TURBULENCE VIA AN INTERMOLECULAR POTENTIAL: THE EFFECT OF VISCOSITY AND THE TRANSITION RANGE OF THE REYNOLDS NUMBER

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Abstract. In our recent works, we proposed and studied a theory of turbulence in gases, which states that turbulent motions are created in an inertial flow via the mean field effect of the intermolecular potential. In the present work, we investigate the effect of viscosity in our model of turbulence via an intermolecular potential. We numerically simulate the inertial air flow at normal conditions in a straight pipe for different values of the Reynolds number, and discover that the transition between the laminar and turbulent flow occurs when the Reynolds number is between 2000 and 4000, which is consistent with practical knowledge. Additionally, as the flow becomes turbulent, the decay rate of the time-averaged Fourier spectrum of the kinetic energy transitions from the inverse eight-thirds to Kolmogorov’s inverse five-thirds power of the wavenumber.

1. Introduction

Reynolds [1] demonstrated that laminar flow of a liquid consistently develops turbulent motions whenever the high Reynolds number condition is satisfied. Later, Kolmogorov [2, 3, 4] observed that the kinetic energy of turbulent air flow decays as the inverse five-thirds power of its Fourier wavenumber. In our recent works [5–7] we proposed a theory of turbulence in a compressible gas flow, where turbulent motions in an otherwise laminar inertial gas flow are created by the mean field effect of the intermolecular potential $\phi(r)$. According to our theory, turbulence in a gas emerges in a compressible flow with density $\rho$ and velocity $u$ at a constant pressure $p_0$ (inertial flow), where the momentum transport equation in the absence of the pressure gradient has a novel forcing term due to the mean field potential $\bar{\phi}$:

\begin{align}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) &= 0, \\
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u^2) + \nabla \bar{\phi} &= 0.
\end{align}

Assuming that the intermolecular potential $\phi(r)$ has the effective range $\sigma$, in [5–7] we estimated the mean field potential $\bar{\phi}$ via

\begin{equation}
\bar{\phi} = \frac{4p_0\rho}{\rho_{HS}},
\end{equation}

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where $\rho_{HS} = 6m/\pi\sigma^3$ is the density of the equivalent hard sphere of mass $m$ and diameter $\sigma$. With (2), we wrote the momentum equation (1b) in the form

\begin{equation}
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u^2) + \frac{4p_0}{\rho_{HS}} \nabla \rho = 0.
\end{equation}

In [5–7], we found that (3), coupled with (1a), produces turbulent flow with Kolmogorov decay of the Fourier spectra of the kinetic energy. Viscous effects were, however, omitted thus far in our initial studies, because we first decided to test our theory in the most basic hydrodynamic limit with infinite Reynolds number.

### 2. The equations for inertial flow with potential forcing and viscosity

In the current work, we add a standard viscous term with the dynamic viscosity $\mu$ into the momentum equation (3):

\begin{equation}
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u^2) + \frac{4p_0}{\rho_{HS}} \nabla \rho = \nabla \cdot (\mu \nabla u).
\end{equation}

According to the kinetic theory of gases [8], $\mu$ is proportional to the square root of the temperature. In the inertial flow, the product of the temperature and density is constant, and thus $\mu$ is inversely proportional to $\sqrt{\rho}$,

\begin{equation}
\mu = \mu_0 \sqrt{\frac{\rho_0}{\rho}},
\end{equation}

where $\rho_0$ and $\mu_0$ are the reference density and viscosity, respectively.

To introduce the Reynolds number, we switch to non-dimensional variables in a standard fashion. We introduce the length scale $L$, velocity scale $U$, and rescale the variables in (1a) and (4) as follows:

\begin{equation}
\tilde{t} = \frac{U}{L} t, \quad \tilde{x} = \frac{x}{L}, \quad \tilde{\rho} = \frac{\rho}{\rho_0}, \quad \tilde{u} = \frac{u}{U}.
\end{equation}

In addition, we introduce the Reynolds number $Re$ and Mach number $Ma$ via

\begin{equation}
Re = \frac{\rho_0 UL}{\mu_0}, \quad Ma = \frac{U}{\sqrt{\frac{\rho_0}{\gamma p_0}}},
\end{equation}

where $\gamma$ is the adiabatic exponent of the gas. In the non-dimensional variables, the density equation (1a) remains the same, but the momentum equation (4) becomes

\begin{equation}
\frac{\partial (\rho \tilde{u})}{\partial \tilde{t}} + \nabla \cdot (\rho \tilde{u}^2) + \frac{4\eta}{\gamma Ma^2} \nabla \tilde{\rho} = \frac{1}{Re} \nabla \cdot \left( \frac{\nabla \tilde{u}}{\sqrt{\tilde{\rho}}} \right),
\end{equation}

where $\eta = \rho_0/\rho_{HS}$ is the packing fraction. It is clear that turbulent flow cannot emerge if the coefficients of the forcing and dissipative terms are balanced, that is,

\begin{equation}
Re_* = \frac{\gamma Ma^2}{4\eta}.
\end{equation}
however, for $Re > Re^*$, the manifestation of turbulent flow depends on the geometry of the domain; in particular, it is known in practice [9] that the transition to turbulent flow in pipes occurs for values of $Re$ between 2000 and 4000.

### 3. Numerical simulation

To confirm whether or not our model predicts the transition to turbulence within a matching range of the Reynolds numbers, here we present numerical simulations of (1a) and (4) for the air flow at normal conditions in a straight pipe. As in our recent works [5–7], we use the appropriately modified rhoCentralFoam solver [10], which uses the central discretization scheme of Kurganov and Tadmor [11], with the flux limiter due to van Leer [12]. The rhoCentralFoam solver is a part of the OpenFOAM suite [13].

#### 3.1. Computational settings

We simulate the flow in a straight pipe of square cross-section. The size of the pipe is $36 \times 5.2 \times 5.2$ cm$^3$. The domain is uniformly discretized in all directions with the step of 0.8 mm, which comprises $450 \times 65 \times 65 = 1,901,250$ finite volume cells in total. The pipe is open-ended at the outlet side, and has a wall at the inlet side, with the circular inlet of 1 cm in diameter located in the middle of this wall. The boundary conditions are the following: the density is set to 1.204 kg/m$^3$ at the outlet, and has zero normal derivative at the inlet and the walls; the velocity has zero normal derivative at the outlet, no-slip condition at the walls, and a radially symmetric parabolic profile at the inlet, with the maximum of 30 m/s in the middle of the inlet, directed along the axis of the pipe. The diameter of the inlet, and the speed of the flow correspond to the experiment by Buchhave and Velte [14]. Initially, the gas inside the pipe is at rest, with zero velocity and uniform density set to 1.204 kg/m$^3$.

The scaling constants in (6) and (7) are: $U = 30$ m/s, $L=5.2$ cm (the width of the pipe), $\rho_{HS} = 1850$ kg/m$^3$ (see [6] for details), $p_0 = 1.013 \cdot 10^5$ Pa, and $\rho_0 = 1.204$ kg/m$^3$, which corresponds to air at normal conditions. For these values of parameters, $Re^* \approx 4.1$.

#### 3.2. Results

We conducted numerical simulations of (1a) and (4) for the values of the Reynolds number $Re = 1000, 2000, 3000$ and 4000, by setting the reference viscosity $\mu_0 = \rho_0 UL/Re$. We found that the flow fully develops by the elapsed time $t = 0.07$ seconds; thus, we computed the statistical averages, presented below, in the time interval between 0.1 and 0.2 seconds. In the left pane of Figure 1, we show four snapshots of the speed of the flow, taken in the longitudinal symmetry plane of the pipe at $t = 0.15$ s, which illustrate the transition between the laminar and turbulent flow. For $Re = 1000$, the flow is laminar and symmetric relative to the axis of the pipe. For $Re = 2000$, this symmetry is broken, and small fluctuations start appearing in the otherwise laminar flow. For $Re = 3000$, the flow is fully turbulent.

The range of the Reynolds number for a turbulent transition in our model agrees with observations and general engineering knowledge [9]. Also, as we noted in [7], the breaking of the flow symmetry during the transition to turbulence is likely associated with the onset of chaos in the dynamics, and happens due to exponentially growing machine round-off errors. The hypothesis that turbulence is a manifestation of nonlinear chaos has also been discussed in the literature (see Letellier [15] and references therein).
Figure 1. Left: speed of the flow (m/s), captured in the longitudinal symmetry plane of the pipe at the elapsed time $t = 0.15$ s for $Re = 1000, 2000, 3000$ and $4000$ (corresponding to $\mu_0 = 1.872 \cdot 10^{-3}, 9.36 \cdot 10^{-4}, 6.24 \cdot 10^{-4}$ and $4.68 \cdot 10^{-4}$ kg/m s, respectively). Right: the Fourier spectra of the kinetic energy, averaged between 0.1 and 0.2 s of the elapsed time, for the same Reynolds numbers. The simulation for air ($\mu_0 = 1.82 \cdot 10^{-5}$ kg/m s), as well as $E_0 k_1^{-5/3}$ and $E_0 k_1^{-8/3}$ power decay slopes, are added for reference. Note that the empirical scaling constant, $E_0 = 20$ m$^2$/s$^2$, is identical for both power decay slopes.

In the right pane of Figure 1, we show time averages of the Fourier spectra of the streamwise component $u_x^2/2$ of the kinetic energy, which were computed as described in our recent works [5–7]. The computation was done within the central core of the pipe of $3.6 \times 3.6$ cm$^2$ in cross-section, extending between 0 and 24 cm of the length of the pipe (300 finite volume cells), and thus largely containing the jet stream. The computed spectra are shown for the same simulated flows with $Re = 1000, 2000, 3000$ and $4000$ in the range $1 \leq k \leq 150$ wavenumbers, which is half of the total number of the finite volume cells. We also show the kinetic energy spectrum for a simulation with $\mu_0 = 1.82 \cdot 10^{-5}$ kg/m s ($Re \sim 10^5$), which corresponds to the viscosity of air at normal conditions [16]. For reference, in Figure 1 we show two power slope lines, given via $E_0 k_1^{-8/3}$ and $E_0 k_1^{-5/3}$, with the empirically chosen scaling constant $E_0 = 20$ m$^2$/s$^2$.

At large scale Fourier wavenumbers ($k \leq 10$), the structures of the kinetic energy spectra of all computed flows are similar, and the major differences start for $k > 10$. For $Re = 1000, 2000$ and $3000$, the kinetic energy spectrum at small scales generally appears to match the $k^{-8/3}$ decay slope, with the following variations. In the $Re = 2000$ regime, the spectrum decays along the $k^{-8/3}$-slope rather monotonously, whereas in the $Re = 1000$ regime (which is fully laminar) the spectrum also exhibits oscillations
around this slope. The latter could be the manifestation of quasi-periodic dynamics at the unstable Fourier wavenumbers, with the periodicity of orbits destroyed by chaos as \( Re \) moves up to 2000. In the \( Re = 3000 \) regime, a peculiar growth of the energy spectrum is observed for \( 100 \leq k \leq 150 \), roughly. The rates of decay of the kinetic energy spectra for the turbulent regime \( Re = 4000 \), as well as that of the air, approach the \( k^{-5/3} \)-slope, which was observed by Kolmogorov [2, 3, 4].

Remarkably, starting at \( Re = 2000 \), the kinetic energy spectra at small scales are largely confined between \( E_0 k^{-8/3} \) and \( E_0 k^{-5/3} \) slope lines, as the flow transitions from laminar to turbulent. This seems to support Kolmogorov’s hypothesis of universality of the turbulent spectra [4], at least for a fixed large scale flow configuration.

4. Summary

In the current work we introduce viscosity into our model of turbulence via an intermolecular potential [5–7]. We numerically simulate the air flow at normal conditions in a straight pipe at different Reynolds numbers. We show that the transition into turbulent flow occurs when the Reynolds number increases from 2000 to 4000, which appears to be consistent with observations, experiments and practical knowledge [9, 15]. Additionally, we find that, in our model, the corresponding rate of decay of the time-averaged Fourier transform of the streamwise kinetic energy at small scales changes from \( E_0 k^{-8/3} \)-slope towards \( E_0 k^{-5/3} \)-slope, as the flow transitions from laminar to turbulent.

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