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Anomalous heat transport by the piston effect in supercritical fluids under zero gravity

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The response to a boundary heating of a very compressible, low-diffusivity, supercritical fluid (CO_2) under zero gravity is studied by solving numerically the full nonlinear one-dimensional Navier-Stokes equations. Both short (acoustic) and long (diffusion) time scales are investigated. A new mechanism of heat transport is seen, where the thermal energy is transformed into kinetic energy in a hot expanding boundary layer (the piston), which in turn is transformed in the bulk into internal energy. Steeply profiled waves are observed. In contrast to the "critical slowing down" behavior, the enhancement of heat transport is so important that it is nearly completed after 1% of the diffusion time.

Because of the increasing number of opportunities for space experiments in material and fluid sciences, there is now a growing interest in understanding the different mechanisms that lead to the transport of heat in fluids under weightlessness. In contrast with the incompressible fluids, for which no driving force for motion can exist when gravity is zero, compressible fluids may generate a flow even in such conditions when they are submitted to a thermal perturbation. This is because[1,2] the hot thermal boundary created near a heated wall expands within the short acoustic time scale and acts as a piston. This acoustic field generated in the bulk provides the initial condition for the long diffusion time-scale equation. When the perturbation is strong and rapid enough, shock waves can be ultimately generated in the bulk phase.[3] This effect should be all the more pronounced when the heat diffuses slowly and the system is compressible, and should therefore become prominent near the critical point[4] of fluids. Note that this effect is not expected to be visible on Earth, because it is hidden in these systems by very strong effects due to gravity.[5] The object of this paper is to investigate the heat transport in a supercritical fluid (CO_2), and to compare it with ideal gases (IG).[6] For this purpose, the fluid was initially set on the critical isobar and at 1 K from the critical temperature (T_c). A thermal perturbation (which mimics a conduction measurement) is imposed at one boundary, and the heat transport is analyzed by numerically solving the Navier-Stokes (NS) equations. Because the classical numerical methods appropriate for compressible flows fail in the low-Mach-number limit, a novel method[7] has been used called PISO for "pressure implicit with splitting of operators." The approximation scheme allows the NS equations to be solved on both acoustic and conduction time scales. A van der Waals equation of state (vdW) has been assumed for the fluid; although this equation fails to reproduce the details of the divergence laws, it catches the essential features of a supercritical fluid. The numerical simulation has been performed on a one-dimensional fluid confined between the abscissa $X=0$ and $X=L=2.5$ mm. Our main findings are very surprising and contrast with the current expectation of a critical slowing down for the heat transport. It is observed that during the acoustic time a steep acoustic wave propagates and induces flows in the system; then the temperature evolves rapidly so that after a time of order 1% of the diffusion time thermal equilibration is nearly completed.

The governing equations are the vdW equation of state and the one-dimensional compressible unsteady NS equations. The initial conditions for CO_2 are (critical) pressure $P_0=P_c=73.8\times10^5$ Pa, and temperature $T_0=T_c+1$ K$=305.2$ K. All numerical data come from Ref. 8. The density $\rho_0=276.2$ kg m^{-3} is computed from the vdW equation

$$\Pi=\tilde{\rho}\left[\frac{\tilde{T}}{1-b\rho_0\tilde{\rho}}-\frac{a\rho_0^2}{P_{01}}\tilde{\rho}\right]. \tag{1}$$

The pressure Π is normalized to the IG pressure under the same density and temperature conditions, i.e., $\Pi=P/\rho_0RT_0$ (R is the IG constant). The decorated quantities are reduced to their initial values ($\tilde{T}=T/T_0$ and $\tilde{\rho}=\rho/\rho_0$) and the subscript 1 refers to IG. The constants are $a=1.89\times10^2$ J m^{3}kg^{-2} and $b=9.75\times10^{-4}$ m^{3}kg^{-1}.[8] The equation of continuity is written as

$$\tilde{\rho}_t+(\tilde{\rho}\tilde{u})_x=0, \tag{2}$$

where $\tilde{u}=u/c_0$ is the fluid velocity normalized to the sound velocity c_0. The subscripts t,x refer to the derivative versus time and space, where t is normalized to the acoustic time t_a defined as L/c_0 and x is normalized to L. The momentum conservation is expressed as

$$\tilde{\rho}\tilde{u}_t+\tilde{\rho}\tilde{u}\tilde{u}_x=-\frac{c_{01}^2}{\gamma c_0^2}\Pi_x+\tfrac{4}{3}\epsilon\tilde{u}_{xx}\,. \quad (3)$$

Here $\gamma=1.4$ is the ratio of specific heats at constant pressure (C_P) and volume (C_V) for IG, and c_{01} is the sound velocity for the equivalent IG ($c_{01}^2 \approx \gamma RT_0$). The parameter ϵ, which is the scaling parameter of the thermal boundary layer thickness in IG,[6] is written as $\epsilon=\mathcal{P}t_a/t_d$. $\mathcal{P}$ is the Prandtl number for the vdW gas and $t_d=L^2/D_0$ is the diffusion time, with D_0 the heat diffusion coefficient. The equation for the conservation of energy is

$$\tilde{\rho}\tilde{T}_t+\tilde{\rho}\tilde{u}\tilde{T}_x=-(\gamma-1)\Pi\tilde{u}_x+\epsilon\left[\frac{C_{P0}}{C_{V0}}\mathcal{P}^{-1}\tilde{T}_{xx}+\tfrac{4}{3}\gamma(\gamma-1)\frac{c_0^2}{c_{01}^2}\tilde{u}_x^2\right]. \quad (4)$$

This equation is a simplified form where the internal energy of the vdW gas is, in first approximation, supposed to be only T dependent. When the exact form of the energy is used, we have checked that, although the numerical values are somewhat changed, this does not modify the interpretation of our results. Moreover, since the system remains far from the critical point, we neglect the variations of C_P, C_V, and $\mathcal{P}$ which are consequently kept to their initial values C_{P0}, C_{V0}, and $\mathcal{P}_0$ and we consider only the temporal evolution of u, P, T, and ρ. The initial conditions correspond to the fluid at equilibrium at T_0, i.e., $\tilde{u}=0$, $\Pi=P_0/\rho_0RT_0$, $\tilde{T}=1$, and $\tilde{\rho}=1$. The boundary conditions $[\tilde{u}(X=0)=\tilde{u}(X=L)=0]$ are those of impermeable walls. The temperature is maintained constant at one boundary: $T(X=L)=0$. It is varied linearly at the other boundary ($X=0$), from T_0 to T_0+13 mK in a time $t_0=1.3$ ms, and is then kept constant. The time $t_0=1.3$ ms has been chosen to be intermediate between the acoustic time ($t_a=11.5$ μs, with $c_0=216$ ms^{-1}) and the diffusion time ($t_d=157$ s, with $D_0 \simeq 4\times10^{-8}$ m^{2}s^{-1}); it appears to be a crucial parameter since it determines in IG the scaling law in the initial boundary layer.[6] The values of $\mathcal{P}$ and ϵ are not very different from the IG case (with $\nu_0 \simeq 1\times10^{-7}$ m^{2}s^{-1} the initial kinematic viscosity, $\mathcal{P}=3.1$, and $\epsilon=2.3\times10^{-7}$); one thus expects a boundary-layer behavior similar to the IG case. However, thermal diffusivity is ten times lower and compressibility fifteen times larger. The main differences in heat transport between vdW and IG gases lie essentially in these values, as will be confirmed by the analysis below.

Two time scales present *a priori* interest; the acoustic time scale, when temperature increases continuously and a boundary layer forms ($t_0>t\sim t_a$), and the scale intermediate between t_0 and t_d once temperature is constant at the boundaries ($t_d \gtrsim t > t_0$).

Acoustic time scale

The velocity behavior is reported in Fig. 1. Near the left wall a thin boundary layer develops in which the velocity gradient is positive: thermal energy is transformed into kinetic energy. The thickness of the layer appears to be of the same order as in IG. This is not surprising since the scaling parameter ϵ is similar to that of the IG case. The pressure disturbance induced by this layer (Fig. 2) exhibits a gradient, corresponding to a propagating wave with a velocity slightly lower than c_0 due to the effect of dispersion. This wave is then reflected by the outer wall ($X=L$), and mixes with other waves that are still generated by the evolution of the boundary layer. As a result, pressure increases in the whole sample and its relative variation decreases.

The fluid velocity increases in the bulk according to the pressure wave; a steep gradient is observed which propagates at the same velocity as the pressure disturbance. The magnitude of the flow velocity, of the order of a few μm s^{-1}, is 2 orders of magnitude larger than for the IG in

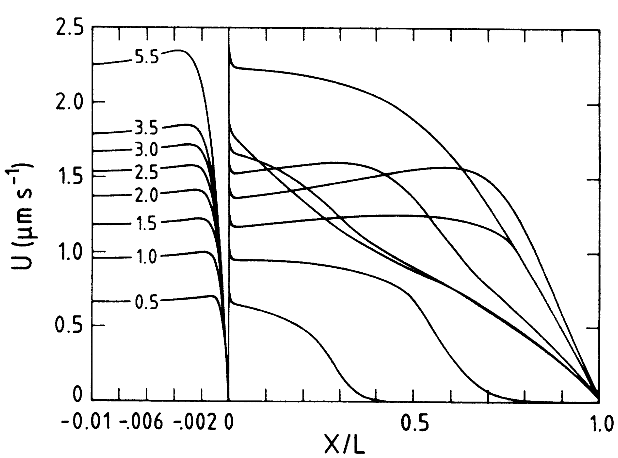

FIG. 1. Velocity profiles for acoustic times. The numbers refer to the ratio t/t_a, with $t_a=11.5$ μs. Negative distances correspond to the magnification of the boundary layer.

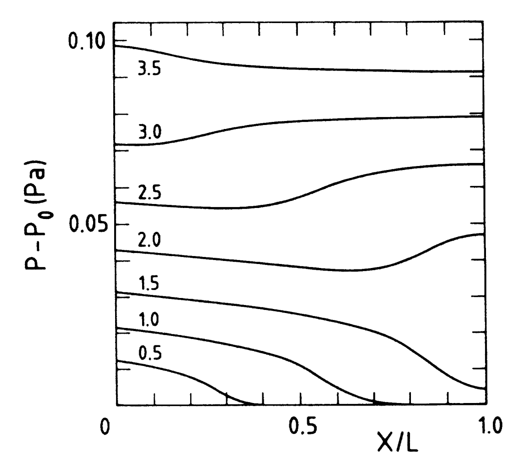

FIG. 2. Pressure profiles for acoustic times (See Fig. 1 caption).

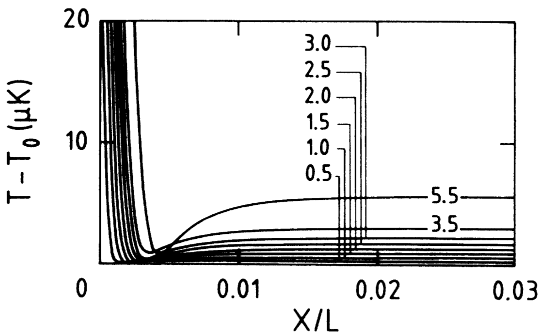

FIG. 3. Temperature profiles for acoustic times (see Fig. 1 caption).

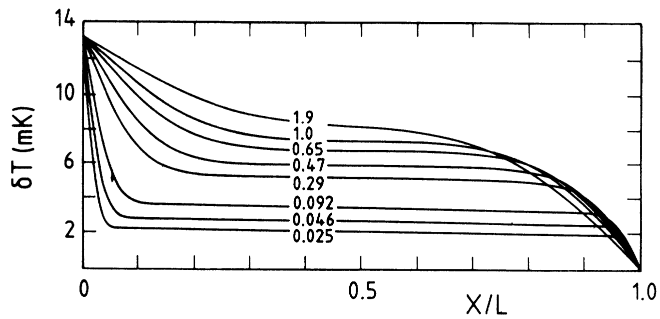

FIG. 5. Temperature increase ($\delta T = T - T_0$) for intermediate times (see Fig. 4 caption).

similar conditions. Temperature (Fig. 3) decreases from the wall and goes to a minimum at the point where velocity exhibits a small peak (Fig. 1). Then, and this is remarkable, the bulk increases in temperature during the acoustic time. This is a phenomenon which has never been detected in IG under the same conditions. We attribute it to the flow produced by the expansion of the thermal boundary layer that slows down in the bulk, causing the kinetic energy to be converted again into heat. It corresponds to the work ($\sim \Pi \tilde{u}_x$) of the pressure forces that act as a source term everywhere in the bulk. This mechanism of direct transfer of energy from the boundary layer to the bulk via an expansion recompression lasts on longer times and is responsible for a fast energy transfer. (Density, not shown, progressively decreases in the boundary layer according to the temperature increase.)

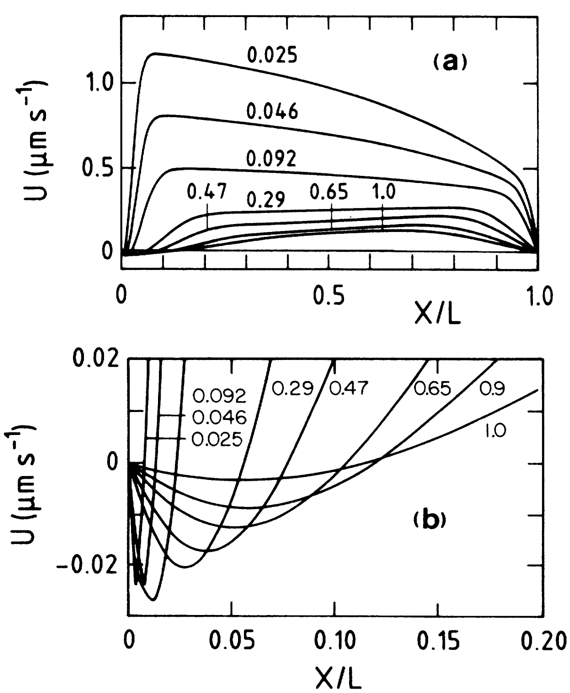

FIG. 4. (a) Velocity profile for intermediate times. The numbers refer to the ratio t/t_d (in percent), with $t_d = 157$ s. (b) Magnification for short distances.

Intermediate time scale

Since the time-dependent thermal perturbation no longer exists, velocity is seen to decrease with time (Fig. 4). There is a change of behavior for a time $t_1 \sim 10^{-3} t_d$; this time determines a period 1 ($t < t_1$), where the velocity gradient in the bulk is still negative and the boundary layer is still expanding due to the momentum conservation, and a period 2 ($t > t_1$), where the velocity gradient becomes positive. One notes the birth, at small X [Fig. 4(b)], of a backward flow ($u < 0$), due to the weakening of the flow momentum which becomes too small to balance the low density in that region.

While pressure is homogeneous, the temperature (Fig. 5) is evolving again according to the same process as before. During period 1 thermal energy is still converted into kinetic energy with time. Near the wall T increases because, in that region, conduction by diffusion is more important than the amount of energy that can be converted into kinetic energy. Deeper in the bulk, where conduction did not have time to occur, the slowing down of the flow produces an homogeneous increase in temperature through the source term $\Pi \tilde{u}_x$. In period 2, the velocity gradient becomes positive and temperature decreases on the right-hand side of the slot, whereas on the left-hand side this effect is balanced by conduction. This effect can thus be visible only on the right-hand side of Fig. 5, where the thermomechanical coupling enhances the transient to equilibrium during this period. (The behavior of density is not markedly different than what can be inferred from temperature variations and is not reported.)

The final equilibrium state is reached by diffusion later on. It must be emphasized, however, that the thermomechanical couplings are responsible for a nearly equilibrium state in a time which represents only 1% of the diffusion time. This acceleration of the heat transport should be more pronounced when the system is close to its critical point, in apparent contradiction to the classical "critical slowing down." This is a surprising result which deserves an experimental verification, presumably under reduced gravity because of the very high instability of supercritical fluids to small temperature disturbances on Earth.

After this work was completed, we received a copy of recent work[9,10] where a pure thermodynamic approach very close to T_c (no flow), has led to a similar speeding up of equilibration.

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