Dynamics of sheared gases

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Abstract

When the characteristic length associated to the gradient of at least one hydrodynamic field becomes comparable to the mean free path, standard hydrodynamics does not apply. Situations like this are particularly evident in sheared gases. A gas-dynamics valid for sheared gases derived from Boltzmann's equation is presented in a compact form in two and three dimensions. The equations are then reduced to the case of stationary planar flow where they are seen to imply highly nonlinear transport equations. The gas-dynamic equations correctly describe, for example, the observed shear thinning and heat flux not orthogonal to the isotherms. The shape of all the hydrodynamic fields can be obtained with extraordinary precision. © 1999 Elsevier Science B.V. All rights reserved.

Keywords:

1. Introduction

Classic fluids represent a special challenge because there cannot be a fundamental theory describing them beyond Liouville's equation. Every effort to describe them necessarily involves assumptions and approximation schemes [1,2]. Since the times of the pioneering articles by Alder and Wainwright (as in [3]) we know that basic properties of classic fluids can be well captured by microscopic *molecular dynamic* computer simulations when simple Newtonian evolution equations are used [4]. Since in this type of microscopic simulations there is no uncertainty about the form of the interaction potential, theoretical results can be tested unambiguously in a manner that is generally impossible with data obtained in experiments with real fluids. It is also possible to obtain information on

quantities of theoretical importance that may not be readily measurable in the laboratory [5].

When a molecular dynamic simulation makes a fluid evolve integrating Newtonian dynamics it is actually integrating the fundamental equation of kinetic theory, namely, Liouville's equation. This equation has precedence over hydrodynamics and certainly over thermodynamics, therefore the information so obtained may have great importance for theoretical developments. Similarly molecular dynamic simulation programs using Newtonian dynamics normally have precedence over those using thermostats.

In this article we begin summarizing the basic theoretical analysis that leads to gas-dynamic equations which are well beyond Navier–Stokes fluid dynamics. Then we proceed to describe the peculiar behaviour which stems from such dynamics. Gases more easily can show a behaviour not described by standard fluid dynamics because the mean free path in them is several orders of magnitude larger than in liquids. In liq-

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uids the characteristic length associated to gradients of any hydrodynamic field X, $(\ell_X = X/|\nabla X|)$ is incomparable larger than the mean free path while in gases they may be of the same order. The implications of this is that in dense fluids local thermodynamic equilibrium usually is a reliable hypothesis while in gases such assumption cannot be sustained in the presence of large gradients. The difference then can be understood first at the level of kinetic theory: the one particle distribution functions $f(\vec{r}, \vec{c}, t)$ is significantly distorted and one has to resort to Boltzmann's equation to re-obtain the balance equations which yield fluid dynamics. In our work we use the moment expansion method developed by Grad [6].

The equations obtained in this way, presented below, are far more complex than those of standard hydrodynamics and we have only scratched the surface of their implications, studying some simple planar laminar flows. Still we have analytically derived, for example, that heat does not flow exactly in the direction of the temperature gradient since there is an *anomalous heat flux* component parallel to the isotherms [7, 8]. The direction of the heat flux depends on ∇T but also on the gradient of the shear rate and on the direction of the external force (e.g., gravity) [9].

Similarly we have derived the law that governs the viscous flow which in hydrodynamics is typically assumed to be Newton's law. In gas-dynamics we have shown that the effective shear viscosity coefficient derived for a planar Couette flow depends on the shear rate and therefore we have a nonlinear dependence of the off diagonal terms P_{ij} of the pressure tensor on the shear rate. The derived effective viscosity describes excellently well the shear thinning of gases observed in simulations. The tensorial nature of P_{ij} is not only determined by terms like $\partial v_i / \partial x_j$ but also by higher derivatives of the velocity field, by the external force and even by derivatives of the temperature field [9].

We have studied the transport laws and have also derived the shape of every hydrodynamic field (density, velocity, temperature, pressure tensor and heat flux vector) for simple planar and laminar flows and have found how well they compare with what we observe in our simulations [7,8].

In the following the gas-dynamic equations are presented and then they are specialized to stationary planar flows. From the latter some results are then obtained: a perturbative 2D solution for a Poiseuille flow, a temperature profile for a Couette flow (given as a table) and a third order generalization of Fourier's law in 3D.

2. The general equations

Starting from a classic system of many point particles interacting via a pair-wise short range central potential it is possible to derive quite generic hydrodynamic equations [2]. They are an incomplete set of equations for the number-density field n, the velocity field $\vec{v}$ and the energy density field u. Such equations involve two unknown fields: the pressure tensor $\mathbf{P}$ and the heat flux vector $\vec{q}$. Standard textbook hydrodynamics is obtained when the following extra ingredients are added: (a) two equations of state, one connecting u with the temperature field T and one connecting the hydrostatic pressure with n and T; (b) two constitutive equations, one linearly relating the pressure tensor with the gradients of the velocity field (thus viscosity coefficients are introduced) and one linearly relating the heat flux vector with the temperature gradient. These are Newton's law and Fourier's law, respectively.

Instead, following Grad, what we do is to assume no constitutive equations whatsoever and derive higher balance equations directly from Boltzmann's equation (hence density is low enough that collisions are uncorrelated) using Grad's moment expansion method [6]. The method further requires to assume that the mean free path is much smaller than any macroscopic length. The last condition is necessary to have a system that is dominated by the bulk behaviour with negligible effects coming from the walls. This is important because Grad's method assumes that the distribution function is analytic in the velocities but it is known that a geometric wall, as the ones we use, implies a non analytic distribution function [10].

Using Grad's moment expansion method [6] we have derived the hydrodynamic equations for hard spheres in dimension $d = 2$ and 3. In the last two dynamic equations (below) a quantity τ is present

$$\tau = \frac{2+d}{2^{d+1}} \frac{1}{p\,\sigma^{d-1}} \sqrt{\frac{m\,T}{\pi}}$$

which is a time scale of the same order as the free flight time of the particles and of the same order as the

relaxation time associated to local fluctuations when all gradients are negligible. The equations are

$$\frac{\mathrm{D}n}{\mathrm{D}t} + n\nabla \cdot \vec{v} = 0,$$

$$m\,n\frac{\mathrm{D}\vec{v}}{\mathrm{D}t} - n\,\vec{F} + \nabla \cdot \mathbf{P} = 0,$$

$$\frac{n\,d}{2}\frac{\mathrm{D}T}{\mathrm{D}t} + \nabla \cdot \vec{q} + \mathbf{P}:\nabla\vec{v} = 0,$$

$$\frac{\mathrm{D}\mathbf{p}}{\mathrm{D}t} + \mathbf{p}\nabla \cdot \vec{v} + \frac{2}{2+d}[\nabla\vec{q}]$$

$$+ [\mathbf{p}\cdot\nabla\vec{v}\,] + p[\nabla\vec{v}\,] = -\frac{1}{\tau}\,\mathbf{p},$$

$$\frac{\mathrm{D}\vec{q}}{\mathrm{D}t} + \frac{d+4}{d+2}\,(\vec{q}\,\nabla \cdot \vec{v} + \vec{q}\cdot\nabla\vec{v})$$

$$+ \frac{2}{d+2}(\nabla\overbrace{\vec{v})\,\vec{q}} + \frac{T}{m}\nabla \cdot \mathbf{p}$$

$$+ \frac{d+4}{m}\mathbf{p}\cdot\nabla T - \frac{1}{m\,n}(\overbrace{\nabla \cdot \mathbf{P})\,\mathbf{p}} + \frac{d+2}{2m}\,p\,\nabla T$$

$$= -\frac{d-1}{\tau d}\,\vec{q},$$

where $\mathrm{D}/\mathrm{D}t \equiv \partial/\partial t + \vec{v}\cdot\nabla$ is the convective derivative, $d = 2$ or 3 is the dimension of space, energy units are such that $k_{\mathrm{B}} = 1$, the square brackets have been used to indicate *symmetric traceless part*, namely

$$[A] = A_{ij} + A_{ji} - \frac{2}{d}\delta_{ij}\sum_a A_{aa},$$

the first over-brace term indicates contraction of the indices of $\vec{v}$ and $\vec{q}$ while the second one is to be understood as $(\partial P_{rs}/\partial x_s)\,p_{kr}$, $\mathbf{p}$ is the symmetric traceless part of the pressure tensor $\mathbf{P}$. Since we are dealing with Boltzmann's equation then $u = (d/2)T$ and the hydrostatic pressure obeys the ideal gas equation of state $p = n\,T$.

The first three equations essentially are the generic balance equations coming directly from Liouville's equation for Hamiltonian systems of many particles interacting pairwise via a short range central potential. The only difference with the most general equation is that u has been replaced by $(d/2)T$, which is true only if the collisional contribution to u can be neglected and this is possible at low density.

The last two equations take the place of the constitutive equations of standard hydrodynamics. They are new *dynamic equations* for the traceless part $\mathbf{p}$ of the pressure tensor and for the heat flux vector $\vec{q}$. Erasing

from these two equations all but the last two terms the standard linear transport equations with the ideal gas shear viscosity coefficient and the ideal gas thermal conductivity coefficient would be recovered.

3. Planar stationary flows

The challenge is to obtain useful information from this large set of hydrodynamic equations in their complete form. So far we have studied stationary cases with laminar planar flow. We have considered a laminar flow in the X direction between two parallel walls (parallel to the XZ plane in 3D and parallel to the X axis in 2D) kept at equal temperature T_0, see figure. The external force $\vec{F}$ is taken to point in the X direction: $\vec{F} = (g, 0, 0)$. Any gradient is in direction Y, namely y is the only relevant coordinate. The only non-vanishing component of the velocity field is $v_x(y)$. Under such circumstances the convective derivative is exactly zero and v_x enters only though its derivative. Instead of dealing with v_x it is more convenient to deal with the adimensional shear rate, $\gamma = \tau\,\mathrm{d}v_x/\mathrm{d}y$. What follows includes the case $g = 0$ and the walls moving with velocities $\pm v_0$ in the X direction, namely a planar Couette flow.

Define the adimensional control parameters:

$$Kn^{2D} = \frac{2}{\sqrt{\pi}\sigma\,N_x}, \quad Kn^{3D} = \frac{1}{\sqrt{2\pi}\sigma^2\,N_{xz}}, \quad \text{and}$$

$$\mathcal{F} = \frac{mg\,L_y}{T_0}\frac{1}{Kn}.$$

Kn is defined in terms of the diameter σ of the particles and the number of particles per unit length, N_x in 2D and N_{xz} is the number of particles per unit
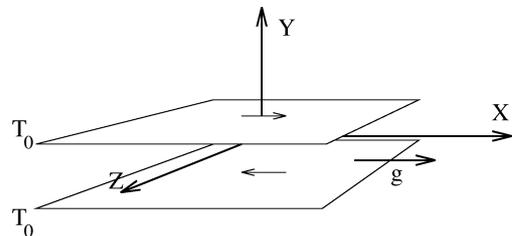
Fig. 1. The text describes a laminar stationary flow in the X direction between two walls orthogonal to the Y axis. There is either gravity g or the walls are moving parallel to the X axis in opposite directions. Under such conditions $P_{yz} = P_{xz} = 0$ and $q_z = 0$.

area in 3D. Kn is a Knudsen number and it serves to characterize the finite nature of the system, it is roughly proportional to the ratio between the mean free path and the width of the channel. The quantity $\mathcal{F}$ serves as the parameter to derive a perturbative solution and it also serves to characterize the intensity of the flow as we show below. Our formalism is valid when Kn is small and $\mathcal{F}$ is at most of order 1. If $g = 0$ then γ is uniform and it serves as the expansion parameter.

The system is defined in such a way that it is symmetric with respect to changing the sign of γ. Since g (or if $g = 0$, γ) is the agent that takes the system out of equilibrium then both g and γ can be taken to be first order quantities. The symmetry implies that the hydrodynamic fields have a well defined parity: T, q_y and the diagonal components of P_{ij} are even while γ, P_{xy} and q_x are odd. The equations then reduce considerably. The mass continuity equation becomes an identity. The momentum balance imply that P_{yy} is uniform and that

$$\tau P'_{xy} = \frac{m\,g}{d}\frac{\tau\,p}{T}. \tag{1}$$

The energy balance equation is

$$\tau q'_y = -\gamma\,P_{xy}. \tag{2}$$

These are all the relations that come from the *standard* hydro*dynamic* equations. The balance equations associated to the pressure tensor yield

$$p = P_{yy} - \frac{6}{2+d}\gamma P_{xy}, \tag{3}$$

$$P_{xx} = P_{yy} - \frac{2(d+4)}{2+d}\gamma\,P_{xy}, \tag{4}$$

$$P_{zz} = (d-2)\,P_{yy} - \frac{4(d-2)}{2+d}\gamma P_{xy}, \tag{5}$$

$$\tau\,q'_x = -\frac{2+d}{2}(\gamma\,P_{yy} + P_{xy}). \tag{6}$$

Consistently, for $d = 2$ automatically $P_{zz} = 0$. From the balance equations associated to $\vec{q}$ it follows that

$$\frac{(d+4)d\tau}{2(d-1)m}P_{xy}T' + d\,T\tau\left[(2+d)P_{yy} + 2((d+4)\gamma - 6)P_{xy}\right]P'_{xy} = -q_x - \frac{(d+4)d\,\gamma\,q_y}{(d+2)(d+1)}, \tag{7}$$

$$\frac{d\,(d+2)\,P_{yy}\,\tau\,T'}{2(d-1)\,m} + \frac{6\,d\,\tau}{(d+2)(d-1)\,m}(T\gamma\,P_{xy})' - \frac{d\,T\,P_{xy}\,\tau\,P'_{xy}}{(d-1)mp} = -q_y - \frac{2d\,\gamma\,q_x}{(d+2)(d-1)}. \tag{8}$$

Eqs. (1), (2), (6), (7) and (8) are five coupled differential equations for γ, T, P_{xy}, q_x and q_y. The uniform field P_{yy} is determined requiring that the integral of the density, $\int p/T\,\mathrm{d}y$, gives N_x in 2D and N_{xz} in 3D, whereas p is evaluated using (3), P_{xx} and P_{zz} are obtained from (4) and (5).

4. Perturbative solution for a 2D Poiseuille flow

As a first illustration let us take the case of a two-dimensional Poiseuille flow in the X direction along a channel of width L_y. Define the following reduced fields: $T^*(\xi) = T(y)/T_0$, $P^*_{ij}(\xi) = P_{ij}(y)/p_0$ and $q^*_k(\xi) = q_k(y)/q_0$ where $\xi = y/L_y$ is the reduced transversal coordinate, $p_0 = N_x T_0/L_y$, and $q_0 = \sqrt{T_0/m}\,p_0/2$. To order $\mathcal{F}^2$ the equations yield,

$$P^*_{xy} = \xi\,Kn\,\mathcal{F},$$

$$\gamma = -\xi\,Kn\,\mathcal{F},$$

$$P^*_{yy} = 1 + \left[\frac{1}{60} - \frac{Kn^2}{4}\right]\mathcal{F}^2,$$

$$p^* = 1 + \left[\frac{1}{60} + \left(\frac{3}{2}\xi^2 - \frac{1}{4}\right)Kn^2\right]\mathcal{F}^2,$$

$$T^*(\xi) = 1 + \left[\frac{1}{48} - \frac{\xi^4}{3} + \left(\frac{3\xi^2}{4} - \frac{3}{16}\right)Kn^2\right]\mathcal{F}^2,$$

$$q^*_x = -\mathcal{F}\,Kn^2,$$

$$q^*_y = \frac{8}{3}\xi^3\mathcal{F}^2 Kn.$$

Already at this order there is an anomalous heat flux q_x parallel to the isotherms, the pressure tensor is not uniform but it is of order $Kn^2\,\mathcal{F}^2$. Newton's law of viscous flow, which in the present notation is $P^*_{xy} = -p^*\,\gamma$ is obeyed, but this is not true at higher orders. The normal component q_y of the heat flux would obey Fourier's law, $q^*_y = -2\,Kn\,\mathrm{d}T^*/\mathrm{d}\xi$, if we drop the term proportional to Kn^2 in the temperature field. From the second order solution written above it can be seen that the reduced velocity field $v^*_x = \sqrt{m/T_0}\,v_x$ to this order is given by $v^*_x = 2\mathcal{F}(1/4 - \xi^2)$ showing that at

Table 1
Comparison of the predicted and observed temperature profile in a 2D Couette flow from the center of the channel ($y/L_y = 0$) to one of the lateral walls, $y/L_y = 0.5$ (the observed profile is almost exactly symmetric). The simulation used $N = 29583$ hard particles in a square box, area fraction occupied by the disks $\rho_A = 0.01$, $Kn = 0.0581$. The temperature imposed on the channel's walls is $T_0 = 1$. The effective value of the shear rate turns out to be $\gamma = 0.026381$. The rightmost column gives the percentage discrepancy between the theoretical and observed values of the temperature. Notice that, except for three values near the wall (which correspond to a region of a size $0.06\,L_y$) the differences are clearly less than 1%

y/L_y	$T_{\text{theor.}}$	$T_{\text{sim.}}$	%
−0.023	1.1917	1.1916	−0.01
0.023	1.1917	1.1917	0.00
0.047	1.1909	1.1912	0.02
0.070	1.1897	1.1897	0.00
0.093	1.1879	1.1880	0.01
0.116	1.1856	1.1860	0.04
0.140	1.1828	1.1832	0.03
0.163	1.1795	1.1799	0.04
0.186	1.1757	1.1764	0.06
0.209	1.1713	1.1726	0.10
0.233	1.1665	1.1680	0.13
0.256	1.1611	1.1629	0.16
0.279	1.1551	1.1573	0.19
0.302	1.1486	1.1511	0.21
0.326	1.1416	1.1436	0.17
0.349	1.1341	1.1358	0.16
0.372	1.1259	1.1268	0.07
0.395	1.1172	1.1164	−0.07
0.419	1.1080	1.1042	−0.34
0.442	1.0981	1.0880	−0.92
0.465	1.0876	1.0617	−2.39
0.488	1.0766	0.9872	−8.30

the center of the channel ($\xi = 0$) the hydrodynamic velocity is proportional to $\mathcal{F}$. This perturbative description can be taken to much higher order. In [8], for example, expressions up to sixth order are given and they describe extremely well the simulation results.

5. Temperature profile

The temperature profile is more dependent on the number of particles than on other fields. Table 1 has a comparison between theory and a simulation with about 30 thousand particles for the temperature profile of a 2D Couette flow for which we have attained an excellent fit. In the Poiseuille flow of the previous paragraph the temperature profile at second order is not parabolic and in the limit $Kn \to 0$ it behaves like ξ^4. The temperature at the center does not have a maximum, as expected, but a shallow minimum, with maxima at $\xi = \pm 3\,Kn/2\sqrt{2}$, namely, in a small region at the center there is heat flux from a cooler center towards the hotter maxima of T^* (!). This minimum has been observed in simulations and an explanation has been presented using the BGK approximation to Boltzmann's equation [11], see also [8]. The temperature difference between the maxima and the center is quite small: $27\mathcal{F}^2\,Kn^4/64$.

6. Third order heat flux law

Besides the perturbative solution presented above it is possible to derive from Eqs. (1)–(8) quite general transport equations. In what follows we show how a heat flux law can be derived from our equations for a planar stationary flow.

To zero order the only non-vanishing fields are the temperature, the pressure and the diagonal terms of the pressure tensor. Since the temperature is even its next contribution is of second order. On the other hand q_x is odd but its first order contribution is uniform, as was seen above, therefore q'_x is of order three. Hence, from (6), the combination $\gamma\,P_{yy} + P_{xy}$ is of third order even though each one is first order. Following this type of reasoning and algebraically solving (7) and (8) in favor of q_x and q_y allows us to obtain up to third order expressions for the heat flux components which, in the three dimensional case, are

$$q_x^* = -\frac{15}{16}Kn\,\mathcal{F}\,\sqrt{T^*} - \frac{157}{80}Kn\,T^{*3/2}(\gamma^3)'$$
$$+ \frac{175}{32}Kn\,\gamma\,(T^{*3/2})',$$
$$q_y^* = -\frac{25}{4}Kn\,(T^{*3/2})' - \frac{21}{4}Kn\,T^{*3/2}(\gamma^2)'.$$

The first component is the anomalous heat flux (parallel to the isotherms) and the second one consists of two terms, the first one is exactly Fourier's term in the case of an ideal gas, the last one comes from gas-dynamics. We would like to mention that an *empirical* transport law of this kind was proposed in [12] (see also [13,14]) to give account of his MD simulations results.

7. Final comment

We have presented a gas dynamics – derived from Boltzmann's equation using a moment expansion method – which is far more complex than the standard Navier–Stokes dynamics. The dynamic fields are the density, the hydrodynamic velocity, the temperature, the pressure tensor and the heat flux vector. No constitutive equations have to be assumed since there are dynamic equations that replace them. The predictions stemming from such framework, when applied to stationary laminar flow, describe extremely well the observations obtained from molecular dynamic simulations. In the case of stationary planar laminar flows a third order modification to Fourier's law has been presented.

Acknowledgements

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