PARTICLE DISPERSION IN INHOMOGENEOUS TURBULENT FLOW

M.P.B. VEENMAN, J.G.M. KUERTEN AND J.J.H. BROUWERS
Department of Mechanical Engineering
Eindhoven University of Technology, The Netherlands

Abstract

A DNS code based on a spectral-element method is developed. The code is applied to calculate Eulerian space-time velocity correlation functions and to study the possibility to describe the dispersion of particles by a Langevin equation for particle velocity. The preliminary results indicate that it is possible to derive the damping coefficients from the correlation functions.

1. Introduction

Particle dispersion can be described by a Langevin equation, but there is no unique way to determine the coefficients in this equation for inhomogeneous flow. A recently developed theory (Brouwers [1]) predicts that these coefficients are related to the Eulerian space-time correlation function in a moving frame. The frame is moved in time with the local average fluid velocity.
The outline of this paper is as follows. In section 2 the numerical methods for the continuum phase and particles are considered. Next, in section 3 the stochastic theory is explained. Then some preliminary results will be presented and discussed in section 4. Finally, the conclusions are made.

2. Numerical Method

2.1. CONTINUUM PHASE

In this section the numerical method used for DNS of turbulent flow in a cylindrical pipe will be described. The equations to be solved are the Navier-

Stokes equations and continuity equation for incompressible flow. Because of the cylindrical geometry the choice for cylindrical coordinates and cylindrical velocity components is natural. Used are r, ϕ and z for the radial, tangential and axial coordinates and u_r, u_ϕ and u_z for the corresponding velocity components. Then the governing equations can be written in the form:

$$\frac{1}{r}\frac{\partial}{\partial r}(ru_r) + \frac{1}{r}\frac{\partial u_\phi}{\partial \phi} + \frac{\partial u_z}{\partial z} = 0 \tag{1}$$

$$\begin{cases} \dfrac{\partial u_r}{\partial t} + \omega_\phi u_z - \omega_z u_\phi + \dfrac{\partial P}{\partial r} = \dfrac{2}{Re}\left(\Delta u_r - \dfrac{u_r}{r^2} - \dfrac{2}{r^2}\dfrac{\partial u_\phi}{\partial \phi}\right) \\ \dfrac{\partial u_\phi}{\partial t} + \omega_z u_r - \omega_r u_z + \dfrac{1}{r}\dfrac{\partial P}{\partial \phi} = \dfrac{2}{Re}\left(\Delta u_\phi - \dfrac{u_\phi}{r^2} + \dfrac{2}{r^2}\dfrac{\partial u_r}{\partial \phi}\right) \\ \dfrac{\partial u_z}{\partial t} + \omega_r u_\phi - \omega_\phi u_r + \dfrac{\partial P}{\partial z} = \dfrac{2}{Re}\Delta u_z + f \end{cases} \tag{2}$$

Here t denotes time, ω_r, ω_ϕ and ω_z are the cylindrical components of the vorticity, Δ is the Laplace operator and the total pressure P is defined as $P = p + \mathbf{u}^2/2$, where p is the static pressure. The forcing term f is adjusted each time step to ensure a constant mass flow through the pipe demanding

$$f = -\frac{4}{Re}\left.\frac{\partial \overline{u}_z}{\partial r}\right|_{r=R}.$$

The equations have been non-dimensionalized by the radius of the pipe R, the kinematic viscosity ν and the bulk velocity u_B. The Reynolds number is defined as $Re = u_B D/\nu$ where D is the diameter of the pipe.
A finite part of a cylindrical pipe of length L is considered, using periodic boundary conditions in the axial direction. Combined with the natural periodicity in the tangential direction there are two periodic directions and the choice for a spectral method is obvious. In the radial direction an expansion based on Chebyshev polynomials is used. However, the distribution of the Gauss-Lobatto collocation points leads to very small cells near the pipe axis and thus necessitates the use of very small time steps. Therefore, the radial direction is divided into several elements and in each element an expansion into Chebyshev polynomials is adopted. At the interfaces between the elements the solution is required to be C^1. Each component of the solution is thus expanded as:

$$u(r,\phi,z) = \sum_{k_\phi=-M_\phi/2+1}^{M_\phi/2-1} \sum_{k_z=-M_z/2+1}^{M_z/2-1} \tilde{u}_{k_\phi,k_z}(r)\exp(ik_\phi\phi + 2\pi i k_z z/L).$$

In this way a hybrid method appears: Fourier-Galerkin in the two periodic directions and Chebyshev-collocation in the radial direction. Derivatives in the periodic directions can easily be calculated in spectral space, whereas derivatives with respect to r follow from the Chebyshev derivative matrix, see [5]. The reduction on the time step is alleviated further by applying 'mode-reduction' in the central element, i.e. the element near the pipe-axis. Here, only half of the available modes are solved, see e.g. [6]. For these modes the boundary conditions for the velocity and pressure at $r = 0$ are translated to the element interface.

The Navier-Stokes equations are integrated in time using a time-splitting method by [4]. We write the Navier-Stokes equations schematically as

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{N}(\boldsymbol{u}) + \nabla P = \boldsymbol{L}(\boldsymbol{u}) + \boldsymbol{f},$$

where $\boldsymbol{N}$ denotes the nonlinear terms on the left-hand side of (2), $\boldsymbol{L}$ the viscous terms on the right-hand side and $\boldsymbol{f}$ the forcing term. A second-order accurate time-splitting method with constant time step Δt is then given by

$$\begin{cases} \boldsymbol{u}^{n+1/3} = 2\boldsymbol{u}^n - \frac{1}{2}u^{n-1} - \Delta t(2\boldsymbol{N}(\boldsymbol{u}^n) - \boldsymbol{N}(\boldsymbol{u}^{n-1})) + \Delta t\boldsymbol{f} \\ \Delta P^{n+1} = \frac{1}{\Delta t}\nabla \cdot \boldsymbol{u}^{n+1/3} \\ \boldsymbol{u}^{n+2/3} = \boldsymbol{u}^{n+1/3} - \Delta t \nabla P^{n+1} \\ \boldsymbol{u}^{n+1} = \frac{2}{3}u^{n+2/3} + \frac{2}{3}\Delta t\boldsymbol{L}(\boldsymbol{u}^{n+1}). \end{cases} \tag{3}$$

In these formulas the superscript denotes the time level. In the first step the nonlinear terms are treated explicitly. The products of vorticity and velocity are calculated in a pseudo-spectral way, where fast-fourier transforms are used to transform from spectral to physical space. Note that the nonlinear terms have to be calculated only once per time step. The latest result is stored and used again in the next time step. Aliasing is prevented by the 3/2-rule.

In the second step a Poisson equation is solved for the pressure to ensure that the solution after the third step satisfies the continuity equation. A point that requires special attention in this step is the boundary condition for the pressure at the wall of the pipe. Following [4] we employ at $r = R$

$$\frac{\partial P^{n+1}}{\partial r} = -\frac{2}{Re}\left(\frac{1}{r}\frac{\partial^2 u_\phi^{n+1}}{\partial r \partial \phi} + \frac{\partial^2 u_z^{n+1}}{\partial r \partial z}\right),$$

where the solution at the new time level is found by linear extrapolation from the solution at the two previous time levels. In order to obtain a unique solution this boundary condition cannot be used for the $(k_\phi, k_z) = (0, 0)$ mode. Instead the mean pressure at the wall of the pipe is prescribed.

In the final step the linear, viscous terms in the Navier-Stokes equations are treated implicitly. In cylindrical coordinates the viscous parts of the equations for u_r and u_ϕ are coupled, but they can be decoupled by introducing $u_\pm = u_r \pm i u_\phi$. Moreover, the equations for the Fourier modes are completely decoupled, so that a one-dimensional equation for each Fourier mode and each velocity component results. These one-dimensional problems are solved by a direct method. At the wall of the pipe a no-slip boundary condition is applied. At the pipe axis the boundary conditions follow from the requirement that the Cartesian velocity components are regular. This results in $\tilde{u}_z = 0$ for $k_\phi \neq 0$, $\partial \tilde{u}_z / \partial r = 0$ for $k_\phi = 0$, $\tilde{u}_\pm = 0$ for $k_\phi \neq \mp 1$ and $\partial \tilde{u}_\pm / \partial r = 0$ for $k_\phi = \mp 1$.
The calculation is started from a random field superposed on an approximate mean field with the axial velocity component given by a logarithmic velocity profile. The random field is chosen in such a way that it satisfies the continuity equation and that the lowest four Fourier modes in both periodic directions are unequal to zero. In the first time step scheme (3) cannot be applied since only one field is available. A first-order time-splitting scheme is used instead. After a large number of time steps a state of fully-developed turbulence is reached. From that time onwards averaged flow quantities can be calculated.

2.2. FLUID PARTICLES

Fluid particles, e.g. particles without inertia, are tracked using this code. The differential equation for the position of such a particle is given by

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{u}(\boldsymbol{x}_i, t), \tag{4}$$

where $\boldsymbol{x}_i$ is the particle position of particle i and $\boldsymbol{u}$ are the three components of the particle velocity derived at the particle position. There are several methods to obtain the particle velocity in the interior of a grid cell. A very accurate method is direct summation of the Fourier series expansion, but this is prohibitively expensive. Linear interpolation gives reasonable results for the velocity, but derivatives of the velocity will be very inaccurate. Alternatively, Hermite interpolation in the radial direction and a fourth order accurate Lagrange interpolation scheme in the periodic directions are used, see [7]. This is done in physical space, since the solution is known there each time step to calculate the nonlinear term. An Euler-forward or 2-stage Runge-Kutta method is used to solve eq. (4) numerically and obtain the new particle position. If a particle leaves the computational domain through the axial boundary the periodicity of the velocity is used to determine its velocity. If a particle leaves the pipe at the outer wall it is reintroduced, using an elastic collision with the wall.

3. Stochastic Approach

3.1. DNS

With this code Eulerian space-time velocity correlation functions are calculated. These are defined as

$$R_{ii}(r,\tau) = \overline{u_i'(r,\phi,z,t)u_i'(r,\phi,z+\overline{u_z}(r)\tau,t+\tau)}, \tag{5}$$

where the overhead bar means time- or ensemble-average, u_i are the fluctuating parts of the three velocity components and τ is the time separation. Since ϕ and z are coordinates in homogeneous directions and the turbulence is stationary, the correlation function depends only on r and τ. As can be seen from eq. (5) the frame is moved in streamwise direction with the local average axial velocity. The Fourier transform of eq. (5) gives the spectral density function for the velocity.

3.2. LANGEVIN MODEL

The Langevin equation for particle velocity can be written as (see e.g. Borgas [2] and Wilson & Sawford [3])

$$\dot{v}' + \tau_s^{-1} v' = (C_0\epsilon)^{1/2} w_1(t), \tag{6}$$

where C_0 is the universal Kolomorov constant, ϵ the mean rate of energy dissipation ,$w_1(t)$ a white-noise term and τ_s the correlation time. The damping coefficient in the Langevin equation corresponds to the correlation time τ_s of the Eulerian correlation function. The determination of τ_s from the correlation function is not a trivial process, since several time scales determine the shape of this function. The smallest scales cause the zero-slope at $\tau = 0$. For high Re-numbers this effect decreases and the correlation function could be described by a single exponential function from which the correlation time can easily be determined. However, in our simulations of moderate Re-numbers a separation of time scales is used. This enables us to quantify the small scale effects.
To model the second (small) time scale, smoothing of white-noise is applied (see e.g. Stratonovic [8]), i.e. the rhs of eq. (6) is replaced by the random process $\zeta(t)$ which obeys the equation

$$\tau_\eta \dot{\xi} + \xi = (C_0\epsilon)^{1/2} w_2(t), \tag{7}$$

where τ_η is the Kolmogorov time-scale and $w_2(t)$ another white-noise term. The resulting spectral density of the particle velocity is

$$S_V(\omega) = \frac{C_0\epsilon}{(1+\tau_\eta^2\omega^2)(\tau_s^{-2}+\omega^2)} \tag{8}$$

The white-noise from the original Langevin equation (eq. 6) is no longer lumped into a delta-correlated process. By decreasing the order of the white-noise, viz. applying eq. (7), the real turbulent process is more accurately described. The process is divided into 2 time scales. If $Re \to \infty$, $\tau_\eta \to 0$ and the original Langevin equation is obtained again. In real flows the Reynolds number is never infinite, so *smoothing the white-noise* is a more realistic approach. The corresponding correlation function is the Fourier transform of eq. (8) and reads

$$\overline{v(0)v(t)} = \frac{\sigma_v^2}{1-\frac{\tau_\eta}{\tau_s}}\left(e^{-\frac{t}{\tau_s}} - \frac{\tau_\eta}{\tau_s}e^{-\frac{t}{\tau_\eta}}\right), \tag{9}$$

where the standard deviation σ_v is given by

$$\sigma_v^2 = \frac{1}{2}C_0\frac{\epsilon\tau_s}{(1+\frac{\tau_\eta}{\tau_s})} \tag{10}$$

The spectral density function for the acceleration, $S_A(\omega)$, can be obtained by multiplying eq. (8) with ω^2.

4. Results

The investigated Reynolds number equals 5300 based on the bulk velocity. The number of Fourier-modes in tangential and axial directions equal resp. 128 and 128. 5 Chebyshev elements are used which contain 28, 28, 21, 28 and 7 collocation points resp., where the element near the pipe axis has 7 collocation points. The code has been extensively tested and compared with DNS and experimental results of others ([6], [9], [10] and [11]). The investigated results, e.g. rms of velocity fluctuations, pressure- and vorticity fluctuations, 2-point velocity spectra and the components of the turbulent kinetic energy equation, are in good agreement. These quantities are merely used to check our code and hence the results are not displayed here.
Some preliminary results on particle dispersion will be discussed now. Special emphasis is put on the tangential velocity component. Due to the symmetry of the flow, the Langevin for this component is decoupled from the axial and radial components which are coupled. So, the tangential direction is a truly homogeneous direction.
Figure 1 shows the Eulerian correlation function for the tangential component, denoted by the solid line, at $r/R = 0.4$. Least-Square-Fitting this result to eq. (9), using τ_c and τ_η as fitting parameters, gives the dashed line as shown in figure 1. This indicates that the assumption of two separate time scales is justified and that this simple model is capable to describe the Eulerian statistics. The correlation function from the DNS, see figure

1, is Fourier transformed to obtain the velocity spectrum, $S_V(\omega)$. For the model eq. (8) can be used. Figure 1 shows the results in *log-log* scale and in figure 2 a linear scale is used. Multiplying these spectra with ω^2 gives the acceleration spectrum as indicated in figure 2. The reciprocal calculated values for τ_η and τ_c are also shown (arrows). The time scales are separated by approximately a factor 10. In the limiting process, where $\tau_\eta \to 0$, the spectrum for the acceleration goes to a constant value (dashdot). This is the true *white-noise approximation.* The actual DNS results are far from this limiting process. Still, by using a relatively simply model, a quantification of the 2 time-scales is possible. In the near future we will analyze the remaining radial and axial directions in the same way, in order to obtain all (damping) coefficients for the 3D Langevin equation. The result will be an *accurate* particle dispersion model for inhomogeneous turbulent flow. It also enables us to calculate the universal Kolmogorov constant C_0.

5. Conclusions

A spectral DNS code is developed to calculate the turbulent flow in a cylindrical geometry. Calculated averaged quantities are in good agreement with DNS and experimental results by others. Eulerian space-time velocity correlations, calculated with this code, can be modeled with a Langevin equation. In this way it is possible to derive the damping coefficients for this equation. Due to the relatively moderate Re-number employed, the white-noise approximation is not obtained.

References

1. Brouwers J.J.H., On Diffusion Theory of Stochastic Inhomogeneous Turbulence, *To be published.*
2. Borgas, M.S. and Sawford B.L., A Family of Stochastic Models for Two-Particle Dispersion in Isotropic Homogeneous Stationary Turbulence, *J. Fluid. Mech*, **279**, 69-99, 1994.
3. Wilson, J.D. and Sawford, B.L., Review of Lagrangian Stochastic Models for Trajectories in the Turbulent Atmosphere, *Bound. Lay. Met.*, **78**, 191-210, 1996.
4. Karniadakis, G.E., M. Israeli, and S.A. Orszag, High-order splitting methods for the incompressible Navier-Stokes equations, *J. Comp. Phys.*, **97**: 414-443, 1991
5. Canuto, C., M.Y. Hussaini, A. Quarteroni, and T.A. Zang, *Spectral methods in fluid dynamics*, Berlin, Springer-Verlag, 1988.
6. Loulou, P., *Direct Numerical Simulation of Incompressible Pipe Flow Using a B-Spline Spectral Method*, Ph.D. Thesis, Stanford University, Department of Aeronautics and Astronautics, 1996.
7. Balachandar, S., Maxey, M.R., Methods for Evaluating Fluid Velocities in Spectral Simulation of Turbulence, *J. Comp. Phys.*, **83**, 96-125, 1989.
8. Stratonovich, R.L., *Topics in the Theory of Random Noise*, Gordon and Breach, New York, 1967.
9. Eggels, J.G.M., Unger, F., Weiss, M.H., Westerweel, J., Adrian, R.J., Friedrich, R., Nieuwstadt, F.T.M., Fully Developed Turbulent Pipe Flow: a Comparison Between

Direct Numerical Simulation and Experiment, *J. Fluid. Mech*, **268**, 175-209, 1994.
10. Wagner, C., Hüttl, T.J., Friedrich, R., Low-Reynolds-Number Effects Derived from Direct Numerical Simulations of Turbulent Pipe Flow, *Computers & Fluids*, **30**, 581-590, 2001.
11. Westerweel, J., Draad, A.A., Hoeven, van der J.G.Th, Oord, van J., Measurement of Fully-Developed Turbulent Pipe Flow With Digital Particle Image Velocimetry, *Experiments in Fluids*, **20**, 165-177, 1996.

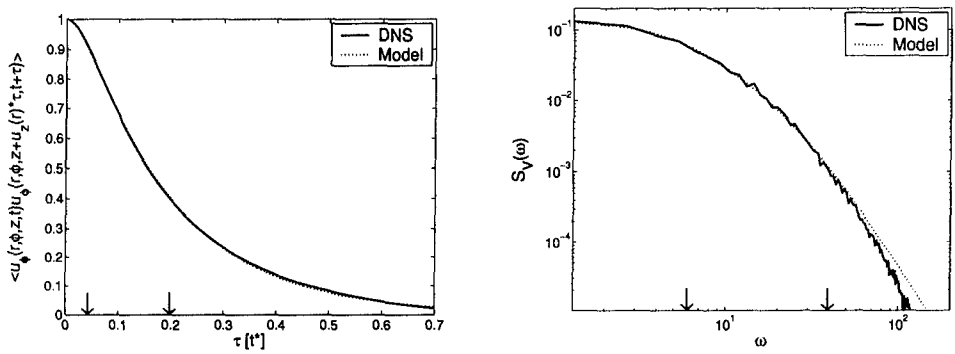

Figure 1. Left: The Eulerian Space-Time correlation function for the tangential velocity component; solid: DNS, dashed: Model. Right: Velocity spectrum; solid: DNS, dashed: Model. In both figures the arrows represent the calculated time-scales.

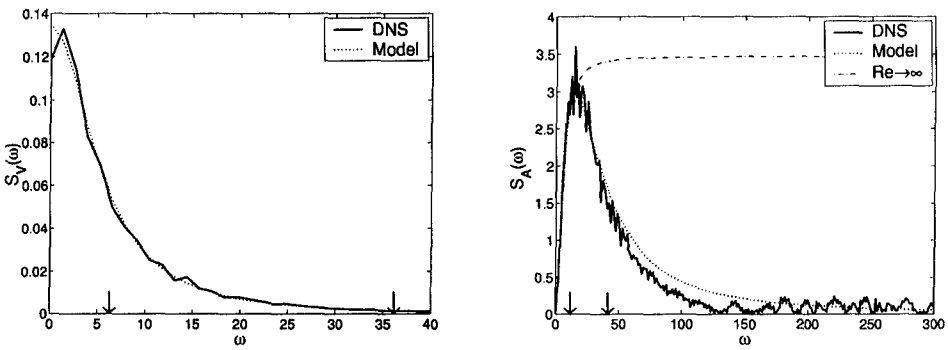

Figure 2. Left: Velocity spectrum; solid: DNS, dashed: Model. Right: Acceleration spectrum; solid: DNS, dashed: Model, dashdot: white-noise approximation. In both figures the arrows represent the calculated time-scales.