SYNOPTIC: Breakdown of Translational and Rotational Equilibrium in Gaseous Expansions,

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Rarefied Flow; Supersonic and Hypersonic Flow

Theme

A numerical study of the breakdown of translational equilibrium in steady expansions and in unsteady rarefaction waves is presented. All results are correlated by a simple nondimensional parameter, leading to the proposal of an empirical breakdown criterion for use in engineering studies of systems involving low-density expansions from continuum to highly rarefied conditions.

Content

An application of the direct simulation Monte Carlo method, which is claimed to give a solution of the full Boltzmann equation. The breakdown of translational equilibrium in steady cylindrical and spherical expansions was studied for both hard sphere and Maxwell molecules. The study of spherical expansions was extended to the combined translational and rotational breakdown in a gas of rough sphere molecules. The breakdown of translational equilibrium in a complete one-dimensional rarefaction wave in a hard sphere gas was also studied. The application of the method generally followed standard procedures, except for the unsteady flow, in which a Lagrangian system of cells moving with the fluid was used in place of the usual Eulerian cells fixed in physical space.

The onset of nonequilibrium was marked by the divergence of the separate kinetic temperatures based on the molecular velocity components parallel and normal to the flow direction. The region of simulation of the steady expansion generally covered only a restricted range of Mach number in the vicinity of the point of breakdown. However, several runs were made over a wide range of Mach number and the temperatures were plotted against radius r in order to obtain an over-all picture of the process. The results gave qualitative support to one of the major predictions of the BGK theory—that the freezing of the parallel temperature T_x occurs gradually over a wide range of Mach number and is much less rapid for Maxwell molecules than for hard sphere molecules. In the case of the normal temperature T_n, there is a qualitative difference between the results for the two molecular models. The Monte Carlo calculation for the Maxwell molecules gave a T_n curve that remains above the $r^{-4/3}$ continuum curve and could well be consistent with the r^{-1} prediction of the BGK theory. However, for the simulation with hard sphere molecules, the T_n curve falls below the continuum curve.

A rarefaction parameter P was defined by the ratio of the logarithmic time derivative of density ρ, following the motion of the fluid, to the collision frequency ν in the gas. That is,

$$P = (1/\nu)D(\ln\rho)/Dt \tag{1}$$

The departure of the temperature ratio T_x/T_n from unity gives the best indication of translational breakdown, and it was plotted against P for all the steady expansion runs. These involved two geometries, three molecular models and Mach numbers ranging from 2 to 20. In all cases, the breakdown of equilibrium occurred at a value of P of approximately 0.04. If the hard sphere formula for collision frequency in terms of viscosity coefficient is substituted into Eq. (1), this leads to the following empirical breakdown criterion for steady expansions

$$\gamma M^2/Re_L = 0.05 \tag{2}$$

Here, γ is the specific heat ratio, M the Mach number, and Re_L the Reynolds number based on density scale length.

The general behavior of P in a steady expansion is that it decreases to a minimum at a Mach number of the order of 1.5 and then increases with M. For very high Mach numbers

$$P \propto M^k \tag{3}$$

where k depends on the geometry and molecular model. This suggests that if a flow is out of equilibrium at supersonic Mach numbers below 1.5, the region of nonequilibrium will extend upstream to the subsonic region. The index k has the value 2.5 for the spherical expansion of a hard sphere gas, leading to a comparatively fast freeze of T_x. However, k becomes zero for a cylindrical expansion of a Maxwell gas and no progressive freeze of T_x would be expected in this case.

The behavior of P in a one-dimensional unsteady rarefaction wave is given by

$$DP/Dt = (P/t)[(\gamma - 1)/(\gamma + 1)](1-2\,\omega) \tag{4}$$

with the coefficient of viscosity assumed to be proportional to T^ω. For a hard sphere gas, $\omega = \frac{1}{2}$ and P remains constant along a particle path. This means that if a fluid element remains in equilibrium when it first enters the expansion, it should remain in equilibrium at all subsequent times. Alternatively, if the element goes out of equilibrium in the very early part of the expansion, it would be expected to remain in much the same state as it progresses along a particle path. A simulation run was carried out for a hard sphere gas and the ratio T_x/T_n was obtained as a function of fluid element at a number of values of time. There was no significant effect of time on the curves, which is exactly as expected from the discussion of Eq. (4). Moreover, the breakdown of equilibrium again occurred at a value of P of approximately 0.4. For more realistic molecules with $\omega > \frac{1}{2}$, P decreases along a particle path and a progressive freeze would not occur. On the contrary, there may be a tendency for a fluid element which initially goes out of equilibrium to move back towards equilibrium at later times.