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Title: BUOYANCY-GENERATED VARIABLE -DENSITY TURBULENCE

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# Buoyancy-generated variable-density turbulence

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Buoyancy-generated turbulence in a fluid with large density fluctuations is studied by direct numerical simulation [Sandoval (1995)]. The flow is incompressible so that acoustic waves are decoupled from the problem, and implying that density is not a thermodynamic variable. The density variations are large such that the Boussinesq approximation is inappropriate and changes in density occur due to molecular mixing. The velocity field is, in general, divergent, and there is no net volumetric flux of velocity. The results of numerical simulations are compared with variable-density model predictions. Both a one-point (engineering) model and a two-point (spectral) model are tested against the numerical data. Some deficiencies in these variable-density models are discussed and modifications are suggested.

We shall restrict our attention to the turbulent interactions of two miscible, incompressible Newtonian fluids of different densities. By the terminology incompressible fluid we mean a fluid whose compressibility coefficient and thermal expansion coefficient are both zero. This decouples acoustic waves from the problem, implying an infinite sound speed and that density is no longer a thermodynamic variable and therefore not a function of the pressure. For a flow to be incompressible, the main criterion is that the Mach number be low, $M \to 0$. In our study, the Mach number is assumed to be zero. It has been illustrated by Joseph (1990) that the velocity field for the mixing of two miscible, incompressible fluids is not in general divergence free, i.e., $\nabla \bullet \vec{u} = 0$. Herein, we refer to the flow in this study as being incompressible due to the low Mach number criterion but not that the divergence of the velocity field is zero. The conservation of mass is

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0.$$

The equations for the conservation of momentum are the Navier-Stokes equations, here given as

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i$$

with the viscous stress tensor defined by

$$\tau_{ij} = \mu \left\{ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_n}{\partial x_n} \right\}$$

Here $\rho(x_i,t)$, $p(x_i,t)$ and $u_i(x_i,t)$ are the density, pressure and velocity fields, respectively, dependent on the spatial coordinate $x_i$ and on time $t$, $g_i$ is an acceleration (e.g., gravity), and $\mu$ the fluid viscosity, assumed constant. Fick's law [see, e.g., Bird, Stewart and Lightfoot (1960)] for the diffusion of two species of different densities gives

$$\frac{\partial \rho}{\partial t} + u_j \frac{\partial \rho}{\partial x_j} = \rho \frac{\partial}{\partial x_n}\left\{\frac{D}{\rho}\frac{\partial \rho}{\partial x_n}\right\}$$

Comparison of the conservation of mass equation with diffusion equation leads to the following result for the divergence of the velocity field:

$$\frac{\partial u_n}{\partial x_n} = -\frac{\partial}{\partial x_n}\left\{\frac{D}{\rho}\frac{\partial \rho}{\partial x_n}\right\}.$$

These equations with periodic boundaries, are solved by a pseudo-spectral algorithm for $128^3$ grid points. Initial conditions are based on the method of Eswaran and Pope (1988). A condition for a mean pressure gradient is also required to correctly specify the problem of a variable-density fluid subjected to an acceleration. This pressure gradient condition ensures zero volumetric flux in the "lab" reference frame. The most common approach to study variable-density flows is to use the Boussinesq approximation [see, e.g., Phillips (1977)]. This approximation is valid when the actual density and pressure fluctuations vary only slightly from their respective means, the vertical scale of motion is small compared with the scale height, and the Mach number of the flow is low.

Departures from the limits of validity of the Boussinesq approximation are examined. An important parameter that characterizes buoyancy driven flow is the initial value of the ratio of the rms density fluctuations to the mean density, $\theta_o = \overline{\rho'\rho'}^{1/2}|_{t=0} / \overline{\rho}$. Two simulations are studied, both with a Schmidt number equal to one. The initial density fluctuations are scaled such that $\theta_o = 0.04$ for one case and $\theta_o = 0.52$ for the other. If this quantity is less than approximately 0.1 then the resulting buoyancy-driven flow is within the Boussinesq approximation. It is observed in this buoyancy-generated problem that the triple correlation, $\overline{\rho'u_i'u_i'}$, which is initially nearly zero, grows to negative values. This reflects the fact that the largest velocities are associated with the negative density fluctuations, and is a result of conservation of momentum. The probability density function (PDF) of the density field, which is initially bimodal, develops a skew to the negative of the mean density due to entrainment behavior. Figure 1 shows the time history of the PDF for the case with $\theta_o = 0.52$. The Boussinesq approximation for this flow predicts symmetric evolution of the PDF because both positive and negative density fluctuations receive the same acceleration. This PDF behavior is seen in the study of isotropic decay [Sandoval (1995)] and occurs only when $\overline{\rho'u_i'u_i'}$ is nonzero.

A consequence of the Boussinesq approximation is that the mean pressure gradient is constant in time and its value is $\overline{\rho}g_i$ i.e., the hydrostatic pressure gradient. This approximation is good

only in the limit of small density fluctuations but, as the initial density fluctuations increase, the mean pressure gradient becomes variable in time. The equation for the mean pressure gradient is

$$\frac{\partial \overline{p}}{\partial x_i} = \frac{1}{\overline{v}}\left\{ g_i - \overline{v'\frac{\partial p'}{\partial x_i}} + \overline{v'\frac{\partial \tau'_{ni}}{\partial x_n}} + \overline{u'_i\frac{\partial u'_n}{\partial x_n}} \right\},$$

where $v = 1/\rho$ is the specific volume. In the limit as the density fluctuations tend to zero, this equation gives the Boussinesq approximation for the mean pressure gradient, i.e., the hydrostatic balance. Figure 2 shows the time evolution of the mean pressure gradient normalized by the hydrostatic value for the cases with $\theta_o = 0.04$ and $\theta_o = 0.52$. For the case with $\theta_o = 0.04$, the mean pressure gradient is nearly constant in time with its value corresponding to the hydrostatic balance. At the instant an acceleration is applied and prior to the development of fluid motion, the mean pressure gradient is

$$\frac{\partial \overline{p}}{\partial x_i} = \frac{1}{\overline{v}}\left\{ g_i - \overline{v'\frac{\partial p'}{\partial x_i}} \right\},$$

Here, the correlation between the fluctuating specific volume and the fluctuating pressure gradient produces a departure from the simple hydrostatic pressure gradient. This correlation increases with increasing initial density fluctuations, and impedes the growth of the turbulent mass flux, $a_i = -\overline{\rho'u'_i}/\overline{\rho}$. This term responds instantaneously to the applied acceleration. Figure 3 shows this correlation plotted as a function of the mass flux for the case with $\theta_o = 0.52$. At early times, this correlation is proportional to the mean pressure. As the flow develops and the density fluctuations decay, this correlation becomes proportional to the mass flux.

The results of the buoyancy-generated turbulence are compared with variable-density model predictions. Both a one-point (engineering) model [Besnard, Harlow, Rauenzahn and Zemach (1992)] and a two-point (spectral) model [Clark and Spitz (1994)] are tested against the numerical data. Some deficiencies in these variable-density models are discussed. In particular, it has been speculated by modelers that the correlation between the fluctuating specific volume and the gradient of the fluctuating pressure is proportional to the mass flux. This speculation is correct within the Boussinesq limit. However, the numerical results show that this speculation, in the limit of large density variations, is incorrect during the early stages of flow development. Modifications to this variable-density model to take into account this behavior are made. Comparison between the model and the numerical results show the inadequacy of the equilibrium assumptions inherent in one-point models as this buoyancy-generated flow is far from equilibrium. Using a two-point (spectral) model, which makes no equilibrium assumption, the one-point statistics of the flow are captured more accurately. Though the one-point statistics from the spectral model are in good qualitative agreement with the numerical data, the spectra from the DNS of the correlation between the fluctuating specific volume and the gradient of the fluctuating pressure do not agree with the spectral model of this quantity.
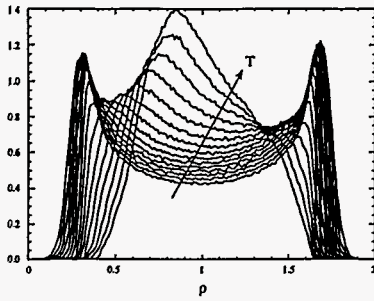
Figure 1: PDF evolution, for T=0.0 to 1.75 by 0.125, for the case with $\theta_o = 0.52$.
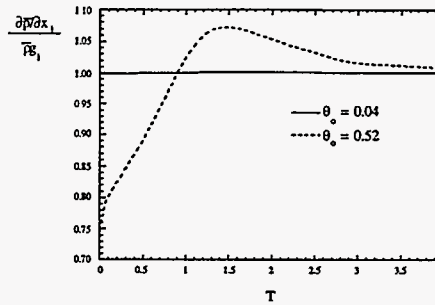


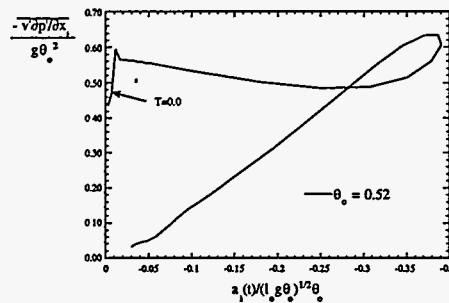Figure 2: Mean pressure gradient histories for the cases with $\theta_o = 0.04$ and $\theta_o = 0.52$.



Figure 3: Correlation between the fluctuating specific volume and gradient of the fluctuating pressure as a function of mass flux in nondimensional form for the case with $\theta_o = 0.52$.

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