were set equal to unity:

$$\tau_\eta = \tau_Q \equiv 1$$

For the Rayleigh-Bénard model we study here (equal kinematic viscosity and thermal diffusivity) the transition from static Fourier conduction to two-roll convection occurs near a Rayleigh number R of 1750:

$$R = g(\partial \ln V / \partial T)_P H^3 \Delta T / (\nu D_T) = H^2 / (\nu D_T).$$

The fluid is confined to a rectangular box, periodic on the sides, with the gravitational constant $g = (1/H)$ chosen to give constant density in the nonconvecting case. H is the

height of the cell, equal here to half the width. ΔT is the difference between the hot temperature at the base ($T_H = 1.5$) and the cold temperature at the top of the cell ($T_C = 0.5$). ν and D_T (chosen equal, for convenience) are the kinematic viscosity and thermal diffusivity (both with units of $[length^2/time]$). For simplicity we choose all values of the relaxation times equal and do not distinguish between the longitudinal and transverse temperatures, $T_{xx} = T_{yy}$. Our model continuum fluid obeys the ideal gas equation of state:

$$P_{eq} = \rho T = \rho e ; \eta_V = 0 ; \eta = 2\kappa_{xx} = 2\kappa_{yy} = 1 .$$

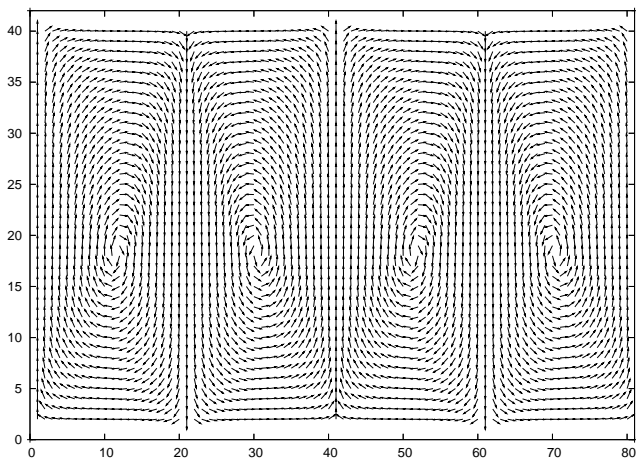


Fig. 6. A fully-converged four-roll structure evolved from the flow field shown in Figure 5. Here the time is 10,000. The Rayleigh number is 40,000 and the viscosity and heat conductivity, $\eta = \kappa = (1/5)$, have equal relaxation times, $\tau_\eta = \tau_Q \equiv 1$. The final kinetic energy is $(K_x/N) + (K_y/N) = 0.001144 + 0.004133 = 0.005277$. The number of computational cells is $N = 80 \times 40$

Numerical results for this model are given as a function of Rayleigh number in References [21] and [22]. Simulations with the various relaxation times all equal to 0.1 reproduced this earlier work perfectly. As an example, the two-roll problem of References [21] and [22], with a Rayleigh number of 40,000 gives per-cell kinetic energies of $(K_x/N) + (K_y/N) = 0.00373 + 0.00357$. We carried out many special cases with a Rayleigh Number of 40,000, which produces stationary steady states. Whether two-roll or four-roll solutions are obtained is sensitive to the initial conditions [22]. We began with a very weak two-roll velocity field as the initial condition in an $H \times W$ box with the coordinate origin at its center:

$$v_x \propto \sin(2\pi x/W) \sin(2\pi y/H) ; \\ v_y \propto \cos(2\pi x/W) \cos(\pi y/H) .$$

We found solutions for $\tau = 5\eta = 5\kappa$ and $\tau = 10\eta = 10\kappa$ but instability when τ was doubled again to $20\eta = 20\kappa$. These additions of relaxation to the Navier-Stokes-Fourier equations lowered the horizontal kinetic energy and raised the vertical, with both effects on the order of parts per thousand.

Thus relaxation in subsonic flows has only relatively small effects in the regime of stable solutions.

V. CONCLUSIONS

Molecular dynamics simulations have established the facts that delay times on the order of a collision time, as envisioned by Maxwell, affect shockwave structure in a substantial way. Cattaneo's approach, with partial time derivatives, has no effect on shockwave structure. Shockwaves are dominated by viscosity, so that stress relaxation must be relatively rapid. Thermal relaxation, important for chemical relaxation, can be either fast or slow.

In ordinary subsonic fluid mechanics the effects of time delays are relatively small. As a result, thermal anisotropy is ordinarily ignored in continuum mechanics. It is a substantial effect in shocks, with repercussions for chemical reaction rates. In our continuum simulations we have assumed relaxation equations with comoving time derivatives,

$$\sigma + \tau_\eta \dot{\sigma} = \eta \dot{\epsilon} , \quad Q + \tau_Q \dot{Q} = -\kappa \nabla T ,$$

rather than partial derivatives. If $\dot{\sigma}$ were replaced with $(\partial\sigma/\partial t)$ there would be no relaxation at all in a stationary problem like the shockwave and Rayleigh-Bénard problems studied here.

The Maxwellian relaxation times cause no trouble solving conventional moderate flow problems like Rayleigh-Bénard convection. The problem areas suggested by this work include (1) formulating optimum choices for locally-averaged hydrodynamic variables with the general goal of maximizing the accuracy of macroscopic descriptions of microscopic results and (2) developing theoretical models for the estimation of the relaxation parameters measured in the dynamical simulations.

A logical approach to problem (1) above would use "entropy production" as a tool [23]. In the Rayleigh-Bénard problem entropy production is proportional to the squares of the nonequilibrium fluxes, σ^2 and Q^2 . If these are computed locally, with a weight function $w(r < h)$ then h can be chosen such that the internal entropy production matches the boundary sources and sinks of entropy. Evidently too small/large an h gives too large/small an entropy production, so that h can be chosen to be "just right". Problem (2) would have to begin with some nonequilibrium simulations tailored to the direct measurement of delay and relaxation.

Finally, the presence of delay has some pedagogical importance. Delay in the results of time-reversible motion equations (molecular dynamics) breaks the time-symmetry which would otherwise lead to a logical contradiction between time-reversible molecular dynamics and conventional irreversible continuum mechanics [12].

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